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APPLICATION OF A ONE-DIMENSIONAL STEADY STATE MODEL FOR SIMULATION THE WATER QUALITY IN A LARGE RIVER: A CASE STUDY OF THE DANUBE RIVER

Alhassan H ISMAIL[1], Diana ROBESCU[2]

The main aim of the study was to explore the applicability of the one-dimensional (1D) steady state model (QUAL2K) for simulating the water quality in large river. Danube River at lower Danube course was chosen as a case study. The model was calibrated using data on April, 2008 (spring season). Validation of the model was performed using data on September, 2008 (autumn season). Moreover, four different scenarios were examined to control the level of CBOD and DO in the river. The model output revealed that the calibration and validation results were in agreement with the observed values, with some exceptions. Although QUAL2K is one-dimensional steady state model, the simulated results were compatible with previous technical reports. Thus, it can be used as a suitable tool for simulating the water quality in large rivers.

Keywords: Mathematical Modeling, Danube River, QUAL2K, DO, BOD.

1. Introduction

Mathematical model is usually used for predicting changes in physico-chemical and biological parameters of water quality due to discharges or location of the point or non-point input sources [1]. Mathematical solution has become an effective tool with the help of computer technology in order to reduce the time required for numerical solutions [2]. Consequently, computer technology has led to significant advancement in the water quality modeling field. A lot of computer water quality models have been developed by different institutions and agencies [3].

In this context, a computer model (QUAL2K) was selected to simulate the water quality of the Danube River. QUAL2K is a one-dimensional, steady-state, river and stream water quality model which developed by Chapra and Pelletier [4]. The model provides uncertainty analysis tools in its process and it has some features such as public domain software, user-friendly, frequent upgrades and has complete documentation materials which makes it widely tested and used in the literature [5,6].

[1] Ph.D. student, Department of Hydraulics and Environmental Engineering, University POLITEHNICA of Bucharest, Romania, e-mail: hassan19851988@yahoo.com
[2] Professors, Department of Hydraulics and Environmental Engineering, University POLITEHNICA of Bucharest Romania, e-mail: diarobescu@yahoo.com

Moreover, QUAL series have been applied mostly for small and medium rivers such as Qiantang River in China [7], Karoon River in Iran [8], Lis River in Portugal [9], Tigris River in Iraq [10], Bagmati River in Nepal [11], and Yamuna River in India [12]. To our knowledge, QUAL2K model has not been applied for large (i.e. deep and wide) rivers. The simulation process in large rivers is preferred using complex models (2D or 3D) to represent the situation more closely [5]. However, complex water quality models such as MIKE-11 and AQUATOX requires extensive data in order to perform the simulation process [2].

In this paper, an attempt has been made to explore the applicability of QUAL2K model for simulating the water quality (i.e. DO and BOD) in large river and to examine the impact of tributaries and other waste loads on the receiving river. The Danube River in Drobeta-Turnu Severin city stretch was chosen as a case study, which has an average discharge of 5600 m^3/sec [13].

2. Materials and Methods

Study area

The Danube River divided into three main parts: the upper Danube course (1060 km), the middle Danube course (725 km) and the lower Danube course (1075 km). The lower Danube course represents Romania's natural border with Serbia, Bulgaria, Ukraine and the Republic of Moldova [14]. In the lower course, the river is flowing through Baziaş and Gura Văii passing the Iron Gate I (located 14 km upstream of Drobeta-Turnu Severin city). The Iron Gate I was constructed in 1971 and considered as the largest dam and reservoir system on the basis of volume, area and hydropower potential among numerous impoundments on the Danube and the tributaries [13].

This study covered 13 km length of the Danube River, starting 2 km downstream of the Iron Gate I and extends to Drobeta-Turnu Severin city (Fig. 1). The importance of this region is emerged due to the lack of proper sewage collection and treatment facilities in the Drobeta-Turnu Severin city, in addition to the effluent discharges from industrial areas in the region. Two major groups of industries exist in the region: south-west industrial area (upstream of Drobeta-Turnu Severin city), and south-east industrial area which (downsterm of Drobeta-Turnu Severin city) [15,16]. In addition to two tributaries (Jidostita and Topolniţa) are connected to the Danube River in the study region.

