The models for the description of highly mineralized brines behavior in surface water bodies

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Abstract

One of the most widely used approaches to the disposal of wastewater, including mine water, is to remove them to surface water bodies in order to reduce pollutant concentration due to dilution process. Most of the dilution methods are based on evaluation of mixing processes with neutral buoyancy while the behavior of heavy highly mineralized brines is fundamentally different. For this reason, most of traditional methods for calculating the dilution which regulate the procedure for the discharge of wastewater to surface water bodies are incorrect. This paper discusses new approach based on hydrodynamic models in 3D formulation in non-hydrostatic approximation.

Introduction

Today one of the world's largest Verkhnekamsk potash and magnesium ore deposits is being actively developed. The main production facilities for the development of this field are located within the Solikamsk-Berezniki industrial hub. Until recently, only PJSC Uralkali was engaged in the development of the field, but at present other large companies are actively involved. As a result, the total production volume can reach more than 20 million tons per year. With the current enrichment system adopted at the considered potash enterprises, the specific volume of excess brines is about 1 m^3 per ton of final products (Lepikhin 2012). Such high production volumes, with the current technologies, will inevitably have a substantial environmental impact, its individual components. Surface water bodies are subject to the greatest load, which is related to the specifics of the adopted technological process of both ore mining and extraction of useful components from it. The task of minimizing the effect of such a large amount of polluted wastewater forms one of the main environmental problems of the Perm region.

This task is strongly complicated by the fact that the behavior of discharged highly mineralized brines differs qualitatively from that of the sewage with neutral buoyancy. Because of that, traditional methods for calculating the dilution processes presented in regulatory documents governing the procedure for the discharge of wastewater to the surface water bodies are incorrect. Our investigations have shown that the discharge of excess brines without their effective initial dilution, due to their high density, results in a significant inhomogeneity of the pollutant depth-distribution in the Kama reservoir. In some areas of the Kama reservoir, the concentration of pollutants in the bottom area is more than an order of magnitude higher than that in the surface horizons. This creates a real danger not only for habitat of benthic hydrobionts, but also for water supply systems. Since the end caps of water intakes, due to the need to ensure their work during the deep winter low water period, are located, as a rule, at a considerable depth, a danger to their stable work is created.

The hydrological regime of the Kamsky reservoir changes very substantially during the year, particularly, the flow rate defining the intensity of hydrodynamical processes in reservoir could vary in more than 20 times. In these conditions, numerical simulation on modern supercomputers becomes the main tool for solving the considered problem. In the present paper we discuss the validity and efficiency of different models and methods for the description of highly mineralized brines behavior in surface water bodies using the example of the Kamsky reservoir. New, very efficient computational technology, combining the calculations in 1D, 2D and 3D formulations, is suggested. The models are verified using the comparison of calculated mineralization fields with the results of field measurements of distribution of specific electric conductivity of water.

Dilution models

In order for dilution models to be sufficiently effective, they must account for the characteristic features not only of water bodies, but also of the effluent itself. Taking into account that the Kama river (Kama reservoir) in the area of the Solikamsk-Berezniki industrial hub has a very complex hydrological regime, being a zone of variable backwater from the Kama hydroelectric station, and the withdrawal brines are characterized by high density, substantially higher than the density of fresh water, a three-level modeling scheme of the processes under consideration was adopted. This three-level scheme has been successfully applied to solve a wide range of water quality formation problems in reservoirs, taking into account density stratification effects (Lyubimova 2010, Lyubimova 2014, Lyubimova 2016, Lyubimova 2018).

The first level is a hydrodynamic model, built on the basis of the Saint-Venant system of equations in one-dimensional formulation for the site covering the entire Kama reservoir from Tulkino to Kama HES with a length of 350 km. For its numerical solution, the software product HES-RAS v.4 was used. As the boundary conditions for this model we used the flow rate in the input section of the Kama river (at Tyulkino settlement), flow rates of the major tributaries: Yaiva, Kosva, Inva, Obva, Chusovaya, Sylva rivers, and water level (and / or flow rate) in the Kama HES upstream. As a result of the calculations, the distribution of the hydraulic characteristics of the flow for the entire computational domain is obtained. On its basis, the boundary conditions for the second level model are estimated.

