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ORIGINAL ARTICLE

Calibration of QUAL2K Water Quality Model in Pattipul Stream (Saran) with Site-Specific Parameters

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ABSTRACT

The study was aimed to sequential calibration for any water quality model using reach-specific estimates of model parameters, which would aid in the prediction of sophisticated river or stream water quality characteristics and accounts for the heterogeneity of stream reaches as diverse estimates. The QUAL2K water quality model with computing MATLAB software provides sequential estimation of reach-wise parameters using a grid-based weighted mean optimization. The Sheetalpur (Saran) segment of the Pattipul stream is selected as river stretch in this study and observations of DO and BOD are used to calibrate and validate QUAL2K model, where desired performance measures are obtained during the calibration and the validation period. This technique proves superior to the existing methods and also captures the system behavior as systematic and efficient approach. This study is expected to help decision-makers in formulating better reach-wise management decisions and treatment policies by providing a simpler and efficient tool to simulate water quality parameters.
Key words: *parameter estimation, QUAL2K, water quality simulation, pattipul stream*

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INTRODUCTION

The recent vast researches on the water quality modeling software and applications attributed improved focus about the water resources and over-exploitation of river or stream reaches due to the rapid increase in pollution. These issues have lead to the development, modification and review of various river water quality models (Chapra *et al*, 2005; Lazar *et al*, 2012; Lindstrom, 2010). Also, the water quality modeling segment has proved an integral part of water resources and environmental management studies (Chiu *et al*, 2016; Lindstrom *et al*, 2016; Wang *et al*, 2016). The majority of these models have not directly related to any physical system components and also difficult due to many inherent coefficients and rate constants that customize the model for different systems with diverse characteristics. The calibration process is based upon physical data of river system that constrained in water quality modeling studies (Liu *et al*, 2007).

The calibration method employing a trial and error approach in most water quality modeling studies, where various combinations of model parameters are considered until the best fit is obtained which is rapid and effective for small parameter sets with sequential process. The sequential calibration means calibration of the river segments one-by-one and river reaches identified stretches with similar hydraulic characteristics. The reach is river segment with constant water quality characteristics in which model parameters of previous reach is applied to next reach until the calibration of entire river stretches. The advantage of this systematic calibration is that it conserves the

heterogeneity of river stretches with an opportunity to adopt different model parameter values for different river segments. This consideration is more efficient to modeling complex river systems with distinct pollution sources entering at different points along the stretch (Parmar and Keshari, 2012; Sharma and Singh, 2009; Zhang *et al*, 2012).
The present study aimed to develop systematic and sequential calibration of a water quality model considering the heterogeneity of pattipul stream reaches coupled with QUAL2K as a water quality simulation tool (Rehana and Majumdar, 2011; Zhang *et al*, 2012) with MATLAB as computing tool. The critical comparison of the methodology with the existing and popular approaches in estimating model parameters is presented and the performance metrics are discussed for convenience of the future projects.

MATERIALS AND METHODS

The water quality modeling tool QUAL2K was selected for reach-specific parameter estimates to Pattipul stream in which stream stretch is divided into smaller reaches which are further sub-divided into smaller computational elements for internal analysis (Chapra *et al*, 2005) through automatic calibration with MATLAB software. The stream stretch was divided into 10 reaches with consideration about diverse hydraulic features and sites of pollution sources, however, hydraulic and biochemical characteristics assumed to be constant within each reach in initialization and headwater boundary conditions were incorporated in terms of flow and pollution load specifications of river flow at initial reach. Also, the flow and pollution load specifications of drains, which describe the energy and mass transfer within the river reach, were input to the model.
The choice of model parameters in a water quality modeling approach based upon the hydrological and biochemical processes considered for simulation. The simulation of DO and BOD levels in rivers, kinetic interactions among various sources and internal sinks of DO and organic matter in the river play a determining role (Chapra *et al*, 2008). The survey of stream clarified Oxygen re-aeration rate, BOD hydrolysis rate and BOD oxidation rate as important to be considered for calibration in this study.
The specifications about range of the parameters obtained by previous study by Chapra *et al* (2008), USEPA (1985) and Zhang *et al* (2012). The range revealed as 0.02-4.1 (day^{-1}) to oxygen re-aeration rate and 0.02-4.2 (day^{-1}) to BOD hydrolysis rate and BOD oxidation rate in this study. The selected model parameters were scrutinized at a smaller interval of 0.1 within their specified range. In the present study, for calibration of three model parameters, i.e., oxygen re-aeration rate, BOD hydrolysis rate and BOD oxidation rate, at each reach, a total of 77,658 possible combinations (21×22×22) of model parameters were generated. MATLAB was used to generate all possible combinations of model parameters. The performance of each of these combinations in simulating the historic water quality conditions of DO and BOD was analysed using different performance measures. MATLAB provided a platform to develop different user-defined performance measurement functions for calibration.
Three model performance metrics, namely, index of agreement (IOA), correlation coefficient (R) and coefficient of efficiency (E) were considered in this study. IOA is the standardized measure of the degree of error in the model simulations. The IOA closer to 1 indicate better model performance and R is the measure of the degree of linear relationship between the observed and simulated data with an ideal value of 1, whereas E represents the degree of improvement in model simulations from the observations.
Finally, the best parameter combinations for the each reach (r_1) were selected by maximizing the optimization function (OFr) as:

$$OF\mathrm{r}_1 = maximize\ [\{IOA+R+E\}DO\mathrm{r}_1+\{IOA+R+E\}BOD\mathrm{r}_1]$$

The steps were repeated by adding the other segments one by-one, until all the segments were calibrated sequentially. The optimization function (OFri) for the i^{th} reach, in general, is:

$$OFri = maximize\ [\{OF\mathrm{r}_{i-1}+IOA+R+E\}DO\mathrm{r}_i+BODr_i+\{IOA+R+E\}BOD\mathrm{r}_i]$$

The calibration of the whole stretch was thus accomplished, ensuring the heterogeneity of each stretch. For calibration, the average conditions of March–June 2020 were used. The QUAL2K model was validated for average conditions of February 2021. The effectiveness of calibrated model parameters in simulating the historic water quality conditions for the validation period was evaluated using the same performance metrics.

RESULTS AND OBSERVATIONS

Calibration of QUAL2K model: Model parameters obtained after the calibration of all 10 reaches of the study stretch are shown in Table 1.

Table 1: Calibrated model parameters for 10 reaches of Pattipul stream

Reach No	Oxygen re-aeration rate (day-1)	BOD hydrolysis rate (day-1)	BOD oxidation rate (day-1)
1	0.40	0.60	4.20
2	0.20	0.20	0.40
3	1.80	3.00	1.20
4	0.80	3.60	0.80
5	1.20	3.60	4.20
6	1.80	0.60	0.60
7	1.20	0.60	0.60
8	4.10	0.60	4.20
9	3.60	0.60	0.60
10	3.60	1.20	1.20

Performance measures estimated during the calibration period using the best model parameter combination for the entire river stretch are shown in Table 2. Oxygen re-aeration rate (day^{-1}) varies from 0.2 to 4.1, with higher values for latter stretches.

Table 2: Model performance measures for calibration and validation periods

Model performance measures	Calibration period		Validation period	
	DO	BOD	DO	BOD
IOA	0.995	0.980	0.972	0.955
Correlation coefficient (*R*)	0.994	0.961	0.954	0.919
Coefficient of efficiency (*E*)	0.982	0.918	0.904	0.839

Reach-to-reach variation in re-aeration rate may be attributed to a change in variables such as flow velocity, water temperature, etc. BOD hydrolysis rate (day^{-1}) was found to be 0.6 for most of the stretches. However, a maximum value of 3.6 and a minimum value of 0.2 were observed for some segments of the stretch. Similarly, BOD oxidation rate (day^{-1}) varied from 0.4 to 4.2, with most of the reaches taking a value of 0.6. However, a few reaches show a steep increase in BOD oxidation rate as 4.2 (day^{-1}), which then rapidly declined to 0.6 (day^{-1}).

The three model parameters selected in this study were also subjected to local sensitivity analysis to find any dormant parameter and each parameters was varied one at a time within their domain and the corresponding effect on DO and BOD simulation evaluated. The formulated DO and BOD profiles for the calibration period are shown in Figure 1, which indicates an acceptable match between simulated and observed data.

The model performance measures (Table 2) also indicate a good fit in DO and BOD simulations. It is observed that due to huge load discharge from the agricultural fields drain into the Pattipul stream, DO concentration drops drastically from 5.5 mg L^{-1} to 0 mg L^{-1} in the upstream stretches. Reduction in BOD load for the latter part of the stream segment results in lesser consumption of oxygen for pollutants decomposition. Also, higher re-aeration rates in latter stretches increase DO values, which results in a moderate gain in DO at latter stretches.