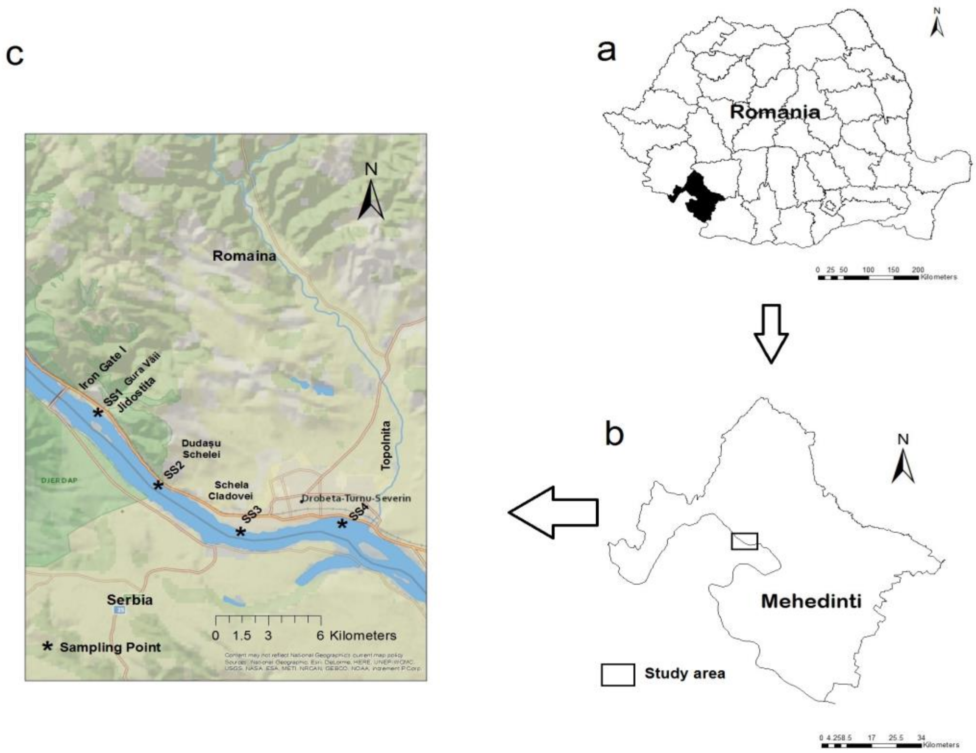

Fig. 1. Map of the study area: a) Romanian Counties, b) Mehedinţi County and c) Sampling Locations

Basic equations

QUAL2K simulates up to 16 water quality indicators and all the indicators are simulated as 1st-order decays except for dissolved oxygen, phosphate and nitrate which are represented in a deeper detail [3]. In this paper, only the BOD, DO and pH were considered for simulation the water quality. The model solves general mass balance equation for all water quality indicators except the bottom algae [4]

$$\frac{\partial C_i}{\partial t} = \frac{Q_{i-1}}{V_i} C_{i-1} - \frac{Q_i}{V_i} C_i - \frac{Q_{ab,i}}{V_i} C_i + \frac{E_{i-1}}{V_i}(C_{i-1} - C_i) + \frac{E_i}{V_i}(C_{i+1} - C_i) + \frac{W_i}{V_i} + S_i \quad (1)$$

where C_i = variable concentration for reach i, t = time, Q_i = outflow from reach i into reach i -1, V_i = volume of i_{th} reach, E_i = bulk dispersion coefficient between reaches i and i -1, W_i = external loading of the constituent to reach i, and S_i = sources and sinks of the constituent due to reactions and mass transfer mechanisms. The detailed description of QUAL2K model can be found in the QUAL2K user’s manual of Chapra and Pelletier [4].

Model Input

The input data required by QUAL2K is flow and concentrations for headwater, discharges of point source pollution and withdrawals, reach segment lengths, hydraulic geometry and weather data parameters [4, 6]. Water quantity and quality data for headwater are available from obtained dataset in four sampling points in the study area. The hydraulic parameters have been obtained from previous technical reports [4, 17, 18]. The meteorological data were obtained from Romanian National Meteorological Administration.