The model of the second level is based on a well-studied system of shallow water equations, including the system of the momentum equations of shallow water momentum and the continuity equation in a two-dimensional formulation. For the numerical solution of this system of equations, the licensed software product SMS v.10 (SMS Tutorial 2006) was used. As the boundary conditions for this model, the flow rate at the upper gauge and the water level at the lower gauge are specified. The morphometry of the computational domain was determined on the basis of our detailed bathymetric investigations. This model was developed for the upper part of the Kama reservoir and includes all the main sources of pollutants from the water users of the Solikamsk-Berezniki industrial hub. A characteristic feature of the studied water body is its complex morphometry. For its adequate setting, the computational grid included more than 40 000 elements. In modeling pollutant transport processes, the flow rate of the discharged brines and the content of pollutants in them were used as input data. At the same time, the calculated parameters themselves, primarily the characteristics of the velocity field, obtained on the basis of this second level model, determine the boundary conditions for the third level model.

In the general case, the use of transport models in the two-dimensional approximation is sufficiently correct, if the discharged wastewater does not form substantial areas with substantial density stratification in water bodies. Otherwise, it is necessary to use transport models in the three-dimensional approximation. These models, because of their much greater complexity, are less frequently used in solving problems of the assessment of anthropogenic impacts on water bodies.

Modeling of the transport of highly mineralized brines in the three-dimensional approach

A characteristic feature of discharged excess brines is their substantial mineralization (about 300 kg / m^3) and, accordingly, high density (about 1200 kg / m^3). Due to the suppression of vertical turbulent pulsations, heavy brines can propagate to considerable distances without decreasing markedly concentrations. To study the effect of density stratification on the processes of dilution and transport of highly mineralized brines, modeling was carried out within the framework of the three-dimensional approach. The discharge of excess brines from a slit-like discharge outlet near the surface oriented across the river bed was considered.

The calculations were performed using the commercial package ANSYS Fluent, which implements the finite volume method. A k-ε turbulence model was used. The equations for turbulent kinetic energy and dissipation rate took into account the contribution of density stratification effects. A detailed description of the calculation algorithm can be found in (Lyubimova 2010, Lyubimova 2014, Lyubimova 2016, Lyubimova 2018). The computational domain was a rectangular parallelepiped containing one source in the form of a rectangular water outlet with the height equal to 1 m and width equal to 1 m located at the surface of the water body in the center of the computational domain relative to the side walls. The height of the computational domain was 10 m, width 40 m, length 300 m.

At the lower boundary of the computational domain corresponding to the bottom, the no-slip conditions and the absence of impurity flux were set. The upper boundary of the region corresponding to the free surface of the fluid was considered undeformable; the conditions for the absence of a normal component of velocity and tangential stresses, as well as the condition for the absence of an impurity flux were set on it.

At the input of the computational domain, a uniform over cross-section velocity of the main stream, having one non-zero component, and a constant concentration equal to the background concentration of the impurity in the river were set. At the exit, the boundary conditions of the vanishing of the derivatives with respect to all variables were set. At the outlet a constant brine flow rate and impurity concentration were set. On the lateral boundaries of the computational domain, the conditions for the equality of the zero derivative of the velocity along the normal and the absence of impurity flux were set.

We considered the quadratic density dependence on concentration, constructed for the brines of potash enterprises (Vostretsov 2008): $\rho(c)=999.993 + 0.6678\, c - 0.00001229\, c^2$ (c is the brine concentration, g / l), while the density changes in depth reached 10%. As the initial state, the background concentration and velocity of the main flow were uniformly distributed over the flow cross section.

The calculations were carried out in the framework of the unsteady approach.

The grid was built using the Gambit 2.4.16 program, while the computational domain was divided into cells with the decrease of grid cell size near the outlet. The main calculations were carried out using a grid consisting of approximately $4 \cdot 10^5$ elements.

When carrying out model calculations, the discharge velocity was taken to be U = 1 m/s, the main flow velocity was V = 0.1 m/s, the salinity of the withdrawn brines varied from 1 to 300 g/L, the background salt concentration in the receiving reservoir water was taken 0.2 g/L.

Calculations showed that brine dilution processes differ substantially from hydrodynamically passive impurities dilution. As can be seen from Fig. 1, there is a substantial non-uniformity of the distribution of the impurity in depth: a heavy impurity accumulates at the bottom and, due to the occurrence of a "blocking" layer, is carried by the flow, almost without decreasing concentration, for very large distances.

For comparison, we present in Fig.2 the results of calculations for the case of neutral buoyancy, when the density of the discharged brines coincides with the density of water in the river.

When organizing the release of wastewater in the warm period, when the water area of the Kama river is not covered with ice, the location of the outlet near the surface is of considerable interest when it is much easier to organize the initial dilution. The performed model calculations for this scheme of organization of the outlet are presented in Fig. 3.

