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Numerical Modeling of a Dilution and Transport of Highly Salty effluent in Water bodies taking into account density stratification effects

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Resume :

L'article est consacré à la simulation des processus de dilution et de transport d'effluents très salés dans un bassin en tenant compte des effets de stratification de densité. Le problème revêt une importance exceptionnelle pour la garantie de la sécurité écologique du réservoir de la Kama à l'échelle du centre industriel de Solikamsk-Berezniki dans les conditions d'extension des mines de sels de potassium et de magnésium de Verhnekams ; une des plus étendues au monde. L'extraction de million de tonnes de sels s'accompagne de la génération d'une quantité équivalente d'effluent très salé.

Abstract :

The paper is devoted to simulation of dilution processes and transport of highly salty brines in water bodies with taking into account density stratification effects. The problem has an exceptional importance for the guarantee of ecological security of the Kama Reservoir on the scale of Solikamsk-Berezniki industrial centre in conditions of extending exploitation of one world-largest Verhnekamsk deposit of potassium and magnesium salts. The output of a million tones of potassium fertilizer is accompanied by generation of the same quantity of brines demanding utilization.

Mots clefs: numerical simulation, 2-D approach, 3-D approach, dilution, salt, Kama river

1 Introduction

With contemporary technologies the desalination of such quantity of brines is extremely energy-consuming and almost inapplicable. That is why, both in Russia and abroad, the main meaning for brine utilization is the release into surface water bodies or underground water-bearing horizons. Since during parameter setting of underground water-bearing horizons the uncertainty level is higher than that for surface water bodies, under the same or close conditions the release into surface water bodies potentially is considerably less dangerous. At the same time due to arising density effects, traditional computational schemes, based on linear diffusion equations for the description of brine behavior, are unfit in essence. Because of suppression of vertical turbulent pulsations, 'heavy' brines can spread to significant distances near bottom slightly reducing their concentration, that's why simulations in the frame of 2-D problem statement on the base of 'shallow water' equations is insufficiently correct in this case and in general case 3-D problem consideration is required. However in the conditions of sophisticated morphometry of water bodies, the direct numerical modeling in the frame of three-dimensional approach demands computational meanings of high level. In this connection, we suggest usage of hybrid computational schemes: to carry out the calculation of distribution of velocity field characteristics within water body area on the base of 2-D approach, while to accomplish the description of brine spreading taking into account density effects with the help of 3-D modeling.

2 Construction peculiarities for the two models

The main water body able to assimilate such huge amounts of removed brines is the upper part of the Kama Reservoir situated within Solikamsk-Berezniki industrial centre. The total extent of the considered sector ~ 40 km, the width of reservoirs on this sector varies from 1.5-2.5 m with average depth ~ 8 m.

2-D (in horizontal plane) model for the considered reservoir sector is created with the help of SMS v10 software by American company AQUAVEO LLC developed by order and with participation of Centre of hydraulic research of USA. It is based on the system of 'shallow water' equations.

The main equations of shallow water momentum and continuity equation are written as follows:

$$\begin{aligned} \frac{\partial q_1}{\partial t} + \frac{\partial}{\partial x_1} \left(\frac{q_1^2}{H} \right) + \frac{\partial}{\partial x_2} \left(\frac{q_1 q_2}{H} \right) &= \frac{\partial}{\partial x_1} (N_{11} - N_p) + \frac{\partial N_{12}}{\partial x_2} + B_1; \\ \frac{\partial q_2}{\partial t} + \frac{\partial}{\partial x_1} \left(\frac{q_1 q_2}{H} \right) + \frac{\partial}{\partial x_2} \left(\frac{q_2^2}{H} \right) &= \frac{\partial}{\partial x_2} (N_{22} - N_p) + \frac{\partial N_{12}}{\partial x_1} + B_2; \\ \frac{\partial q_1}{\partial x_1} + \frac{\partial q_2}{\partial x_2} + \frac{\partial(\rho H)}{\partial t} &= 0, \end{aligned} \quad (1)$$

$$B_1 = f q_2 + \gamma^2 \rho_a W \cos \theta - \frac{g}{c^2} \frac{1}{\rho} \frac{q_1 (q_1^2 + q_2^2)^{\frac{1}{2}}}{H^2} + \rho_a \frac{\partial H}{\partial x_1} + \rho g H \frac{\partial h}{\partial x_1}; \quad (2)$$

