Simulation adequacy assessment of water quality of Rosetta Branch

Aiman M. El Saadi

ABSTRACT

Quality status of fresh waterways in Egypt, especially those that receive agricultural drainage water such as Rosetta Branch (RB), is critical for most of its water uses. However, the country depends on this marginal quality water to fill the gap between demand and supply. Therefore, the need for effective/economic water management tools turn into an obligation. Mathematical models can be considered as effective and practical tools for the quality assessment of water bodies. This paper carries out a statistical comparison between simulated and observed data, error quantification and simulation efficiency in order to assess the functionality of water quality (WQ) models for simulating the WQ of RB. This approach was set up to evaluate the cost-effective RB simulation adequacy using different WQ models and assess the gap between simulation simplicity and results accuracy. The simulation case of RB was compared using advanced MIKE-11 and simple QUAL2K WQ models. Despite the simplicity of the QUAL2K model, it showed a good adequacy compared to MIKE-11. Both mathematical models outputs showed a good agreement against field observations. However, MIKE-11 gives results that are more precise in general and for nutrients specifically.

Key words | goodness-of-fit, model calibration, surface water, water quality modelling

INTRODUCTION

Rosetta Branch (RB) is one of the critical surface water bodies of Egypt regarding its water quality (WQ). The WQ of the branch suffers from the seasonal variation of agriculture pollution sources discharging into its water as well as the limited amounts of fresh water released into the branch. The branch should be effectively simulated under current and future development scenarios in the context of the policy of the Ministry of Water Resources and Irrigation, even though the WQ is described by physical and chemical analysis of samples. Other questions need to be answered, such as understanding the relationships among WQ parameters, prediction of WQ and assessing the effects of WQ management. This makes WQ models the most applicable interpretation tools for answering those questions.

Chapra & Canale (2010) defined the WQ mathematical model as an idealized formulation that represents the response of aquatic ecosystems to external pollution sources. They are designed to simulate/compute quality in the receiving water as a function of pollutant effluents to explain and predict the effect of the neighbouring activities on water recourses.

As described in the manual (DHI 2004), MIKE-11 is a one-dimensional hydrodynamic modelling tool (see Table 1) for rivers and channels and contains the following modules: hydrodynamic (HD), advection-dispersion, sediment transport, ECO-lab including WQ modelling. The formulation can be applied to branched and looped networks and quasi-two-dimensional flow simulation on floodplains (Paudyal 2002). The hydraulic resistance is based on the bed slope from the empirical equation of Manning or Chezy. The model is well suited to complex systems and has been applied as a WQ model to rivers in northern India and England (Crabtree et al. 1996; Kazmi & Hansen 1997). MIKE-11 requires large amounts of input data for its deterministic equations.

The HD module, which is the core of the MIKE-11 model, simulates dynamic flows in rivers. This module...
assumes that the flow conditions are homogeneous within the channel. The model solves the full HD equations of Saint-Venant with an implicit finite difference method developed by Abbott & Ionescu (1967) for the computation of flows in rivers. It can model subcritical as well as supercritical flow conditions. Chowdhury (2000) described the basic concept of MIKE-11 HD model briefly.

MIKE-11 is an advanced model of flow and WQ in-stream and can simulate solute transport and transformation in complex river systems. However, it has its limitations: (1) there is a need for a large amount of data and it is difficult to simulate some determinants well if the data are lacking; and (2) channel cross sections are needed at reach boundaries, which makes the calibration and evolution of the results a substantial task and requires long computational times (Cox 2003).

According to the user manual (Brown & Barnwell 1987), QUAL2K (or Q2K) is a river and stream WQ model. QUAL2K is neither a stochastic nor dynamic simulation model. It is a one-dimensional, steady-state model (Table 1) of WQ and in-stream flow. The QUAL2K model can simulate up to 16 WQ indicators along a river and its tributaries and is suitable for modelling pollutants in freshwater that rely on sediment interactions, especially as a sink of inorganic and organic substances. The initial step of the standard QUAL2K is to divide the river system into reaches (up to 50), and each of these is then divided into a number of computational elements of equal length. The data requirements of the model in terms of flow and WQ include single values of each pollutant modelled (Tsakiris & Alexakis 2012).

Zhang et al. (2012) identified QUAL2K as an effective tool for the relative evaluation of potential WQ improvement programmes through simulating the effects of a range of WQ improvement scenarios in the Hongqi River.

