



## CALIBRATION OF WATER-QUALITY MODEL "WODA" – CASE STUDY OF THE WARTA RIVER

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**Abstract.** The main feature of the proposed model implemented by a computer package WODA, that distinguishes it from other commonly used models like QUALE 2E or WASP5, is a possibility of its automatic calibration i.e. parameter estimation taking into account simultaneously several sets of measured concentration data. Model WODA, developed by A. Kraszewski and R. Soncini-Sessa, enables fitting simulated values to measured concentrations of *BOD* and *DO* based on the least-square criterion. This model was applied for parameter estimation of the Warta River in Poland. Measured concentration data used for parameter estimation were obtained from monthly monitoring. The results are presented in the form of *BOD* and *DO* lines against measured concentrations along the analysed stretch of the Warta River. Adaptation of the model simulation results to measured data is described by quantifying characteristics. They indicate relatively good adjustment. The reasons of some differences are discussed and explained.

**Keywords:** *BOD*, *DO*, least-square criterion, model calibration, nonpoint pollution.

### 1. Introduction

Mathematical water quality models were developed since 1920. In 1925, the well-known model of Streeter and Phelps [1] described the balance of dissolved oxygen in rivers. In 1970, package DOSAG-1 was developed by the Texas Water Development Board to simulate point and distributed sources of carbonaceous and nitrogenous oxygen demand and their impact on the *DO* concentration in stream. DOSAG-1 was modified for EPA by Water Resources Engineers as DOSAG-3 by increasing the number of simulated constituents. In the same year Mash et al [2] developed the first version of probably the most popular model – QUAL-1 which allows for simulation of *DO* and *BOD*. QUAL model was improved and extended several times throughout the following years. In 1972, QUAL-1 was extended by Camp Dresser & McKee [3] by adding the option for computing algae, nutrients, and non-conservative pollution. In 1987, Brown and Barnwell [4] introduced two new versions: QUAL 2E and QUAL2E UNCAS. QUAL 2E contains an enhancement to algae-nutrient-*DO* interaction, whereas QUAL2E UNCAS enables uncertainty analysis including three options: sensitivity analysis; first-order, second-moment analysis; and Monte Carlo simulations. The second most popular water quality model is probably WASP5. Its first version was developed in 1983 by Di Toro [5] and modified in 1993 by Ambrose et al [6]. Model WASP5 consists of two engines: DYNAHYD5 [7] used for simulation of unsteady flow and WASP5 which simulates transport of pollution in the river.

Majority of models, including the most popular QUAL2E and WASP5, use the traditional calibration technique involving trial and error. Model WODA (Water Oxidation Deoxidation Assessment) developed by Kraszewski and Soncini-Sessa [8] belongs to a newer generation of models that use automatic calibration techniques employing genetic algorithms. WODA is one-dimensional steady-state water quality model that uses the advanced version of Streeter-Phelps model [1]. The model takes into account sedimentation, photosynthesis, and respiration of aquatic organisms as well as reaeration and biodegradation. All processes are described by the first-order equations, hence the model involves a group of linear models. The unique feature of this model is that *BOD* loads in non-point sources can be considered as unknown variable and can be estimated during the automated calibration process.

The purpose of the paper is to present an automatic calibration method employing the least-square criterion in water-quality model WODA [8] as well as the model application to the Warta River studies. An exemplary calibration was performed for the middle stretch of the Warta River (between 333 km and 218 km a mile from the river mouth) in the central-west region of Poland. Model calibration was aimed on a model parameter adjustment to measured parameters (*BOD* and *DO*), i.e. fine-tuning of the parameters until the model represents field conditions within acceptable limits. Measured concentration data used for this calibration were obtained from the State Inspectorate of Environmental Protection (WIOS) database containing the results of monthly monitoring of

the Warta River and its tributaries. Flow data were obtained from the database generated by the Institute of Meteorology and Water Management (IMGW). Information about *BOD* and *DO* loads from wastewater treatment plants effluent discharges was obtained from the local Water Works.

Distributed pollution sources of Poznan city urban area were considered as unknown variables and evaluated within the calibration procedure. Due to the influence of temperature on reaction rates, the calibration was performed separately for the summer and winter periods.

