Research Journal of Recent Sciences ISSN 2277-2502
Vol. **3(6),** 6-14, June **(2014)** *Res.J.Recent Sci.*

Application of QUAL2Kw for water quality modeling in the Tunggak River, Kuantan, Pahang, Malaysia

Hossain M.A., Sujaul I.M. and Nasly M.A.[*]
Faculty of Civil Engineering and Earth Resources, University Malaysia Pahang, Kuantan, MALAYSIA

Available online at: www.isca.in, www.isca.me
Received 2nd September 2013, revised 20th November 2013, accepted 11th December 2013

Abstract

The Tunggak River receives waste water from the Gebeng industrial estate (GIE) and from some agricultural and homestead areas in Kuantan, Malaysia. Discharges of industrial effluents containing conventional and non-conventional pollutant with degradable organics and nutrients are the major cause of water quality deterioration in this river. Degradable organic and nutrients have resulted in decrease in DO concentrations along the river. With the objective of modeling of the water quality of the river a one- dimensional river and stream water quality model QUAL2Kw was calibrated and confirmed using the data for the period of 2012-13. With some exceptions it represented the collected data quite good. Simulation of various water quality constituents was done applying the model during dry and wet season. The result shows that the DO concentration was very low in all parts of the river. BOD and COD was very high compare to standard level of Malaysia. Due to industrial wastewater the pollution was high and without taking improve management based on the simulated results, the scenario will not change.

Keywords: QUAL2kw, Tunggak river, simulation, dissolved oxygen, calibration, water quality.

Introduction

The anthropogenic activities like industrialization homestead and agricultural practices introduces significant amount of organic matters and nutrients into the river flow that resulted contamination of surface water[1]. Pollutants in degradable wastewater caused decrease in dissolved oxygen due to their metabolism by the action of microorganism and other biota; chemical oxidation of reduced pollutant and plant respiration also results reduction in DO concentration[2,3],[4]. Water flow is influencing the availability and reduction of dissolved oxygen too; decreasing is clearly visible during low flow periods. It is essential to maintain the threshold level of the key parameters like dissolved oxygen (DO), carbonaceous biochemical oxygen demands (CBOD), ammoniacal nitrogen (NH_3-N), nitrate nitrogen (NO_3-N), inorganic phosphorus (PO_4^{3-}), temperature and pH for a better river health[2]. To maintain the minimum standard of the water quality, efficient water management including monitoring and research is necessary[5].

Nowadays, surface water management includes some mathematical models for evaluating the impact of pollutant. Water quality models are being used for water management as an important tools; which are able to predict long and short term variation of water quality parameters [5-6].

Among the water quality models, QUAL2E was the widely used mathematical model for river and stream water quality to evaluate the conventional pollutant impact[2,7,3]. However, due to some limitations it was modified by Park and Lee[8] and they developed QUAL2K, 2000, which included the addition of new water quality interactions. It was further developed by Chapra and Pelletier[9] with the name QUAL2K, 2003. By modifying the QUAL2K, 2003, Pelletier et al.[10] developed QUAL2Kw, which is the modernized version of QUAL2E[2].

QUAL2Kw has many new features, including Software Environment and Interface, Model segmentation, carbonaceous BOD speciation and others[11]. Similar to QUAL2K, it is a one-dimensional, steady flow stream water quality model and useful even in data limited condition[2]. The software of QUAL2Kw is freely available and can be used for both small and big river[5]. It can simulate a number of constituents including temperature, pH, carbonaceous biochemical demand, sediment oxygen demand, dissolved oxygen, organic nitrogen, ammonia nitrogen, nitrite and nitrate nitrogen, organic phosphorus, inorganic phosphorus, total nitrogen, total phosphorus, phytoplankton and bottom algae. Kannel et al.[2] applied the model for Bagmati River, Nepal and the model represented the field data quite well. Gardner et al.[12] also used the model for better understanding of the water quality status in Rio Blanco watershed in Jalisco, Mexico. As a tool for water quality management of small river basin, Oliveira et al.[13] used this QUAL2Kw in Portugal. In Malaysia, QUAL2K model was used by Zainudin et al.[14] for Sungai Tebrau and found as an outstanding tool in managing the river basin.

Regarding the present study, Tunggak River is a small river having no tributary. It is being polluted due to the vicinity of industrial zone of Gebeng, Kuantan, Malaysia. Gebeng industrial areas discharging their wastewater to the river flow that causing heavy pollution; it act as an important factor to contribute DO reduction as well as increasing of other water quality parameters in the river water. In this study QUAL2Kw model is calibrated and confirmed with the observed data. The objective of the study is to calibrate the QUAL2Kw model with water quality data of Tunggak River and to simulate the water environment of the river for better water management.

