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Model structure sensitivity of river water quality models for urban drainage impact assessment

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Abstract: Numerical modeling of physicochemical conditions in rivers influenced by urban drainage and other pressures is increasingly used as supportive method for an integrative environmental impact assessment. In various European countries, protocols for water quality based impact assessment (WQA protocols) are in use, of which many propose the use of water quality models. Despite the increased effort to study uncertainty issues in river water quality modeling in recent years, identifying and differentiating model structure uncertainty remains a challenging task. This study elaborates upon a key conflict in model development: the need to simplify and to still ensure structural adequacy to obtain reliable modeling results. The paper evaluates the adequacy of diverse river water quality modeling approaches when subjected to a changing model structure. This evaluation is achieved by applying a set of calibrated candidate models to two different river case studies under varying pollution conditions. The term 'model structure sensitivity' is introduced to quantify the output variation as a result of a changing model structure. Sensitivity is here, in contrast to previous works, positively interpreted as model flexibility. The study illustrates that the interdependence between model sensitivity and model error is conditional upon complexity, but model adequacy differs depending on the pollution dynamics in the modeled system. Results show that model structure uncertainty has a composite nature: effects related to transport and conversion model contribute with varying shares. Two actions should be considered to improve model structure characterization: i) use of a variety of model structures combined with an analysis of structure and parameter sensitivity, and ii) acquisition of high-resolution reference data to capture varying pollution load dynamics.

***Keywords**:* Candidate models; environmental impact assessment; model structure sensitivity; urban drainage impacts; river water quality modeling

1 INTRODUCTION

Today development and optimization of urban drainage systems is driven by a two-sided objective: to guarantee urban drainage safety while preserving the ecological compatibility with regard to receiving water quality. The idea of considering aquatic ecology is clearly put forward by the implementation of the EU WFD (Europe) and the Clean Water Act (U.S.) addressing emission and water quality based aspects in the same manner ('combined approach'). To handle these requirements in urban drainage management practice, various protocols for water quality based impact assessment (WQA protocols) have been established, mostly on a national basis (cf. Blumensaat et al., 2012). In this respect, numerical models are increasingly used to describe the present water quality status and to predict future situations, e.g. driven by a globally changing environment (climate, demographic, societal change). Misled by the apparent easiness of the usage, water quality models are often applied disregarding uncertainties associated with the model-based assessment of aquatic ecosystems.

The need for a systematic uncertainty assessment in the field of water quality modeling is particularly relevant against the background that the number of aspects related to water quality based analysis of urban wastewater systems has increased towards more complex approaches with a generally higher level of uncertainty (Freni et al., 2009). Besides rather well established methods to estimate input and parameter uncertainty (e.g. through a global sensitivity analysis), the assessment of model structure uncertainty plays an extra role, independent of the modeling purpose (hydrology or quality). Here a key conflict in model development is exposed: balancing structural adequacy and model complexity to minimize the total modeling error of the model application. Snowling and Kramer (2001) refer to this interdependence as structural uncertainty in a simulation model depending on model complexity, sensitivity and error.

In practice however, this aspect is often disregarded due to its intangible character. A foremost (and also legitimate) objective of modelers is to reduce complexity and to develop and use models that are as simple as possible. A critical point is that such simplification is often solely driven by the constraint that computationally demanding approaches, e.g. probabilistic concepts for individually quantifying parameter uncertainty, can be applied. The objective of this study is to discuss the relationship between the model sensitivity (flexibility), error and complexity in order to allow the modeler to make an informed decision, particularly with regard to a water quality based assessment of urban drainage impacts.

2 LITERATURE REVIEW

Typically modeling uncertainty is attributed to three main sources: uncertainty in model input data, parameter uncertainty, and model structure uncertainty. Having recognized that differentiating various uncertainty sources appears problematic, Refsgaard et al. (2007) formally distinguish modeling uncertainty in: i) context and framing, ii) input uncertainty, iii) model structure uncertainty, iv) parameter uncertainty, and v) model technical uncertainty. More recently Deletic et al. (2012) suggest a revised concept introducing the term "calibration uncertainty" whereas model parameters are given a central role as they are, according to the authors, impacted by all different uncertainty sources.

Model structure uncertainty (MSU) is typically interpreted as deficiencies in the model concept, such as the disregard of key processes or scaling issues, both potentially introduced due to the need to simplify. MSU can be considered a *conceptual uncertainty* caused by an incomplete understanding and a simplified description of modeled processes (Refsgaard et al., 2007). According to Oberkampf et al. (2004), MSU is only related to the mathematical equations that are chosen to describe the system of interest.

