Identifiability and uncertainty analysis of the River Water Quality Model No. 1 (RWQM1)

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Abstract State of the art models as used in activated sludge modelling and recently proposed for river water quality modelling integrate the knowledge in a certain field. If applied to data from a specific site, such models are nearly always overparameterised. This raises the question of how many parameters can be fitted in a given context and how to find identifiable parameter subsets given the experimental layout. This problem is addressed for the kinetic parameters of a simplified version of the recently published river water quality model no. 1 (RWQM1). The selection of practically identifiable parameter subsets is discussed for typical boundary conditions as a function of the measurement layout. Two methods for identifiable subset selection were applied and lead to nearly the same results. Assuming upstream and downstream measurements of dissolved substances to be available, only a few (5–8) model parameters appear to be identifiable. Extensive measurement campaigns with dedicated experiments seem to be required for successful calibration of RWQM1. The estimated prior uncertainties of the model parameters are used to estimate the uncertainty of model predictions. Finally an estimate is provided for the maximum possible decrease in prediction uncertainty achievable by a perfect determination of the values of the identifiable model parameters.

Keywords Identifiability analysis; sensitivity analysis; uncertainty analysis; river water quality modeling; collinearity index; Fisher information matrix

Introduction

The integration of knowledge in the form of mathematical models is useful for various reasons: (i) such models make it possible to test hypotheses on functional interactions in the system. (ii) they are compact and transparent archives of knowledge about a system that facilitate communication among engineers and scientists, and (iii) they can be used for predicting future states of the system or its responses to assumed or expected changes in driving conditions. Because of the request to include as much knowledge as possible in such "state of the art" models, there is a trend that such models become larger and larger (Beck, 1999). This makes the parameters of such models usually non-identifiable for any single application to a real system.

In the field of water quality modelling, the parameters of such "state of the art" models are usually not universal enough to make it possible to describe different systems with the same values of all model parameters. Hence, site-specific model parameters must be obtained by calibration to experimental data. Obviously, trying to estimate all model parameters from those data is utopian. Rather, a subset of parameters should be selected that, with the proper data, can yield a well-calibrated model for a given application of the model to a real system. However, this raises the question of how to select such a subset of parameters to be adjusted. Important aspects to be considered for answering this question are:

i. Prior knowledge on parameter values, universality and uncertainty.
ii. The experimental and initial conditions and the measurement layout used for data collection.
iii. The measured data if already available.

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iv. Information on the identifiability of model parameters for the given measurement layout (the model structure is assumed to be given; the aspect of structural uncertainty is not addressed here).

Most of the techniques designed to find practically identifiable subsets of model parameters for a given model structure and a given experimental layout are based on an investigation of sensitivity functions. However, there are different possibilities of how to apply techniques of this class. Graphical analyses of sensitivity functions (Holmberg, 1982; Reichert *et al.*, 1995) are only possible for very simple models. For this reason we concentrate on numeric criteria for magnitude and approximate linear dependence of sensitivity functions (Belsley, 1991; Brun *et al.*, 2001) and on techniques based on scalar functions calculated from the Fisher information matrix (Walter and Pronzato, 1990; Söderström and Stoica, 1989; Weijers and Vanrolleghem, 1997; Hidalgo and Ayesa, 2001).

In order to summarise the knowledge about modelling of oxygen and the most important nutrients in rivers, to introduce a basis for scientific exchange, and to facilitate practical application of river water quality modeling, Shanahan *et al.* (2001), Reichert *et al.* (2001) and Vanrolleghem *et al.* (2001) introduced the river water quality model no. 1 (RWQM1). It is obvious (and clarified by the two field studies by Borchardt and Reichert (2001) and Reichert (2001)) that this model belongs to the category of models that are too large for a unique parameter identification in a typical field application. Because this model will possibly be applied to various field studies, it is important to know for which parameters information can be gained under which measurement layout and how large the uncertainties of the model predictions can be expected to be. It is the goal of this paper to give answers to these questions for a typical river and for typical measurement layouts and to demonstrate methodically how such answers could be found for other situations. We concentrate in this analysis on the kinetic part of the model because the uncertainties are larger than in the stoichiometric part. Nevertheless, an analysis of the stoichiometric part is also of interest. Such an analysis is also in progress.

