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Conceptual river water quality model with flexible model structure

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ABSTRACT

Physically-based river water quality models are valuable tools for river basin management and planning. However, their long computational times pose many difficulties for applications that involve a large number of model iterations. This paper addresses this problem by developing a faster, surrogate conceptual model based on the detailed reference models. The hydrodynamic information and water quality process equations from different detailed models are considered as ensembles in the developed model. The model conceptualizes rivers using cascades of reservoirs and lumps the advection-diffusion and physico-biochemical processes. We tested the model by comparing its performance for the Molse Neet river, Belgium, with two popular reference models, namely, MIKE 11 and InfoWorks RS. Results show that the conceptual model performs equally well as the reference models, but with simulation time 10^4 times faster. The successful testing of this model opens a development avenue towards problem solving in the context of water quality control and management.

Software availability

Name: COnceptual RIver WAter Quality (CORIWAQ)
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Hardware required: General-purpose computer. We recommend using a high-speed processor and at least 4 GB of RAM
Software required: MATLAB, a C compiler and DHI MATLAB toolbox
Programming language: MATLAB and C
Availability: upon request or through the following website of the Hydraulics Section, KU Leuven (www.kuleuven.be/hydr/pwtools.htm)

1. Introduction

Clean water is an increasing concern to our society because poor water quality both directly and indirectly causes many water-related diseases. United Nations Development Programme (2006) announced that the people with water-related diseases contribute to 50% of hospitalized patients in the world. This type of diseases leads to nearly 20% of all deaths under 5-years old children (WHO/UNICEF, 2009). To keep our surface waters clean, it is crucial to effectively control and manage its quality, which requires quantitative knowledge on water quantity and quality status both in time and space. Information on the water quality status can be obtained from monitoring systems (Shrestha and Kazama, 2008; Haji Gholizadeh et al., 2016). However, such systems are expensive and usually insufficient to cover the high spatio-temporal variability of water quality variables (Bartley et al., 2012; Lessels and Bishop, 2015). An efficient alternative solution is the use of mathematical water quality (WQ) models. Such models give decision makers insights in the cause-effect relationships and guidance in the design of water resources management strategies (GWP, 2013). By comparing simulation results of different scenarios, decision makers can easily derive evidence-based decisions.

Many WQ models have been developed, ranging from lumped conceptual models to more detailed physically-based models, from

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models describing single components of the integrated water system to holistic models (Chapra, 2008). However, simulations obtained by different models do not always lead to similar findings. This is because different models have different model structures, which are based on specific hypotheses and tested for selected case studies. Because of data limitations, validation of the complete model structure is in most cases impossible. For this reason, it would be useful to take into account in the decision making process the uncertainty in the model results as a consequence of the model structure assumptions (Lindenschmidt et al., 2007; Nguyen and Willems, 2016). At current, in most model applications, just one software package is applied, e.g. SWAT (Neitsch et al., 2011), HEC-5Q (Willey, 1986) or InfoWorks ICM (Innovyze, 2012), which involves one fixed model structure. Moreover, the WQ modules in most of the packages only accept the hydrodynamic results of their own packages as input. The InfoWorks package solely allows to import networks and results from HEC-RAS. Meanwhile, MIKE11 ECO Lab (DHI, 2011) permits integration with other hydrodynamic models albeit only after modifications in the source code. This inflexibility does not allow a complete analysis of the uncertainty in the WQ simulation results. Therefore, we plead for the development and application of decision support tools that involve a flexible model structure including different model structures and that allows to modify and combine physico-biochemical processes from different physically-based models.

River WQ models, as many types of models, may involve a detailed representation of the modelled system (detailed physically-based models) or a simplified one (simplified models). Simplified modelling involves the use of a lumped conceptual model that is based on a lumping of the processes in space and conceptualized representation of the most dominant processes (Cox, 2003). For instance, TOMCAT and QUAL2E simulate physico-biochemical processes with non-uniform and steady flow at daily scale (Warn, 1987; Brown and Barnwell, 1987). With the advantage of short computational times, these models allow implementation of sensitivity analysis, parameter optimization and uncertainty analysis, e.g. QUAL2Kw (Pelletier et al., 2006). Lumped conceptual river WQ models have the disadvantage that their processes and parameters are less explicit, hence are less directly linked to measurable system properties. Meanwhile, the detailed physically-based models, e.g. MIKE 11 (DHI, 2011), InfoWorks RS (Innovyze, 2012), CALHIDRA 3.0 (Cardona et al., 2011), simulate the hydrodynamic, advection-diffusion and physico-biochemical processes. The long simulation time poses difficulties on applications that involve huge number of model runs, iterations and/or long-term simulations, such as model uncertainty analysis, auto-calibration, real-time control, optimization, etc. The difficulties are larger for applications in larger river catchments. For instance, a water quality simulation for a 1-year period at a time step of 1 h for a river system with the total rivers' length of 139 km and cross-sections at distances of approximately 50 m takes about 4 days on a standard PC (Keupers and Willems, 2017).