Despite its known relevance, little attention is paid to uncertainty attributed to model structure in most modeling studies (Refsgaard et al., 2006). Several studies emphasize the general relevance (Deletic et al., 2012; Engeland et al., 2005) but few actually attempt to estimate the impact of structural uncertainties on modeling results. McIntyre (2004) underlines the difficulty to avoid structural uncertainty particularly in river water quality models due to the complexity and the variability of boundary conditions of the modeled systems. Underlining the fact of interdepending uncertainties, the same author states that model structure errors increase the risk of distorted parameter estimations, which consequently results in an underestimation of the total model error. In the same line Reichert and Omlin (1997) state that disregarding structural uncertainty leads to an underestimation of total uncertainty in the model prediction. Further studies discuss i) model sensitivity towards specific processes (Vandenberghe et al., 2006), ii) corresponding uncertainty sources (van Griensven and Meixner, 2006; Lindenschmidt, 2006) and iii) strategies for assessing structural, i.e. conceptual uncertainty (Refsgaard et al., 2006) by applying water quality models of different complexity and scale (tools used: QUAL2E, RWQM1, WASP, SWAT). Even though having a different focus, the studies concordantly conclude that a major problem with distributed water quality modeling (transport and conversion) lies in the structure of these models.

Overall, it can be concluded i) that individual sources of uncertainties are strongly interrelated and can therefore not be considered separately and ii) that there is a clear trend in acknowledging modeling uncertainty as a complex problem due to this interdependence. In water quality modeling studies, the issue of model structure uncertainty is more and more understood, increasingly better defined, but still very hard to identify and hence, especially in practice, very often neglected.

3 METHODOLOGY

3.1 Assessment framework

The here proposed sensitivity assessment is based on a comparative analysis of model outputs (based on the idea of alternative candidate model structures; cf. Beck and van Straten, 1983) reflecting the sensitivity due to model structure changes.

Modifications are attributed to the conversion model concept and to transport model concept on the one hand and to multivariate changes of selected model parameters on the other hand (see Fig. 1). For this, three different water quality models are applied to and calibrated for two different real-life case studies (i.e. rivers), where each river is subjected to two different pollution load situations. Model input and reference data remain unchanged for each case and each loading situation; data uncertainty is, relatively seen, not decisive as it does affect all simulations in the same manner. Still, this framework does not account for measurement uncertainty associated with measured data. Simulations for each river and loading situation are performed under defined boundary conditions and for a period of 4 days with a computation step size of 10s. Different model implementations are grouped according to the type of model structure that is changed: i) the conversion model, ii) the approach describing physical re-aeration, iii) the longitudinal and iv) cross-sectional representation of the riverbed (see Fig. 1).

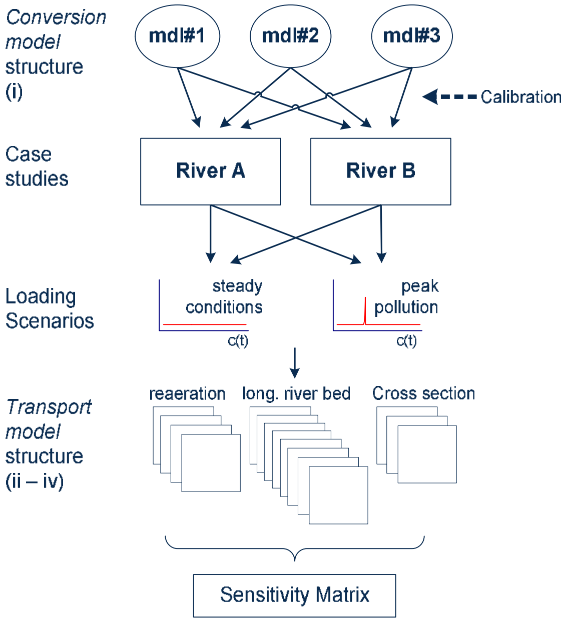

Figure 1: Model structure sensitivity analysis

In a second step (not shown in Fig. 1), the parameter sensitivity is examined through multivariate changes of relevant model parameters. The resulting variation is then confronted with the sensitivity resulting from structure changes (sensitivity matrix).