The paper is structured as follows. First, the techniques used for selecting identifiable parameter subsets and for uncertainty analysis are briefly reviewed. Then the submodel of the RWQM1 used for the analyses is introduced and the measurement layouts are discussed. Then the results of identifiability and uncertainty analyses are presented and discussed. Finally, the key results are summarized and conclusions are drawn.

Techniques

Selection of subsets of identifiable model parameters

In this section, we briefly review and compare two recently proposed techniques for identifiable parameter subset selection for large environmental simulation models. The first technique was proposed and applied to the activated sludge wastewater treatment model no. 1 (Henze *et al.*, 2000) by Weijers and Vanrolleghem (1997). The second technique was proposed and illustrated by Brun *et al.* (2000) and it was applied to modelling oxygen, nutrient and plankton dynamics in Lake Zürich (Omlin *et al.*, 2000a) by Omlin *et al.* (2000b) and to biological phosphorus removal in activated sludge systems by Brun *et al.* (2001).

We assume the outputs of a deterministic model be described by the function

$$\boldsymbol{y}(\boldsymbol{\theta}) \tag{1}$$

where $\boldsymbol{y} = (y_1,...,y_n)^T$ is the vector of model outcomes that correspond to the measured output variables and $\boldsymbol{\theta} = (\theta_1,...,\theta_m)^T$ is the vector of model parameters. Note that for state-space models Eq. (1) combines the state equations with the observation equations. In addition to the deterministic model, Eq. (1) also contains the experimental layout specifying which variables are measured at which points in space and time. The observation vector

$\boldsymbol{y}$ contains all observed variables at all observation locations in space and time. The mathematical form of the model is not relevant. It can consist of algebraic equations, ordinary or partial differential equations and/or integral equations.

Both techniques for the selection of identifiable model parameter subsets are based on sensitivity functions. It is useful to define the following two nondimensional sensitivity functions

$$s_{i,j} = \frac{\Delta\theta_j}{sc_i}\frac{\partial y_i}{\partial \theta_j}, \quad \tilde{s}_{i,j} = \frac{s_{i,j}}{\sqrt{\sum_{k=1}^{n} s_{k,j}^2}}, \tag{2}$$

the matrices $\boldsymbol{S} = (s_{i,j})$ and $\tilde{\boldsymbol{S}} = (\tilde{s}_{i,j})$, and the column vectors $\boldsymbol{s}_j = (s_{i,j},...,s_{n,j})^T$ and $\tilde{\boldsymbol{s}}_j = (\tilde{s}_{i,j},...,\tilde{s}_{n,j})^T$.

Note that the vectors $\tilde{s}_j$ are constructed from by normalisation: $\tilde{s}_j = s_j / \| \tilde{s}_j \|$. The dimensional scaling parameters in Eq. (2), $\Delta\theta_j$ and sc_i, are very important for the analysis. $\Delta\theta_j$ represents the uncertainty range of the parameter θ_j according to prior knowledge and is a characteristic scale of the variable y_i. In this paper, $\Delta\theta_j$ is assessed by dividing the model parameters into three uncertainty classes by prior knowledge and provide relative uncertainties. If no prior knowledge on parameter uncertainty is available, the parameter value itself can be used for $\Delta\theta_j$. This results in an analysis of the same relative identifiability of the model parameters. The parameters sc_i represent typical magnitudes of the variables y_i. Here, we use the inflow concentration of the substance represented by y_i. A reasonable alternative for sc_i would be the measurement accuracy of y_i. If the number of measurements for different variables differ significantly, this could also be considered by an appropriate choice of the scaling factor. Note that the normalised sensitivity functions, $\tilde{s}_j$ are independent of $\Delta\theta_j$ and of a common multiplicative factor in all sc_i.

Poor identifiability of model parameters can be caused by a small sensitivity of the model results to a parameter, or by an approximate linear dependence of sensitivity functions of the results with respect to the parameters.

