Modelling of stratified flows in the problem of the morphological behaviour of a sandpit

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Abstract. The problem of the removal of brines from underwater sand pits is studied. The intensity of the removal of brines from the pits due to the changes in the hydrological regime of the river is calculated in three-dimensional approach. It is found that for the flow rates typical for the summer, the removal of brines collected in underwater pits does not occur. At flow rates typical for the spring, there is a fairly intensive removal of accumulated brines. Numerical experiments have shown that the underwater pits can serve as brines batteries, becoming an additional source of river pollution under certain hydrological conditions.

1. Introduction
The production of non-metallic building materials (NBM) from the river channel pits is one of the most widely used methods of producing NBM. In spite of the large number of investigations, associated with the evaluation of the impact of such developments on rivers, many important aspects remain open. As a rule, evaluation of the impact of mining is focused primarily on the analysis of changes in the velocity regime of the river. In most cases, these indicators adequately define the parameters governing the use of the river. The studies of changes in water level and velocity regimes due to the large-scale mining are carried out quite successfully using the one-dimensional (1D) [1-5] and two-dimensional (2D) [6-8] models. However, for areas of high anthropogenic impact on rivers it is necessary to evaluate not only the hydraulic flow parameter changes, but also hydrochemical regimes of the river. To correctly solve these problems the use of three-dimensional models (3D) is needed.

Until now 3D hydrodynamic models did not receive wide distribution in river hydraulics because of their complexity. One an example of application of such models for the solution of problems of increasing the efficiency of water supply and regulating wastewater can be found in [9]. In this study, one of the most powerful software packages CFD Fluent was used for the development of 3D-models. 3D calculations were performed on a supercomputer «URAN» of the Institute of Mathematics and Mechanics, Ural Branch of the Russian Academy of Sciences. Characteristics of the model according to the tasks of river hydraulics can be found in [10].

The present study is dedicated to the simulation of dilution and transport of highly mineralized brines in rivers taking into account density stratification effects. This problem is of high significance for ecological safety due to the growth of the exploitation of salt depositions. The production of one million tones of fertilizer is accompanied with the same quantity of highly mineralized brines demanding utilization. The desalination of such quantity of highly mineralized brines under current
conditions requires extremely high power inputs and is practically impossible. That is why in Russia and abroad the main method of brine utilization is the dumping into surface water bodies or underground. Numerical investigation of the dilution and transport of highly mineralized brines in rivers in the framework of two-dimensional models is sufficient only when there is no significant density stratification, in this case it is applicable to use depth-averaged characteristics.

The problem configuration for the investigation of underwater pit washing is shown in Fig. 1.

Figure 1. Problem configuration for the investigation of underwater pit washing: h – the thickness of the water layer above the pit; H & L are the depth and length of the pit

Input hydrodynamical characteristics needed to implement 3D model, were calculated on the basis of 2D-hydraulic model, realized for the whole Kama reservoir: Kama river (Tyulkino village) – the backwater of Kama hydroelectric power station. Now even with the use of powerful computational tools, such as the cluster “URAN” is not possible to build 3D models for the considered site because of the very large area of the river system under consideration.

2. Governing equations and boundary conditions.

We implement the Reynolds-averaged Navier-Stokes equations:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_i}{\partial x_i} \delta_{ij} \right) \right] +
\]

\[
+ \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \left( \rho k + \mu \frac{\partial u_i}{\partial x_i} \right) \delta_{ij} \right] + \rho g_i.
\]

Here, \( \rho \) is the density, \( x_i \) are coordinates (we use Cartesian coordinate system), \( u_i \) are the velocity components, \( \mu \) is the kinematic viscosity, \( \mu_t \) is the turbulent viscosity.

The turbulence kinetic energy \( k \) and rate of its dissipation \( \epsilon \) are obtained from the following transport equations:

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho ku_i) = \frac{\partial}{\partial x_i} \left[ \mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_i} \right] + G_k + G_b - \rho \epsilon,
\]

\[
\frac{\partial}{\partial t} (\rho \epsilon) + \frac{\partial}{\partial x_i} (\rho \epsilon u_i) = \frac{\partial}{\partial x_i} \left[ \mu + \frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_i} \right] + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k}.
\]
In equations (3)-(4), $G_k$ represents the generation of turbulence kinetic energy due to the mean velocity gradients $G_k = \mu S^2$ where $S$ is the modulus of the mean strain rate tensor, defined as $S = \sqrt{2S_{ij}S_{ij}}$, $S_{ij} = 0.5 \left( \partial u_j / \partial x_i + \partial u_i / \partial x_j \right)$, $G_h$ is the turbulence kinetic energy due to buoyancy, which is calculated as

$$G_h = g \frac{1}{\rho} \left( \frac{\partial \rho}{\partial c} \right) \mu_s \frac{\partial c}{\partial x_i},$$

(5)

i.e. taking into account the dependence of the density on concentration, $\beta$ is the concentration expansion coefficient, $\mu_s$ is the parameter of density stratification due to the concentration, $Pr_t$ is the turbulent Prandtl number, $g_i$ is the component of the gravity vector in $i$-th direction; $C_{1e}, C_{2e}$, and $C_{3e}$ are constants, $\sigma_k$ and $\sigma_\varepsilon$ are the turbulent Prandtl numbers for $k$ and $\varepsilon$ respectively. The turbulent viscosity $\mu_s$ is computed as follows: $\mu_s = \rho C_{\mu} k^2 / \varepsilon$, where $C_{\mu}$ is a constant.