Water quality data were obtained for the year of 2008 in four sampling points namely, Gura Văii (SS1) which is about 2 km downstream of Iron Gate I, Dudașu Schelei (SS2), Schela Cladovei which is located upstream of Drobeta-Turnu Severin (SS3), and downstream of Drobeta-Turnu Severin (SS4). Table 1 shows the water quality datasets used in this study. Water quality and quantity datasets for April (spring) and September (autumn), 2008, were used for model calibration and verification respectively. Recent data on the Danube water quality were not available and data sets obtained during 1 year (2008) were provided by National Administration of Romanian Waters “Administrația Națională Apele Române” (ANAR).

The total length of the study region (13 km) was divided into 4 reaches with further subdivided into 17 segments ranging between 0.43 – 1.24 km. Fig. 2 shows the river discretization along with the locations of point and non point sources pollution. The two tributaries existing in the study area have been considered as point sources. Discharges of non-point sources pollution loads in the study area were assumed to be 1 m^3/sec as a maximum. The diffuse loads cannot be estimated and however, the most way for taking these sources into consideration is the assumption [19]. The assumed value would be the appropriate value for lowland rivers such as the Danube River in the study area.

A trapezoidal cross-section channel was considered for modeling with a channel slope of 0.001 and a bottom width 210 m [20]. Manning roughness coefficient was assumed as 0.035, since the Danube River is a natural stream channel, clean and straight [21].

In QUAL2K, the model simulates the ultimate CBOD (CBODu) instead of 5 day CBOD ($CBOD_5$) and therefore, the observed $CBOD_5$ was converted to (CBODu) using the following relationship [9]:

$$CBOD_u = \frac{CBOD_5}{1 - e^{-5k}} \qquad (2)$$

where, k is the CBOD decomposition in the bottle, 1/day. The polluted water and wastewater contaminated with organic carbon has a k values in the range 0.05–0.3 1/day [19]. The value of k was calculated as 0.13 1/day, assuming the CBODu/$CBOD_5$ ratio as 2.05 which is the reference value proposed by [22].

Table 1

Headwater quality and quantity of Danube River

Stations	Location (km)	Q m^3/s	Water Temperature °C	DO mg/L	BOD mg/L	pH	TSS mg/L	Total P mg/L	NO_3 mg/L	NH_4 mg/L
April, 2008										
SS1	0.00	8730	11	9.11	2.2	7.3	25	0.43	1.549	0.165
SS2	4.66	8630	13	8.72	1.99	7.4	24	0.44	1.46	0.172
SS3	7.23	8550	12	8.83	2.02	7.7	26	0.48	1.578	0.144
SS4	10.13	8270	14	8.89	2.07	7.4	26	0.45	1.529	0.16
September, 2008										
Stations	**Location (km)**	**Q m^3/s**	**Water Temperature °C**	**DO mg/L**	**BOD mg/L**	**pH**	**TSS mg/L**	**Total P mg/L**	**NO_3 mg/L**	**NH_4 mg/L**
SS1	0.00	2870	21	7.7	1.56	7.7	28	0.74	1.232	0.251
SS2	4.66	2650	23	7.26	1.53	7.3	28	0.86	1.232	0.165
SS3	7.23	2890	22	7.34	1.77	7.5	28	1.05	1.029	0.204
SS4	10.13	2960	22	7.43	1.62	7.6	25	0.883	1.164	0.207