## 2. Description of Model WODA

Model WODA [8] belongs to a group of relatively simple water-quality models. The model is based on the following assumptions:

- one-dimensional flow – Concentration varies only along the length of the river and is homogenous in cross-section;
- negligible horizontal dispersion – Mass transport is performed only due to advection. This assumption is justified by fulfilling Dobbins [9] criterion;
- aerobic condition for biochemical processes – Only aerobic biochemical processes are considered, which are described by the first-order biochemical reactions.

In model WODA, as in the majority of similar models developed on the basis of Streeter-Phelps equation, change in *BOD* concentration is described by the following equation:

$$\frac{dBOD}{dt} = \frac{S_q}{A} BOD - k_d BOD - k_s BOD + \frac{1}{A} (L_{n-p}^{BOD} + u \cdot L_{n-p}^{u-BOD}), \quad (1)$$

where *BOD* – biological oxygen demand, g/m<sup>3</sup>; *t* – time, h;  $S_q = \frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t}$  for steady state  $S_q = q = \frac{\partial Q}{\partial x}$  – lateral non-point inflow along a reach, m<sup>3</sup>/s; *A* – cross-sectional area of the river, m<sup>2</sup>; *k<sub>d</sub>* – *BOD* reduction rate due to biodegradation, h<sup>-1</sup>; *k<sub>s</sub>* – *BOD* reduction rate due to sedimentation and washing out organic mass from bottom deposits, h<sup>-1</sup>;  $L_{n-p}^{BOD}$  – *BOD* load in the lateral nonpoint inflow, g/(s·km);

$$L_{n-p}^{BOD} = q \cdot BOD_q, \quad (2)$$

$BOD_q$  – *BOD* concentration (g/m<sup>3</sup>) in the lateral nonpoint inflow *q* distributed uniformly along a reach length  $\Delta x$   $L_{n-p}^{u-BOD}$  – unknown *BOD* load in the lateral nonpoint inflow, (g/s·km) adjusted for each data set individually; *u* – scaling factor of  $L_{n-p}^{u-BOD}$  adjusted simultaneously for all data sets (–).

Equation 1 takes into account advection (the first term on the right side of this equation) and two basic biochemical processes: biodegradation and sedimentation of organic mass in the stream (the second and third terms).

The unique feature of model WODA that distinguishes it from the others, such as QUAL 2E, WASP5, is in the last term of Equation 1. It describes *BOD* load in the nonpoint lateral inflow and is divided into known  $L_{n-p}^{BOD}$  and unknown  $L_{n-p}^{u-BOD}$  load which is adjusted during calibration.

In model WODA change in *DO* concentration driven by intensity of processes occurring in rivers, such as advection, biodegradation, reaeration, respiration, and photosynthesis is expressed in the following equation:

$$\frac{dDO}{dt} = \frac{S_q}{A} \cdot DO - k_d \cdot BOD + k_a \cdot (DOS - DO) + \frac{1}{A} L_p^{DO} + \frac{1}{A} (k_{res} DO + k_{ph} DO), \quad (3)$$

where *DO* – dissolved oxygen concentration, g/m<sup>3</sup>; *DOS* – saturation of dissolved oxygen, g/m<sup>3</sup>; *k<sub>a</sub>* – aeration rate, h<sup>-1</sup>; *k<sub>res</sub>* – respiration rate, 1/s; *k<sub>ph</sub>* – photosynthesis rate, 1/s.

Calibration technique used in model WODA includes automated optimization algorithm aiming to estimate the parameters of the model. An objective function, described by Equation 4, is based on the least-square criterion [8, 10]:

$$\min_p \sum_{i=1}^m \sum_{j=1}^{n_i} [(BOD_{ij} - \overline{BOD}_{ij})^2 + (DO_{ij} - \overline{DO}_{ij})^2], \quad (4)$$

where  $BOD_{ij}$  – *BOD* calculated concentration in *j*-cross-section in *i*-data set, g/m<sup>3</sup>;  $DO_{ij}$  – *DO* calculated concentration in *j*-cross-section in *i*-data set, g/m<sup>3</sup>;  $\overline{BOD}_{ij}$  – *BOD* measured concentration in *j*-cross-section in *i*-data set, g/m<sup>3</sup>;  $\overline{DO}_{ij}$  – *DO* measured concentration in *j*-cross-section in *i*-data set, g/m<sup>3</sup>; *m* – number of data sets used to estimate the parameters; *n<sub>i</sub>* – number of *BOD* and *DO* sampling points in *i*-data set; *p* – vector of estimated model parameters.

