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Grey-box modelling of pollutant loads from a sewer system

Henrik Bechmann [a,b,*], Marinus K. Nielsen [a], Henrik Madsen [b], Niels Kjølstad Poulsen [b]

[a] *Krüger A/S, Gladsaxevej 363, DK-2860 Søborg, Denmark*

[b] *Department of Mathematical Modelling, Technical University of Denmark, Building 321, DK-2800 Lyngby, Denmark*

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Abstract

Using a compact measuring unit with on-line meters for UV absorption and turbidity, it is possible to determine concentrations of organic load (chemical oxygen demand (COD) and suspended solids (SS)) anywhere in a sewer system. When measurements of the flow are available as well, the pollutant mass flow at the measuring point can be calculated.

The measured data are used to estimate different models describing the load of pollutants in the sewer. A comparison of the models shows that a grey-box model is most informative and best in terms measured by the multiple correlation coefficient. The grey-box model is a state-space model, where the state represents the actual amount of deposition in the sewer, and the output from the model is the pollutant mass flow to the wastewater treatment plant (WWTP). The model is formulated by means of stochastic differential equations. Harmonic functions are used to describe the dry weather diurnal load profiles. It is found that the accumulation of deposits in the sewer depends on previous rain events and flows.

By means of on-line use of the grey-box models, it is possible to predict the amount of pollutants in a first flush at any time, and hence from the capacity of the plant to decide if and when the available detention basin is to be used for storage of wastewater. The mass flow models comprise an important improvement of the integrated control of sewer and WWTP including control of equalisation basins in the sewer system. Further improvements are expected by the introduction of an additive model where dry weather situations and storm situations are modelled separately before addition to the resulting model.

Keywords: Pollutant deposition; Sewer system; First flush; Grey-box models; Statistical identification; On-line measurements

1. Introduction

On-line measurements of organic pollution in terms of biological, chemical or total oxygen demand (BOD, COD or TOD) and suspended solids (SS) by means of UV absorbance and turbidity sensors are now well described (Dobbs, Wise & Dean, 1972; Mrkva, 1975; Kanaya, Fujita, Hayashi, Hiraoka & Tsumura, 1985; Ruban, Marchandise & Scrivener, 1993; Nowack & Ueberbach, 1995; Matsché & Stumwöhrer, 1996; Reynolds & Ahmad, 1997; Wass, Marks, Finch, Leeks & Ingram, 1997). When on-line measurements of COD and SS are available a better characterization of the wastewater can be achieved, and this leads to a better understanding of the processes in the sewer system.

The sewer system is often modelled by means of deterministic modelling as a configuration of storage volumes connected with pipes of different dimensions (Mark, Appelgren & Larsen, 1995; Dempsey, Eadon & Morris, 1997; Heip, Assel & Swartenbroekx, 1997; van Luijtelaar & Rebergen, 1997). As these models are formulated as a large collection of differential equations with many parameters, it is difficult to estimate the parameters on the basis of available measurements.

Data based models are also common in the literature (Capodaglio, 1994; Delleur & Gyasi-Agyei, 1994; Ruan & Wiggers, 1997; Young, Jakeman & Post, 1997). These models have few parameters, which can then be estimated on the basis of available data. However, as the models are most often formulated in discrete time, the parameter estimates depend on the sampling time.

In this paper a data based grey-box modelling approach is used. A grey-box model is a physically based macroscopic model with stochastic terms to count in uncertainties in model formulation and measurement values. The introduction of stochastic terms enables maximum likelihood estimation of the model parameters. The maximum likelihood method provides

* Corresponding author. Tel.: +45-3969-0222; fax: +45-3969-0806.
E-mail address: hnb@kruger.dk (H. Bechmann)

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estimates of the variances of the parameter estimates, which are used to evaluate the uncertainty of the parameters. The proposed models are formulated here in continuous time. Measurements of pollutant mass flows in the inlet to a wastewater treatment plant (WWTP) are modelled by means of models of differing complexity. Pollutant deposition in the sewer can for instance be included, to make it possible to quantify the amounts of pollutants in a first flush.