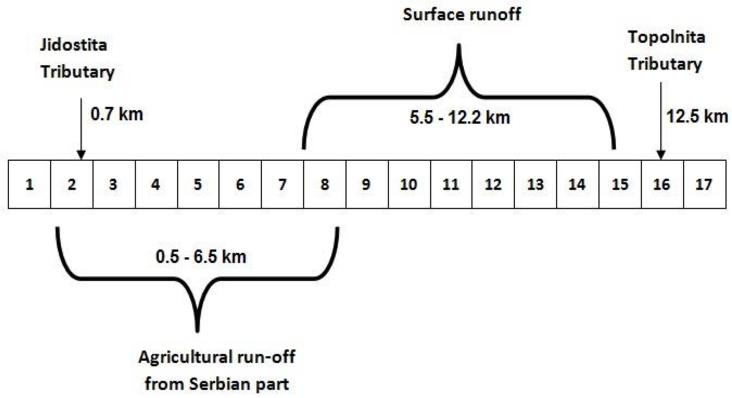

Fig. 2. Segmentation of Danube River with location of pollution sources

The model rates were obtained from various technical sources: the default values presented by the QUAL2K user manual [4], the Environmental Protection Agency [17], and literature from QUAL2E and QUAL2E-UNCAS [18]. The stoichiometry parameters such as carbon (gC), nitrogen (gN), phosphorus (gP), dry weight (gD) and chlorophyll (gA) were specified according to the default values given in the QUAL2K user manual as 40, 7.1, 1, 100 and 1, respectively. The slow CBOD hydrolysis rate and fast CBOD oxidation rate were calibrated as 1.53 and 3.56 respectively. The model offers three options for estimating the reaeration rate coefficient: O'Connor and Dobbins [23], Churchill et al., [24] and

Owens et al., [25]. Churchill et al., [24] formula was chosen to estimate the reaeration rate for Danube River, since this formula was developed for large rivers with mean depths ranging from 0.65–3.48 m and mean velocities ranging from 0.56–1.52 m/s [26]. The algae and bottom SOD coverage were assumed 20%. This percent tends to be the most accepted assumption for deep and wide rivers like the Danube [19]. The exponential model was chosen for oxygen inhibition for CBOD oxidation, nitrification and denitrification [9,11]. The input data of headwater parameters were temperature, flow, pH, DO, BOD, NH4-N, NO3-N, organic phosphorus and inorganic phosphorus. Alkalinity was assumed as 100 mg/L of CaCO3 (default value for QUAL2Kw). Other water quality parameters (inorganic suspended solids, conductivity, detritus, phytoplankton and pathogen) were left blank as they were not available.

Model Run

The model was calibrated using data on April, 2008 (spring season). The calculation step for the model was set at 0.015 hour, to increase the model stability. In order to maximize the goodness of model fit between the simulated results and observed data, the model was run iteratively until the model coefficients were adjusted and the reasonable agreement were achieved. Furthermore, the model was validated using data on September, 2008 (autumn season) without changing the calibrated system parameters in order to test the ability of the calibrated model.

3. Results and discussion

QUAL2K model was calibrated and validated for two different seasons: spring (April 2008) and autumn (September 2008). The model calibrated and validated results for the water quality data at four sampling sites are shown in Fig. 3 and Fig. 4, respectively. Both the calibration and validation results were in agreement with the observed values, with some exceptions. The relative error is used for estimation the errors in simulation. The relative error of calibrated and validated results between the simulated and observed values for flow rate, CBODu, DO and pH are shown in Table 2.

Generally, the results revealed that the BODu concentration were below 5 mg/L and DO concentration above 7 mg/L which reflect a good quality of the river in the study area. pH values were ranging between 7.29 - 7.70 in the study area. Furthermore, it was observed that the flow rate (Q) values did not fluctuate along the 13 km of river distance. Although QUAL2K is steady state model, the simulated results were compatible with previous technical reports [27, 28].