To solve Equation 4, package WODA employs the Gauss-Newton method. The values of estimated parameters obtained by the Gauss-Newton method give the best-fitted *BOD*- and *DO*-line to all the data sets. The goodness of adjustment can be estimated by quantifying characteristics.

## 3. Case Study

### 3.1. Description of the Warta River

The Warta River is the biggest river of Great Poland (Wielkopolska) and the biggest right-bank tributary of the Odra River. The tributary area of the Warta River has approximately 55,000 km<sup>2</sup> what corresponds to almost 17 % of the area of Poland. Water in the Warta River is classified by European Standards to class A3, due to fecal coliform contamination as well as nutrients and organic matter concentration [11]. The water quality of the Warta River is impacted by several industrial, municipal wastewater discharges, polluted water blending from the Warta River's tributaries as well as non-point sources of organic matter and nutrients from agri-cultural areas.

Approximately 140 km of the middle stretch of the Warta River (from Nowa Wies Podgorna – 342,5 km upstream from the mouth of the Warta River, to Oborniki – 206,3 km upstream from the mouth of the Warta River), was chosen for water quality study [12]. The selected stretch for water quality study is shown in Fig 1.

### 3.2. Input Data

Data required for water quality modeling can be classified [12] as follows:

#### A. Hydraulic Input Data

- Boundaries – cross-section Nowa Wies Podgorna (342,6 km) is the upstream boundary.
- Flow measured in four selected cross-sections – Nowa Wies Podgorna (342,6 km), Srem (291,8 km), Poznan (243,6 km) and Oborniki (206,3 km) – was obtained from daily hydrologic monitoring of the Warta River performed by IMGW – Poznan Division.
- Relationship between discharge  $Q$  and cross-sections area  $A$  for each reach  $Q = f(A)$ . This relationship was obtained from SPRuNeR [13] – a hydraulic model of the Warta River developed at the Agricultural University of Poznan.

#### B. Water-Quality Input Data

- Boundaries – cross-section Nowa Wies Podgorna (342,6 km) is the upstream boundary.
- Point Sources – the following point sources were considered in this study:
  - (1) larger tributaries of the Warta River as listed in Table 1, and
  - (2) wastewater treatment plants discharging to the Warta River as listed in Table 2.

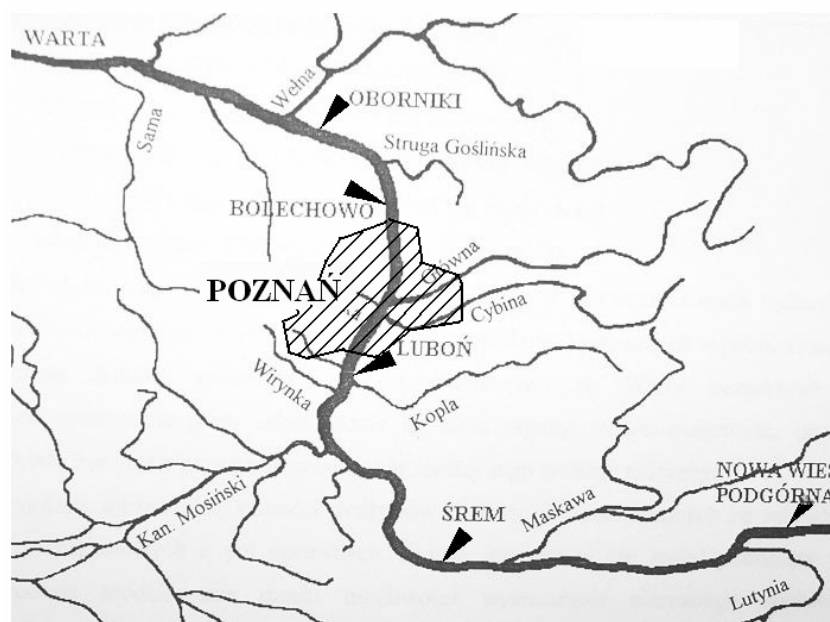
- Nonpoint sources of pollution –  $BOD$  load in runoff from the urban area of Poznan, which involved storm drainage outflows, combined sewer overflows and unregistered foul sewer outflow.