<u>*Evaluation criterion:*</u> Emphasis is put upon dissolved oxygen (DO), representing a relevant indicator for short-term and delayed impacts. Modeled time series are analyzed focusing on *global* and *local DO minima* – see example in Fig. 2. To address potentially irregular extreme concentrations, e.g. due to numerical instabilities, the 1%ile DO concentration is used as representative evaluation criterion (single-objective – see Fig. 3). This criterion is evaluated for each simulation run resulting in a *range of values* for all simulations, suggesting that this variation serves as indicator for (model structure and parameter) sensitivity. It should be noted that in this study the focus is *not* primarily on the absolute magnitude of oxygen dissolved in the bulk liquid. The main stress is put upon a comparative analysis of the DO minima level and its variations.

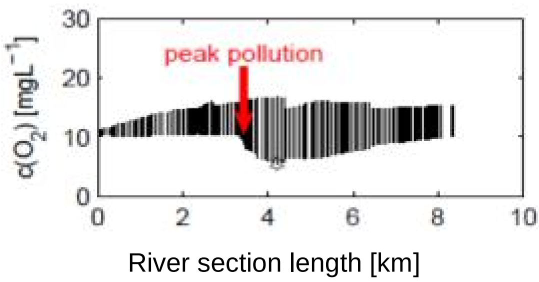

Figure 2: DO concentrations (incl. daily variations) along the river course. Local DO minimum is indicated with '☼'.

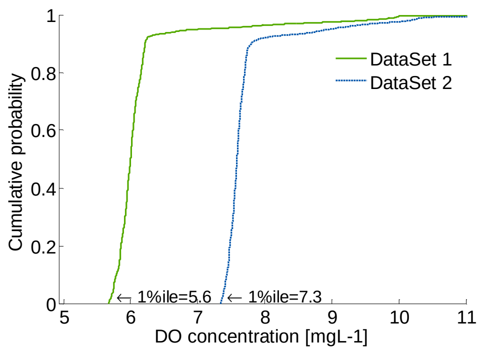

Figure 3: Cumulative distributions of DO concentration including the 1%ile.

3.2 Model error

Anchor of the sensitivity analysis are six calibrated model implementations applying three different conversion models to each of the two river case studies (see Fig. 1). The model error is quantified for calibrated implementations by comparing observed and simulated DO concentrations for a defined analysis period (see Fig. 3). To measure the 'Goodness of Fit' the root mean squared error (RMSE) is applied. Validation against measured reference data has been carried out for all implementations *before* subjecting them to systematic changes.

3.3 Model sensitivity - Definition

Model structure sensitivity: The model's structure sensitivity (i.e. variations of the model output as a result of changes made to model structure) is estimated by quantifying the range of 1%ile DO concentrations for each group of implementations that is subjected to a particular model structure change. In case simulations reveal a large range within a group, high structure sensitivity can be assumed, likewise underlining a model's flexibility. This flexibility may be exploited as it improves model adequacy, i.e. the model better corresponds to reality.

Parameter sensitivity: A model is considered uncertain with regard to its parameters in case the prior knowledge on the parameter(s) is poor (wide distribution) and the posterior correction based on reference data (calibration) is poor if no or little reference information is available. Knowing the sensitivity of a modeling output due to parameter variations alone prior to calibration, helps the modeler to determine which parameters are the key drivers of a model's result. Measured reference data is needed to identify if the output range matches reality. In case no data is available one cannot judge whether the *'a priori'* defined parameter range (e.g. taken from literature) covers reality.

3.4 Model structure changes (transport model)

The model's structure sensitivity is differentiated into i) sensitivity related to the transport model and ii) sensitivity stemming from the conversion model complexity. Factors that influence the transport model structure refer in particular to the spatial representation of the riverbed channel but also to the physical reaeration modeling approach. Univariate changes (changes to one particular structure type while leaving the remaining model structure in the original state) regarding i) the reaeration model (Churchill et al., 1962; Owen & Gibbs, 1964; O'Connor-Dobbins, 1956; Wolf, 1974), ii) the spatial resolution along the river reach and iii) the detail of representation of the cross section profiles (detailed, parabolic, trapezoidal) have been applied to each river for each WQ modeling concept.

3.5 Model structure changes (conversion model)

Model structure sensitivity stemming from conversion models of different complexity is analyzed. Here, three modeling concepts, different in complexity and characteristics, have been selected to cover at least a wider 'slot' of the diversity of available modeling approaches (see Tab. 1). The underlying concept for water transport (hydraulics) is based on the St. Venant approach and remains unchanged for all simulations.