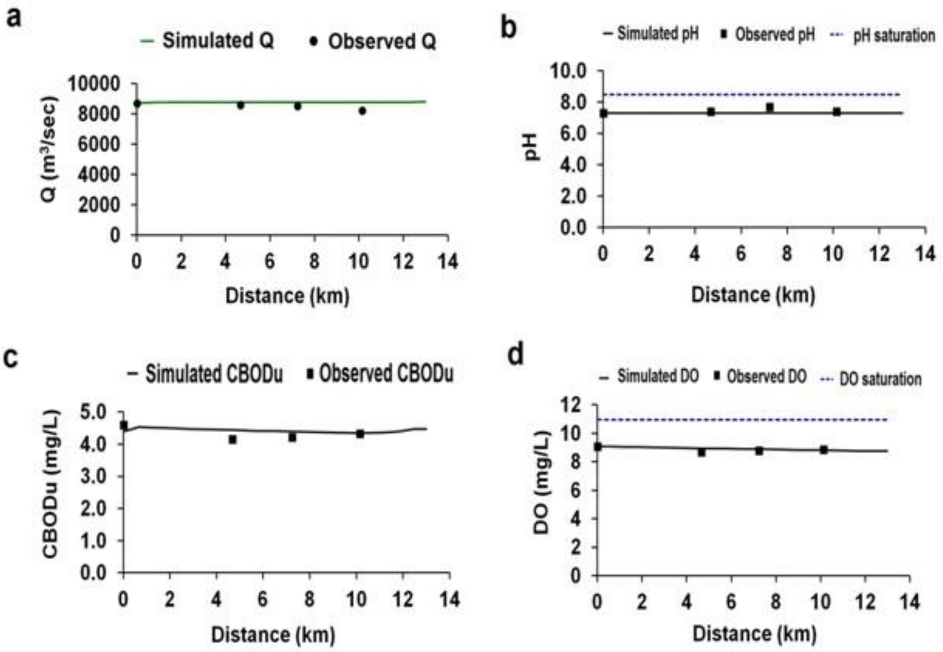

Fig. 3. Calibrated results in spring season for Danube River: a) flow rate, b) pH, c) ultimate CBOD, d) dissolved oxygen (DO), (April 2008)

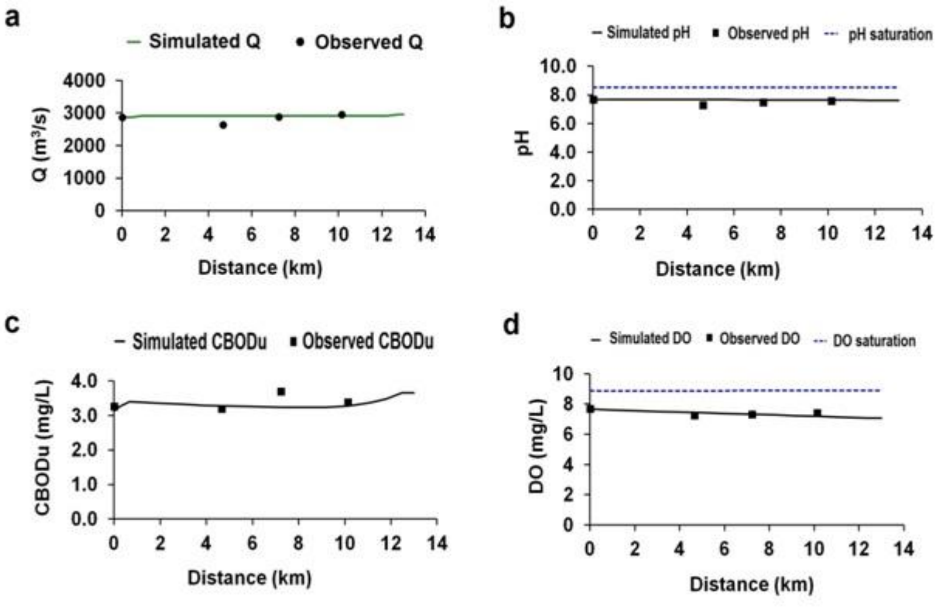

Fig. 4. Validated results in autumn season for Danube River: a) flow rate, b) pH, c) ultimate CBOD, d) dissolved oxygen (DO), (September 2008)

The model results showed that the concentrations of DO were above the limits of 4 mg/L in the study region [5]. Moreover, the variations in simulation for BODu and DO concentration along the 13 km distance were insignificant due to the fact that the pollution load connected to the river such as the two tributaries (Jidostita and Topolniţa) have low discharge compared to the flow of the river.