Bahadur et al. (2013) identified and researched 65 surface water and ocean models; both MIKE-11 and Qual2k were involved. Eight definite criteria to evaluate each model were reviewed and itemized in a single table. Both models are similar as they are 1D models, work in a river environment, have advanced degrees of analysis; the main difference regarding availability is that Mike-11 is proprietary while QUAL2K is in the public domain.

Most WQ models including QUAL2K and MIKE-11 contain sub-models that calculate water temperature. These sub-models use short and long wave solar and atmospheric radiation, evaporation and sensible heat fluxes. Despite the similarity of both QUAL2K and MIKE-11 models, the most important difference is the division of organic matter into dissolved, suspended and sediment fractions in MIKE-11, while in QUAL2K, the organic matter is divided into dissolution and sediment fractions. A minor difference between QUAL2K and MIKE-11 is the simplified treatment of nitrification in MIKE-11 that ignores nitrite as an intermediate product (Rauch et al. 1998). Table 1 furnishes the general characteristics of MIKE-11 and QUAL2K models.

Chapra (1997) theoretically identified the trade-offs between model complexity, uncertainty and information. In principle, with an unlimited budget, a more complex model will be more reliable by adding complexity to the model (i.e., more equations with more parameters), assuming there are sufficient funds to perform the necessary field and laboratory studies to satisfy the additional parameters. There are always limits to the ability to totally characterize a natural water system; at that point there are two extreme outcomes: one extreme is a very simple unrealistic model that does not yield reliable predictors and the other, a very complex detailed model that outpaces available data because of uncertainty of the parameters. Conversely, there is an intermediate point where the model is consistent

<table>
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with the available level of information; at this point, a third dimension must be interjected, that is the reliability required to solve the problem.

The main objective of this research is to assess the satisfactoriness of the advanced MIKE-11 and simple QUAL2K WQ models for simulating the WQ of RB throughout scaling correlation, efficiency and error magnitude. To achieve this objective both models were calibrated using the same field observations and equivalent boundary conditions. Afterwards, statistical techniques were applied to investigate the acceptability of both models’ results compared to field observations.

**METHODOLOGY**

The methodology of this research was focussed on a specific study area (i.e., RB). The required data for simulating RB with both selected models were collected and prepared. Afterwards, both simulation cases were calibrated using standard procedure for a selective number of WQ variables followed by simulation of WQ parameters. Then, and in order to assess the adequacy of both models in simulating RB, the framework below was followed:

1. Measure the correlation between field observations and simulation results.
2. Estimate the magnitude of error between field observations and simulation results.
3. Assess the accuracy of model outputs by the means of efficiency.

**Site description**

On its way to the Mediterranean Sea, the River Nile splits into the Damietta and Rosetta branches. The RB starts downstream of the Delta Barrages (N 30° 11’ 20.08″, E 31° 06’ 34.14″) flowing in a northerly direction and ends at Idfina Barrages (N 31° 18’ 20.87″, E 30° 31’ 08.48″) which regulates the excess flow of the branch to the Mediterranean Sea, as shown in Figure 1.

The RB is considered to be the major source of freshwater for the western side of the Nile Delta, where several water treatment plants are located (i.e., Mahallet Abu Ali, Desouk, Fowwa and Mahmoudia 1 and 2) to supply adjacent cities with potable water. However, there are three main sources of pollution which degrade the quality of the water along the RB. The first source is the agricultural point sources, which comes from five agriculture drains located along the branch (i.e., Rahawy drain, Sabal drain, Tala drain, Tahrir drain and Zawyet El-Bahr drain), as seen in Figure 1. The second source is treated industrial wastewater, which is discharged from industrial companies at Kafr El Sheikh District. The third source is the effluent of wastewater treatment plants that is mixed with drainage water as happens in Rahawy drain. El Bouraie et al. (2011) provided the seasonal WQ of RB of the Nile River at its upstream then concluded that Rahawy drain is the significant source of water pollution to RB, especially during the winter season. The cross sections and hydraulic characteristics of RB were surveyed and profiled by the field team...
of the Nile Research Institute of the National Water Research Centre (NWRC) of Egypt.