Table 1: Comparison between different modeling concepts used.

	Model #1	*Model #2*	*Model #3*
Reference	Streeter and Phelps (1925)	Lijklema et al. (1996)	Reichert et al. (2001) - *constX*
Cause-effect rel's	Effect focused	Cause focused	Cause focused
Biomass	No	Suspended	Sessile
Structure	Fixed	Fixed	Adaptive
Complexity	Low	Moderate	High
Processes	Degradation of organics	Degradation of organics, nitrification	Degradation of organics, nitrification
No. of parameters	1	11	26
Mass balance	Not closed	Not Closed	Closed

3.6 Model calibration

Model fitting with regard to the conversion model has been accomplished by manually adapting the degradation rate k_1 in the Streeter-Phelps approach (model#1), k_{dr} in the approach of Lijklema et al. (1996) (model#2) and the constant biomass densities (X_n) in the constX approach (model#3). The RMSE is used as objective function. For *River A*, reference data were obtained from regular monthly measurements at different locations (2004 – 2007; LfULG, 2009), whereas for *River B* detailed online monitoring was conducted (6 months field campaign; hourly resolution; see Blumensaat et al., 2008).

3.7 Case study characteristics

The simulation analysis has been conducted for two different rivers to cover different river characteristics and scales: River A, a small, coarse material-rich, siliceous highland creek (average base flow: 0.03 m^3s^{-1}; course length: 8.4 km) and River B, a section of a medium-scale, coarse material-rich, siliceous highland river (base flow: 0.3-1.0 m^3s^{-1}; course (section) length: 128 (8.5) km). The examined river sections are both affected by various urban drainage impacts: treatment plant effluent discharges, combined sewer and stormwater overflows, which is why both sites were previously subject to detailed field and model investigations (cf. Blumensaat et al., 2008; Blumensaat et al., 2009).

3.8 Loading scenarios and model input

Model-based analysis is carried out for two distinct loading scenarios to differentiate the impact of influencing factors under changing pollution dynamics: a. unpolluted, b. peak pollution. The scenario ‘unpolluted’ describes a steady dry weather situation without any pollution impact, while the ‘peak pollution’ scenario mimics a short-term pollution shock load, e.g. induced by a combined sewer overflow (CSO), into an unpolluted stream. Background conditions in River A stem from regular monthly grab sampling of the environmental authority (2004 – 2007; LfULG, 2009), while a long-term online monitoring campaign forms the basis for background water quality in River B (cf. Blumensaat et al., 2009). Characteristics of the ‘pollution peak’ scenario are derived from CSO events actually monitored for case study B (online monitoring of 30 spill events). The analysis is additionally verified by a large data set on CSO data published in Brombach et al. (2005).

3.9 Parameter variation

The sensitivity stemming from parameter variations is quantified and compared with model structure sensitivities to rank different sensitivity sources in an overall context. This comparison is based on the assumption that both parameter value ranges and different model structures are realistic and based on the same knowledge base as expressed in literature. The quantification of parameter sensitivity using the Monte-Carlo (MC) method has been split into two phases:

1. Univariate change of organic matter degradation rates, as this is the only model parameter that is equally used in all modelling concepts. 1000 parameter values were randomly sampled from a triangular distribution.
2. Multivariate change of the four most relevant model parameter in model#2 (k_{d1}, k_{d2}, k_n, β – see Lijklema et al., 1996) and the five most influential parameters in model#3 (sensitivity identified in Reichert and Vanrolleghem, 2001) to estimate the main share of the total parameter uncertainty.1000 parameter sets were sampled from multiple triangular distributions - parameters were assumed non-correlative.

Key values for distributions are taken from Lijklema et al. (1996) and Reichert & Vanrolleghem (2001).

4 RESULTS AND DISCUSSION

4.1 Calibration results

For calibrated model implementations (both Rivers) the model error is quantified through the RMSE between observations and simulated data (see results in Tab. 2).

Table 2: Model error RMSE of calibrated model implementations.

Model Error / Calibration	RMSE in [mg DO L^{-1}] Model#1	RMSE in [mg DO L^{-1}] Model#2	RMSE in [mg DO L^{-1}] Model#3
River A	0.39	0.50	0.63
River B	1.18	1.02	0.78

Considering the low pollution level in *River A*, modeled and observed DO minima are in a very similar range for all three implementations - the model error is similarly low (RMSE: 0.39 – 0.63 mgL^{-1}).