The technique proposed by Brun *et al.* (2000) is based on two different $\tilde{s}_j$ measures of sensitivity and "compensability" to quantify the two problems separately. First a sensitivity ranking of parameters is done using

$$\delta_j^{msqr} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} s_{i,j}^2} = \frac{1}{\sqrt{n}}\|\boldsymbol{s}_j\| \quad \text{or} \quad \delta_j^{mabs} = \frac{1}{n}\sum_{i=1}^{n}|s_{i,j}|. \tag{3}$$

Then the "compensability" is quantified for interesting parameter subsets by the "collinearity index"

$$\gamma(\boldsymbol{\theta}) = \frac{1}{\min_{||\beta||=1}\|\tilde{\boldsymbol{s}}_1\beta_1 + \mathrm{L} + \tilde{\boldsymbol{s}}_m\beta_m\|} = \frac{1}{\min_{||\beta||=1}\|\tilde{\boldsymbol{S}}\boldsymbol{\beta}\|} = \frac{1}{\sqrt{\min\left(EV\left[\tilde{\boldsymbol{S}}^T\tilde{\boldsymbol{S}}\right]\right)}} \tag{4}$$

which quantifies the minimum achievable norm of a linear combination of the normalised sensitivity functions with normalised coefficients (γ is unity for linearly independent sensitivity functions and approaches infinity with increasing degree of dependence). Note that the γs are characteristics of a single parameter whereas the δs give information on problems due to "compensability" within the subset of parameters.

A set of identifiable parameters is constructed from the sensitivity ranking by starting with the most sensitive parameter and adding less sensitive parameters unless the collinearity

index becomes too large (larger than a threshold of the order of 10 to 15). Parameters that lead to a too severe increase in the collinearity index are omitted and the procedure continues until either no additional parameter is found that leads to a moderate value of the collinearity index or the sensitivity becomes too small. This technique can be viewed as a quantification of the visual assessment of sensitivity functions (Holmberg, 1982, Reichert *et al.*, 1995; and many more). It does not depend on statistical assumptions with regard to parameter estimation. However, for least squares estimation, δ_j^{msqr} is the more logical choice in Eq. (3).

The technique proposed by Weijers and Vanrolleghem (1997) also starts with a sensitivity ranking that we will perform with the same measure (3) as for the technique described above. The ranking is, however, only used for a preliminary selection of a set of about 15 parameters (depending on the problem) and final subset selection from those parameters is done by a criterion based on the determinant or the condition number of the Fisher information matrix (FIM):
(we calculate the Fisher information matrix using the same scaling as used above). The first

$$cn = \sqrt{\frac{\max\left(EV\left[\boldsymbol{S}^T\boldsymbol{S}\right]\right)}{\min\left(EV\left[\boldsymbol{S}^T\boldsymbol{S}\right]\right)}} \quad \text{or} \quad \sqrt{\det\left[\boldsymbol{S}^T\boldsymbol{S}\right]} \tag{5}$$

measure, *cn*, in (5) is a measure of the shape, the second is a measure of the size of the confidence region (small size for large values of det) if the parameters would have been estimated by the method of least squares.

Both techniques described above are local analyses that use only derivatives of model results with respect to model parameters for a specified set of parameter values. The techniques can be extended to regional or global analyses by calculating the results for a suitable sample of parameter values (Weijers and Vanrolleghem 1997). Weijers and Vanrolleghem (1997) did not provide critical values for *cn* or the $\sqrt{\det}$, but rather applied routine parameter estimation algorithms to find out at what set size convergence problems started to occur. In this study, however, it is attempted to provide a more universal measure by calculating the 2*m*th root of the determinant of FIM, where *m* is the number of parameters in the set. This corresponds to an effective extension of the confidence region in one dimension.

Uncertainty analysis

Uncertainty analysis is most often done by linear error propagation or by Monte Carlo simulation (Hammersley and Handscomb, 1964; Rubinstein, 1981). The advantage of linear error propagation is its computational efficiency. If the sensitivity functions have already been calculated for identifiability analysis according to Eq. (2) no further simulations are required to get an error estimate. However, if model nonlinearities are significant within the uncertainty range of the parameters, the results of linear error propagation are inaccurate. Monte Carlo simulation is a simple technique to consider nonlinearity. However, due to the very large number of simulations required, this technique is computationally very demanding. Convergence can be improved by using latin hypercube sampling (McKay *et al.*, 1979).

Implementation

All simulations were performed with the simulation and data analysis programs AQUASIM (Reichert, 1994; *http://www.aquasim.eawag.ch*) and WEST (Vangheluwe *et al.*, 1998; *http://www.hemmis.be*).