Material and Methods

Study area: The study was conducted in the Tunggak River basin and surrounding surface water of Gebeng Industrial Estate (GIE), located in the eastern part of peninsular Malaysia. The Tunggak river basin is under continuous degradation process due to rapid industrialization and urbanization[15]. This study covered lower 7.51 km length of the river where, the mid-zone is densely populated industrialized and residential areas and the lower part is with mangrove plantation (figure 1). In the industrial zone wastewater discharge line are directly connected with the river flow. The water quality of the river is deteriorating due to low DO concentration, presence of other toxic parameters and metal contamination[16].

Figure-1
Map of the study area indicating monitoring station on Tunggak River

Monitoring stations and data collection: For this study seven monitoring stations was selected along the river namely: Eastman chemical (EC); British petroleum (BPL); AsturiSdn. Bhd. (Ast); Mieco Manufacturing (MF); Taman balo 9k makmur (TBM); Seberang balok (SB) and Lower stream (LS). The detail summary of the monitoring stations is given in table-1. The monitoring, water samples and data collection were done on March-August for dry season and on September- February for wet season; as these two seasons are prevailing in the area. In this study observed water quality parameters were: water flow, temperature, pH, electrical conductivity (EC),dissolved oxygen (DO), total suspended solids (TSS), inorganic phosphorus(PO4-P), ammoniacal nitrogen (NH4-N), nitrate nitrogen (NO3-N), 5 days biochemical oxygen demand as mgO2/L (CBOD or BOD) and chemical oxygendem and as mgO2/L (COD).

During collection, transportation, preservation and analysis of water samples the methods of the American Public Health Association[17] and HACH[18] were followed. For BOD, water samples were collected in separate black bottles (300 ml) and were stored in ice-boxes. The data of physical parameters: water flow, temperature, pH, EC and DO were collected in-situ using YSI and other portable devices. Flow was observed using current meter and other physical parameters were measured using YSI. All other data were measured in the environment laboratory.

TSS determination was done by gravimetric method using temperature controlled oven. The concentration of BOD was measured by reading out the DO concentration before and after the incubation. BOD samples were incubated for 5 days at 20±30C in BOD bottle and after the incubation period BOD5 was calculated with the final reading of DO. COD determination was done in reactor digestion method using HACH spectrometer 5000. Nitrogen (NH4) was measured in nessler method; nitrate was estimated in cadmium reduction method, PO4-P was determined in ascorbic acid method. In those determination calorimetric method (APHA, 2005) was used.

Modeling tool: In the study a one dimensional mathematical model QUAL2Kw was used. It can be used for river water quality simulation when the river water flow is steady but non-uniform and the pollution loading into it remain roughly constant[13,19]. It considers the influence of point source and non-point source pollution loads during simulation[19]. Moreover, the model has a number of new elements that make it usable for shallow and small river besides relatively large river basin[18-21].

The QUAL2Kw model has a general mass balance equation for all constituent concentration(Fig. 2) in the water column (except bottom algae) of a reach i(excluding hyporheic) is written as [10]:

$$\frac{dc_i}{dt} = \frac{Q_{i-1}}{V_i}c_{i-1} - \frac{Q_{ab,i}}{V_i}c_i + \frac{E_{i-1}}{V_i}(c_{i-1}-c_i) + \frac{E_i}{V_i}(c_{i+1}-c_i) + \frac{W_i}{V_i} + S_i \qquad (1)$$

Where, ci = constituent concentration, Qi =flow at reach i (m3/d), Vi =volume of reach i (m3/d), Qab,*i* = abstraction flow at reach i (m3/d), Ei = bulk dispersion coefficient between reaches (m3/d), Ei−1, Ei are bulk dispersion coefficients between reaches i−1 & i and i & i + 1, Wi =external loading of the constituent (mg/day) and Si= sources and sinks of the constituent due to reactions and mass transfer mechanisms (mg/L/day). The detail description of interacting water quality state variables process is described in Pelletier and Chapra[11].

For auto calibration QUAL2Kw maximize the goodness of fit of the model results compared with measured data by using genetic algorithm (GA). It is the reciprocal of the weighted average of the normalized root mean squared error (RMSE) of the difference between the model predictions and the observed data for water quality constituents. The GA maximizes the fitness function f(x) as:

$$f(x) = \left[\sum_{i=1}^{n} w_i\right] \left[\sum_{i=1}^{n} \frac{1}{w_i} \left[\frac{\left(\sum_{j=1}^{m} O_{ij} / m\right)}{\left[\sum \left(p_{ij} - O_{ij}\right)^2 / m\right]^{1/2}} \right]\right] \quad (2)$$

Where, O*ij* = observed values, P*ij* = predicted values, m=number of pairs of predicted and observed values, w*i* = weighting factors, and n =number of different state variables included in the reciprocal of the weighted normalized RMSE. Pelletier et al.[10] described details about auto-calibration method in their publication, 'QUAL2Kw – A framework for modeling water quality in streams and rivers using a genetic algorithm for calibration'.