Analyzing the situation in *River B* it becomes clear that model#1 and model#2 fail in realistically describing oxygen depletion phenomena due to peak overflow pollution: oxygen sags are underestimated. While model error differences are numerically still moderate (RMSE: 0.78 – 1.18 mgL^{-1}), it is obvious that, despite calibration, short-term DO dynamics (identified through high-resolution online monitoring) can only be reproduced by the most complex model (model#3).

4.2 Model structure sensitivity – transport model

Fig. 4 illustrates the effects of model structure changes on the DO concentration for individual model implementations (here exemplary for different reaeration concepts). The 'bars' shown in sub-charts in each of the figures show the simulated DO concentration *range*. The upper end of the bar indicates the absolute DO maximum, the lower end the DO minimum (1%ile), whereas in case of the 'peak pollution' scenario (right part in each sub-chart) the 1%ile minimum due to the induced peak pollution pulse is extra indicated through '☼'. Under 'unpolluted' conditions, different re-aeration concepts lead to similar results, i.e. to 'no-effect' as models operate close to full saturation (left-sided part in sub-charts in Figure 4). However, under 'peak pollution', the DO minima vary considerably depending on the reaeration concept applied. Comparing the simulations for the two rivers, it becomes evident that physical reaeration strongly depends on existing hydraulics, i.e. individual bed characteristics. Still, no clear trend can be observed when assessing the performance of reaeration models in different rivers.

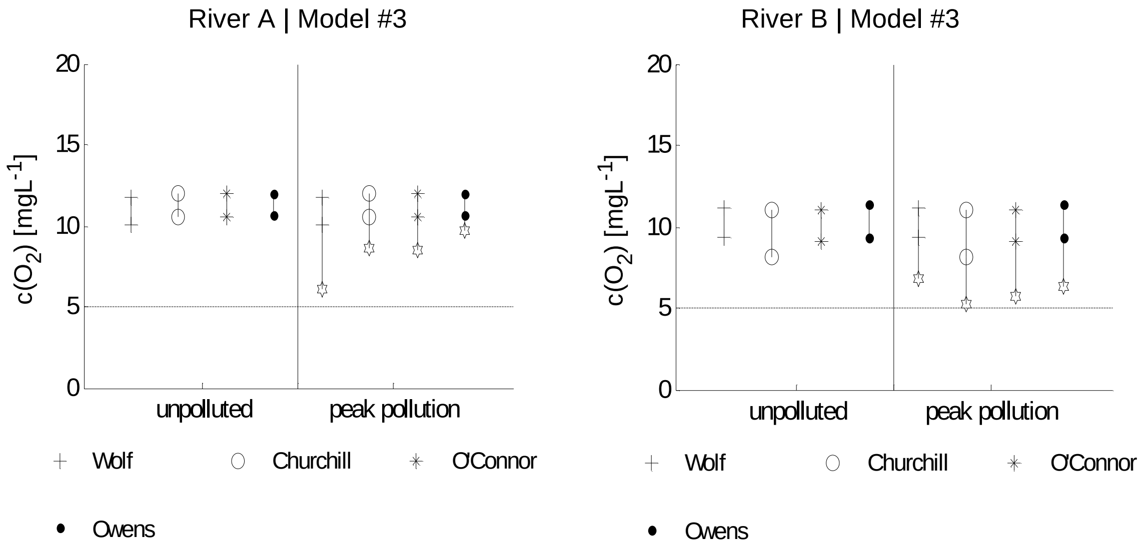

Figure 4: structure sensitivity (reflected by the variability of the DO range) when changing the reaeration concept (here shown for model#3).

4.3 Model structure sensitivity – conversion model

Fig. 5 summarizes results of the model sensitivity analysis by illustrating the modeled variation of the 1%ile DO minima for all different model implementations. Results are visualized in four groups: each of the two rivers is evaluated for unpolluted (upper two rows) and 'peak pollution' (lower two rows) conditions. In each group, model sensitivity stemming from model structure changes (top three) and parameter variations (lower two) is illustrated individually for each of the three conversion models.