2. The measurement system

A compact portable measuring box, developed by Krüger A/S, Denmark, has been used to collect measurements of UV absorption and turbidity from the inlet to the Aalborg East WWTP in Northern Jutland, Denmark, in the late 1997 and in the beginning of 1998. The Krüger measuring box consists of a Grant SQ-1003 datalogger, a Dr. Lange UV absorbance sensor model LSV 109 and a Dr. Lange SOLITAXplus LSV 121 turbidity sensor. The Aalborg East WWTP is equipped with the STAR control system (Nielsen & Önnerth, 1995; Önnerth & Bechmann, 1995) which supplies estimates of the inlet flow, based on measurements from the inlet pumping station. Fig. 1 shows the data used in the present work. Laboratory analyses of COD and SS are also available.

3. Models of the pollution concentrations and fluxes

The relationships between on-line measurements of UV absorbance (A) and turbidity (T) and laboratory analyses of COD and SS concentrations (C_{COD} and C_{SS}, respectively) are assumed to be:

$$C_{\mathrm{COD}} = \alpha_{\mathrm{COD}} A + \beta_{\mathrm{COD}}, \tag{1}$$

$$C_{\mathrm{SS}} = \alpha_{\mathrm{SS}} T + \beta_{\mathrm{SS}}, \tag{2}$$

where α_{COD}, β_{COD}, α_{SS} and β_{SS} are parameters, which have to be estimated on the basis of measurements of

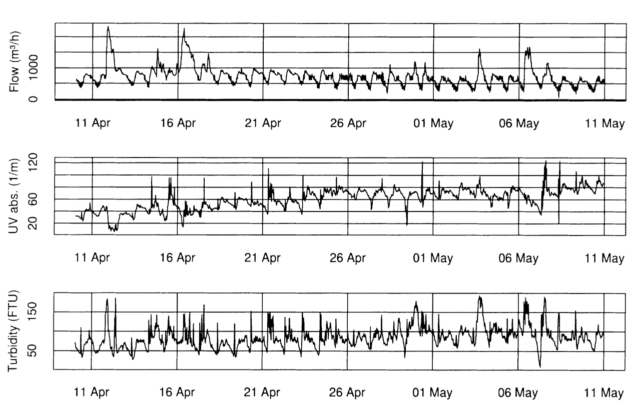

Fig. 1. The measurements of flow, UV absorbance and turbidity.

C_{COD}, C_{SS}, A and T, as the parameters depend on the actual operating conditions and the wastewater composition (Dobbs et al., 1972; Mrkva, 1975; Kanaya et al., 1985; Ruban et al., 1993; Nowack & Ueberbach, 1995; Matsché & Stumwöhrer, 1996; Reynolds & Ahmad, 1997; Wass et al., 1997). When these parameters are estimated, it is possible to consider the observation at time t of pollution flux:

$$y(t) = Q(t)C(t) \tag{3}$$

with $Q(t)$ and $C(t)$ denoting the flow and the pollution concentration (C_{COD} or C_{SS}), respectively. This quantity can be modelled using:

$$y(t) = \hat{y}(t) + \epsilon(t). \tag{4}$$

Here $\hat{y}(t)$ is the predictable part of the model, and the residual $\epsilon(t)$ is a stochastic part, which is the difference between the data observed and the prediction obtained from the model.

The first approach considered is to model the pollution flux using a fixed diurnal profile expressed as an nth order harmonic function with a 24-hour period (model 1):

$$\hat{y}(t) = a_0 + \sum_{k=1}^{n} \left(a_k \sin\left(2\pi k \frac{t}{24\ \mathrm{h}}\right) + b_k \cos\left(2\pi k \frac{t}{24\ \mathrm{h}}\right)\right), \tag{5}$$

where a_0, a_k and b_k $(1 \leqslant k \leqslant n)$, are the unknown parameters.

Another approach is to model the flux as a mean value and a term proportional to the flow (model 2):

$$\hat{y}(t) = c_0 + c_1 Q(t), \tag{6}$$

where c_0 and c_1 are positive parameters.

These two approaches can be combined to (model 3):

$$\hat{y}(t) = a_0 + \sum_{k=1}^{n} \left(a_k \sin\left(2\pi k \frac{t}{24\ \mathrm{h}}\right) + b_k \cos\left(2\pi k \frac{t}{24\ \mathrm{h}}\right)\right) + cQ(t). \tag{7}$$

Note that the parameter values of the Fourier expansion in Eqs. (5) and (7) are in general not the same, as some of the harmonic variation in $y(t)$ is most likely explained by the harmonic variation of $cQ(t)$.

These approaches all result in static models.