Table 2

Relative Error (%) of calibrated and validated results between the simulated and observed values for water quality of Danube River, approximate values

Calibrated Results	**% Relative Error**			
Parameters	**SS1**	**SS2**	**SS3**	**SS4**
Q	0	1.5	2.5	6
BODu	4	6.5	3.5	0.5
DO	0	2.5	0.5	0.5
pH	0	1.5	5	1.5
Validated Results	%Relative Error			
Parameters	SS1	SS2	SS3	SS4
Q	0	10	1	1.5
BODu	4	2	12.5	2
DO	0	2	0.5	3
pH	0	5	2	1.5

The model was also used to predict the BODu and DO of the river in different scenarios as a proactive management. Four different scenarios were examined; Case 1: low flow period (1000 m^3/s), Case 2: high flow period (Q = 10000 m^3/s), Case 3: low flow period (Q = 1000 m^3/s) with BOD = 70 mg/L and DO = 0 mg/L for point sources, and Case 4: high flow period (10000 m^3/s) with BOD = 70 mg/L and DO = 0 mg/L for point sources. The water quality modelling results in four different scenarios for BOD and DO is shown in Fig. 5.

The dissolved oxygen concentrations along the river in all cases were correct the minimum dissolved oxygen standard of 4 mg/L, which reflect a good health for the river in this region. As for the CBODu, it can be noticed that the highest concentration for the simulated CBODu in cases 1, 2, 3 and 4 were 5, 3, 8, 3.5 mg/L respectively. The highest values were noticed close to Drobeta-Turnu Severin city in which Topolniţa tributary was the major sources influencing the water quality of the river in the study region. Moreover, the discharge (Q) is the main factor influencing the variation of CBOD concentration than DO in the Danube River.

The model was able to predict the water quality in different scenarios, in spite of some limitations which can be found when modeling a large river such as the estimation of organic loading from non-point sources like livestock and discharges from agricultural activities [9].

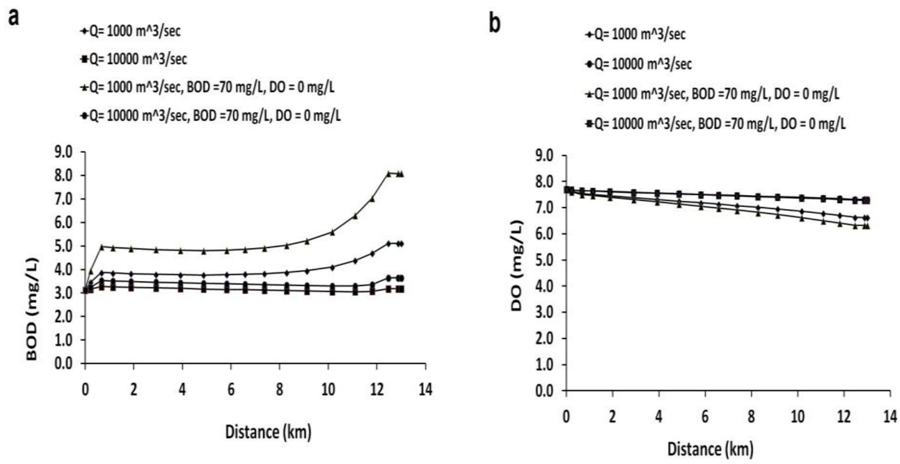

Fig. 5. Water quality simulation of Danube River in different scenarios: a) BODu, b) DO

4. Conclusions

One-dimensional steady state model (QUAL2K) was applied to simulate the water quality in Danube River. This study covered 13 km of the lower Danube course. QUAL2K model was able to predict the water quality in different scenarios. The simulated results showed good fit with the observed values with some exceptions. CBODu and DO showed some differences between simulated and measured data sets at some points, however, the results could be acceptable. The results showed that the DO was correct the minimum dissolved oxygen standard of 4 mg/L, which reflect a good health for the river in the study area. Simulation results for CBODu were below 5 mg/L. Furthermore, the discharges have a significant effect in the water quality of Danube River and the Topolniţa tributary was the major sources influencing the water quality of the river in the study region. In spite of some limitation, it can be concluded that QUAL2K can be used as a suitable tool for simulating the water quality in large river.

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