For this research, the field survey and sampling collection were expanded to cover the whole stream of the RB and all point sources as illustrated in Figure 1. WQ samples were collected from RB at 13 sampling locations in the winter season (January 2010), as well as five samples being collected from the five major agriculture drains and two from industrial sources during the same period. The water samples were analysed at the Central Laboratory for Environmental and Water Quality Monitoring of the NWRC of Egypt according to Standard Methods for the Examination of Water and Wastewater (APHA 1989). Four WQ parameters, biochemical oxygen demand (BOD), dissolved oxygen (DO), nitrate (NO₃) and ammonia (NH₄) were considered for study due to their significance for water health. The DO was measured in field using an in-situ membrane electrode DO meter. BOD, NO₃ and NH₄ were measured using standard laboratory analysis applied on water samples that were collected from the same locations. NO₃ was analysed and measured in the laboratory using ion chromatography instrument, the NH₄ analyses were measured using selective electrode method and the BOD determined using a 5-day BOD test.

Model application

Hydraulic characteristics of RB such as flows, velocity and cross-sectional details at different locations were collected. The velocity varies according to the change in the cross section of the stream, as the discharge is steady. Considering the stability of pollution sources, the major influence on WQ status of the branch is the change in the barrages’ discharge that changed seasonally. The applied simulation case used information of the winter season of the year 2010 for both models in order to study the effect of irrigation closure period on RB. The total length of RB is 225 km with an average width of 150–200 m. The water average depth is in the range of 2–2.5 m. The branch water is used for drinking, irrigation, industry and fishery.

With the purpose of presenting most of the morphological changes of RB, 40 cross sections with an intermediate distance of about 5 km over the stream were implemented in MIKE-11. The implemented cross sections give a complete overview of the morphology of the branch as a requirement of MIKE-11. The RB network was digitized in Arc-GIS software to build up a shape file for it that could be imported to the MIKE-11 model. Three modules inside MIKE-11 were used for the simulation of RB, namely, HD, advection-dispersion and ECO-lab modules. The last two modules were used for WQ analysis of RB. For equivalency of both model cases, the simulation mode in MIKE-11 was set to quasi-steady hydraulics.

For QUAL2K, cross sections were applied using the bottom width and side slopes as required by the model. The branch was divided into 40 reaches (simulation segments), each about 5 km in length, illustrating the variation in hydraulic characteristics of RB.

Both models were set up for simulating 200 km excluding the reaches near the barrages at upstream and downstream ends of RB. Equivalent time step of 15 minutes in MIKE-11 and 0.25 hours in QUAL2K was used with a simulation period between 1 January and 4 January.

The RB receives pollution from several point sources, representing the boundary conditions of the branch. Five out of the seven pollution point sources that discharge into the branch are agriculture drains. The average discharge of Rahawy drain, Sabal drain, Ganoub Tahrir drain, Zawiet El Bahr drain and Tala drain are 3.0 Mm³/day, 1.0 Mm³/day, 0.75 Mm³/day, 0.4 Mm³/day and 0.9 Mm³/day, respectively. The other point sources are two industrial effluents. Both discharge directly into the branch at Kafer El-Sheikh. The average discharge of the Salt & Soda Factory (detergents) is 0.022 Mm³/day and the average discharge of the Maliya Factory (superphosphates) is 0.028 Mm³/day.

Model calibration is the first stage testing or tuning of the model to a set of field data used in the original construction of the model. Such tuning is to include a consistent and rational set of theoretically defensible parameters and input (Thomann & Muller 1982). Patro et al. (2009) calibrated MIKE-11 using river water level and discharge data of various gauging sites for the monsoon period in the delta region of Mahanadi River basin in India. They found that the calibration and validation results of MIKE-11 show that the model performs quite satisfactorily in simulating the river flow for the delta region of Mahanadi River basin.

For RB simulation, both models were manually calibrated by fine tuning the model results to fit closer to the field
measured data set. This was done by adjusting the model kinetic parameters to obtain an optimal agreement between the model results and the field data set. Equivalent boundary condition, which has been used for calibration of both models, was as similar as the field conditions of RB that were surveyed and furnished previously in this paper. After the hydraulic calibration, the WQ calibration procedure used to calibrate MIKE-11 and QUAL2K models followed the next steps:

1. BOD-DO relations
   - Degradation rate
   - Re-aeration
2. Ammonia-nitrate
   - Nitrification
   - De-nitrification.

The bed resistance of RB was calibrated using the Manning coefficient. The Manning coefficient calibrated to values between 0.04 and 0.045 in QUAL2K and MIKE-11 along the RB. Regarding WQ calibration in the MIKE-11 case, the number of re-aeration expressions was set to three. The constants of the O’Connor-Dobbins (1958), Owens et al. (1964) and Churchill et al. (1962) formulas were used. The three re-aeration formulas were provided with their constants by Chapra & Pelletier (2003). Also in QUAL2K, the re-aeration formula was set to internal selection that chooses automatically, based on water level, between the same three formulas that were used in MIKE-11 (i.e., O’Connor-Dobbins, Owens-Gibbs and Churchill) for oxygen budget calculations. Re-aeration temperature coefficient was then adopted in both models. The hydrolysis rate of BOD was calibrated then its temperature coefficient was adopted in QUAL2K; however, the first order decay rate was selected and calibrated then its temperature coefficient was adopted in MIKE-11. The ammonia decay rate of the nitrification process was calibrated then its temperature coefficient was adopted in both MIKE-11 and QUAL2K models. The calibration processes were concluded by adopting the de-nitrification coefficients.

The calibration is based on the error, namely, the difference between the calculated and measured values of most significant terms. It is therefore necessary to adopt a suitable range of acceptability of the error, with a pre-established threshold, exceeding which, the result of the model cannot be accepted (Benedini 2011).

Model adequacy

To assess the efficiency of the models, goodness-of-fit techniques were applied. Goodness-of-fit statistics can be computed for continuous and categorical dependent variables. Most of these statistics are discussed in detail in Helsel & Hirsch (2002) and Witten & Frank (2005). Krause et al. (2005) compared different efficiency criteria for hydrological model assessment including the approaches used in this research. With the aim of assessing the adequacy of simulated cases of RB, evaluation algorithmic methods were used. Initially, Spearman’s rank correlation was used to measure the power of the agreement between field observations and simulation results. Then, mean absolute error (MAE) was used to estimate the magnitude of error between field observations and simulation results. Finally, Nash-Sutcliffe model efficiency was used to assess the predictive power of the models comparing field measurements to simulation results.

Spearman’s rank correlation coefficient (Equation (1)), named after Charles Spearman, is a nonparametric measure of statistical dependence between two variables (Berthouex & Brown 2002; Helsel & Hirsch 2002). It assesses how well the relationship between two variables can be described using a monotonic function. If there are no repeated data values, a perfect Spearman correlation of +1 or –1 occurs when each of the variables is a perfect monotone function of the other.

\[
\rho = \frac{\sum_{i=1}^{n} (R_{xi} - R_{yi}) - n \left( \frac{n + 1}{2} \right)^2}{n(n^2 - 1)/12} \tag{1}
\]

where \( R_{xi} \) and \( R_{yi} \) are the ranks of the two compared variables and \( (n + 1)/2 \) is the mean rank of both \( x \) and \( y \).

As a goodness-of-fit, the MAE measures how much the field observations vary (i.e., error magnitude) from its modelled predicted values. The MAE (Equation (2)) reported the average magnitude of the errors in the same units as the original values.

\[
\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} |X_{\text{mod}} - X_{\text{obs}}| = \frac{1}{n} \sum_{i=1}^{n} |e_i| \tag{2}
\]

The MAE is an average of the absolute errors \( e_i \), where \( X_{\text{mod}} \) is the prediction and \( X_{\text{obs}} \) is the true value.
Nash–Sutcliffe model efficiency coefficient ($E$) is commonly used to assess the predictive power of hydrological discharge models (Nash & Sutcliffe 1970). However, it can also be used to quantitatively describe the accuracy of model outputs for variables other than discharge (such as nutrient loadings, temperature, concentrations, etc.). The mathematical definition of the coefficient is presented in Equation (3):

$$E = 1 - \frac{\sum_{i=1}^{n} (X_{\text{obs}, i} - X_{\text{mod}, i})^2}{\sum_{i=1}^{n} (X_{\text{obs}, i} - \bar{X}_{\text{obs}})^2}$$  \hspace{1cm} (3)

where $X_{\text{obs}}$ is the observed value and $X_{\text{mod}}$ is the modelled value at time/place $i$.

Nash–Sutcliffe efficiencies can range from $-\infty$ to one. An efficiency of one (i.e., $E = 1$) corresponds to a perfect match between model and observations. An efficiency of zero indicates that the model predictions are as accurate as the mean of the observed data, whereas an efficiency less than zero ($-\infty < E < 0$) occurs when the observed mean is a better predictor than the model. Essentially, the closer the model efficiency is to one, the more accurate the model is (Krause et al. 2005).