The final approach considered is model 4 which is a dynamic model formulated as a state-space model. This model takes the deposition of pollutants in the sewer system and on impervious areas of the catchment area into account.

The model is based on the assumption that pollutants deposit gradually in dry weather and that the deposited pollutants are flushed out during rain incidents and into the inlet of the treatment plant. Let $x(t)$ denote the deposition of pollutants at time t. Then a simple first-order linear ordinary differential equation:

$$\frac{d\hat{x}}{dt} = a(\hat{x} - \bar{x}) + b(Q - \bar{Q}) \tag{8}$$

can be used to describe the dynamics of the pollution deposition. The time derivative of $\hat{x}$ is the estimated growth rate at which pollution is built up in the sewer, and $\bar{x}$ and $\bar{Q}$ are the mean values of $\hat{x}$ and Q. The parameters a and b are assumed to be negative, and hence a flow larger than the average flow during the period will decrease the growth rate and a flow lower than the mean flow will increase the growth rate. Similarly a deposited amount larger than the mean will decrease the growth rate, and vice versa.

The pollution flux observed at the measuring point in the inlet to the WWTP, is assumed to consist of a fixed diurnal profile, which describes the pollutants that enter the sewer system, minus a contribution to the depositions in the sewer. This is formulated in the observation equation:

$$\begin{aligned}\hat{y}(t) &= a_0 + \sum_{k=1}^{n}\left(a_k \sin\left(2\pi k\frac{t}{24\ \text{h}}\right) + b_k \cos\left(2\pi k\frac{t}{24\ \text{h}}\right)\right) \\ &\quad - \frac{d\hat{x}}{dt} \\ &= a_0 + \sum_{k=1}^{n}\left(a_k \sin\left(2\pi k\frac{t}{24\ \text{h}}\right) + b_k \cos\left(2\pi k\frac{t}{24\ \text{h}}\right)\right) \\ &\quad - a(\hat{x} - \bar{x}) - b(Q - \bar{Q}).\end{aligned} \tag{9}$$

Besides a better description of the available data, this approach also provides information about the practically unmeasureable amount of deposits in the sewer and impervious areas of the catchment. Hence, besides the parameter estimates, the model also provides an estimate of $x - \bar{x}$. This means that the model does not give information about the actual deposition level x, but only about the difference from the mean level of deposition. This does not pose any practical limitations on the use of the model, as, for instance, it is still possible to quantify the amount of pollutants in a first flush.

All the proposed pollution flux models can be applied to both SS and COD flux.

4. Estimation methods

The parameters of the concentration models (1) and (2) as well as the parameters of the static pollution flux models (5)–(7), can be estimated by ordinary least-squares methods, as these models are all linear in the parameters.

The method used to estimate the parameters of the dynamic pollution flux model (4) and (8), (9) is a maximum likelihood method for estimating parameters in stochastic differential equations based on discrete time data given by (4). For a more detailed description of the method refer to Madsen and Melgaard (1991) or Melgaard and Madsen (1993).

In order to use the maximum likelihood method, some stochastic terms have to be introduced. Hence, the first-order differential equation (8) turns into a stochastic differential equation, where the continuous time equation describing the dynamics of the pollution deposition can be written as the so-called Itô differential equation (Øksendal, 1995).

$$dx(t) = f(x, u, t)\,dt + g(u, t)\,dw(t), \tag{10}$$

where x is the state variable, u an input (e.g., control) variable, w a standard Wiener process (see e.g., Kloeden & Platen, 1995), and f and g are known functions. The function $g(u, t)$ describes any input or time-dependent variation related to how the variation generated by the Wiener process enters the system. Note, that in order to illustrate the flexibility of the method Eq. (10) represents a generalization of the ordinary state equation (8).

For the observations we assume the discrete time relation

$$y(t) = h(x, u, t) + e(t), \tag{11}$$

where $e(t)$ is assumed to be a Gaussian white noise sequence independent of w, which can be seen as a generalization of (4) and (9). All the unknown parameters, denoted by the vector $\boldsymbol{\theta}$, are embedded in the continuous–discrete time state-space model (Eqs. (10) and (11)).