The following pollution sources were not considered as input due to lack of data:

- (1) nonpoint pollution loads from agricultural areas,
- (2) untreated wastewater outflows from a combined sewer system occurring after rainfall events (CSOs), and
- (3) untreated runoff from storm drainage systems discharging.

**Table 1.** Main tributaries of the Warta River included in the study

Tributary	River mile from the Warta River mouth (km)
Lutynia	333,0
Maskawa	307,2
Kanal Mosinski	265,1
Wiryńska	257,7
Kopla	254,6
Strumien Junikowski	251,4
Cybina	242,7
Bogdanka	240,6
Główna	239,6
Struga Goslińska	218,5



**Fig 1.** Location of reach of the Warta River included in the study with denoted cross-sections of water quality measurements

Water quality data were obtained from WIOS – Poznan Division database containing monthly the Warta River water quality monitoring results. Pollution loads were calculated based on known discharge and concentration measurements from monthly monitoring conducted between 2000 and 2002.

Available data enabled modeling the Warta River only for steady-state conditions.

**Table 2.** Wastewater treatment plants (WWTP) discharges into the Warta River included in the study

Wastewater treatment plant	River mile from the Warta River mouth (km)
Srem	290,6
Mosina	263,1
Poznan COS– the central WWTP	238,3
Poznan LOS – the left bank WWTP	239,8
Oborniki	226,6

Assumed in the program WODA relationship between discharge  $Q$  and the cross-section area of the stream  $A$  has a form of exponential function [1]

$$Q = \alpha \cdot A^\beta \tag{5}$$

in which  $\alpha$  and  $\beta$  are regression coefficients.

Regression coefficients were evaluated for all the cross-sections for which the measurement results were available (altogether 117 cross-sections). In order to reduce the number of reaches included in the model WODA, a procedure of cross-section elimination and aggregation was applied [12]. In the first stage cross-sections, for which the correlation coefficient satisfied the relationship  $R^2 < 0,98$ , were eliminated. Then aggregation of similar cross-section was performed on the basis of comparison and averaging of quantifying characteristics.

As a result of this application procedure the number of cross-sections, hence the number of reaches enclosed among them, was reduced from 117 to 12.

### 3.3. Model Calibration

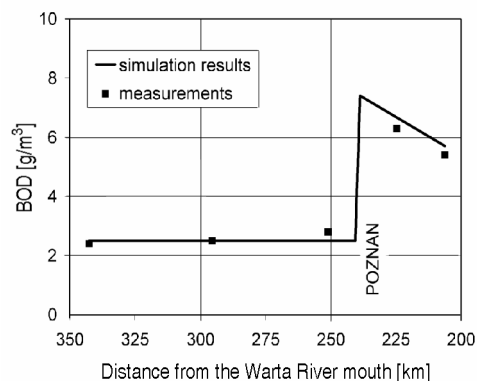
The calibration was performed separately for the summer (since May till August) and winter (since September till April) periods. Each period was represented by nine different data sets that are not presented in the paper.

In the first approximation only the processes of biodegradation and aeration were considered. Based on the results of the first approximation, the considered reach of the Warta River was divided into two sub-reaches to account for differences in intensity of biodegradation and aeration upstream and downstream from Poznan. To improve agreement between measured and simulated  $DO$  and  $BOD$  concentrations, nonpoint  $BOD$  loads from Poznan area were considered unknown and estimated using an automatic calibration method included in package WODA. Unknown  $BOD$  loads were estimated for each of the nine data sets, to fine-tune the model until it simulated

field conditions within acceptable limits. In the following steps the first-order reaction coefficients, describing sedimentation, photosynthesis and respiration processes, were estimated. The model accuracy to predict system behavior can be measured by the following quantifying characteristics: mean square error, average deviation and coefficient of correlation.