Reading Fig. 5 row-wise allows comparing model sensitivities of different conversion models for one particular pollution load situation, while a column-wise evaluation compares model sensitivities for one particular conversion model under different pollution situations. The main findings are:

1. The full scope of model sensitivity becomes only obvious under 'peak pollution' conditions, independent from the conversion model and the case study under consideration. In turn, model sensitivity is generally low for the scenario 'unpolluted', since substrate is limited and conversion rates are rather low, DO levels are close to saturation and structure changes do not significantly affect the oxygen balance. This becomes particularly relevant during the initial model selection process as the full model functionality (i.e. flexibility) may only become obvious under dynamic pollution situations.

Data on dynamic situations are (still) rare, and models are often tested for unpolluted steady state situations in which the complete functionality of the models cannot be overlooked.

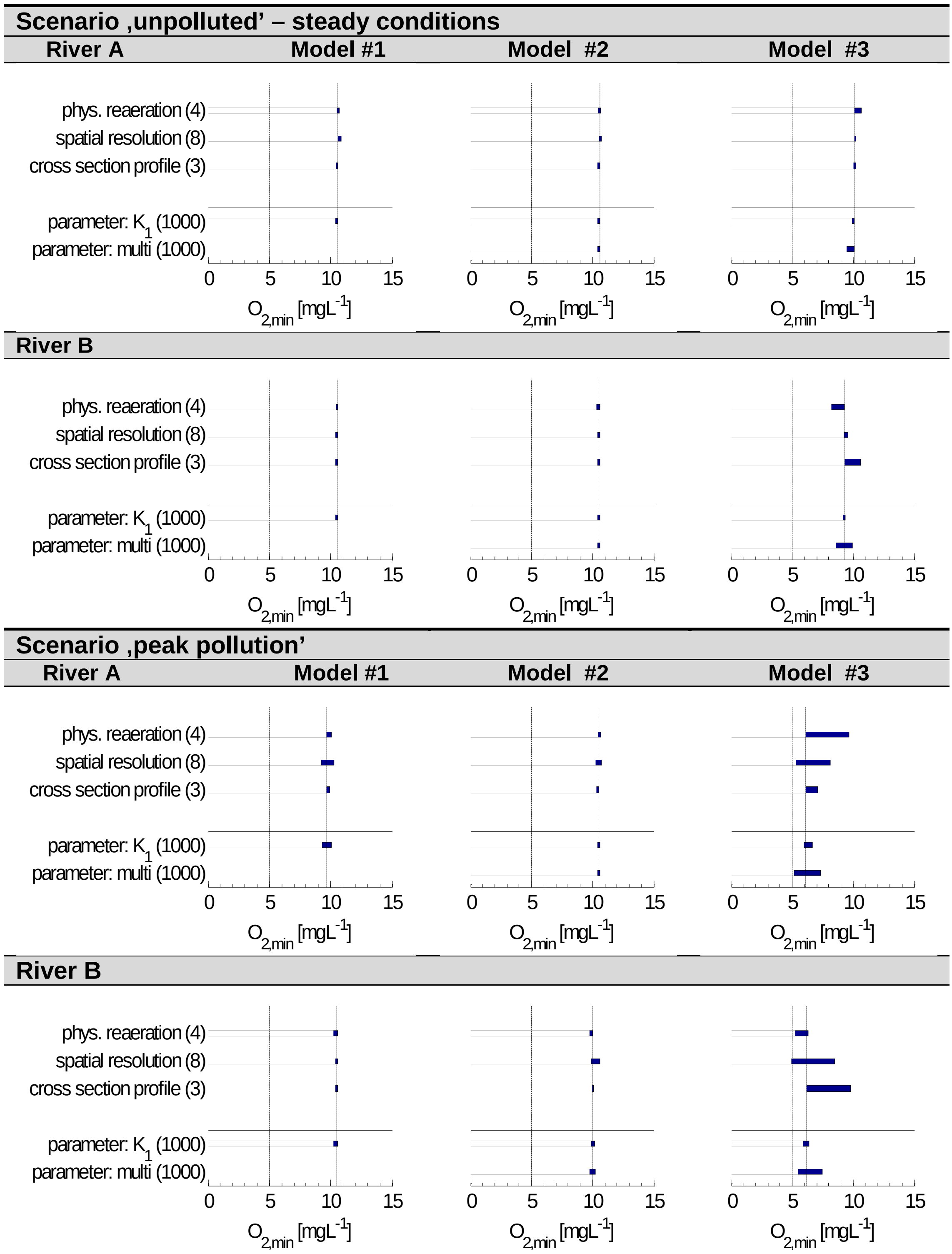

Figure 5: Sensitivity matrix expressing the 1%ile DO range (horizontal bars) for different WQ concepts, different rivers, different loadings. The dashed line (- -) represents an ecologically critical DO concentration (5 mgL^{-1}, LAWA, 1998); the dotted line (…) represents the value of the calibrated reference model in its original configuration.