Model calibration and confirmation: River segmentation: The total 7.51 km length of the lower part of the Tunggak River was segmented into 7 reaches that are shown in Fig. 3. The figure shows the reaches of the river along with the locations of point sources of pollution loads.

Input data: The input data of water quality parameters were flow, temperature, conductivity (EC), pH, DO, BOD, COD (as generic constituent), ammoniacal nitrogen, nitrate nitrogen, inorganic phosphorus, inorganic suspended solid (ISS). Regarding phytoplankton and pathogen, those data were not measured. The bottom plants were assumed 40%. These diment/ hyporheic zone thickness was assumed 10 cm. The water qualities for the point and diffuse source of pollutions were other input to the model. The data were collected for one time in a day of each month both in wet and dry season. Average data for the dry season and wet season were used as the input data.

Table 1
Water quality monitoring stations in the Tunggak River

Station No.	Name of Stations	Distance from upper stream (km)	Location
1.	Upper Stream (US)	0.00	Near the bridge on JalanGebeng 2/6
2.	Eastman (EC)	1.27	Besides Eastman Chemical sdn.bhd
3.	British Petroleum (BPL)	1.17	50 meters from BP Chemicals Sdn. Bhd
4.	Astro (Ast)	0.87	Near AstroSdn. Bhd.
5.	Mieco Factory (MF)	0.90	Near the bridge on JalanPintasanKuantan
6.	Taman Balok (TBM)	0.85	50 meters from Taman BalokMakmur
7.	SeberangBalok (SB)	0.85	Near PerumahanSeberangBalok
8.	Lower Stream (LS)	1.60	Besides the bridge on JalanGebeng 2 (Port road)

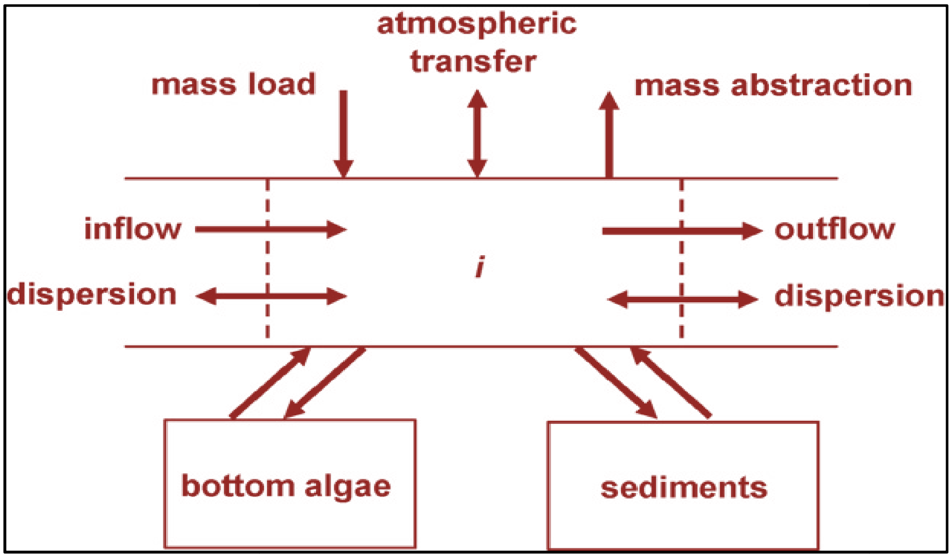

Figure- 2
Mass balance in a reach segment *i*.

