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Lessons learned by modelling impounded river water quality with QUAL2E

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Abstract

A series of impoundments have been designed to contain hydroelectric power plants (HEPP) on the River Sava. Impoundments will change the velocity of the river, its depths, nutrients cycling, buffering and self-purification capacity. In addition, settling will increase and eutrophication will probably worsen, etc. The US EPA QUAL2E water quality model has been used to simulate and predict possible changes in water quality and the consequent influence on the aquatic ecosystems. The first HEPP in the series is already constructed and operating. Measurements in this impoundment already show a perceivable change in water quality. In this article we discuss the lessons learned by the use of the QUAL2E model. It seems in our case that the QUAL2E model can not take into account all relevant factors and thus use of the models is limited. On consideration of the 2D or 3D model, allowances have to be made for the possible shift in the ecosystem composition, as this seems to be the main source of difficulty if the model is to be properly calibrated for all circumstances, i.e. the flow conditions in different seasons.

1 Introduction

Planned impoundments for hydroelectric power plants (HEPP) on the River Sava will change the former natural water regime of the river and its riparian land. Consequently, conditions which influence the River Sava water quality will also be changed.

Effects of river impoundments on water quality can be positive or negative. Decrease of dissolved oxygen concentration, increase of water temperature and, in some special conditions, enlarged algae production are main negative effects. On the other hand, decreased quantity of suspended substances and decreased organic and bacteriological load in river downstream the impoundments can be seen as a positive effect on water quality. These positive contributions directly contribute to the natural (nonimpounded) water self purification capacity [5].

The intention of our study was quantitative determination of the River Sava water quality changes in existent impoundment Vrhovo in average and extreme hydrological conditions using QUAL2E water quality model [1]. Simulations have been done with stationary model option. Calibration, verification and validation of the model have been done with experimental measurements in impoundment in years 1996 and 1998. After that the model has been used for quantitative prognosis of dissolved oxygen and biochemical oxygen demand in the impoundment for average and extreme hydrological conditions.

2 Data

2.1 Basic data on hydroelectric power plant (HEPP) Vrhovo

HEPP Vrhovo, which construction started in 1987, represents the first HEPP in the series of HEPP on the River Sava section between Zidani most and border with Croatia. The role of the HEPPs will be production of peak energy and therefore they will work in daily accumulation regime [4]. HEPP Vrhovo has started operation in August 1994 and it is still in the phase of test operation.

The river basin of HEPP Vrhovo comprises 7 189 km^2, average discharge is 235 m^3/s. Impoundment lies at 191.00 m above sea level, lowest water level is 182.88 m a.s.l., gross fall is 8.12 m. The surface of the impoundment is 1.43 km^2 and the volume is $8.65*10^6$ m^3. Retention time of water in the impoundment is (depending of the discharge) from some hours up to a few days [6].

2.2 Sampling

For the determination of water quality we designed sampling of three hours average samples on the locations at the inflow into impoundment (for River Sava in Suhadol and for River Savinja in Veliko Širje) and at the output from the impoundment (on dam of the Vrhovo HEPP). First sampling campaign was carried out from 16.9.1996 to 20.9.1996. A new sampling campaign to acquire additional data for model validation, was carried out in August 1998.

Discharges for the first sampling campaign were got from daily log of the Vrhovo HEPP. Regarding characteristic discharges for the period 1961-1990 [2, 3], discharges of River Sava at the inflow into the impoundment (at sampling point Hrastnik) were ranged from average low period discharge to maximal low period discharge and discharges of River Savinja (at sampling point Veliko Širje) have been in class of minimal average period discharge. Discharges during sampling in 1998 were obtained from the database of the Hydrometeorological

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Institute of Republic of Slovenia. Regarding characteristic period discharges, discharges at measuring points Hrastnik and Veliko Širje were ranged from average low period discharge to maximal low period discharge.

3 QUAL2E calibration and validation

3.1 The QUAL2E model

The model used was QUAL2E, perhaps the most widely used computer model for simulating stream-water quality. In this model, the stream is conceptualised as a string of completely mixed reactors linked sequentially by advection and dispersion. Sequential groups of these reactors are defined as reaches. Each reach is divided into computational elements with identical length, hydrogeometric properties and biological rate constants; the last two may change between reaches, but the computational element length remains constant throughout the simulated stream. The model is capable to model up to 15 water quality constituents in streams that are well mixed laterally and vertically. Constituents that can be simulated in the model are dissolved oxygen, carbonaceous biochemical oxygen demand, temperature, algae as chlorophyll a, components of nitrogen cycle as nitrogen (organic nitrogen, ammonium, nitrite, and nitrate), components of the phosphorus cycle as phosphorus (organic phosphorus and dissolved inorganic phosphorus), coliforms, an arbitrary nonconservative constituent, and three arbitrary conservative constituents [1].