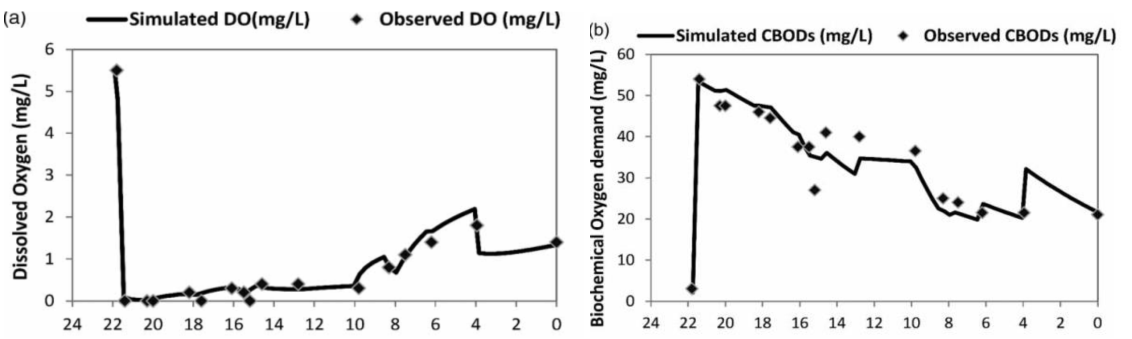

Fig. 1: Simulated (a) DO and (b) BOD profiles for the calibration period.

Except for the upstream segment of the Pattipul stream stretch, the DO concentration falls below 2 mg L^{-1} reaching a negligible DO concentration in most of the reaches. The permissible DO and BOD concentrations for the aquatic ecosystem, i.e., DO values greater than 4 mg L^{-1} and BOD lesser than 5 mg L^{-1} was found to be violated throughout the stream stretch.

The calibrated model was then validated using the data for February 2021. Figure 2 presents the profiles of simulated and observed DO and BOD. The validation results indicate that the calibrated model is able to effectively simulate the system characteristics, along with its heterogeneity.

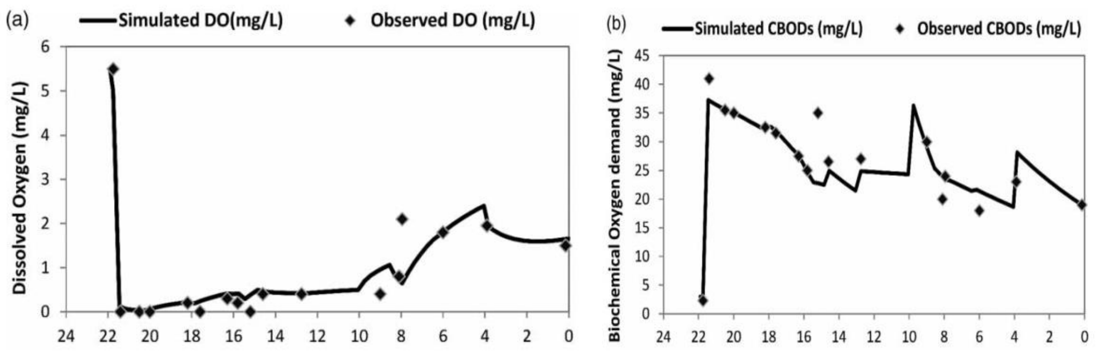

Fig. 2: Simulated (a) DO and (b) BOD profiles for the validation period.

A good agreement is observed between the simulated and observed data of DO and BOD values, with high model performance measures (Table 3). The simulations of the present approach gave the closest match to the observed DO and BOD values for both the periods. Table 6 shows various model performance measures from present and past studies for the selected periods.

Table 3: Comparison of different calibration approaches

References	Water quality parameters	Calibration period		Validation period	
		IOA	R^2	*IOA*	R^2
Walling (2014)	DO	0.999	0.951	0.996	0.932
	BOD	0.842	0.779	0.876	0.733
	DO and BOD	0.921	0.865	0.936	0.833
Parmar and Keshari (2012)	DO	0.976	0.898	0.954	0.897
	BOD	0.843	0.838	0.712	0.849
	DO and BOD	0.910	0.868	0.833	0.873
Present study	DO	0.995	0.988	0.972	0.910
	BOD	0.980	0.924	0.955	0.845
	DO and BOD	0.988	0.956	0.964	0.878

In the present study, DO and BOD have been jointly considered for determination of model parameters, which was the case of other studies too. Therefore, in order to compare different calibration approaches, the collective model performance in simulating DO and BOD should be taken into consideration. The calibration approach of the present study gave the highest IOA values of 0.988 and 0.964 for the periods of calibration and validation periods respectively.