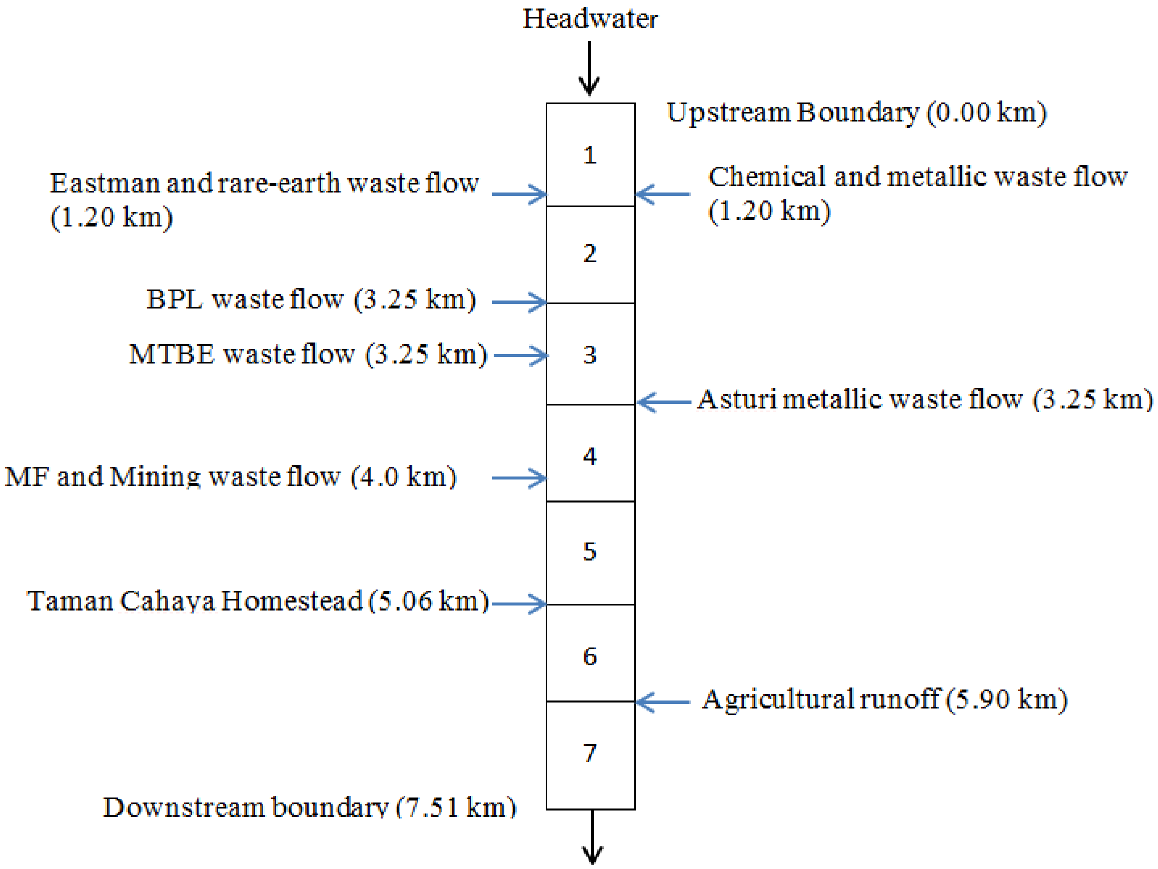

Figure- 3
QUAL2Kw segmentation scheme with location of pollution sources along Tunggak River

System parameters: The system parameters required by QUAL2 Kw for calibration are shown in table-2. These parameters were obtained from a numbers of studies and literatures including: Environment Protection Agency (EPA) guidance document[22], user manual of QUAL2Kw [11]and documentation for the enhanced stream water quality model QUAL2E and QUAL2E-UNCAS [7]. Internal calculation method was used to calculate re-aeration rate; which was also applied by Zhang et al.[19].

Exponential model was chosen for oxygen inhibition of CBOD oxidation, nitrification and phyto-respiration; and also for oxygen enhance of de-nitrification and bottom algae respiration. The range of CBOD oxidation rate was assumed as 0–5, which was also used by Oliveira et.al [13]; Cho and Ha[21] and Camargo et al.[23] for small river. The other parameters were set as default value in QUAL2Kw.

Model implementation: Model calibration was run with the measured data of dry season. To avoid instability in the model calibration, the calculation step was set at 5.625 min[2,24]. Euler's method was set for the solution of integration; Newton–Raphson method was used for pH modeling. The sediment digenesis simulation was done for level I option. To perform goodness of fit different weighting factors were given to different parameters. The weight 50 was given for DO as it is the most influential parameter[2,23]. Weight 2 was given for temperature, pH, CBOD and COD; and for other parameters 1was given as weighting factor. Model was run for a population size of 100 with 50 generations in the evolution (model runs in a population). It was because, according to Pelletier et al.[10] a population size of 100 performs better than smaller numbers and as nearly as a population size of 500.

Results and Discussion

Calibration and confirmation: Figure 4 shows the calibration and figure 5 shows the confirmation results of modeling respectively. Figure 4 denotes that, calibration result of temperature, pH and DO were in accordance with the observed values and other parameters were little bit different. The studied river water qualities were hard to reach the minimum DO requirement in all reaches of the river (figure 4). The low DO concentration that was below 3.0 mg/L in all reaches is an indication of entering wastewater from different point sources through wastewater drains and channels from the industrial areas; those wastewater add high organic and inorganic materials resulted low DO [15].