3.2 Input data for the QUAL2E model

Input data for the QUAL2E model are discharges on water gauge station Hrastnik on Sava and discharges on water gauge station Veliko Širje on Savinja, results of physical-chemical analyses (water temperature, the concentration of dissolved oxygen, biochemical oxygen demand, chlorophyll a, concentrations of organic nitrogen, ammonium, nitrite, nitrate, dissolved orthophosphate and organic phosphorus) on sampling site Suhadol on Sava and on sampling site Veliko Širje on Savinja, data about daylight average solar radiation and number of daylight hours per day in Slovenia.

3.3 Hydraulics

First step in the modelling with QUAL2E model was division of modelling reach of River Sava from Suhadol to river dam Vrhovo in total length of 9.88 km into a number of subreaches and computational elements. It has been divided into 26 subreaches of different length and into computational elements, each of length 130 meters. Savinja is the tributary of the river Sava. It is modelled as point source to the main stream Sava.

Hydraulic characteristics of the stream subreaches are determined in a functional form. For different discharges (Q) from 65 m^3/s to 150 m^3/s average ($\overline{u}$)velocity and depth (h) to corresponding cross-sections are known. From this

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the empirical constants a, b, α, β in equation $\bar{u} = a \cdot Q^b$ and $h = \alpha \cdot Q^\beta$ for each reach are calculated with mathematical programme NONLIN [7].

3.4 Model calibration

For the year 1996 we have results of physical-chemical analyses for 22 samples from each sampling point. These results represent 3-hour average samples for 5 days sampling. The set of the last 15 samples was used for model calibration, while the set of remaining 7 samples was used for model validation. Sampling results from 1998 were used as a new, independent event for additional model validation in changed meteorological and hydraulic conditions.

Input data for single simulation are three-hour average values. Therefore, three-hour average state of flow and water quality on modelled section of River Sava was followed (simulated) with model calculations.

Satisfactory agreement between measured and modelled results was achieved for BOD_5, dissolved O_2 and chlorophyll a. This is proved by calculated integral of the variable along the river stretch and by average value of measured and calculated variable, as shown in Table 1.

Table 1. Simulated versus measured values for BOD_5, DO and chlorophyll a concentration at the Vrhovo dam.

Variable	BOD_5 (mg O_2/l)		DO (mg O_2/l)		chl a (µg/l)	
Sample	Measured	Simulated	Measured	Simulated	Measured	Simulated
1	1,87	1,91	9,62	9,38	2,75	2,86
2	2,00	1,81	9,57	9,62	2,76	2,83
3	2,02	1,79	9,49	9,47	2,71	2,62
4	2,01	1,89	9,47	9,37	2,69	2,89
5	1,78	2,02	9,26	9,26	1,89	2,02
6	1,95	2,46	9,18	9,18	1,75	1,85
7	2,03	2,00	9,23	9,26	1,63	2,16
8	1,82	1,94	9,47	9,34	2,03	1,64
9	1,55	1,48	9,55	9,44	2,72	2,67
10	1,48	1,78	9,44	9,21	2,79	2,20
11	1,44	1,36	9,38	9,11	2,82	2,74
12	1,33	1,31	9,3	9,01	2,52	3,30
13	1,27	1,31	9,16	9,05	2,08	1,16
14	1,31	1,35	9,12	9,19	2,11	1,53
15	2,92	1,97	11,1	9,80	-	1,50
Integral	**24,39**	**24,44**	**131,98**	**130,10**	**30,82**	**30,28**
Average	**1,79**	**1,76**	**9,49**	**9,31**	**2,38**	**2,32**

For ammonium such good agreement between measured and calculated results could not have been reached (Table 2). It can be concluded that there are unknown sources and sinks of ammonium in the accumulation lake, which are not included in the model. However, modelled results are in an acceptable range. Comparison of modelled and measured results for nitrite and nitrate on the Vrhovo dam shows that the model is successfully calibrated for these two variables.

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Table 2. Simulated versus measured values for ammonium, nitrite and nitrate concentration at the Vrhovo dam.