Water quality submodel and measurement layouts

As in Reichert (2001) we used a simplified version of the RWQM 1 that is based on constant benthic densities of bacteria, algae and consumers. Similarly to Omlin *et al.* (2000a, b)

Table 1 Values, uncertainty classes and uncertainty ranges of the conversion model parameters (for an explanation of these model parameters, see Reichert et al., 2001)

Name	Value	Uncertainty cl.	range	Unit	Name	Value	Uncertainty cl.	range	Unit	Name	Value	Uncertainty cl.	range	Unit
$k_{death,ALG,20}$	0.1	3	0.050	d^{-1}	$k_{hyd,20}$	3	3	1.5	d^{-1}	$k_{resp,H,anox,20}$	0.1	3	0.05	d^{-1}
$k_{death,CON,20}$	0.05	3	0.025	d^{-1}	K_I	2000	3	1000	W/m^2	$k_{resp,N1,20}$	0.05	3	0.025	d^{-1}
$k_{eq,1}$	100000	3	50000	d^{-1}	$K_{N,ALG}$	0.1	3	0.05	gN/m^3	$k_{resp,N2,20}$	0.05	3	0.025	d^{-1}
$k_{eq,2}$	10000	3	5000	d^{-1}	$K_{NH4,ALG}$	0.1	3	0.05	gN/m^3	$K_{S,H,aer}$	2	3	1	$gCOD/m^3$
$k_{eq,N}$	10000	3	5000	d^{-1}	$K_{N,H,aer}$	0.2	3	0.1	gN/m^3	$K_{S,H,anox}$	2	3	1	$gCOD/m^3$
$k_{eq,P}$	10000	3	5000	d^{-1}	$K_{NH4,N1}$	0.5	3	0.25	gN/m^3	X_{ALG}	500	3	250	gCOD/m
$k_{eq,s0}$	2	3	1	d^{-1}	$K_{NO2,H,anox}$	0.2	3	0.1	gN/m^3	X_{CON}	100	3	50	gCOD/m
$k_{eq,w}$	10000	3	5000	$m^3/gH/d$	$K_{NO2,N2}$	0.5	3	0.25	gN/m^3	X_H	200	3	100	gCOD/m
$k_{gro,ALG,20}$	2	2	0.4	d^{-1}	$K_{NO3,H,anox}$	0.5	3	0.25	gN/m^3	X_{N1}	10	3	5	gCOD/m
$k_{gro,CON,20}$	0.0002	2	0.00004	$m^3/gCOD/d$	$K_{O2,ALG}$	0.2	3	0.1	gO/m^3	X_{N2}	5	3	2.5	gCOD/m
$k_{gro,H,aer,20}$	2	2	0.4	d^{-1}	$K_{O2,CON}$	0.5	3	0.25	gO/m^3	X_S	100	3	50	gCOD/m
$k_{gro,H,anox,20}$	1.6	2	0.32	d^{-1}	$K_{O2,H,aer}$	0.2	3	0.1	gO/m^3	β_{ALG}	0.046	2	0.0092	$^oC^{-1}$
$k_{gro,N1,20}$	0.8	2	0.16	d^{-1}	$K_{O2,N1}$	0.5	3	0.25	gO/m^3	β_{CON}	0.08	2	0.016	$^oC^{-1}$
$k_{gro,N2,20}$	1.1	2	0.22	d^{-1}	$K_{O2,N2}$	0.5	3	0.25	gO/m^3	β_H	0.07	2	0.014	$^oC^{-1}$
$K_{HPO4,ALG}$	0.02	3	0.01	gP/m^3	$k_{resp,ALG,20}$	0.1	3	0.05	d^{-1}	β_{hyd}	0.07	2	0.014	$^oC^{-1}$
$K_{HPO4,N1}$	0.02	3	0.01	gP/m^3	$k_{resp,CON,20}$	0.05	3	0.025	d^{-1}	β_{N1}	0.098	2	0.0196	$^oC^{-1}$
$K_{HPO4,N2}$	0.02	3	0.01	gP/m^3	$k_{resp,H,aer,20}$	0.2	3	0.1	d^{-1}	β_{N2}	0.069	2	0.0138	$^oC^{-1}$

Table 2 Values, uncertainty classes and uncertainty ranges of input and system parameters. Light intensity was modelled as $I = I\max \sin(\pi(0.5+(t \bmod 1d - 0.5d)/t_{light}))$ for $0.5(1d - t_{light})) < t \bmod 1d < 0.5(1 + t_{light}))$ and elsewhere 0