Table 2
Calibrated parameters for the Tunggak River in 2012

Parameters	Values	Units	Auto-calibration	Min. value	Max. value
Carbon	40	gC	No	30	50
Nitrogen	7.2	gN	No	3	9
Phosphorus	1	gP	No	0	4.2
Dry weight	100	gD	No	100	100
Chlorophyll	1	gA	No	0.4	2
ISS settling velocity	0.01	m/day	Yes	0	2
O2 reaeration model	Internal		No		
Slow CBOD hydrolysis rate	2.7636	day−1	Yes	0	5
Slow CBOD oxidation rate	0.213085	day−1	Yes	0	0.5
Fast CBOD oxidation rate	3.0658	day−1	Yes	0	5
Organic N hydrolysis	2.27565	day−1	Yes	0	5
Organic N settling velocity	1.67572	m/day	Yes	0	2
Ammonium nitrification	0.1505	day−1	Yes	0	10
Nitrate denitrification	0.98572	day−1	Yes	0	2
Sed. denitrification transfer coefficient	0.09598	m/day	Yes	0	1
Organic P hydrolysis	2.112	day−1	Yes	0	5
Organic P settling velocity	0.72152	m/day	Yes	0	2
Inorganic P settling velocity	1.38792	m/day	Yes	0	2
Sed. P oxygen attenuation half sat constant	1.81956	mgO2/L	Yes	0	2
Bottom plant					
Growth model	zero-order				
Max Growth rate	72.631	mgA/m2/day	Yes	0	100
First-order model carrying capacity	100	mgA/m2	No	50	200
Basal Respiration rate	0.48434	day−1	Yes	0	0.5
Excretion rate	0.47967	day−1	Yes	0	0.5
Death rate	0.062045	day−1	Yes	0	0.5
External nitrogen half sat constant	193.179	ugN/L	Yes	0	300
External phosphorus half sat constant	31.623	ugN/L	Yes	0	100
Inorganic carbon half sat constant	1.13E-04	moles/L	Yes	1.30E-06	1.30E-04
Light model	Half saturation				
Light constant	24.59071	langleys/day	Yes	1	100
Ammonia preference	61.74442	ugN/L	Yes	1	100
Subsistence quota for nitrogen	61.87110	mgN/gD	Yes	0.072	72
Subsistence quota for phosphorus	6.3753283	mgP/gD	Yes	0.01	10
Max. uptake rate for nitrogen	1303.12	mgN/gD/d	Yes	350	1500
Max. uptake rate for phosphorus	79.1345	mgP/gD/d	Yes	50	200
Internal nitrogen half sat ratio	3.7176325		Yes	1.05	5
Internal phosphorus half sat ratio	3.260499		Yes	1.05	5
Detritus dissolution rate	1.4653	day−1	Yes	0	5
Detritus settling velocity	0.94975	m/day	Yes	0	5
COD decay rate	0.8	day−1	Yes	0.8	0.8
COD settling velocity	1	m/day	Yes	1	1

The concentrations of CBOD, COD was higher and beyond the standard level in all reaches. These two parameters decreased steadily up to 6.5 km from downstream boundary (Fig. 4). The head water was relatively better regarding BOD and COD. This was because of the amount industrial wastewater increased with the distance due to the dense of industries at the mid region of the river (after 1 km from upstream)[16].The concentration of ammoniacal-N decreasedsteadily and sharply increased after 6 km from downstream. On the contrary inorganic phosphorus was almost similar up to 5 km and after that it increased sharply.

With some exception, the outcomes of the model calibration were in well agreement with the observed data. Table-3 shows the root mean square errors (RMSE) between the simulated and observed values of water quality parameters in calibration (dry season) and confirmation (wet season). The table also shows the difference of RMSE from calibration to confirmation (%). Calibration and confirmation had similar RMSE value, if the difference is less than 20%; it indicated the good matching between the observed and predicted values[23]. During calibration, the RMSE of temperature, pH, DO, CBOD, COD,NH_4-N, PO_4-P and ISS were 2.67, 0.69, 1.55, 34.58, 37.93, 0.510.44 and 21.18%, respectively (table 3).

In the confirmation, the RMSE for temperature, pH, DO, CBDO, COD, NH_4-N, PO_4-P and ISS were observed 3.07, 0.56, 1.20, 33.10, 32.48, 0.56, 0.39 and 7.51% respectively (Table 3). On the basis of the difference of RMSE (%) temperature, pH, CBOD, COD NH_4-N and PO_4-P had very good match between observed and predicted values. The more difference indicated that, the environmental condition especially for those parameters was different between the two periods[23].

In spite of some errors, as some errors in this modeling are inevitable due to time variation of sample collection; the simulation results were quite good and acceptable to achieve modest management goals. Nevertheless, more accuracy could be attained through adding various input variables including bottom algae, sediment oxygen demand, organic nitrogen, total and organic phosphorus, etc. in monitoring program; and also sophisticated 2D or 3D models can be applied to achieve the better management.