Variable	NH_4^+ (mg N/l)		NO_2^- (mg N/l)		NO_3^- (mg N/l)	
Sample	**Measured**	**Simulated**	**Measured**	**Simulated**	**Measured**	**Simulated**
1	0,18	0,40	0,05	0,06	1,96	2,07
2	0,19	0,26	0,05	0,05	1,96	2,08
3	0,23	0,25	0,05	0,05	1,99	2,07
4	0,24	0,24	0,05	0,04	1,99	2,03
5	0,22	0,37	0,05	0,06	1,99	2,04
6	0,28	0,37	0,06	0,06	1,99	2,04
7	0,34	0,41	0,06	0,06	2,05	2,05
8	0,49	0,37	0,06	0,06	2,09	2,01
9	0,49	0,20	0,05	0,05	2,15	2,00
10	0,50	0,18	0,05	0,04	2,15	2,04
11	0,51	0,16	0,05	0,04	2,15	2,03
12	0,42	0,19	0,05	0,04	2,15	2,18
13	0,59	0,31	0,06	0,06	2,15	2,18
14	0,64	0,30	0,06	0,06	2,15	2,08
15	0,63	0,26	0,06	0,05	2,12	2,08
Integral	**5,55**	**3,94**	**0,76**	**0,73**	**29,00**	**28,91**
Average	**0,40**	**0,28**	**0,05**	**0,05**	**2,07**	**2,07**

Concentrations of orthophosphate and organic phosphorus calculated by the model are in most profiles lower than the measured concentrations. Higher values could not have been obtained with only varying parameters, which have influence on these two variables.

On the base of comparison of modelled and measured results it was concluded that calibration of the model regarding the given input (measured) data was successfully accomplished. Causes of larger differences between calculated and measured values of ammonium and organic phosphorus should be researched with additional quality and systematic measurements in the impoundment Vrhovo. Determination of organic phosphorus should be done also in unfiltered water samples, because in that way dissolved and particular organic phosphorus would be determined. Then, a new calibration exercise should be done to obtain better agreement with measurements [8].

3.5 Model validation

In the first phase model validation was performed with the set of 7 measurements, which belonged to the same measurement campaign, from which a different set of 15 measurements was used for model calibration. We were forced to use distinct data of the same campaign for calibration and validation, because at that time we did not have two distinct measurement campaigns. Suitable quantitative agreements between simulated and measured values were obtained for BOD_5, DO, chlorophyll a, ammonium, nitrite and nitrate.

Simulated concentrations of orthophosphate and organic phosphorus are in most profiles lower than the measured concentrations. Regarding the results of this validation we cannot reliably apply the model for quantitative prediction of orthophosphate and organic phosphorus in the impoundment. We think that the reason for these differences is systematic error, i.e. total phosphorous is not measured, and P is determined only in filtered samples.

In the second phase, model validation was performed with a set of 6 measurements, which were done in August 1998 at low discharges and at pronounced summer meteorological conditions. Suitable quantitative agreement between simulated and measured results was obtained only for dissolved oxygen (Table 3). For all other simulated variables the agreement is not so good.

Table 3. Simulated versus measured values for BOD_5, DO and chlorophyll a concentration at the Vrhovo dam

Variable	BOD_5 (mg O_2/l)		DO (mg O_2/l)		chl a (µg/l)	
Sample	**Measured**	**Simulated**	**Measured**	**Simulated**	**Measured**	**Simulated**
1	3,21	1,47	8,12	7,89	9,92	3,85
2	3,47	1,54	7,87	7,78	10,56	3,92
3	3,19	1,52	8,12	8,29	9,80	4,23
4	3,38	1,76	7,75	8,84	11,30	3,75
5	2,73	1,67	7,75	9,03	10,27	4,49
6	2,55	1,47	8,19	8,90	16,56	4,62
Integral	**15,65**	**7,96**	**39,65**	**42,34**	**55,17**	**20,63**
Average	**3,09**	**1,57**	**7,97**	**8,46**	**11,40**	**4,14**

The results of model validation are shown in Figures 1, 2 and 3.

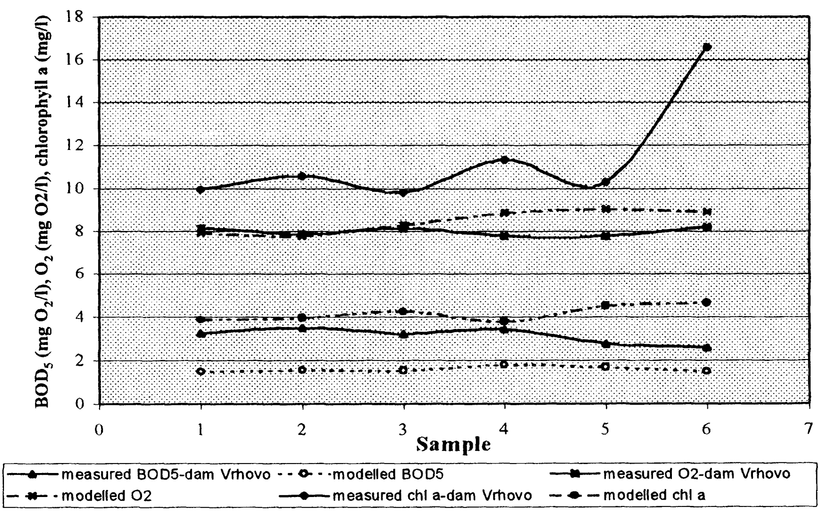

Figure 1. Modelled versus measured BOD_5, DO, and chlorophyll-a.

