Modeling of Water Quality Evolution with Advanced Hydroinformatic Tool. Study Case: Bega Channel Sector

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Abstract. Water quality evolution modeling is very important to predict the changes in surface water quality for water resources and environmental management in the world. Worldwide, in the last decades, hundreds of surface water quality models have been developed. Water quality models based on advanced hydroinformatic tools are an efficient way to simulate and predict the pollutant transport in water courses, lakes and reservoirs, which can contribute to saving the cost of labors and materials for a large number of sampling and chemical experiments to determine the degree of pollution of water bodies. Surface water quality models are useful tools to simulate and predict the levels, distributions, and risks of chemical pollutants in a given water body, in different scenarios of pollution (point source, distributed source and accidentally pollution). The modeling results from these models are very important components of environmental impact assessment and can provide a basis and a technique support for specialists from the water resources and environmental management authorities to make the right decisions. For the case study, we use MIKE11 advanced hydroinformatic tool. MIKE11, part of the DHI software products, is a professional engineering software package for the simulation of flows, water quality and sediment transport in estuaries, rivers, irrigation systems, channels and other water bodies. MIKE11 is a user-friendly, fully dynamic, one-dimensional modeling tool for the detailed analysis, design, management and operation of both simple and complex river and channel systems. The used modules for modeling are Hydrodynamic Module and ECOLab module. The case study was realized on Bega channel sector (city of Timisoara – state border with Serbia), Timis county, Romania.

1. Introduction

Water quality is fundamental for river and adjacent ecosystems good health. Water quality sustains ecological processes that support native fish populations, vegetation, wetlands and birdlife. Water quality is important not only to protect public health, but also many of human needs depend on the water quality that is suitable for drinking, irrigation, watering stock, fishing and recreation, and to meet cultural and spiritual needs. If water quality is not maintained or decreasing, it is not just the environment that will suffer. The economic and recreational value of water resources will also diminish. [1]

Water quality objectives recognize the economic and environmental values of water resources and are established for different scopes that the community wants to see protected. These include water for drinking and irrigation, for the food industry, recreational use, and healthy aquatic ecosystems. These
objectives have been established following consultation with communities, for surface and ground water resources. Water quality is managed and assessed in terms of indicators for levels of bacteria, physio-chemical properties of water (dissolved oxygen, biochemical oxygen demand, concentration of various chemicals, suspensions etc.). [1]

Water quality evolution modelling is very important to predict the changes in surface water quality for water resources and environmental management in the world. Worldwide, in the last decades, hundreds of surface water quality models have been developed. Water quality models based on advanced hydroinformatic tools are an efficient way to simulate and predict pollutant transport in water courses, lakes and reservoirs, which can contribute to saving the cost of labors and materials for a large number of sampling and chemical experiments to determine the degree of pollution of water bodies. These models offer efficient tools for water quality managers to protect public health support the economy and maintain rich and healthy ecosystems.

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2. MIKE 11 advanced hydroinformatic tool
MIKE11 advanced hydroinformatic tool, part of the DHI software products, is a professional engineering software package for the simulation of flows, water quality and sediment transport in estuaries, rivers, irrigation systems, channels and other water bodies. MIKE11 is a user-friendly, fully dynamic, one-dimensional modeling tool for the detailed analysis, design, management and operation of both simple and complex river and channel systems. The used modules for modeling are Hydrodynamic Module and ECOLab module. [2]

\[
\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = q
\]  

(1)

\[
\frac{\partial Q}{\partial t} + gA \frac{\partial h}{\partial x} + \left( \alpha \frac{Q^2}{A} \right) + \frac{g |Q| Q}{C^2 A R} = 0
\]  

(2)

where: Q is discharge, x is longitudinal channel distance, A is cross-sectional area, q is lateral inflow, t is time, h is flow depth, C is the Chezy coefficient and R is the hydraulic radius.