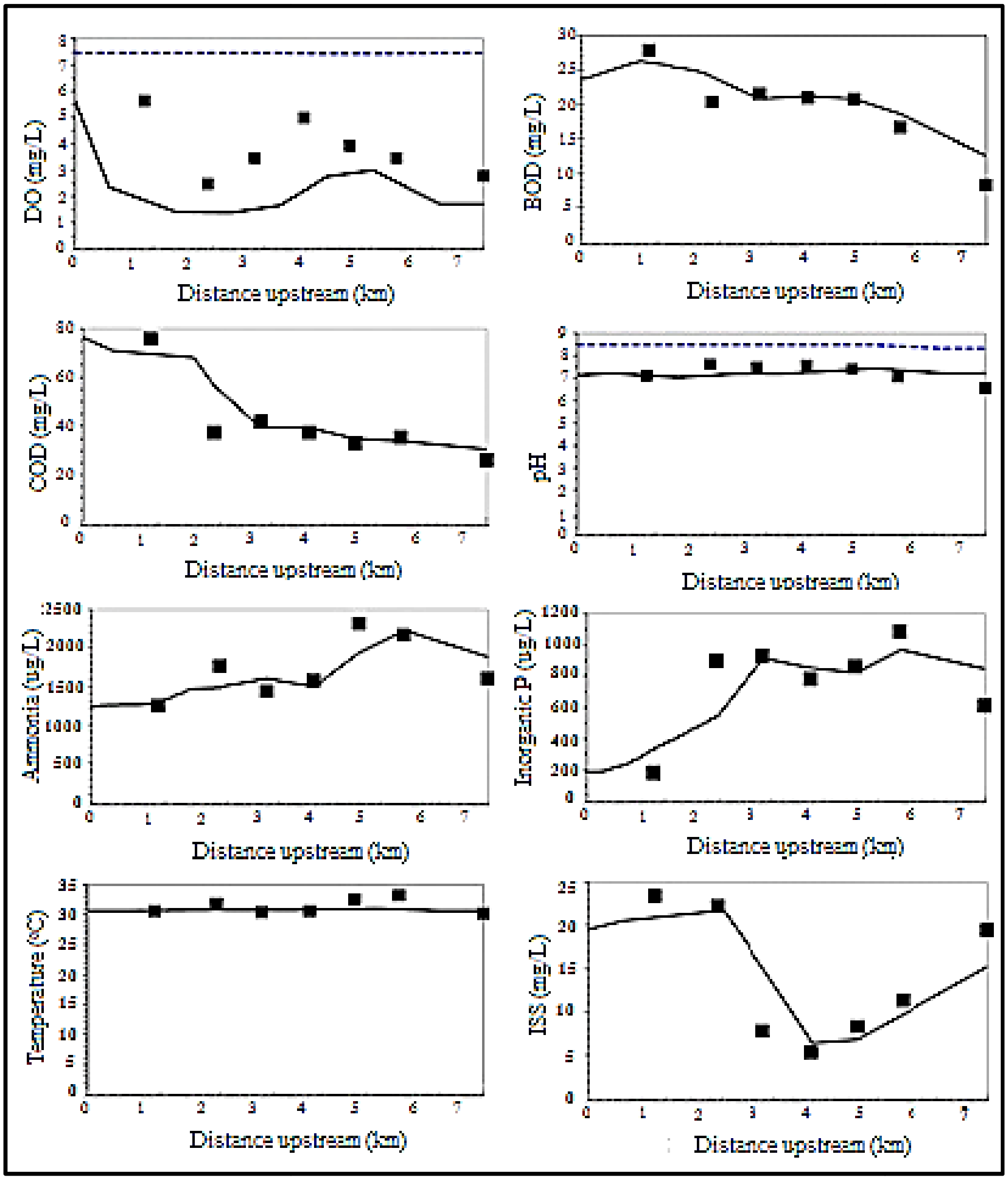

Figure-4
Model calibration of water qualities in Tunggak River for dry season's data