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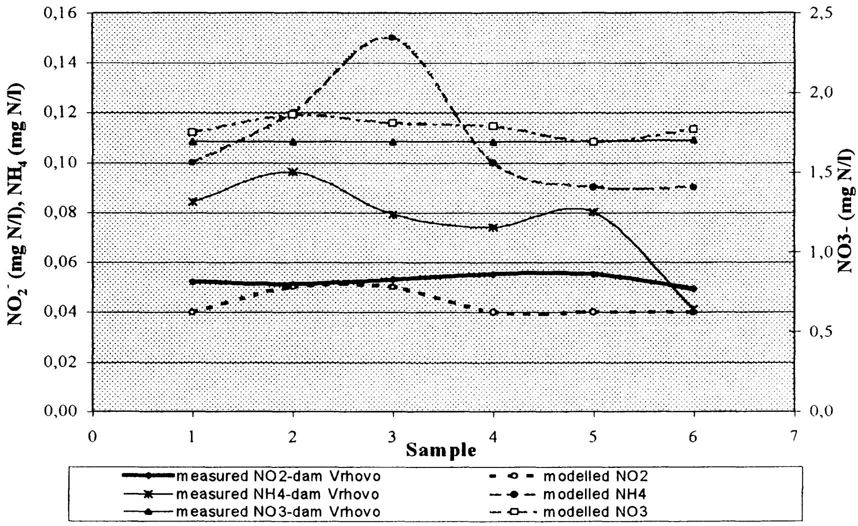

Figure 2. Modelled versus measured NH_4^+, NO_2^-, and NO_3^-.

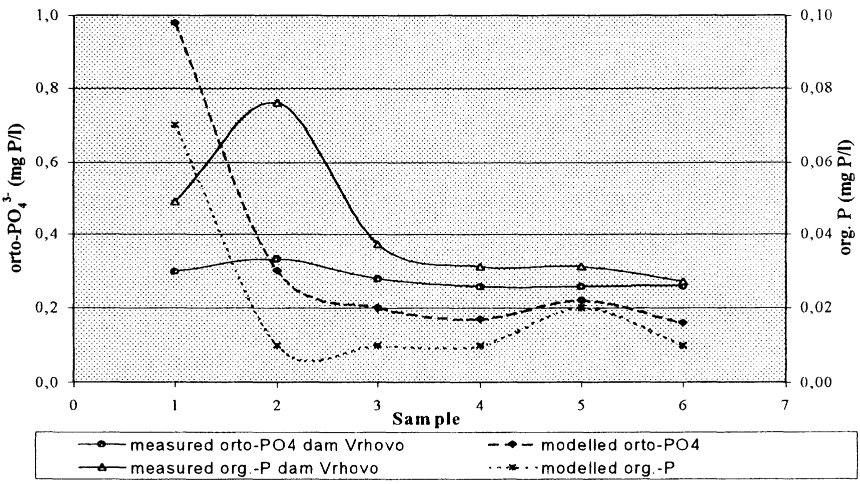

Figure 3. Modelled versus measured orto-PO_4^{3-} and org-P.

4 Prediction of water quality changes in the impoundment Vrhovo

Quantitative water quality prediction of River Sava in the Vrhovo impoundment was performed only for DO and BOD_5. It has to be pointed out that the BOD_5 values calculated by the model do not include newly grown decomposable algae biomass, which could be a serious systematic error (compared to measurements) in the case of intensive algae growth (eutrophication). Instead, this additional oxygen consumption is included in the determination of the DO in the impoundment. Model thus assumes the BOD_5 only as the external load, while all load (external and internal) is properly conceptualised in the DO term.

Predictions were performed for extreme and average hydrological conditions, i.e. for minimal low discharge in a period (simulation A), average low discharge in a period (simulation B) and maximal low discharge in a period (simulation C).

Table 4. Results of simulated DO concentrations at the Vrhovo dam according to the measured DO concentrations at the inflow into the impoundment.