As follows from the presented results, at high concentrations of discharged brines

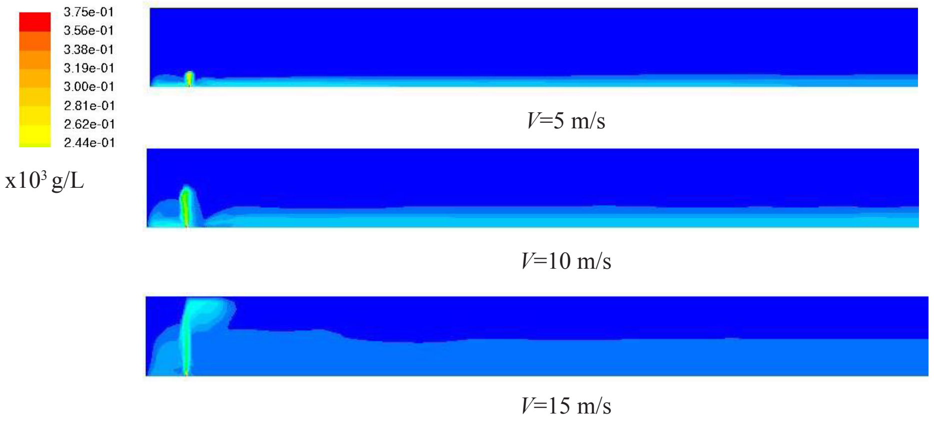

***Figure 1** Pollutant concentration fields in vertical cross-section along the main stream. Diameter of outlet is 0.1 m. Concentration of the discharged brines is 375 g/L.*

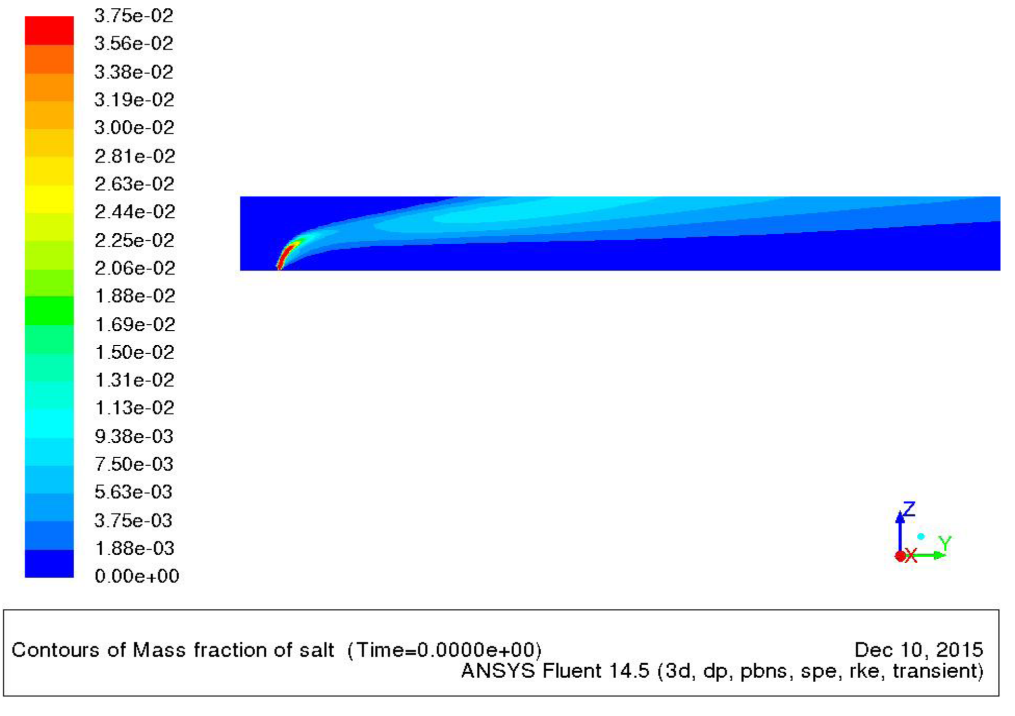

***Figure 2** Pollutant concentration fields in vertical cross-section for the case of neutral buoyancy. Diameter of outlet is 0.025 m, discharge velocity is U=10 m/s.*

without special measures in the bottom areas, stable zones of unacceptably high pollution will be formed, propagating to long distances.