$$B_2 = -f q_1 + \gamma^2 \rho_a W \sin \theta - \frac{g}{c^2} \frac{1}{\rho} \frac{q_2 (q_1^2 + q_2^2)^{\frac{1}{2}}}{H^2} + \rho_a \frac{\partial H}{\partial x_2} + \rho g H \frac{\partial h}{\partial x_2},$$

$$N_p = \int_{-h}^{\eta} p dx_3 = \rho g \frac{H^2}{2} + H \rho_a; \quad N_{11} \approx 2 \varepsilon_{11} \frac{\partial q_1}{\partial x_1}; \quad (3)$$

$$N_{22} \approx 2 \varepsilon_{22} \frac{\partial q_2}{\partial x_2}; \quad N_{12} \approx \varepsilon_{12} \left(\frac{\partial q_1}{\partial x_2} + \frac{\partial q_2}{\partial x_1} \right),$$

$$q_k = \int_{-h}^{\eta} \rho v_k dx_3 = \rho \int_{-h}^{\eta} v_k dx_3, \quad H = h + \eta$$

where q_k — fluid flux (fluid mass per units of length time); ε_{ik} — generalized coefficients of vertical density; for isotropic flow $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{12} = \varepsilon$; x_1, x_2, x_3, t — Cartesian coordinates and time; η — deflection of free water surface (fig. 1.1); h — depth, measured from base surface (not necessarily horizontal one); $f = 2H\omega \sin \varphi$ — Coriolis effect, where ω — angular velocity of the earth rotation, φ — local latitude; g/c^2 — dimensionless value; g — gravity acceleration; c — friction coefficient, or Shezy coefficient; ρ — density of water. γ^2 — dimensionless coefficient, or coefficient of wind stress, approximately equal 0,0026; ρ_a — density of air; W — speed of wind; θ — angular between axe x_1 and wind direction.

For the correct set of morphometry of the considered water body, the materials of a detailed survey done with echo depth-sounder with GPS conjugated sensing elements were compared to large-scaled snapshots. Processing of primary materials was carried out using software complex ArcGIS. We did the digitization of gotten maps, obtained vector data (of banks, isolines, points of water body depth, points of

horizontal lines and heights of the area). Then the data were transformed into TIN data. The information lets get such characteristics as coordinates and heights of any chosen point from these data.

On the base of obtained vector and TIN data, with the usage of SMS v10 software application, orthogonal finite-element mesh of modeled water body is generated. Note, for the generating, setting of boundary conditions of the modeled water body, vector data of the water body banks in the view of shape-files and TIN data are used.

As an example fig.1 pictures modeling results for one of the considered sectors with initial and boundary conditions given in table 1. The modeling results are presented in fig.1 as distribution of pollution zones.

Table 1. Given water flow, water level and concentration of polluting substances

Water level in the Kama river above Berezniki, Q, cub.m. / s.	Water level in the Kama river lower Berezniki, H, abs. m.	Water flow in the Zyryanka river Q, cub.m. / s.	Water flow at pumping station, Q, cub.m. / s.	Concentration of polluting substance at pumping station, g/l.
2250,0	106,4	1,0	2,5	10,0