**RESULTS AND DISCUSSION**

After the calibration procedure presented in the Methodology section was followed, the WQ parameters for RB (i.e., DO, BOD, NH$_4$ and NO$_3$) were simulated for verification. Figure 2 shows the calibration results of MIKE-11 for the hydraulic characteristics of RB.

Thirteen field observations were collected from the main stem of RB for model calibration. Their locations were distributed over the simulated reaches of RB, as seen in Figure 1. The statistical characteristics of the models’ output and field measurements are presented in Table 2.

Figures 3–6 represent the spatial results of the simulation of the WQ parameters DO, BOD, NH$_4$ and NO$_3$, respectively, for both MIKE-11 and QUAL2K models compared to the field measurements. Figures 3–6 show reasonable agreements between models’ results and field measurements.
observations; however, the MIKE-11 results showed a better agreement with field results than those of QUAL2K. Regarding the effect of the point sources (i.e., drains discharging into the branch), the results of MIKE-11 showed better peaking response to them, as seen in Figures 3–6, than those of QUAL2K.

Table 3 presents the nonparametric Spearman’s correlation between both model results and field observations for each calibrated WQ parameter. The Spearman’s rank order correlations presented in the following tables are pairwise deleted in the case of missed records and significant at $p < 0.05$. Overall, the results of the MIKE-11 showed better correlation to field observations than those of QUAL2K. However, both models’ results showed high correlation to field observations except for nitrate, which showed a moderate correlation. The Spearman’s correlation between MIKE-11 and QUAL2K results for DO, BOD, NH$_4$ and NO$_3$ are 0.818, 0.918, 0.981 and 0.533, respectively, indicating high correlation except for nitrate that showed a moderate correlation.
The MAE is scaled with the same units of the variables presented. Comparing the MAE results presented in Table 4 to the statistical characteristics presented in Table 2 (i.e., mean and standard deviation) of each variable, all MAE between modelled values and field measurements showed acceptable results; however, the MAE for MIKE-11 showed better results than those computed for QUAL2K results. Comparing all MAE results to the average of field observations (as seen in Table 5), the MIKE-11 showed better results than those of QUAL2K.

As shown in Table 6, the Nash–Sutcliffe efficiency ($E$) results for simulating DO, NH$_4$ and NO$_3$ with both MIKE-11 and QUAL2K indicated adjacent perfect match between modelled and field data (i.e., $E$ is close to 1). Nevertheless, DO results of QUAL2K showed a moderate match between modelled and field data. For both models, the ($E$) value of
BOD results indicated that the model predictions are as accurate as the average of the observed data (i.e., $\bar{E}$ is close to zero). The efficiency of simulating DO with MIKE-11 is obviously better than with QUAL2K, as seen in Table 6. However, simulation efficiency ($E$) of both models for BOD and NO$_3$ showed a close efficiency.

CONCLUSIONS

MIKE-11 is a commercial advanced WQ model that needs a massive amount of detailed input data, whereas QUAL2K is an open-source simple WQ model that needs relatively limited input data. The RB has unique conditions that require modelling assessment for WQ. In view of the RB simulation, the results of both models showed good agreement with the field observations, however, MIKE-11 showed better agreement versus field observations. Regarding efficiency ($E$), both models showed a perfect match between modelled and field data, nevertheless, MIKE-11 showed better efficiency than QUAL2K.

Bearing in mind the significance of DO as a major parameter in all biological WQ processes, the efficiency of MIKE-11 in simulating DO showed the finest results among all simulated WQ variables. In addition, nitrate simulation results of MIKE-11 showed better correlation to the field data than those of QUAL2K. The MIKE-11 and
QUAL2K models are slightly different in efficiency regarding the simulation of biological WQ variables. The MIKE-11 is more preferable in simulating the nutrients, yet the QUAL2K gives reasonable simulation.

Both MIKE-11 and QUAL2K models can effectively simulate irrigation and drainage canals of Egypt; however, the choice depends on the acceptability of uncertainty in results represented in model efficiency and mean error. Regarding the cost-effective dimension of the RB simulation, QUAL2K is very economically reasonable, yet, provides reasonable and satisfactory results for decision-making.

REFERENCES


First received 25 August 2014; accepted in revised form 29 April 2015. Available online 26 May 2015