The observations are given in discrete time, and, in order to simplify the notation, we assume that the time index t belongs to the set $\{0, 1, 2, \ldots, N\}$, where N is the number of observations. Introducing

$$\mathcal{Y}(t) = [y(t), y(t-1), \ldots, y(1), y(0)]' \tag{12}$$

i.e., $\mathcal{Y}(t)$ is a vector containing all the observations up to and including time t, the likelihood function is the joint probability density of all the observations assuming that the parameters are known, i.e.,

$$\begin{aligned}L'(\boldsymbol{\theta}; \mathcal{Y}(N)) &= p(\mathcal{Y}(N)|\boldsymbol{\theta}) \\ &= p(y(N)|\mathcal{Y}(N-1), \boldsymbol{\theta})p(\mathcal{Y}(N-1)|\boldsymbol{\theta}) \\ &= \left(\prod_{t=1}^{N} p(y(t)|\mathcal{Y}(t-1), \boldsymbol{\theta})\right)p(y(0)|\boldsymbol{\theta}),\end{aligned} \tag{13}$$

where successive applications of the rule $P(A \cap B) = P(A|B)P(B)$ are used to express the likelihood function as a product of conditional densities.

In order to evaluate the likelihood function it is assumed that all the conditional densities are Gaussian. In the case of a linear state-space model as described by (4) and (8), (9), it is easily shown that the conditional densities are actually Gaussian (Madsen & Melgaard, 1991). In the more general nonlinear case the Gaussian assumption is an approximation.

The Gaussian distribution is completely characterized by the mean and covariance. Hence, in order to parameterize the conditional distribution, we introduce the conditional mean and the conditional variance as

$$\hat{y}(t|t-1) = E[y(t)|\mathscr{Y}(t-1), \boldsymbol{\theta}]$$

and

$$R(t|t-1) = V[y(t)|\mathscr{Y}(t-1), \boldsymbol{\theta}], \tag{14}$$

respectively. It should be noted that these correspond to the one-step prediction and the associated variance, respectively. Furthermore, it is convenient to introduce the one-step ahead prediction error (or innovation)

$$\epsilon(t) = y(t) - \hat{y}(t|t-1). \tag{15}$$

For calculating the one-step ahead prediction and its variance, an iterated extended Kalman filter is used. The extended Kalman filter is simply based on a linearization of the system equation (10) around the current estimate of the state (see Gelb, 1974). The iterated extended Kalman filter is obtained by local iterations of the linearization over a single sample period.

Using (13)–(15) the conditional likelihood function (conditioned on $y(0)$) becomes

$$L(\boldsymbol{\theta}; \mathscr{Y}(N)) = \prod_{t=1}^{N} \left(\frac{1}{\sqrt{2\pi}\sqrt{R(t|t-1)}} \times \exp\left(-\frac{\epsilon(t)^2}{2R(t|t-1)} \right) \right). \tag{16}$$

Traditionally, the logarithm of the conditional likelihood function is considered

$$\log L(\boldsymbol{\theta}; \mathscr{Y}(N)) = -\frac{1}{2}\sum_{t=1}^{N} \left(\log R(t|t-1) + \frac{\epsilon(t)^2}{R(t|t-1)} \right) + \text{const.} \tag{17}$$

The maximum likelihood estimate (ML-estimate) is the set $\hat{\boldsymbol{\theta}}$, which maximizes the likelihood function. Since it is not, in general, possible to optimize the likelihood function analytically, a numerical method has to be used. A reasonable method is the quasi-Newton method.

An estimate of the uncertainty of the parameters is obtained by the fact that the ML-estimator is asymptotically normally distributed with mean $\boldsymbol{\theta}$ and covariance

$$\boldsymbol{D} = \boldsymbol{H}^{-1}, \tag{18}$$

where the matrix $\boldsymbol{H}$ is given by

$$\{h_{lk}\} = -E\left[\frac{\partial^2}{\partial\theta_l \, \partial\theta_k} \log L(\boldsymbol{\theta}; \mathscr{Y}(N)) \right]. \tag{19}$$

An estimate of $\boldsymbol{D}$ is obtained by equating the observed value with its expectation and applying

$$\{h_{lk}\} \approx -\left(\frac{\partial^2}{\partial\theta_l \, \partial\theta_k} \log L(\boldsymbol{\theta}; \mathscr{Y}(N)) \right)_{|\theta=\hat{\theta}}. \tag{20}$$

The above equation can be used for estimating the variance of the parameter estimates. The variances serve as a basis for calculating t-test values for test under the hypothesis that the parameter is equal to zero. Finally, the correlation between the parameter estimates is readily found, based on the covariance matrix $\boldsymbol{D}$.