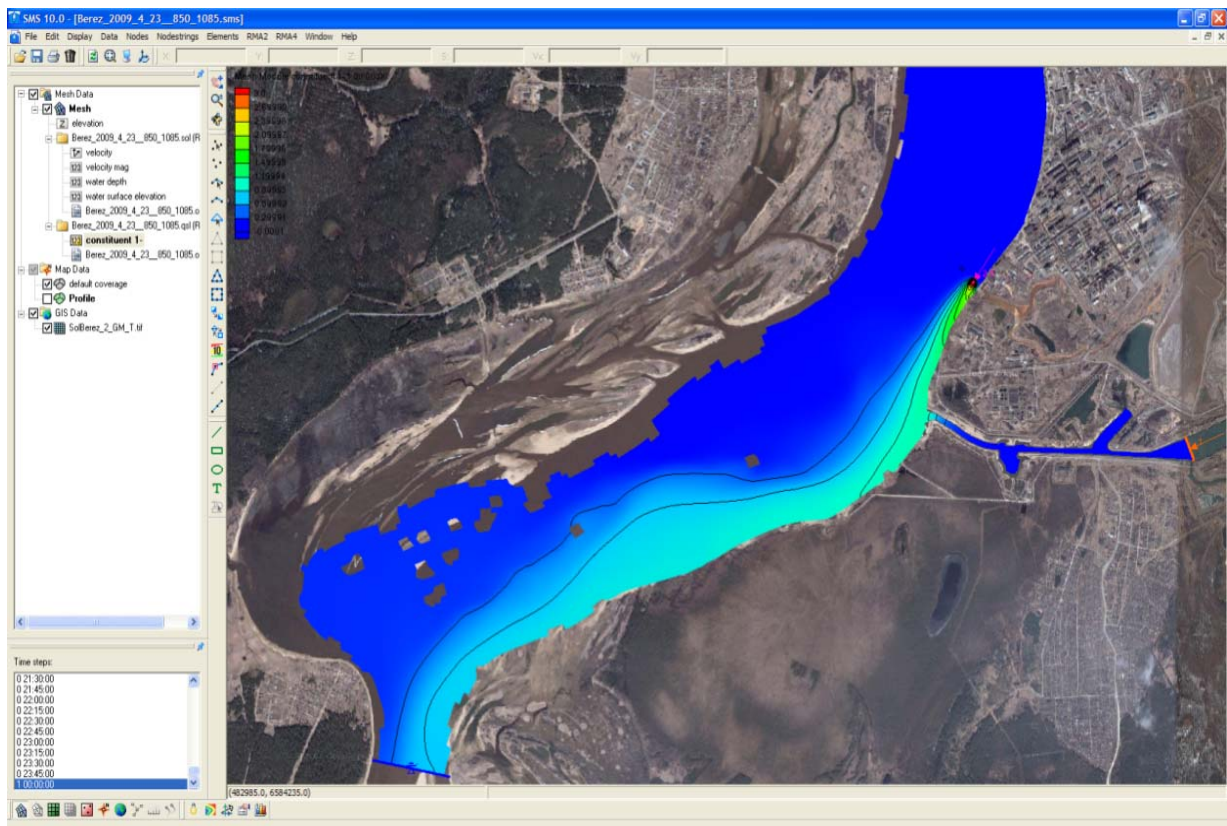


FIG. 1 – Pollution zone of water object at given water flow, water level and concentration of polluting substances at Berezniki pumping station

Estimation of the modeling results was carried out by comparing the results of the modeling to the data of production monitoring and large-scaled cosmic snapshots done on specific dates. Thanks to essential difference in optical density of released effluents and water in the reservoir, comparing of distribution of computational and observed pollution zones is suggested to be

possible. It is necessary to accentuate, even with stable hydrologic characteristics of flow and constant regime of pollutant supply, the content of considered ingredients in any point of water flow is quite complicated chance process, characteristics of which are determined by the turbulent regime of water body. At the same time, diffusion models give some average value with averaging scale $TD \gg T$ (where T is characteristic scale of turbulent pulsations). This has very serious importance for the estimation how computational and observed values coincide. Since in large water objects characteristic averaging scale during probe selection $T_{pr} \ll TD$, to obtain correct assessments it is necessary to employ automatic observation stations letting to estimate the content of computational ingredients with sufficient frequency during long time intervals or usage of integral schemes of probe selection. Unfortunately, the two approaches are used very seldom because of both organizational difficulties and cost price.

3 Three dimensional modeling

Numerical modeling in the frame of 3-D approach was carried out with the help of commercial software package Fluent 6.3.26. Calculation domain and mesh were built in Gambit 2.3.16 software. 3-D modeling was performed with building the exact construction of scattering releasers. To improve the effluent scattering and to provide the strongest mixing of the effluents with water flow of the Kama river, the pumping station is designed in such a way that water conduits on their edges have scattering releasers, representing steel tubes with diameter $D_y = 1.4 \text{ m}$, each tube is furnished with five cone nozzles $D_y = 0.5 \text{ m}$. The nozzles are situated on the side opposite to the river stream, on the distance of $r_y = 5 \text{ m}$ from each other, at angle 45° to the vertical line.