Name	Value	Uncertainty cl	range	Unit	Explanation
I_{max}	900	1	45	W/m^2	Maximum light intensity at noon
K_{st}	25	1	1.25	$m^{1/3}/s$	Friction coefficient according to Strickler
$K_{2,CO2,20}$	16	1	0.8	d^{-1}	Gas exchange coefficient for carbon dioxide
$K_{2,O2,20}$	20	1	1	d^{-1}	Gas exchange coefficient for oxygen
p	101325	1	5066	Pa	Atmospheric pressure (used for O_2 saturation)
pH_{in}	8	1	0.4		pH in inflow
Q_{in}	5	1	0.25	m^3/s	River discharge
S_0	0.001	1	0.00005		Slope of river bed
$S_{Ca,in}$	60	1	3	gCa/m^3	Calcium concentration in the inflow
S_{Cl}	20	1	1	gCl/m^3	Chloride concentration (used for conductivity)
$S_{HPO4+H2PO4,in}$	0.5	1	0.025	gP/m^3	Phosphate concentration in the inflow
S_K	4	1	0.2	gK/m^3	Potassium concentration (used for conductivity)
S_{Mg}	15	1	0.75	gMg/m^3	Magnesium concentration (used for conductivity)
S_{Na}	15	1	0.75	gNa/m^3	Sodium concentration (used for conductivity)
$S_{NH4+NH3,in}$	1	1	0.05	gN/m^3	Ammonia concentration in the inflow
$S_{NO2,in}$	0.5	1	0.025	gN/m^3	Nitrite concentration in the inflow
$S_{NO3,in}$	5	1	0.25	gN/m^3	Nitrate concentration in the inflow
$S_{O2,in}$	10	1	0.5	gO/m^3	Oxygen concentration in the inflow
$S_{S,in}$	10	1	0.5	$gCOD/m^3$	Dissolved substrate concentration in the inflow
S_{SO4}	20	1	1	$gSO4/m^3$	Sulfate concentration (used for conductivity)
t_{light}	0.6	1	0.03	d	Length of day ($\sin^2$ shape of light intensity)
T_{max}	20	1	1	^oC	Maximum temperature during the day (sin shape)
T_{min}	18	1	0.9	^oC	Minimum temperature during the day (sin shape)

Table 3 Experimental layouts 1–7 with the list of variables assumed to be measured at the downstream site and the values of the scales (sc_i) used to make the outputs non-dimensional. The scales were chosen to be equal to the input concentration at the upstream end of the river reach

Layout 1	Layout 2	Layout 3	Layout 4	Layout 5	Layout 6	Layout 7	sc_i
S_{O2}	S_{O2}	S_{O2}	S_{O2}	S_{O2}	S_{O2}	S_{O2}	10 mgO/l
	$S_{NH4}+S_{NH3}$	$S_{NH4}+S_{NH3}$	$S_{NH4}+S_{NH3}$	$S_{NH4}+S_{NH3}$	$S_{NH4}+S_{NH3}$	$S_{NH4}+S_{NH3}$	1 mgN/l
		S_{NO2}	S_{NO2}	S_{NO2}	S_{NO2}	S_{NO2}	0.5 mg N/l
			S_{NO3}	S_{NO3}	S_{NO3}	S_{NO3}	5 mgN/l
				$S_{HPO4}+S_{H2PO4}$	$S_{HPO4}+S_{H2PO4}$	$S_{HPO4}+S_{H2PO4}$	0.5 mgP/l
					pH	pH	8
						S_{cond}	500 µS/cm

we divided the uncertainty ranges of the parameters into three classes: accurately known parameters (class 1), $\Delta\theta_j$=5%; very poorly known parameters (class 3), $\Delta\theta_j$=50%; and an intermediate class 2 with $\Delta\theta_j$=20%. All external and input parameters are assigned to class 1, and all kinetic parameters with exception of growth rates and temperature dependence coefficients (that were assigned to class 2) were assigned to class 3. The class 3 parameters are half-saturation concentrations and specific death and respiration rates that are very poorly known. Uncertainty in stoichiometric coefficients is not considered in the present analysis. Table 1 gives an overview of model parameters (from Reichert *et al.* (2001), with exception of K_I, that was increased in order to account for the use of water surface instead of *in situ* light intensities), Table 2 on input and system parameters.