2. The most complex model (model#3) generally shows a higher sensitivity regarding model structure changes. On the other hand, model #1 and model#2 are rather rigid and inflexible. In fact, DO minima

simulated under 'peak pollution' with the two simpler models are just little lower than for 'unpolluted' conditions. This leads to the conclusion that, even if sufficient reference data is available, model#1 and #2 are extremely difficult to adapt to meet case-study and pollution load characteristics. In case of insufficient reference data, simpler models may just pretend a level of validity, which is not given in reality.

Generally, for all conversion models the highest model sensitivity stems from changes of the resolution of the longitudinal description of the river bed channel affecting the transport of dissolved compounds through the channel system (CSTR approach). While this type of sensitivity is *not* dependent on actual river characteristics, the sensitivity originating from different cross section simplifications and varying reaeration concepts is river specific.

4.3 Parameter sensitivity

Parameter sensitivity typically appears in the same order of magnitude as sensitivity stemming from model structure changes (high structural sensitivity -> high parameter sensitivity). In absolute terms, the sensitivity is the highest for the most complex model (model#3). Comparing univariate changes of individual degradation parameters (k_1, kd_r, k_1), the model sensitivity is generally lower and is in the same range for all analyzed models. Model calibration for simpler models is therefore 'a priori' limited since the 'tuning range' of these concepts is limited.

4.3 Limitations of the study

Despite the different river characteristics, the analysis remains limited since the examined cases represent only a selected range of river types. Conclusions, particularly with regard to large streams, require an extra analysis.

The study solely covers model sensitivity regarding dissolved oxygen as one characteristic indicator for urban drainage impacts. However, further water quality constituents relevant to urban drainage (e.g. NH_3-N, TSS) may need to be similarly examined to cover the full range of model sensitivity.

5 SUMMARY AND CONCLUSIONS

The present study describes and discusses a model-based sensitivity analysis for different river water quality models focusing on the influence of model structure and parameter changes on dissolved oxygen minima. The method coherently addresses the issues of model sensitivity (flexibility), model complexity, and system scale dependency under varying pollution dynamics.

1. The analysis shows that the interdependence between sensitivity and model error is conditional upon complexity, which confirms the findings of Snowling and Kramer (2001) regarding the analysis of groundwater models and Lindenschmidt (2006) regarding WQ modeling of large streams. Hence, it can be concluded that this phenomenon is generally *scale independent*. However: relevance clearly differs depending on the pollution dynamics in the modeled system. The model structure sensitivity is generally higher for the more complex model, and it becomes only obvious under varying pollution.

2. The model error is low for all candidate models under steady unpolluted conditions. Still, the error of simpler models significantly increases under peak pollution, while structure (and parameter) sensitivity remains low. This inflexibility of the simpler models underlines the fact that they appear inadequate to describe effects of pollution dynamics. In turn, the higher sensitivity of the more complex models allows a distinct model adaptation which reduces the model error to a minimum in case adequate reference data exist. The results clearly show that model structure uncertainty has a composite nature: effects related to transport and conversion model contribute with varying shares and partly depend on river characteristics.

3. The study furthermore shows that model structure sensitivity and parameter sensitivity are in the same order of magnitude assuming that different model structures and parameter ranges are based on established knowledge expressed in literature. This leads to the conclusion that analyzing structural sensitivity is as important as the quantification of parameter sensitivity and an isolated quantification of parameter uncertainty (using rather simple models being less demanding in terms of their required computing capacity) is not enough to obtain higher confidence in the modeling result.

Two options should be considered to optimize model structure characterization: i) candidate modeling approaches should be applied including the evaluation of structure and parameter sensitivity, and ii) the acquisition of high-resolution reference data should be foreseen to address varying pollution load dynamics and to so help differentiating different sources of uncertainty (cf. Medici et al., 2012).

The proposed framework should further be applied to examine model structure sensitivity with regard to water quality variables other than dissolved oxygen. Hence, the present work may be seen as a contribution towards a better understanding of the interdependence of model complexity, model sensitivity and structural adequacy in river water quality modeling, which ultimately allows the modeler to make an informed decision.

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