DISCUSSION

The water quality parameters was tested with QUAL2K modeling approach with sequential calibration techniques for different reaches of the Pattipul stream in this study which showed most prominent variation in oxygen re-aeration rate followed by BOD oxidation rate and BOD hydrolysis rate. The variations in BOD hydrolysis rate and BOD oxidation rate along different stretches of the river can be attributed to (i) the difference in biochemical characteristics of pollution loads contributed by different drains and (ii) variations in water temperature (Chapra *et al*, 2005). The BOD decay (oxidation and hydrolysis) rate depends on the nature of the organic matter added to the river, which in turn depends on the source of organic matter (Chapra *et al*, 2005).

Walling (2014) also observed an increase in the re-aeration rate for latter stretches. The increase in oxygen re-aeration rate for latter stretches may be attributed to an observed steep temperature increase in the downstream of river reaches. Previous studies on the Yamuna River have also reported that re-aeration rate (day^{-1}) varied from 0.02 to 4.0 (Paliwal *et al*, 2007; Parmar and Keshari, 2012; Singh *et al*, 2007).

The highest R2 values (0.964 and 0.878) were observed in the present study followed by Parmar and Keshari (2012) and Walling (16). Therefore, on an overall scale, the model parameters of the present study simulated DO and BOD better than previous studies for both the analysis periods. Improvements in the performance measures of the present approach, when compared with those from previous studies, may be attributed to the consideration of heterogeneity of stream reaches while determining model parameters for the entire stream stretch. In Pattipul stream, drains are the major contributor of organic matter and carry pollutants from different domestic or agricultural sources. The decay rate of organic matter from these domestic or agricultural sources would necessarily vary. Therefore, the BOD decay rate should not be conveniently assumed to be constant throughout the stream stretch. This is equally applicable in the case of other parameters.

The proposed technique offers a local calibration approach in which the river reaches are individually calibrated in sequence. In the past, automated calibration techniques proposed by various studies offered a global method of calibration i.e., the whole stretch was calibrated together. The proposed technique offers a simpler approach to determine the model parameters for simulating river water quality conditions.

It is important to note here that the number of model parameters selected for calibration of the water quality model does not constrain the utility and applicability of the proposed framework. However, the inclusion of greater numbers of model parameters would not only augment the complexity and execution time of the calibration process, but might also introduce identification problems. Therefore, it is suggested to identify the parameters playing a negligible role and exclude them from the calibration process. The final selection of the best-fitting model parameters largely depends on the user-specified ranges of model parameters. Therefore, it is essential to accurately specify the ranges of model parameters selected for calibration. Inclusion of very broad ranges of model parameters would merely add to the complexity and time-consumption factors, without benefitting the quality of the results.

Conclusion

The pollution study was applied to simulate the water quality characteristics of reach-specific behavior by considering different parameter values for different stream reaches.

A sequential calibration technique was proposed to consider the heterogeneity of river reaches while determining model parameters in water quality modeling studies. Three model parameters, namely, oxygen re-aeration rate, BOD hydrolysis rate and BOD oxidation rate were considered in the calibration process. The effects of other parameters such as nitrification rate, phytoplankton respiration and growth rate, benthic algal growth and respiration rate, zooplankton respiration rate, zooplankton death and excretion rate, phytoplankton death rate and benthic algal death rate were not considered for DO and BOD simulation, because they were found to have a negligible role in the present study region. A sensitivity analysis of model parameters can be adopted to choose the major parameters affecting the DO and BOD simulations.

The present calibration approach is data-intensive and needs water quality data downstream of each river reach. The approach also assumes the data to be error-free for every reach and selected parameters only play a significant role in DO and BOD simulation process over the study stretch. The range of selected model parameters derived in the present study is specific to study region and their upper or lower bound may vary for other regions. In the present study, weighted average optimization function was adopted, in which some of its component objectives fit better than others. Nevertheless, the proposed approach is generic and can be implemented to calibrate water quality models of any river stretch for any number of model parameters. The step-wise framework of the proposed approach helps in setting up the structure and considering the heterogeneity of reaches. The proposed approach substantially improves the efficiency of the water quality model by closely replicating the physical system, which in turn aids in the efficient management of water resources and in deriving reliable treatment policies for any river stretch.

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