Measurement layouts considered in this analysis and scale factors are summarised in Table 3. Upstream inflows are assumed to be constant. The values used are given in Table 2. Downstream measurements according to the experimental layouts listed in Table 3 are assumed to be used for parameter estimation.

Identifiability analysis

Table 4 shows the results of the identifiability analysis technique described by Brun *et al.* (2001). The table shows the parameters in decreasing order of δ^{msqr}. Only those parameters with a δ^{msqr} of at least 10% of the maximum of δ^{msqr} are retained for further analysis. The first parameter (with highest value of δ^{msqr}) was selected and additional parameters added as long as the value of γ remained below 10. Other parameters were skipped. If γ was close to 10 after adding a new parameter, it was checked if adding a parameter with a slightly smaller value of δ^{msqr} led to a significantly smaller value of γ. If this was the case, the other parameter was selected instead. In some cases, as shown for layout 4, the selection of a new parameter was not unique: to the selection in the first column, the parameter K_I could be added (second column) or one of the parameters X_{CON}, $k_{resp,ALG,20}$ or $k_{resp,H,aer,20}$. The first parameter is more sensitive but leads to a larger value of γ than the second choice.

In Table 5 the results for the determinant technique proposed by Weijers and Vanrolleghem (1997) are summarised. In order to make the application of the determinant technique transparent and comparable to the other technique, the same scaling was used as described by Eqs. (2) and (5). In all cases we obtained parameter sets of given size that contained the parameters identified for the smaller subset sizes. For this reason in Table 5 only the additional parameter is listed in each case. Horizontal lines divide values for γ below 10 (interpreted as identifiable), and below 15 (interpreted as possibly identifiable) from larger values of γ (interpreted as not identifiable). We did not apply the condition number technique also proposed by Weijers and Vanrolleghem (1997) (see Eq. (5)), because we do not expect meaningful results only from the shape of the confidence region without reference to its size and orientation. For the current application, this technique would lead to

Table 4 Results for the values of δ^{msqr} and γ for the experimental layouts 1–4. The layouts 5–7 essentially lead to the same results as layout 4. The row "offset" contains the value of γ corresponding to the selected parameters (marked with "x"). The other values of γ correspond to the set consisting of the marked parameters plus the current one

Layout 1			Layout 2			Layout 3			Layout 4				
	δ^{msqr}	γ		δ^{msqr}	γ		δ^{msqr}	γ		δ^{msqr}	γ	γ	γ
Offset:		**1.7**	**Offset:**		**2.2**	**Offset:**		**2.5**	**Offset:**		**2.4**	**10.3**	**5.5**
X_{ALG}	0.124	x	X_{N1}	0.119	x	X_{N2}	0.126	x	X_{N2}	0.110	x	x	x
K_I	0.081	14.0	X_{ALG}	0.109	x	X_{N1}	0.116	x	X_{N1}	0.101	x	x	x
$k_{gro,ALG,20}$	0.052	197	K_I	0.079	13.7	$K_{NO2,N2}$	0.092	53	$K_{NO2,N2}$	0.080	53	53	53
X_H	0.048	x	$k_{gro,ALG,20}$	0.049	116	X_{ALG}	0.091	x	X_{ALG}	0.080	x	x	x
X_S	0.017	12.8	$k_{gro,N1,20}$	0.048	355	K_I	0.066	13.0	K_I	0.058	10.3	x	13.9
X_{N1}	0.015	11.2	$K_{NH4,N1}$	0.047	26.9	$k_{gro,N2,20}$	0.053	343	$k_{gro,N2,20}$	0.046	329	329	333
$k_{gro,H,aer,20}$	0.014	51	X_H	0.038	x	$K_{NH4,N1}$	0.047	12.7	$K_{NH4,N1}$	0.041	12.7	13.4	12.7
$k_{hyd,20}$	0.014	10.9	X_{CON}	0.023	43.6	$k_{gro,N1,20}$	0.047	311	$k_{gro,N1,20}$	0.041	301	309	329
			$k_{resp,ALG,20}$	0.019	116	$k_{gro,ALG,20}$	0.041	52	$k_{gro,ALG,20}$	0.036	18.4	22.2	130
			$k_{resp,H,aer,20}$	0.018	39.7	X_H	0.031	x	X_H	0.027	x	x	x
			$K_{NH4,ALG}$	0.016	x	X_{CON}	0.019	18.6	X_{CON}	0.017	5.6	13.9	47.9
			X_S	0.012	12.3	$k_{resp,ALG,20}$	0.016	19.9	$k_{resp,ALG,20}$	0.014	5.5	13.9	x
						$k_{resp,H,aer,20}$	0.015	19.1	$k_{resp,H,aer,20}$	0.013	5.4	14.1	64
						$K_{NH4,ALG}$	0.013	x	$K_{NH4,ALG}$	0.012	x	x	x