The model constants $Pr_t$, $C_{1e}, C_{2e}, C_{\mu}, \sigma_k$ and $\sigma_\varepsilon$ were taken to have the following values:

$Pr_t = 0.85$, $C_{1e} = 1.44$, $C_{2e} = 1.92$, $C_{\mu} = 0.09$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$.

The equation of mass transfer has the form

$$\frac{\partial}{\partial t} (\rho c) + \nabla \cdot (\rho \vec{v} c) = -\nabla \cdot \vec{J},$$

(6)

where $\vec{J} = -\left( \rho D + \mu_s / Sc_l \right) \nabla c$, is the mass flux, $Sc_l = \mu_s / \rho D_l$ is the turbulent Schmidt number, and the turbulent diffusion parameter $D_l$ describes turbulent mass transfer.

The dependence of density on concentration is defined according to the linear law $\rho = \rho_0 - \rho_0 \beta (c - c_0)$, where $\rho_0$, $c_0$ are the density and concentration of the water in the absence of brines.

We set the no-slip condition, zero mass flux condition on the rigid boundaries (bottom of the river):

$$u_x = u_y = u_z = 0, \quad \frac{\partial c}{\partial n} = 0$$

(7)

At the entrance of computational domain we impose the velocity of river, in which a component (perpendicular to the outfall axis) is the only non-zero constant $\left\{ v, 0, 0 \right\}$; the concentration is set equal to the background concentration of pollutant in the river water.

$$x = 0: \quad u_x = V, \quad u_y = u_z = 0, \quad c = c_0$$

(8)

The conditions on the other boundaries of the computational domain are:

$$\frac{\partial u_x}{\partial n} = 0 \quad (i = x, y, z), \quad \frac{\partial c}{\partial n} = 0$$

(9)

At the beginning of the calculation we impose the constant or linear distribution of brines concentration:

$$c_{max} = a + b z.$$  

(10)

The computations were made using the ANSYS Fluent package of computational fluid dynamics and the k- $\varepsilon$ model describing the turbulent pulsations. The problem was solved by applying the non-stationary isothermal approach. The second-order accuracy scheme was used to perform spatial discretization of equations. The temporal evolution was simulated using the explicit scheme of the second order. To study the effect of the computational mesh size we have performed test calculations using four meshes: with 163000, 269000, 639000 and 1258000 nodes. On the basis of the results of
these test calculations, in main calculations we used the mesh with 269000 nodes. The number of grid nodes throughout the depth of the computational domain was taken equal to 30.

3. Results of modelling

The calculations included two stages. During the first stage the accumulation of brines ejected from the rectangular outlet device of the dimension 1 m x 1 m, located near the bottom at a distance of fifty meters from the front edge of the pit was simulated. The discharge of brines with the concentration $c_{\text{inlet}} = 300$ g/l (0.3 wt%) was considered. It lasts 2 hours then stops. When the discharge occurs the accumulation of brines in the pit takes place. During the second stage of calculations the removal of accumulated brines from the pit was simulated.

The pit has the following dimensions: 100 m width, 400 m length (in the direction of flow), 6 m depth, the depth of the river $h = 6$ meters.

The simulations were carried out for two velocities of the river according to the summer period 0.3 m/s and to the spring period 1.2 m/s. In the first case the velocity in the river during the second stage was taken to be the same as in the stage of brines accumulation in the pit $v = 0.3 \text{ m/s}$, the results of calculation for this case are presented in Figures 2 and 3. In Figure 2 the concentration fields in the middle of the vertical section of the computational domain are presented. Figure 3 presents the vertical distributions of the brines concentration at a distance 40 meters from the pit for different time moments.

![Figure 2](image_url)

**Figure 2.** The intensity of washing the underwater pit in summer $v = 0.3 \text{ m/s}$. Mineralization of water: blue – less than 0.5 g/l; yellow – 10 g/l; green – transition zone

![Figure 3](image_url)

**Figure 3.** Vertical distribution of brine concentration in the middle of computational domain at a distance of 40 m from the pit at different time moments. Case $v = 0.3 \text{ m/s}$
As one can see from Figures 2 and 3, during the first stage the brines are carried away from the river bottom along the river, while the brines in the pit are not washed away with time. The stage of quick changes in the concentration in the river is observed within 2 hours and then the concentration field becomes stationary, brines concentration in the computational domain is not varied.

In simulations for the spring season the velocity of flow in the river was taken to be four times larger than in the calculations for summer (\(v = 1.2 \, m/s\)). In this case, the most part of the brines is washed out from the pit (figure 4 shows the concentration of brines in the pit). The washing time is reduced with the growth of the river velocity: at the same period of time greater amount of brines is removed from the pit in spring than in the summer (see figures 3 and 5 for comparison).

Figure 4. The intensity of washing underwater pits during the spring. Case \(v = 1.2 \, m/s\). Mineralization of water: blue – less than 0.5 g/l; yellow – 10 g/l; green – transition zone.

![Figure 4](image)

Figure 5. Vertical distribution of brine concentration in the middle of computational domain at a distance of 40m from the pit at different time moments. Case \(v = 1.2 \, m/s\)

![Figure 5](image)

4. Conclusion

Thus, at flow rates typical for the summer period, there is no removal of brines accumulated in the underwater pits. At flow rates typical for the spring season there is a fairly intensive discharge of accumulated pollutants. Numerical experiments have shown that the underwater pits created in the process of large-scale production of non-metallic building materials, can serve as original batteries of brines becoming an additional tense source of river pollution under certain hydrological conditions.
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