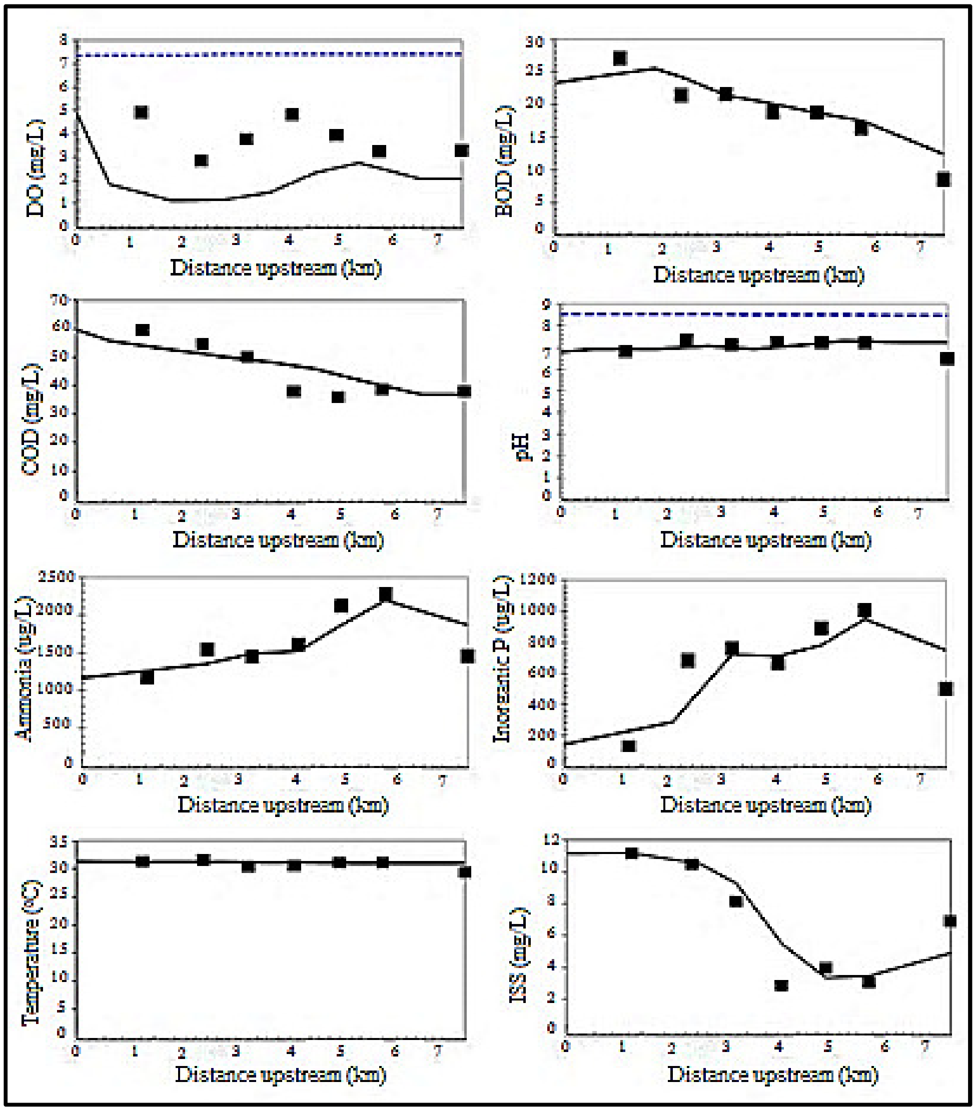

Figure-5
Model confirmation of water qualities in Tunggak River for wet season's data

Table 3
Root mean squared errors (RSME) between predicted and measured values of water quality parameters during calibration (dry) and confirmation (wet season)

SL No.	Parameters	RMSE (%)		Difference (%)
		Calibration	Confirmation	
1.	Temperature	2.57	3.07	19.5
2.	pH	0.69	0.56	18.8
3.	DO	1.55	1.20	22.6
4.	CBOD	34.58	33.10	4.3
5.	COD	37.93	32.48	14.4
6.	NH_4-N	0.51	0.56	9.8
7.	Inorganic Phosphorus	0.44	0.39	11.4
8.	ISS	21.18	7.51	64.5

Conclusion

River and stream water quality QUAL2Kwwas calibrated using the data in dry season of 2012 and confirmed with wet season's (2012-13) data. RMSE showed good match between observed and predicted value of maximum parameters except ISS. The model was applied to simulate various water quality parameters. The result shows that, the water quality parameters did not differ greatly from dry season to wet season. RMSE denoted that, the ISS differed significantly and it was due to runoff at wet season. However, the model QUAL2Kw adequately represented the field data of Tunggak River and the modeled data (Simulation) expressed that, the DO concentration was very low and due to increase amount of waste water it cannot be fixed without taking improved management based on the simulated results.

Acknowledgments

Authors are grateful to the university Malaysia Pahang and the Faculty of Civil Engineering and Earth Resources for their supporting and funding through the research project RDU 110354 and GRS 120363.

Reference

1. S.S., A. and B.N., S. Effect of Anthropogenic Activities on Zooplankton Population of Sogal Pond, Belgaum District, Karnataka, India, *Res.J.Recent Sci.,* **2,** 81–83 **(2013)**

2. Kannel P.R., Lee S., Lee Y.S., Kanel S.R. and Pelletier G.J., Application of automated QUAL2Kw for water quality modeling and management in the Bagmati River, Nepal, *Ecol.Model.*, **202,** 503–517 **(2007)**

3. Drolc A. and Končan J.Z., Water quality modelling of the river Sava, Slovenia, *Water Res.,* **30,** 2587–2592 **(1996)**