Table 5 Parameter sets with the largest value of of all parameter subsets of given size together with the values of $\sqrt[2n]{\det}$ and γ for layouts 1 to 4. Again layouts 5–7 essentially lead to the same results as those for layout 4

Setsize	Layout 1			Layout 2			Layout 3			Layout 4		
	new par.	$\sqrt[2n]{\det}$	γ	**New par.**	$\sqrt[2n]{\det}$	γ	**New par.**	$\sqrt[2n]{\det}$	γ	**New par.**	$\sqrt[2n]{\det}$	γ
1	X_{ALG}	0.57	1.0	X_{N1}	0.77	1.0	X_{N2}	1.00	1.0	X_{N2}	1.01	1.0
2	X_H	0.31	1.7	X_{ALG}	0.74	1.0	X_{N1}	0.88	1.5	X_{N1}	0.90	1.4
3	K_I	0.15	14.0	X_H	0.47	1.6	X_{ALG}	0.82	1.5	X_{ALG}	0.83	1.5
4	X_{N1}	0.079	15.2	$K_{NH4,ALG}$	0.30	2.2	X_H	0.57	1.8	X_H	0.58	1.8
5	$k_{hyd,20}$	0.050	18.2	K_I	0.21	13.7	$K_{NH4,ALG}$	0.38	2.5	$K_{NH4,ALG}$	0.39	2.4
6	$K_{NH4,ALG}$	0.029	26.8	$K_{NH4,N1}$	0.13	27.6	K_I	0.28	13.0	KI	0.30	10.3
7							$K_{NH4,N1}$	0.21	15.2	$K_{NH4,N1}$	0.22	13.4
8							$K_{NO2,N2}$	0.14	94.1	X_{CON}	0.17	14.8
9										$K_{NO2,N2}$	0.13	93.5

significantly different results as the two other techniques; e.g. growth rates would be selected instead of bacterial concentrations although they have a smaller prior uncertainty and similar sensitivity functions). Such deviating results were also found in the subset selections performed on ASM1 by Weijers and Vanrolleghem (1997).

Note that the subset selection results presented in Tables 4 and 5 are remarkably similar. This means that the determinant technique makes a similar weighting of the two criteria δ and γ as the systematic application of the technique by Brun *et al.* (2000). In other words, the determinant criterion can be used as a simple technique that could allow automation of this selection procedure. Parameter sets with slightly lower values of the determinant would represent alternative identifiable parameter sets (not shown in the table).

The results clearly show how the size of the identifiable parameter subset increases with additional measurements for layouts 1–3 (from 2–3 to 5–8). However, the addition of four

more measured variables in the layouts 4–7 does only to a very small degree increase the size of the identifiable parameter subset. The essential parameters identifiable from the data are bacteria and algae concentrations responsible for primary production, nitrification (2 steps) and respiration. In addition, depending on the parameter values and the measurement accuracy, some half-saturation concentrations may be identifiable.

These poor identifiability results are not very astonishing because the dominating processes can be described by 5–8 parameters and are identifiable from oxygen, ammonia and nitrite measurements. The dominating processes in the studied river are primary production, respiration and two nitrification steps. The additional measurements give information on process stoichiometry, which was assumed to be known in the present application. The results from the identifiability analysis imply that a large effort is necessary in collecting highly informative dynamic data in order to make a calibration of RWQM1 possible. Experimental design techniques (Vanrolleghem *et al.*, 1999) may support the design of adequate measuring campaigns.

