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Modeling and simulation of pollutants transport in rivers

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Abstract

This paper is devoted to mathematical modeling and computer simulation of diffusion and transport of chemicals in rivers. We present one-, two-, and three-dimensional models in terms of time-dependent convection–diffusion–reaction differential equations, further we give the finite difference approximation and appropriate numerical algorithms for these models, and finally we discuss briefly the computer implementation of this methodology in a user friendly software package. To verify the model and the computer code we have used it to study the diffusion and transport of chemicals, in this case NO_3 and PO_4, in two rivers in Western Georgia flowing into the Black Sea. Namely, we considered the river Khobistskali subject to pollution sources Ochkhomuri and Chanistskali river Choga polluted with NO_3.

In order to evaluate the quality, the accuracy, and the performance of the methods and the developed software we have applied one-, two- and three-dimensional models to the same case, for which we had data from measurements. By analyzing the difference between the measured and the simulated values of controlled chemicals in the rivers, we have estimated the effect of agricultural activities along the banks of the river (in the interval between two sections) on the pollution degree of the Khobistskali river. In this sense, the example is schematic, since the number, the arrangement, and the capacities of pollution sources of Khobistskali only partially correspond to the real situation. Though, the geometry of the rivers, the arrangement of the control sections, and the concentrations of polluting substances in the rivers matches well the real data.

Keywords: Modeling; Simulation; Pollutant; Transport; River water; Software package

1. Introduction

The evaluation and analysis of water pollution from both technological and economic points of view is a very important issue in the ecology. Fast and reliable estimates of the damages on the water quality due to

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pollution could play essential role in establishing governmental regulations for environmental protection. Introduction and utilization of such measures are impossible without knowledge of various processes, e.g. formation of a water line in rivers, transport of pollutants, capability of self-cleaning, etc. The mathematical models and computer systems could be applied also at both the pre-designing stage of measures and facilities and in the process of practical use of the facilities. In this respect mathematical modeling of water levels in rivers and the processes of transport and diffusion of chemicals could play a major role in establishing scientifically justified and practically reasonable programs for long-term measures for a rational use of water resources, reduction of pollutants discharge from particular sources, estimation of the impact in the environment of possible technological improvements, development of methods and monitoring facilities, prediction and quality management of the environment, etc. Further, systems for automated monitoring and control open up possibilities to application of new mathematical and computer methods for analysis and rational use of natural resources. The success of the mathematical methods and automated systems in solving practical problems in many respects depends on the adequacy of the models and the quality of the software used for the simulation of the real processes.

We consider our work as a part of a substantial effort and research activities in the area of mathematical modeling and computer simulation of the water line in rivers and river pollution (cf. [1–8]). In [5] an eutrophication models for simulation of seasonal algae concentrations prior to fertilizer application are developed. These models led to computer implementation of the methodology developed in [7,8] and a number of computer simulations. Further in [6] a three-dimensional numerical eutrophication model has been developed. This model also integrates the hydrodynamics with the water quality and simultaneously incorporates the sediment oxygen demand and the nutrient releases from sediments.

The objective of current work is to put together in one effort the full cycle of mathematical modeling, numerical methods and approximations, computer implementation, and simulation of time-dependent transport of substances in a water media during the eutrophication process. The proposed mathematical models and numerical methods are implemented in a user friendly software package and have been used to repeat the numerical simulation presented in [5,6] for appropriate choice of the initial data and boundary conditions.

One of our main goals is to give the practitioners in environmental and in particular in water protection agencies a user friendly, accurate, and relatively simple software tool. The developed code provides a reliable tool for quick analysis of the water quality in rivers. Also it is applicable to other fields of science and engineering. The software package we have developed is based on modeling distribution of the concentration of polluting substances in rivers due to multiple sources and polluting substances. We have developed one-, two- and three-dimensional advection–diffusion models under various initial and boundary conditions. Some of the important features of the model include: (1) advection–diffusion equation with a non-local boundary condition at the end of the controlled section which incorporates a capability of natural self-cleaning of the river and a boundary condition of complete mixing at the end of controlled section; (2) a diffusion equation with a non-local boundary condition at the end of the controlled section which models natural self-cleaning of the river and a boundary condition of complete mixing. It is assumed, that the studied river section contains some point or/and volume sources of pollution, for example, ends of pipes, through which enterprises discharge industrial wastes into the river, underground sources or other rivers running into the river within the section, etc. We assume that at the upper end of the river section under control, i.e. at the beginning of the given cross-section, the concentrations of the polluting substances are known.

The paper is organized as follows. In Section 2 we give a brief description of the mathematical model, a general three-dimensional advection–diffusion–reaction equation for advection in the longitudinal direction and reaction describing the self-cleaning properties of the river. Next, we give two simplified, one-dimensional and two-dimensional, models that proved to be excellent mathematical tool for many practical situations. A novelty in our model are the boundary conditions described in Section 2.3. We have included a non-local boundary condition that gives better modeling capabilities in the case of significant possibility of a river to self-purify. In this case the modeling process corresponds better to the real situation. Here instead of theoretically infinite (or practically enough long) river section we use only a particular section of the river. This substantially decreases the simulation time and improves the accuracy. Further, we describe the coordinate system that is used to model adequately the geometry of the river channel. Finally, in Section 2.5 we briefly describe the discretization and the numerical algorithms that were implemented in the computer system.