4. Haribhau M.G., Trace Metals Contamination of Surface Water Samples in and Around Akot City in Maharashtra, India, *Res.J.Recent Sci.,* **1,** 5–9 **(2012)**

5. Bottino F., Ferraz I.C., Mendiondo E.M. and Calijuri M.D.C., Calibration of QUAL2K model in brazilian micro watershed: effects of the land use on water quality, *Acta Limnologica Brasiliensia,* **22,** 474–485 **(2010)**

6. Sardinha D. and Conceição F., Evaluation of the water quality and auto-purification from the meio stream, Leme (SP), *Engenharia Sanitaria e Ambiental*, **13,** 329–338 **(2008)**

7. Brown L. and Barnwell, T., *The enhanced stream water quality models QUAL2E and QUAL2E-UNCAS: documentation and user manual.* (U. S. Environmental Protection Agency, Athens, GA, **1987**).

8. Park, S. S. and Lee, Y. S., A water quality modeling study of the Nakdong River, Korea. *Ecol.Mode.*, **152,** 65–75 **(2002)**

9. Chapra S. and Pelletier G., *QUAL2K:* A Modeling Framework for Simulating River and Stream Water Quality: Documentation and Users Manual, (Civil and Environmental Engineering Dept., Tufts University, Medford, MA., **2003**)

10. Pelletier G.J., Chapra S.C. and Tao H., QUAL2Kw – A framework for modeling water quality in streams and rivers using a genetic algorithm for calibration, *Environ. Model. Soft.,* **21,** 419–425 **(2006)**

11. Pelletier G. and Chapra S., QUAL2Kw theory and documentation A modeling framework for simulating river and stream water quality, (Environmental Assessment Program Olympia, Washington 98504-7710, **(2008)**

12. Gardner S., Griggs B., Handy J., Lemme N. and Paudel M.A, Qual2k water quality analysis of the Blanco watershed near Jalisco, Mexico, Department of Civil and Environmental Engineering, Brigham Young University **(2007)**

13. Oliveira B., Bola J., Quinteiro P., Nadais H. and Arroja L., Application of Qual2Kw model as a tool for water quality management: Cértima River as a case study, *Environ. Monit. Assess.*, **184,** 6197–210 **(2012)**

14. Zainudin Z., Rahman N., Abdullah N. and Mazlan N.F., Development of water quality model for Sg. Tebrau using QUAL2K, *Journal of Applied Sciences,* **10,** 2748–2750 **(2010)**

15. Sujaul I., Hossain M., Nasly M.A. and Sobahan M.A., Effect of Industrial Pollution on the Spatial Variation of Surface Water Quality, *Am. J. Environ. Sci.*, **9,** 120–129 **(2013)**

16. Nasly M., Hossain M. and Islam M., Water Quality Index of Sungai Tunggak: An Analytical Study, in *3rd International Conference on Chemical, Biological and Environment Sciences (ICCEBS'2013)* 40–45 **(2013)**

17. Andrew D., Standard methods for the examination of water and wastewater, 1200, American Public Health Association, (**2005**)

18. HACH, Water analysis guide **(2005)**

19. Zhang R., Qian X., Yuan X., Ye R., Xia B. and Wang Y., Simulation of water environmental capacity and pollution load reduction using QUAL2K for water environmental management, *Int. J. Environ. Res. Public Health*, **9,** 4504–21 **(2012)**

20. Anh D.T., Bonnet M.P., Vachaud G., Van Minh C., Prieur N., VU DUC L., and LAN ANH L., Biochemical modeling of the Nhue River (Hanoi, Vietnam): Practical identifiability analysis and parameters estimation, *Ecol.model.*, **193,** 182–204 **(2006)**

21. Cho J.H. and Ha S.R., Parameter optimization of the QUAL2K model for a multiple-reach river using an influence coefficient algorithm, *Sci. Total Environ.,* **408,** 1985–91 **(2010)**

22. Bowie G.L., Mills W.B., Porcella D.B., Campbel Carrie L., Pagenkop, James R., Rupp, Gretchen L., Johnson, Kay M., Chan, Peter W.H., Gherini, Steven A., Chamberlin and Charles E., Rates, constants, and kinetics formulations in surface water quality modeling, *EPA* (U. S. Environmental Protection Agency, Athens, GA, **1985**)

23. Camargo R.D.A., Calijuri M.L., Santiago A.D.F., Couto E.D.A. De and Silva M.D.F.M.E., Water quality prediction using the QUAL2Kw model in a small karstic watershed in Brazil, *Acta Limnologica Brasiliensia*, **22,** 486–498 **(2010)**

24. Zhang, R., Qian, X., Li, H., Yuan, X. and Ye, R., Selection of optimal river water quality improvement programs using QUAL2K: a case study of Taihu Lake Basin, China, *Sci. Total Environ.,* **431,** 278–85 **(2012)**