Uncertainty analysis

Figure 1 shows model predictions and uncertainty estimates using prior uncertainties from Tables 1 and 2 and assuming zero uncertainty for the five identifiable parameters. With the exception of nitrite, the uncertainty bounds using linear error propagation are not extremely different from those based on Monte Carlo simulation. Estimation of the five identifiable parameters leads to a significant reduction in prediction uncertainty. However, prediction

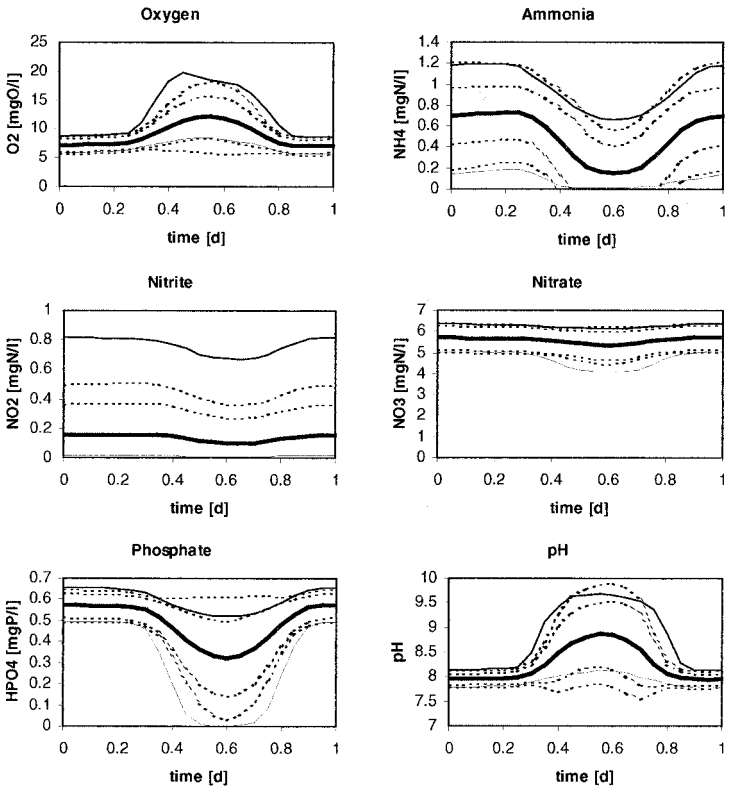

Figure 1 Downstream (after 10 km) model results (thick solid line) and uncertainty ranges: 95% prior uncertainty estimates with linear error propagation (outer dashed lines), 95% prior uncertainty estimates for lognormal distributions calculated by Monte Carlo simulation (thin solid lines), and 95% uncertainty estimates (inner dashed lines) calculated with linear error propagation assuming no uncertainty for the 5 identifiable parameters

uncertainty still remains very large (with the exception of nitrate that is not significantly affected by the conversion processes).

Conclusions

Both identifiability analysis techniques used in this study can easily be used and lead to nearly the same results. The collinearity index used by Brun *et al.* (2000) seems to be a sensitive indicator of nonidentifiability. The determinant of the Fisher information matrix used by Weijers and Vanrolleghem (1997) seems to be an excellent ranking tool for identifiable parameter sets. However, it can only be used if results and parameters are carefully made nondimensional. The scaling factors used for this purpose should always be reported.

Measurements of oxygen, ammonia and nitrite over a few days in a rather steady state river system where the only dynamics are induced by the diurnal variation in light intensity lead to the identifiability of only about 5–6 kinetic parameters of a simplified version of the river water quality model no. 1. The parameters that could be identified are the biomass densities (assumed to be constant) and some half-saturation concentrations. The availability of data on nitrate, phosphate, pH, dissolved ions and conductivity does not significantly increase the number of identifiable kinetic parameters (5–8) for the boundary conditions used in this study. Nevertheless, such measurements are useful in order to identify stoichiometric parameters and to test the model structure (which was assumed to be correct in the present analysis). More information can only be gained by improved experimental designs, for instance under more dynamic conditions and/or with more difficult measurements, such as the quantification of benthic biomass. Also, microcosm experiments in the laboratory may yield additional information to support the calibration of the RWQM1. An uncertainty analysis of model results based on rough estimates of prior uncertainties revealed a very large uncertainty in model predictions, which could only partially be decreased with the measurements described above.

The result obtained in this simple, hypothetical case study challenges the use of complicated river water quality models as quantitative predictive tools without comprehensive and well-designed measuring campaigns. In particular, more knowledge on the dynamics of benthic biomass is necessary; an aspect that was not even considered in this study. Despite of those problems, the models may still be useful as knowledge archives, for didactical purposes and for qualitative or short-term predictions.

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