The advection-dispersion model (AD) is based on the one-dimensional (vertically and laterally integrated) equation for the conservation of mass of a substance in solution, i.e. the one-dimensional advection-dispersion equation:

\[
\frac{\partial (AC)}{\partial t} + \frac{\partial (QC)}{\partial x} - \frac{\partial}{\partial x} (AD \frac{\partial C}{\partial x}) = -A \cdot K \cdot C + C_2 q
\]  

(3)

where: C is the concentration, D the dispersion coefficient, A the cross-sectional area, K the linear decay coefficient, C2 the source/sink concentration, q the lateral inflow, x the space coordinate and t the time coordinate. The advection-dispersion equation is solved numerically using an implicit finite difference scheme which, in principle, is unconditionally stable and has negligible numerical dispersion.
The equation reflects two transport mechanisms:

- advective (or convective) transport with the mean flow;
- dispersive transport due to concentrations gradients.

The main assumptions underlying the advection-dispersion equation are:

- the considered substance is completely mixed over the cross-sections, implying that a source/sink term is considered to mix instantaneously over the cross-section;
- the substance is conservative or subject to a first order reaction (linear decay);
- Fick's diffusion law applies, i.e. the dispersive transport is proportional to the concentration gradient.

The module requires output from the hydrodynamic module, in time and space, in terms of discharge and water level, cross-sectional area and hydraulic radius. [2]

ECOLab is a numerical lab for Ecological Modeling. It is an open and generic tool for customizing aquatic ecosystem models to describe water quality, eutrophication, heavy metals and ecology. The module is mostly used for modeling water quality as part of an Environmental Impact Assessment (EIA) of different human activities.

The user can use predefined ECOLab (WQ) templates containing the mathematical descriptions of ecosystems or can choose to develop own model templates. The module is developed to describe chemical, biological, ecological processes and interactions between state variables and also the physical process of sedimentation of components can be described. The ECOLab is integrated with the advection-dispersion module. [3]

Biological Oxygen Demand, BOD - the carbonaceous biological oxygen demand - is an expression of the water’s organic matter content, that is to say, the biodegradable part of the organic matter which gives rise to oxygen consumption. The organic matter content is measured by registering the oxygen consumed during the degradation for a period of 5 days. Degradation in the environment of the organic matter expressed as BOD gives rise to an equivalent consumption of oxygen. The BOD degradation terms will, therefore, be a part of the oxygen balance. Degradation of BOD is also a source of nutrients (nitrogen and phosphorus) since these are part of the organic matter. The inorganic nutrients (ammonia) being products of the BOD degradation can be oxidized and give rise to the additional oxygen consumption. [4]

Dissolved Oxygen, DO - oxygen in the aquatic environment is produced by photosynthesis of algae and plants and consumed by respiration of plants, animals and bacteria, BOD degradation, sediment oxygen demand and oxidation of nitrogen compounds. The main reason for modeling the dissolved oxygen concentration is to ensure that it is above acceptable levels for biota in the area under consideration. In ECOLab the variations in the concentration of DO are described differently for each model level. In the simplest level, variations of DO concentration are described as a function of the naturally occurring processes (photosynthesis, respiration and reaeration) and degradation of organic matter (BOD). A number of processes affect the oxygen concentration: [4]

- Re-aeration: (dissolved oxygen is re-aerated through interchange with the atmosphere)

  \[ \frac{d\text{DO}}{dt} = K_2(C_s - \text{DO}) \]  

  where: \( C_s \) - saturation concentration of DO, \( T \) - water temperature (0C) \( K2 \) - re-aeration constant at 20°C (1/day).
• **Nitrification:**

\[
\frac{dNH_3}{dt} = K_4 \cdot NH_3 \cdot \theta^{(T-20)} \cdot \frac{DO_2}{K_s+DO_2^n}
\]  

where: NH3 - concentration of ammonia (mg/l), K4 - nitrification rate at 20ºC (1/day or ((mg/l)½/day), θ - Arrhenius temperature coefficient, Ks - half-saturation constant.

• **Photosynthesis:**

\[
P = P_{\text{max}} \cdot \cos 2\pi \frac{\tau}{\alpha} \quad \text{if} \quad \tau \in [t_{\text{up}}, \ t_{\text{down}}] ; 0 \quad \text{if} \quad \tau \in [t_{\text{down}}, \ t_{\text{up}}]
\]  

where: P - actual production (g O2/m²/day), P_{\text{max}} - maximum production at noon (g O2/m²/day), τ - actual time of the day related to noon, α - actual relative day length, tup,down - time of sunrise and sunset.