The modeling was carried out in the frame of stationary approach. In Fluent package the following models were chosen: k-epsilon model for turbulent flows, Species Transport model for admixture distribution. Momentum, continuity and mass transfer equations were solved. As boundary conditions for the velocity we used non-slip boundaries at bottom and banks and set the absence of tangential stress on free river surface. The absence of mass flux was set for concentration on rigid and free boundaries. Inlet velocity and initial concentration of admixture in water were constant.

Figs. 2 and 3 presents the results of calculations at the parameters given in Table 1 for the computational domain with the width 190 m and length 300 meters (the height of the domain in all the calculations corresponded to the river depth 10 m). In this case, to set the mesh, taking into account different scales from 0.2 m to 1 m, size function with growth rate 1.2 was applied. The total greed consisted of more than 400 000 tetrahedron cells. The distribution of depth-inhomogeneity for concentration is plotted in fig.2 for the distances 100 and 200 meters from the admixture source. As one can see, the distribution of admixture is inhomogeneous in depth. The distribution of turbulent kinetic energy on the distances 100 and 200 meters from the admixture source is presented in fig.3.

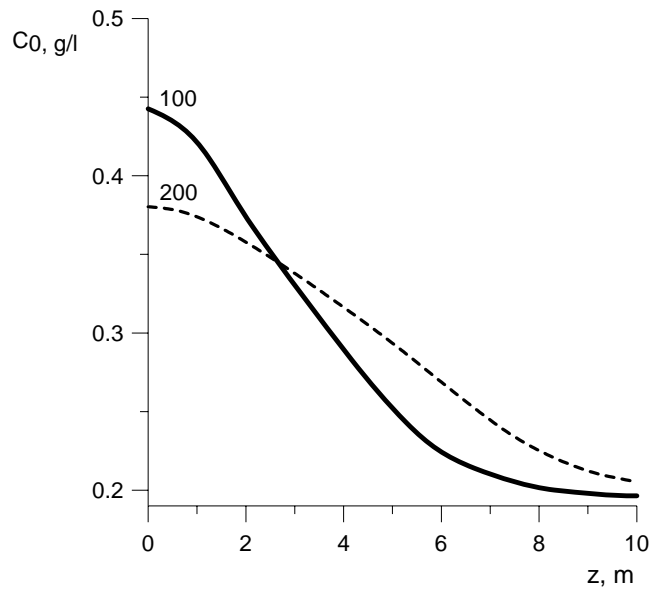


FIG. 2 – The depth-distribution of admixture concentration on the distance 100 (solid line) and 200 (stroked line) meters from the admixture source

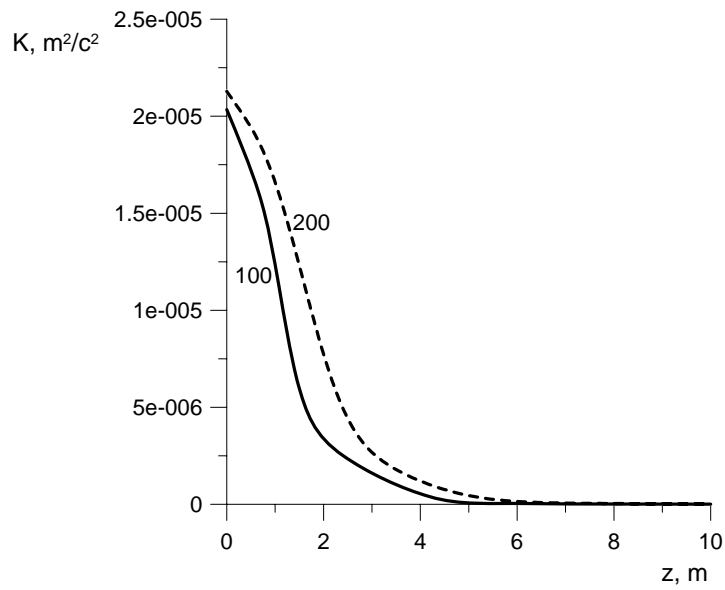


FIG. 3 – The depth-distribution of turbulent kinetic energy on the distance 100 (solid line) and 200 (stroked line) meters from the admixture source