Emulation modelling is known as a low-order approximation of the detailed physically-based models to reduce their computational complexity (Castelletti et al., 2012). In this manner, the most relevant variables are taken into account in the emulator. The variables are identified by data-based or structure-based approaches. In the data-based approach, the variables can be selected by a statistical measure of input-output relationship, e.g. partial mutual information (Bowden et al., 2005; Li et al., 2015) and minimum redundancy maximum relevance (Peng et al., 2005; Hejazi and Cai, 2009). In the structure-based approach, a model formulation is derived for each possible combination of the variable replacement by constants (e.g. Crout et al., 2009; Reichert et al., 2011; Machac et al., 2016). The model performances are evaluated by criteria such as residual sum of squares, Akaike's information criterion and Bayesian information criterion. The advantage of the former approach is that it has much less computational cost. However, the ignorance of physical mechanisms can lead to low accuracies when the sample size is small. Therefore, this paper opts for the structure-based approach, but after simplification of existing model structures in order to reduce the computational times.

Considering the above-mentioned needs of a flexible, physically-based, but reduced complexity model structure with reduced computational time, this paper builds further on the recent advances by the development of the flexible version of the conceptual river water quality model CORIWAQ (COnceptual RIver WAter Quality). CORIWAQ is a hybrid of conceptual and physically-based models to obtain more accurate simulations than the traditional lumped conceptual models, but with shorter computational times than detailed physically-based reference models. Accordingly, hydrodynamic information for CORIWAQ is obtained from detailed physically-based models. The equations used to simulate the biochemical transformation processes in CORIWAQ are taken the same as in the physically-based models. The hydrodynamic characteristics in the CORIWAQ process equations are directly taken from the detailed full hydrodynamic reference models after applying correction factors. Considering the same inputs as the detailed reference models, the lumped model is implemented for the motions of determinant concentrations. The advection and diffusion processes along river segments are conceptualized using a reservoir-type approach. The physico-biochemical processes along the river segments are presented by a set of equations with the incoming concentrations at the first cross-sections and outcoming concentrations at the last cross-sections of the corresponding river segments. With this approach, each river segment is characterized by one time series for each hydraulic characteristic and WQ variable. This approach has been widely used to transform precipitation to runoff (Pedersen et al., 1980; Chow et al., 1988; Weiler et al., 2003; Chetan and Sudheer, 2006; Nourani et al., 2009), groundwater recharge to discharge (Peters et al., 2003) and for river or tidal river or sewer hydraulics (Wolfs et al., 2015; Meert et al., 2016; Wolfs and Willems, 2017). However, there are only few studies on the application of lumped conceptual models for river WQ modelling (e.g. Whitehead et. al 1997; Willems and Berlamont, 2002; Radwan et al., 2003, 2004; Willems, 2008). Two detailed physically-based models, implemented in the software packages, MIKE 11 and InfoWorks RS (hereafter denoted shortly as "RS"), with different numerical schemes and different equations to simulate biochemical transformations, are selected as reference models. This research is a follow-up of the initial CORIWAQ developments based on MIKE 11 (CORIWAQ-MIKE11) by Keupers and Willems (2017). CORIWAQ-MIKE11 was applied to simulate the influence of combined sewage system overflow on river WQ (Keupers et al., 2015) and analyze the global analysis sensitivity of WQ parameters (Keupers and Willems, 2015). In this paper, CORIWAQ has been extended for InfoWorks RS (CORIWAQ-RS). The developed model is tested by simulating the water quality for the Molse Neet river in Belgium and by comparing its results with those obtained in both MIKE 11 and RS. In the calibration stage, the CORIWAQ parameters are calibrated to minimize the misfit between the WQ output of CORIWAQ and the reference models. In the validation stage, the calibrated parameters are used to reproduce the WQ variables and compare with those of the spatially more detailed reference models. The calibration and validation are complemented within different flow conditions, i.e. wet, mean and dry conditions. Finally, how robust the CORIWAQ model is to changes in the process settings, is also tested.