The estimation methods are implemented in the CTLSM program, which are available from http://www.imm.dtu.dk/~hm/.

5. Results and discussion

The parameters of Eqs. (1) and (2) are found by linear regression. It turned out that β_{COD} and β_{SS} were insignificant, and therefore they were eliminated in the final estimation. The estimated parameters and their standard deviations are shown in Table 1. The degrees of explanations (multiple correlation coefficients) of the COD and SS concentration models are $R^2 = 0.98$ and $R^2 = 0.97$, respectively.

For the models, which include a diurnal profile modelled as a harmonic function (models 1, 3 and 4), it was found that second-order harmonic functions were suitable, as the higher order coefficients were insignificant. In Tables 2 and 3 it can be seen that some of the parameters of the harmonic functions are insignificant, as their estimated values are smaller or comparable in absolute values to their estimated standard deviations. Especially b_1 of COD flux model 3, b_1 of SS flux model 3 and b_2 of SS flux model 4 are very uncertain. Usually insignificant parameters should be excluded from the final estimation, to make the estimation of the remaining parameters better. However, we have chosen to include these parameters for comparison with the other models.

Comparison plots of measured and modelled pollution fluxes of the 4 models are shown in Figs. 2–5. Note, that the modelled pollution fluxes shown in the figures

Table 1
Parameters of Eqs. (1) and (2) (the β parameters are insignificant and are therefore not estimated)

Parameter	α_{COD}	β_{COD}	α_{SS}	β_{SS}
Unit	$(\text{g } O_2/\text{m}^3)/\text{m}^{-1}$	$\text{g } O_2/\text{m}^3$	$(\text{g SS/m}^3)/\text{FTU}$	g SS/m^3
Estimate	10.57	–	3.05	–
Standard deviation	0.40	–	0.13	–

Table 2
Parameter estimates of the COD flux models

Model 1							
Parameter	a_0	a_1	b_1	a_2	b_2		
Unit	kg O_2/h	kg O_2/h	kg O_2/h	kg O_2/h	kg O_2/h		
Estimate	443.5	−148.6	−39.22	17.94	53.94		
Standard deviation	3.8	5.34	5.34	5.34	5.34		
Model 2							
Parameter	c_0	c_1					
Unit	kg O_2/h	kg O_2/m^3					
Estimate	190.1	0.3464					
Standard deviation	10.3	0.0130					
Model 3							
Parameter	a_0	a_1	b_1	a_2	b_2	c	
Unit	kg O_2/h	kg O_2/h	kg O_2/h	kg O_2/h	kg O_2/h	kg O_2/m^3	
Estimate	270.8	−114.3	−29.29	19.25	36.04	0.2361	
Standard deviation	9.4	5.07	4.79	4.76	4.85	0.0120	
Model 4							
Parameter	a	b	a_0	a_1	b_1	a_2	b_2
Unit	h^{-1}	kg O_2/m^3	kg O_2/h	kg O_2/h	kg O_2/h	kg O_2/h	kg O_2/h
Estimate	−0.08775	−0.4448	444.4	−93.50	1.403	24.67	22.69
Standard deviation	0.00864	0.0175	3.0	4.65	4.690	4.12	4.34

Table 3
Parameter estimates of the SS flux models

Model 1							
Parameter	a_0	a_1	b_1	a_2	b_2		
Unit	kg SS/h	kg SS/h	kg SS/h	kg SS/h	kg SS/h		
Estimate	198.8	−65.91	−16.62	−10.55	32.10		
Standard deviation	3.3	4.70	4.70	4.70	4.70		
Model 2							
Parameter	c_0	c_1					
Unit	kg SS/h	kg SS/m^3					
Estimate	−77.11	0.3772					
Standard deviation	5.25	0.0066					
Model 3							
Parameter	a_0	a_1	b_1	a_2	b_2	c	
Unit	kg SS/h	kg SS/h	kg SS/h	kg SS/h	kg SS/h	kg SS/m^3	
Estimate	−67.96	−12.96	−1.268	−8.536	4.445	0.3647	
Standard deviation	5.60	3.01	2.846	2.830	2.882	0.0071	
Model 4							
Parameter	a_{SS}	b_{SS}	a_0	a_1	b_1	a_2	b_2
Unit	h^{-1}	kg SS/m^3	kg SS/h	kg SS/h	kg SS/h	kg SS/h	kg SS/h
Estimate	−0.01192	−0.4147	204.3	−3.945	4.002	−6.357	−0.1627
Standard deviation	0.00090	0.0086	1.7	2.663	2.429	2.339	2.476

are not one-step ahead predictions, but simulations from the estimated models. The simulations are based only on the measured input to the models, which is time of day (models 1, 3 and 4) and inlet flow (models 2–4). In Tables 2 and 3 the parameter estimates of the proposed models are listed, and in Table 4 the correlations between measured and simulated fluxes R^2 of the models are listed.