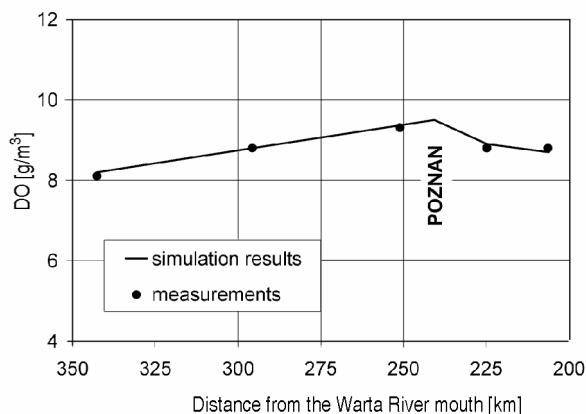
**Table 3.** Values of quantifying characteristics obtained in the study

Function	BOD		DO	
	Winter	Summer	Winter	Summer
Mean Square Error	3,78	1,68	0,36	0,73
Average Deviation	0,02	0,18	0,20	-0,02
Coefficient of Correlation	0,49	0,78	0,93	0,78



**Fig 2.** Comparison of measured and simulated  $BOD$  concentrations in analysed reach of the Warta River for 2 July 2002

Summary of the Warta River model calibration results for the summer and winter calibration periods are presented in Table 3.



**Fig 3.** Comparison of measured and simulated  $DO$  concentrations in analysed reach of the Warta River for 2 July 2002

An example of graphical comparison of measured in summer and simulated water quality parameters (*BOD* and *DO* concentrations) is presented in Fig 2 and Fig 3.

The corresponding adaptation of the model to the July 2, 2002 subset is characterized by quantifying characteristics as listed in Table 4.

**Table 4.** Values of quantifying characteristics for 2 July 2002

Function	BOD	DO
Mean Square Error	0,18	0,05
Average Deviation	-0,14	-0,13
Coefficient of Correlation	0,98	0,96

### 3.4. Results

Monitoring of *BOD* concentrations along the Warta River indicates considerable increase in *BOD* concentration on around the area of Poznan. It was found that the point sources, such as Bogdanka Stream, LOS-Poznan WWTP, are not responsible for this increase. The reason should be sought in nonpoint sources from Poznan area. In order to account for nonpoint sources, a distributed nonpoint pollution load was assumed between 241,0 km and 239,0 km of the Warta River. Magnitude of this load varied for different simulations to represent different field conditions for each calibration period.

In most simulations faster drop of *BOD*-and *DO*-line was noticed downstream from Poznan comparing to upstream from Poznan, which means that self-cleaning processes in reach downstream from Poznan occur with greater intensity (Table 5). Greater intensity of biodegradation may be caused by higher organic matter concentration and consequently higher bacteria activity. In this reach the biodegradation rate has higher value comparing to the reach upstream from Poznan. Both monitoring data and model results indicated almost constant *BOD* concentration in upstream reach (compare with Fig 2). To let *BOD*-line follow measured *BOD* concentrations, biodegradation process was neglected in this reach of the Warta River. Although biodegradation coefficient was assumed zero, biodegradation surely occurs in this reach, but changes in *BOD* concentration are unnoticeable due to balance between *BOD* concentration increase due to inflow from agricultural area and decrease due to biodegradation.

The model indicates that reaeration is more intense downstream than upstream from Poznan. As increase in biodegradation rate causes increasing decay rate of *DO*-line (based on Streeter-Phelps relationship), acceptable adaptation of *DO*-line to measured values of dissolved oxygen concentration requires limited decay rate for *DO*-line which can be obtained by increasing reaeration coefficient. As agricultural activity is not observed during the winter period, the trend discussed above is not observed for this period. Biodegradation and reaeration rates during winter were found to be very low (most likely far below a threshold of model sensitivity, hence it is difficult to talk about any tendency).

Calibrated photosynthesis and respiration coefficients show that biological activity of microorganisms is very limited because of low temperatures in winter. Moreover, in summer, higher oxygen uptake rate during respiration was observed comparing to oxygen release from photosynthesis. This may indicate the superiority of fauna over flora in the Warta River ecosystem.

### 4. Conclusions

Calibration of the middle reach of the Warta River (between Nowa Wies Podgorna – 342,5 km, and Oborniki – 206,3 km) using program WODA allowed determination of biodegradation, reaeration, respiration and photosynthesis rates characterizing relevant processes.

