Model of surface water quality

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Abstract. To predict the variation in Dissolved Oxygen, as well as ammonia concentration in streams, several computer-based mathematical models have been used. How can we control this process using statistical data about, predict, analyze, prevent the critical period, those are some goals for this review.

Keywords: simulate; modeling; predict extreme events; water quality

1 Introduction

Mathematical models in the study of environmental phenomena keep up with the latest results in the mathematical domain which could provide solutions for controlling, analyzing, predicting and study of risk phenomena. Water quality model usually consist of a set of mathematical expressions relating one or more water quality parameters. In any set of environmental measurement, the subjects of accuracy and precision of the measurements are always beneath the surface. Most environmental discharge permits embody normally distributed statistics for environmental events. This is incorrect and rarely realized. Mathematical model of the evolution of the Danube surface water quality parameters and the mathematical accepted structures can help the establishing of a more comprehensive map of risk factors, the imagine of the complex system of Danube River which live like a human entity, permanently monitored, [1].

2 Study area

Study area is located in the terminal of the Danube river basin, in contact with Delta and only 80 km from flowing into the Black Sea. This area is known as Romanian Danube Shipping Sector. Framed in terms of the mathematical modeling, area of study is an imaginary quadrilateral, in latitude of 18 and in longitude by about 1' , around latitude: 45.28 and longitude: 27.97. The evaluation of Danube water quality was conducted in two control locations 183 km and 166 km, which are the entry and exit locations of the river water in Brăila County. From this study, monitored data archive during four years ago (2004-2007) was used. Initial data table was structured and used for data interpolation of each function with twelve values per each year for each monitored element, obtaining time series with a lot of data. These data are confirmed by the real evolution in time.

3 Surface water quality model

The evolution of such series could give important results about phenomena which usually are not viewed analyzing the data using other methods like excel maps. First step was to use the interpolation with Spline function for initial data table of twelve values for one year, developing structure of graphical analysis for parameters like Dissolved Oxygen (DO), degree of saturation of DO, (DOs), or the coefficient of adsorption for Oxygen in water K, temperature T and connections between. This has produced a theoretical evolution for (DO) and water temperature and others monitored parameters for surface water as functions of time, giving the possibility to consider that the evolutions could be modeled as C1 class function of time. We consider that our results show a strong spatial structure for water characteristic on a given day and temporal structure from day to day, using a high degree of division, and the function $f(x) = (\sin x + \cos x)^{\frac{4}{3}}$, (eq.1) it is an inspired function in this case. If a spline function will interpolate the data using a fine norm, one could see for obtained data that between the second and the third month in 2006, there is a maximum of 9.9 (mg/l), not visualized in data table with twelve values monitored by stations, [2]. Many cases like this can be present during an annual decade so, we could accept the real evolution representing in graph could show some periods out of accepted level of concentration of (DO). A simplified model with some identified substances in water could be described by the concentration of these chemicals species: (DO), algae in water, (BOD), (SOD), (BOD) including carbonaceous BOD (CBOD), nitrogenous group involved in nitrification, NH_4^+, NO_2^-, NO_3^-. The DO in water has an important impact on aquatic animals and plants. The two major sources of oxygen in water are from diffusion from the atmosphere across the water surface and photosynthetic oxygen production from aquatic plants such as algae and macrophytes. Important factors that affect DO in water may include water temperature, aquatic plant photosynthetic activity, wind and wave mixing, organic contents of the water, and sediment oxygen demand. Excessive growth of algae (bloom) or other aquatic plants may provide very high concentration of DO, so called supersaturation. On the other hand, oxygen deficiencies can occur when plant respiration depletes oxygen beyond the atmospheric diffusion rate.

One can identify three reactions in the molecular soup, for the chemical species considered in the simplified model and these reactions give us information about rules for the model. Reduced nitrogen species (NH_4^+, NO_2^- and NO_3^-) can be oxidized aerobically by nitrifying bacteria which can utilize carbon compounds but always require nitrogen as an energy source. The two-step nitrification can be expressed as:

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\begin{array}{ll}
NO_2^- + \frac{1}{2}O_2 \leftrightarrow NO_3^- & R1 : a + 2b = 2c \\
NH_4^+ + \frac{3}{2}O_2 \leftrightarrow NO_2^- + 2H^+ + H_2O & R2 : 3a + 2d = 2b + 4e \quad \text{(eq.2)}. \\
NH_3 + H^+ \leftrightarrow NH_4^+ & R3 : f + e = d.
\end{array}
$$

Molecules present in one unit of water at any time t will be considered like elements of some multisets. The idea of using multisets in the representation of biochemical reactions was present in G. Paun and V. Manca research since 1997, [4]. Biological processes are subjected to noise, fluctuation, external influxes, but at large, they are essentially deterministic (V. Manca, 2009).The reactions which are present between chemical species present the transition from one stage to another and will be represented by rules but this could be a not easy process, [3]. The fluxes we could consider stoichiometric coefficients of equations of chemical reactions. The flux function could describe the equilibrium formulas. The real data taken and the possibility of data interpolation could produce a much large beach data which could be used in specialized programs of simulation. The experimental data and the control of the concentration of the species, the real evolution of the concentration of chemical species, could propose a structure of a P-System as follow: $P = (V, T, C, m, w_1, w_2, w_3, (R_1, p_1, f_1), (R_2, p_2, f_2), (R_3, p_3, f_3))$ where: V is an alphabet (elements of different chemical species presented in a unit, notated in (eq.2) with a,b,c,d,e,and f)); T is the output alphabet; C catalysts could include the influence of X-raises or level of rainfall; m is the membrane structure, in our case $[[\ ]_2[\ ]_3]_1$; R_i denote reaction (2) as there were described above and which are theoretical reaction not possible in natural condition and as p_i "the power" of these reaction this are possible in a sense or in other sense; f_i are function of control and these show that in one transition a rule R_i could be applied to a number of times. We assume that there is a connection between functions f_i and obtained functions by interpolation, (see eq.1). These functions show a periodical evolution.

However, for the investigation of environmental condition in the sediment, an additional sediment investigation must be analyzed, [2]. The situation must be upgraded considering growth of Algae with $NH4^+$, growth of Algae with $NO3^-$, death of consumers, reversible reactions, anoxic processes, etc.

Biological denitrification is the conversion of nitrate to gaseous nitrogen species and to cell material by the ubiquitous heterotrophic facultative aerobic bacteria and some fungi. denitrifiers include a broad group of bacteria. These groups of organisms can use nitrate or oxygen as electron acceptor (hydrogen donor) for conversion of nitrate to nitrogen gas.

The main characteristic of water courses is the variable load with materials in suspension and organic substances load directly proportional to the weather and climatic conditions. For waters of the river Danube, 800 organic and inorganic compounds have been highlighted. These increase during rain falls, reaching a maximum level during the period of great high floods and a minimum level during freezing periods. Considering this, one could accept that the proposed P-System must contain more than three cell in the membrane structure and one of this which must contain elements of living organism present in water will be an important one. We consider that if we have the evolution in time of this system and its transition through a lot of stages, reversely the transition rules will be better defined.

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