When comparing Figs. 2–5, it is seen that the simple harmonic model 1 is good at describing most of the dry weather situations, but not the wet weather situations. Models 2–4 are better than model 1 at following the peaks in pollution flux in wet weather, as they include a term proportional to the flow. Besides a better correlation between measured and modelled pollutant fluxes expressed by the degree of explanation R^2, application of the dynamic model provides information about the pollutant depositions in the sewer. In Fig. 6 the estimated deviations from the mean levels of COD and SS deposits are shown. From this figure it is seen that

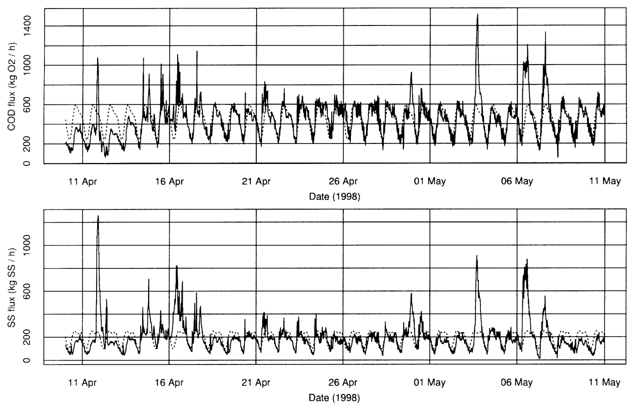

Fig. 2. The pollutant flux modelled as a diurnal profile. Solid lines: measured flux, dashed lines: modelled flux.

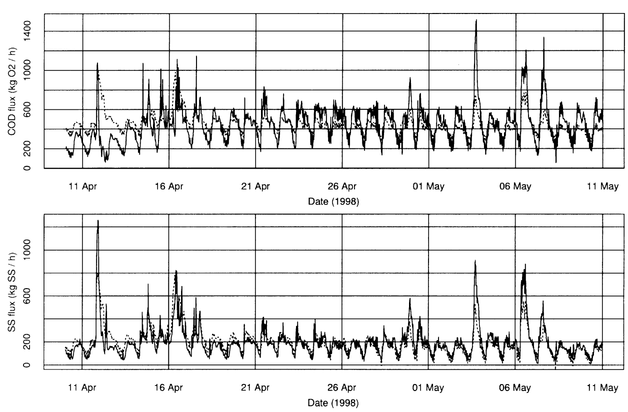

Fig. 3. The pollutant flux modelled as proportional to the flow. Solid lines: measured flux, dashed lines: modelled flux.

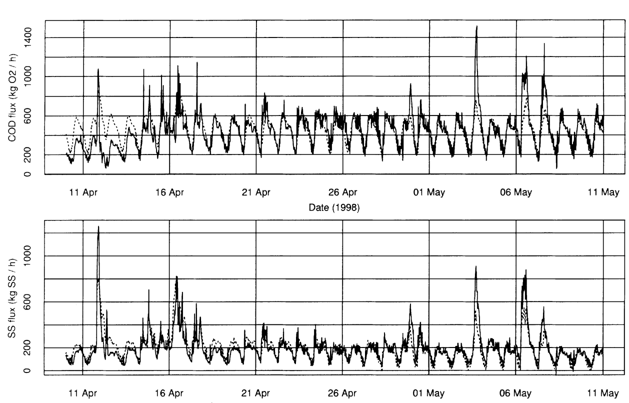

Fig. 4. The pollutant flux modelled as a diurnal profile plus a term proportional to the flow. Solid lines: measured flux, dashed lines: modelled flux.

pollutants build up in the sewer during dry weather periods and are flushed out during rain. The amounts of deposits in a first flush can also be quantified on the basis of Fig. 6: The first and second rain incidents contain approximately 3000 kg O_2 (COD) and 6000 kg