• **Respiration:**

\[
R = R_{20} \cdot \theta_2^{(T-20)}
\]  

where: R - actual respiration rate of plants, bacteria and animals (g O2/m²/day), R20 - respiration rate at 20ºC (g O2/m²/day), θ2 - Arrhenius temperature coefficient.

• **Oxygen consumption from degradation of organic matter:**

\[
\frac{dBOD}{dt} = K \cdot BOD \cdot \theta^{(T-20)} \cdot \frac{DO_2}{K_s+DO_2^n}
\]  

where: BOD - actual concentration of organic matter (mg O2/l), K - degradation constant for suspended organic matter at 20ºC (1/day), θ - Arrhenius temperature coefficient, Ks - half-saturation constant (dissolved/suspended/deposited organic matter).

• **Sediment oxygen demand (B1)** is assumed to be constant in time.

As a basis for the description of the water quality conditions, the AD calculates the conservative transport of the modeled components. The WQ (water quality) processes in combination with the AD transport give the final result. [4]

3. **Study Case**

The water quality evolution was modeled on Bega Channel sector (the City of Timisoara to Romanian - Serbian border, Bega Channel is transboundary water course), in order to Bega Channel sustainable development.

The data required for modeling are: longitudinal profile of studied river sector (Figure 1); 13 cross-sections (where was performed over time bathymetric measurements by Banat Water Basin Administration) (Figure 2); time series: discharge hydrograph – average monthly discharge for 2005 in cross-section upstream of Timisoara – duration of simulation 1 year; boundary conditions: Q-H curve in cross-section situated downstream, on the state border (Figure 3). [5]
Figure 1. Area plan of Bega Channel and studied sector

Figure 2. Cross sections between upstream Timisoara and RO-SRB border

Figure 3. Average monthly discharges hydrograph and variation of OD, BOD and temperature in upstream and downstream cross sections
4. Results and discussions

For water quality modeling, WQ model level 1 with state variables was used: BOD, oxygen and temperature. When calculating the oxygen balance the nitrification component is not included. Suspension and sedimentation are not included in the BOD balance, and only immediate oxygen consumption is taken into account. At this level, the problem under study relates to oxygen depletion due to discharges of readily degradable organic matter into the river. Phosphorus and coliforms are optional. The differential equation describing the effects of these processes on the dissolved oxygen concentration (oxygen balance) is the following: [4]

\[
\frac{d\text{DO}}{dt} = +K_2(C_s - \text{DO}) - K \cdot \text{BOD} \cdot \theta^{(T-20)} \cdot \frac{\text{DO}^2}{K_s + \text{DO}^2} - R_{20} \cdot \theta_{(T-20)} + P_{\text{max}} \cdot \cos 2\pi \left( \frac{\tau}{\alpha} \right) - B_1
\]

The obtained results from modeling with MIKE11 – ECOLab are shown in figures 4, 5, 6 and 7.

Figure 4. Water level in longitudinal profile and discharge in cross-sections

Figure 5. Variation of dissolved oxygen and BOD
5. Conclusions

Water is a key environmental factor for the life of humans, animals and plants, representing an indispensable resource for the economy, to be important both quantitatively and qualitatively. The use and effective protection of water resources and ecosystems of the world against pollution and climate change requires a coordinated action, worldwide. In particular, the EU Member States are obliged to adopt the management plans and programs of measures appropriate for each water body with taking into account the result of analyses and studies. Special attention should be paid to cross-border water bodies, which, in addition to EU directives and regulations, are also subjects to the international treaties concluded between riparian states.
An important step to achieve the management plans of water resources is the quality evolution forecast in watercourses. Understanding of physical, chemical and biological processes in water bodies plays an important role in the design, development and implementation of performant water quality models. The advanced hydroinformatic modeling tools for the water quality provide satisfactory results with regard to the status of water quality, both in normal periods and in case of accidental pollution.

The detailed results obtained from modeling and forecast increase general understanding of the evolution of water quality in water bodies and support authorities to act (in time and space), in case of accidental pollution, according to the plans of action in emergency situations, based on plans of risk management of watercourses’ pollution.

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