Simulation	Q (m^3/s)	Σt (h)	DO (mg/l)		BOD_5 (mg/l)	
			Input Measured	Output Simulated	Input Measured	Output Simulated
A	39,7	54,6	8,53	7,70	2,54	1,00
B	58,8	37,4	8,53	7,82	2,54	1,30
C	84,0	27,1	8,53	7,91	2,54	1,55

In spite of the fact, that due to the unfavourable validation results, quantitative predictions by model could not have been reliably done for all planed water quality parameters, an approx. information about changes of the most critical variables for estimation of River Sava quality changes is got with the calculation of dissolved oxygen concentrations in the impoundment. Results of calculations are given in Table 4. Concentration of the dissolved oxygen is the most reduced at minimal low period discharge, where reduction amounts to 0,83 mg O_2/l. Organic pollution expressed as BOD_5 is also reduced the most at this discharge. Reduction of oxygen and BOD_5 concentrations are smaller at bigger discharges. Of course, smaller BOD_5 reduction at bigger discharges is not a result of smaller self-purification capacity of water but is a consequence of shorter retention time of the observed element between the input and output profile.

5 Discussion

To find the possible sources of bad fit we checked the data, the analytical procedures, the model assumptions and the model concepts. We ended up with this list of possible reasons for relatively unsuccessful model validation:

1. Not enough data for quality model calibration. For more accurate quantitative modelling water quality parameters in the Vrhovo impoundment it would be

necessary to do more accurate model calibration. For this it would be surely necessary to perform more series of quality measurements in different hydrological and meteorological conditions, for which the calibrated model has to be used for prediction of change of water quality of the River Sava in the impoundment.

2. Hydrodynamics of the model is not completely known. However, velocity distribution is of vital importance for pollution transport and transformation. We found out that 1D (one-dimensional) modelling is questionable for summer conditions, when horizontal and vertical temperature gradients form in the impoundment.

3. Likewise, measurements of water quality constituents show in summer period non-homogeneous horizontal and vertical distribution. It means we do not deal with complete mix of pollutants in cross sections. This statement again points out that 1D model (in longitudinal direction) is not appropriate. So, at least vertical dimension should be included in the modelling of water quality parameters, which means, that water quality in the impoundment should be modelled with (at least) two-dimensional model.

4. Average daily solar radiation for absolutely sunny August day in Slovenia is 564 ly. Maximal input value for average daily solar radiation allowed by model is 400 ly, which means that calculations have been performed with this truncated value, instead with the true one.

5. Among the model parameters is the light extinction coefficient (λ) the one which has the most dominant influence on the system behaviour in the Vrhovo impoundment (e.g. observed primary production, measured as chlorophyll a).

6. The newly originated biologically decomposable algae biomass is not considered in model calculation of BOD. Because of this the calculated values of BOD_5 are lower than the measured values.

7. With regard to model results and field measurements, achieved at low discharges and on condition of intensive primary production in dam it can be concluded that excessive decrease of dissolved oxygen concentration, which could have negative influence on impounded water quality does not appear in the impoundment Vrhovo. But it is clear, that in summer time when water temperature is high and discharges are low, intensive primary algae production can be expected and consecutively secondary pollution, which is reflected in decreased oxygen concentration and in increased value of BOD.

8. At higher discharges and shorter retention times of water in the impoundment conditions for increased primary production cannot fully develop. Thus, the decrease of DO is minimal, while the influence on the BOD_5 reduction can still be seen. This means positive contribution to river self purification capacity. From model calculations it is seen, that organic pollution, expressed as BOD_5, at discharge of 39.7 m^3/s is reduced by 1.54 mg/l. This is equivalent to wastewater treatment plant of almost 90.000 PE (one population equivalent, PE, means load of one person per day, and is 60 g BOD_5/day). At discharge of 84.0 m^3/s the reduction of BOD_5 is equivalent to wastewater treatment plant of 120.000 PE.

9. It is also not clear how much the parameters with which we calibrated the model, change along the flow length and in time, i.e. during the year. We

calibrated the model with unique values of the parameters for all profiles and for all seasons. In the future a proper measurements campaign shall be designed to get an answer to this question.

6 Conclusions

In this paper we described the problems we faced modelling impounded river water quality with the use of the popular 1D (one-dimensional) QUAL2E model. We learned that a better measurements program has to be set up to properly assess all relevant parameters and their changes in place and time. Some conceptual changes have to be done in the QUAL2E model to realistically simulate the BOD profile (secondary pollution not taken into account). Perhaps also introduction of a 2D or 3D model will have to be done.

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