It is found that the intensity of self-cleaning processes is greater in summer than in winter, showing that temperature is a limiting factor for microorganisms' activity in the Warta River.

The Warta River seems to be a clean river in terms of *BOD* and *DO* concentrations. The intensity of self-cleaning processes in the Warta River is low or even seasonally undetected by the model (for instance, respiration during the winter season).

To justify estimation of unknown nonpoint *BOD* loads by the automated calibration process, additional information should be gathered for verification purposes. Data required for verification should be collected along a characteristic line, i.e. downstream the main river with a lag time equivalent to transport time of a pollutant. Additionally, discharge measurements and concentration necessary for pollution load computation in runoff from storm drainage network, untreated runoff from CSO, and outflow from municipal and industrial WWTPs should be considered in further studies.

**Table 5.** Reaction rates of self-purification processes in the Warta River middle stretch estimated by program WODA

Process	Unit	Summer period		Winter period	
		Upstream from Poznan	Downstream from Poznan	Upstream from Poznan	Downstream from Poznan
Biodegradation	h <sup>-1</sup>	0	0,026	0,008	0,023
Reaeration	h <sup>-1</sup>	0	0,096	0,014	0
Respiration	g/(s·km)	0,050		0	
Photosynthesis	g/(s·km)	0		0	

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## VANDENS KOKYBĖS PROGRAMOS MODELIO WODA TIKRINIMAS PAGAL WARTA UPĖS PAVYZDĮ

M. Sowinski

Santrauka

Svarbiausia kompiuterio programos WODA modelio savybė, išskirianti jį iš kitų dažnai taikomų modelių, pavyzdžiui, QUALE 2E arba WASP5, – tai galimybė jį patikrinti automatiškai būdu, t. y. parametrų nustatymas, atsižvelgiant į tuo pačiu metu gautus rezultatų rinkinius. Modelis WODA, kurį sukūrė A. Kraszewski ir R. Soncini-Sessa, leidžia priderinti modeliuotas vertes prie BDS ir ištirpusio deguonies kiekio pagal mažiausiųjų kvadratų metodą. Šis modelis buvo pritaikytas Lenkijos Warta upės parametrams įvertinti. Išmatuotos koncentracijos, naudotos parametrus įvertinti, buvo gautos po mėnesio stebėjimų. BDS ir ištirpusio deguonies kiekio vertės pateikiamos kartu su išmatuotomis koncentracijomis pagal upės ilgį. Modeliavimo rezultatų ir išmatuotų verčių skirtumas įvertintas statistiniais metodais. Tai parodė atitiktį tarp modelių ir matuotų verčių. Aptartos priežastys, galėjusios turėti įtakos kai kuriems skirtumams.

**Reikšminiai žodžiai:** BDS, ištirpusio deguonies kiekis, mažiausiųjų kvadratų metodas, modelio pritaikymas.

## ПРОВЕРКА МОДЕЛИ „WODA“ КОМПЬЮТЕРНОЙ ПРОГРАММЫ ПО КАЧЕСТВУ ВОДЫ НА ПРИМЕРЕ РЕКИ ВАРТА

M. Совински

Резюме

Важным свойством компьютерной программы „WODA“ по сравнению с другими часто применяемыми программами, например, QUALE 2E или WASP5, является возможность проверить ее автоматическим способом, т. е. установить параметры с учетом полученных в то же время результатов. Модель „WODA“, созданная А. Крашевским и Р. Сончини-Сесса, позволяет соотнести смоделированные значения с BDS и количеством растворенного кислорода по методу наименьших квадратов. Этот метод был применен для оценки параметров польской реки Варта. Концентрации, примененные для оценки параметров, были определены после месяца наблюдений. Значения BDS и количества растворенного кислорода были представлены вместе с измеренными концентрациями по длине реки. Разница между результатами моделирования и измеренными данными оценивалась статистическими методами. Это подтвердило соответствие смоделированных и измеренных значений. Выявлены причины, которые могли оказать влияние на некоторые различия.

**Ключевые слова:** BDS, количество растворенного кислорода, метод наименьших квадратов, применение модели.

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