Conclusions

As a working tool for evaluating the efficiency of various brine removal schemes, a complex hydrodynamic model of the Kama river (Kama reservoir) has been developed on the basis of a combination of one-, two- and three-dimensional formulations. Near brine releases, the calculations are carried out within the framework of a three-dimensional model, taking into account the substantial

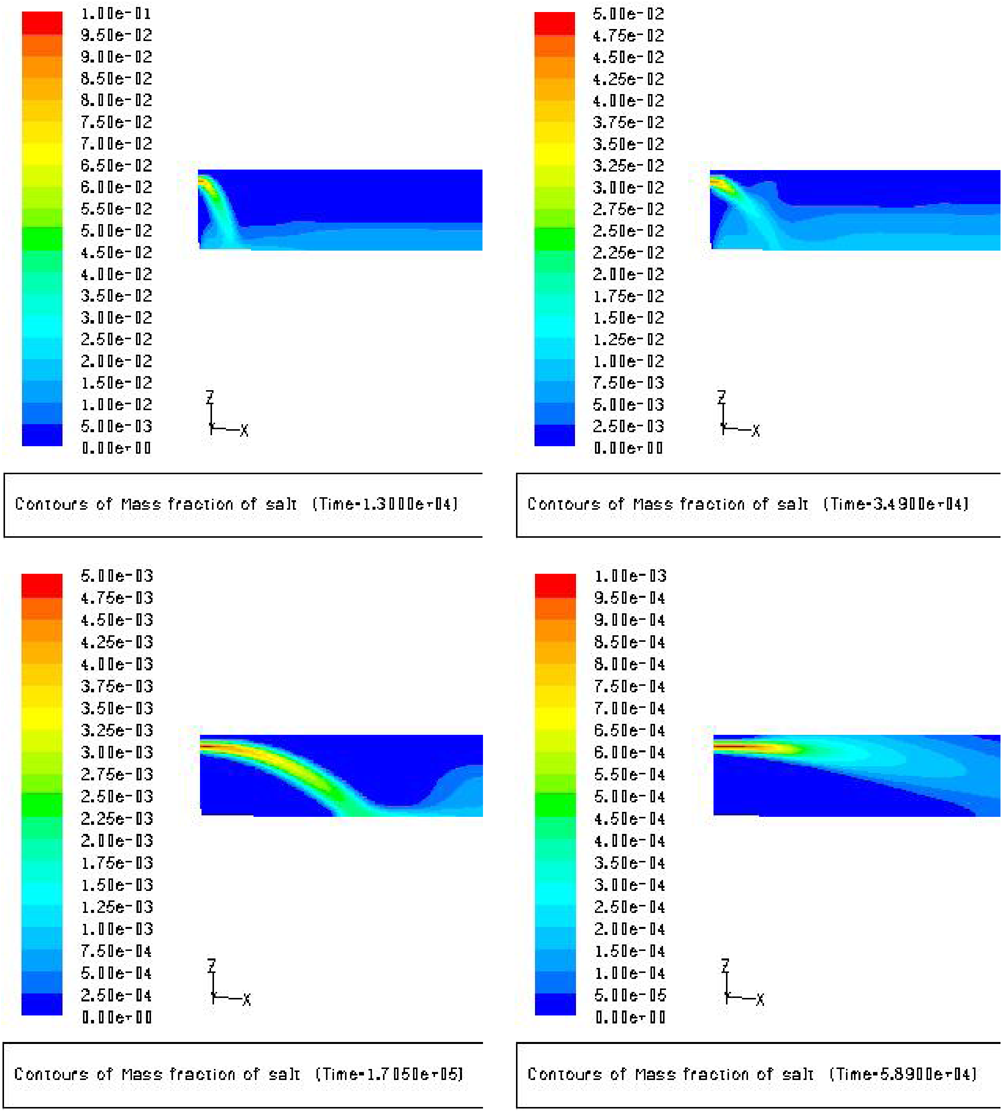

Figure 3 *Behavior of highly mineralized brines in the reservoir-receiver at different concentrations of the discharged brines (c=100, 50, 5, 1 g/L). Velocity of flow in water body is V=0.2 m/s.*

inhomogeneity of the calculated parameters over the depth. At larger distances, when the concentration of contaminating ingredients is more homogeneous in depth, it is most efficient to use models in a two-dimensional approximation. At the same time, the results of simulation in two-dimensional approximation determine the boundary conditions for the model in three-dimensional approximation. In turn, the boundary conditions for the model in two-dimensional approximation are determined on the basis of model calculations in the framework of one-dimensional approximation.

The computational experiments carried out in a three-dimensional formulation allowed us to reveal the specific features of the behavior of highly mineralized wastewater in water bodies. Due to their high density, the behavior of brines discharged in water bodies differs substantially from the behavior of wastewater with a density of 1000 kg / m^3, therefore, it is necessary to take into account the existing depth-inhomogeneity of the chemical composition of water. At the same time, traditional systems for organizing scattering water outlets require substantial adjustments.

It is important to work out the configuration of the scattering water outlets most effective for specific structural conditions on the basis of three-dimensional hydrodynamic modeling.

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