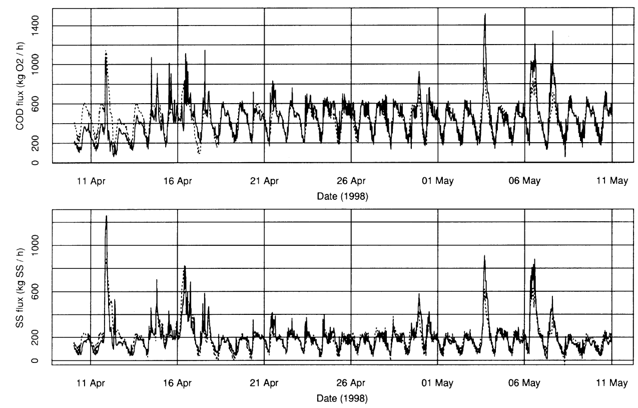

Fig. 5. The pollutant flux modelled by a dynamic grey-box model. Solid lines: measured flux, dashed lines: modelled flux.

Table 4
Degrees of explanation of the different models

Model	R^2	
	COD model	SS model
1	0.39	0.15
2	0.32	0.69
3	0.51	0.69
4	0.61	0.76

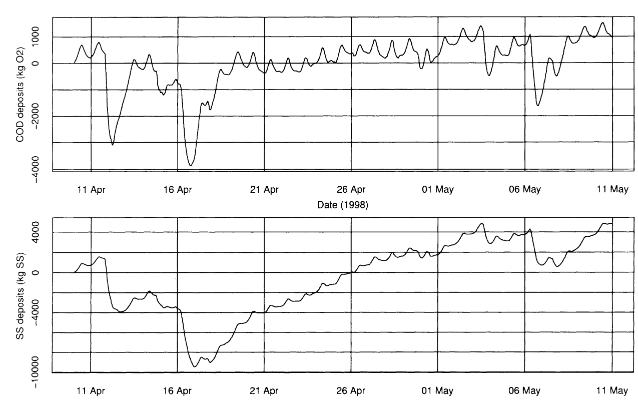

Fig. 6. Estimated depositions of COD and SS in the sewer and on impervious areas.

SS which are 14% and 63% of the diurnal load of COD and SS, respectively. As it is expected that deposited COD stabilizes in the sewer this is considered realistic. The stabilization of COD will lead to a smaller amount of COD in a first flush compared to the normal load of COD than the amount of SS compared to the normal load of SS, as deposited SS are not expected to stabilize in the sewer.

The time constants of the dynamic COD and SS models are $-1/a = 11.4$ h and $-1/a = 83.9$ h, respectively. This means that after a considerable change in the flow, the COD and SS depositions will reach 63% of the steady state level in 11.4 and 83.9 h, respectively. The dynamics of the COD deposition is thus about seven times faster than the dynamics of the SS deposition.

As the data used for estimating the models are dominated by dry weather situations, the fluxes are underestimated during rainful events. A separation of the models into dry weather models and storm models, which are added to each other, might be a significant improvement.

6. Conclusions

Linear relationships between UV absorption and COD and between turbidity and SS are derived. These relationships are used to compute the COD and SS concentrations from on-line measurements of UV absorption and turbidity. Using available measurements of the flow in the inlet to Aalborg East WWTP the pollution flows of COD and SS are used to estimate models of differing complexity. It is shown that the estimated dynamic grey-box models, which include the deposition and flush out of pollutant masses in the sewer, describe the data better than the other models proposed. Furthermore, these dynamic models estimate the amounts of deposits in the sewer at any time. Hereby the amounts of pollutants in a first flush are found. This information is very useful when control algorithms for the use of the available detention basin at the WWTP are designed. However, when the models are to be used to enable better operational control of available detention basins, predictions of the wastewater flow to the WWTP are required. When flow forecasts are available, the models suggested can be used to predict the pollutant load with the same time horizon as the flow predictions.

With degrees of explanation (multiple correlation coefficients) $R^2 = 0.76$ and $R^2 = 0.61$ for the dynamic grey-box COD and SS flux models, respectively, there are still variations in the data that are not described by the models. Hence, there is still a need to develop better models. Improvements could be a separation into dry weather models and storm models, and the introduction of limitations on the depositions in the sewer and on impervious areas. However, introduction of limitations on the depositions will require measurement data that covers the limits sufficiently to estimate the parameters that describe the bounds.

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