Numerical modeling of the flow of polluted groundwater into the Vyatka River

T P Lyubimova¹,² and Ya N Parshakova¹

¹Institute of Continuous Media Mechanics, Ural Branch of the Russian Academy of Science, 614013 Perm, Russia
²Department of Theoretical Physics, Perm State University, 614990 Perm, Russia

E-mail: parshakova@icmm.ru, lyubimovat@mail.ru

Abstract. In the formation of the hydrochemical regime of water bodies and adjacent territories, a significant role is played by the density stratification effects caused by the heterogeneity of the distribution of mineralization fields. When the concentration of the heavy solute is larger than one ppm under terrestrial conditions, these effects have a great influence on the nature of the flow. Such effects cannot be described using hydrodynamic models within the framework of shallow water equations; for their correct description, it is necessary to use hydrodynamic models in a full three-dimensional non-hydrostatic formulation. The present paper presents the results of numerical modeling of the formation of diffuse pollution of the Vyatka River during washing of floodplain water bodies (quarries, lakes) in the region of the Kirovo-Chepetsk industrial complex. The assessment of the scale and intensity of the supply of nitrogen-containing compounds was made. The calculation results form the basis for the development of a number of possible measures aimed at both reducing diffuse runoff and ensuring the standard water quality at the main drinking water intake in Kirov, Russia.

1. Introduction
The process of diffuse pollution of water bodies is caused by the combination of several independent hydrological and geochemical processes [1] and, as a rule, is formed by large industrial complexes. These contaminants are characterized by a high specific density, since they are not formed due to the functioning of actual production processes, but are spread from previously accumulated waste substances. A typical example of such a process is the Kirovo-Chepetsk industrial complex located on the Vyatka River. The source of diffuse pollution formed by this complex is not its current production activity, but the implementation of previously accumulated pollution. Downstream from this production complex along the Vyatka river the main drinking water intake in the city of Kirov is located, therefore, the task of assessing the scale of this pollution based on numerical modeling is urgent. The required input parameters and conditions for the numerical experiment are determined on the basis of the data of field measurements [1].

At present, the Kirovo-Chepetsky industrial complex is a group of enterprises leading in Russia in the production of a wide range of polymers (fluoroplastics, fluoroelastomers, etc.), mineral fertilizers,
ammonium nitrate, freons and other chemical products. These city-forming enterprises have a common long history of industrial production (until 2003, JSC Kirovo-Chepetsk Chemical Plant). The date of foundation of the unified enterprise is October 8, 1946, when it was decided to create industrial facilities for the production of chemical products based on chlorine and fluorine.

Over a long period of operation of enterprises in the adjacent territory (floodplain of the Vyatka river), several large waste disposal facilities were organized, among which it should be noted: a site for disposal of waste of 3-4 hazard classes, a three-section sludge accumulator, a chalk tailing dump, an underground disposal site for industrial wastewater others [1]. Until 1987, wastewater was discharged into surface water bodies; from 1987 to the present time, injection into underground horizons has been used (the reservoir is located at depths of 1125-1287 m).

The specific features of the formation of the hydrochemical regime of water bodies and the state of natural complexes under the conditions of filtration processes in geological media were considered earlier in the works [2-4]. In these works, the problem of pollution of the hydrosphere by objects located on the territory of existing and abandoned industrial plants is considered. In this regard, the development of hydrodynamic models describing the transport of pollution and making it possible to predict changes in the ecological situation over a long period of time is urgent [5]. It is also important to assess the impact on the hydrosphere of household and industrial waste landfills, due to their large size and high risks of pollution penetration into groundwater with precipitation and melt water [3].

The development of complex analytical and numerical models of large water bodies and industrial reservoirs is an urgent task [6,7]. Currently, the processes of liquid infiltration from storage facilities into the surrounding soil and groundwater [3,8,9] are being actively investigated, and monitoring of the state of groundwater and surface waters adjacent to industrial reservoirs is carried out [9,10]. Observation data reliably show that there is an increased concentration of soluble waste components in the adjacent hydrosphere. Possible local violations of the integrity of the waterproofing of waste storage facilities require the development of models of pollution infiltration, which would make it possible to predict the intensity of the infiltration process. In addition to the direct contamination of objects in the hydrosphere, one should also take into account the change in soil characteristics during adsorption of contaminants and the nature of the spread of contaminants in porous media [11-13].

2. Mathematical model of contamination propagation in the geological environment

In order to describe the propagation of contaminants in groundwater, a porous medium model is used that considers the momentum diffusion. For numerical modeling of the spread of pollutants in the rock mass, it is possible to use a model of laminar flow in a porous medium at a flow rate characterized by low Reynolds numbers \( \text{Re} = \frac{v_a h}{\nu} < 2000 \), where \( v_a \) - average flow rate, \( h \) - characteristic size of the study area, \( \nu \) - kinematic fluid viscosity. In this study \( v_a = 10^{-7} \text{ m/s}, h = 2000 \text{ m}, \nu = 1e-06 \text{ m²/s}, \) with such parameters \( \text{Re} = 200 \). Therefore, the modeling was carried out within the framework of the laminar model.

The problem was solved within the framework of a nonstationary isothermal approach. To solve the problem, a spatial grid was generated with condensation near the lower aquifer.

The equations of motion in tensor form are as follows:

\[
\frac{\partial (m \rho)}{\partial t} + \frac{\partial}{\partial x_i} \left( m \rho v_i \right) = 0, \tag{1}
\]

\[
\frac{\partial}{\partial t} \left( \frac{1}{m} \rho v_i \right) + \frac{\partial}{\partial x_j} \left( \frac{1}{m} \rho v_i v_j \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \frac{\mu}{m} \frac{\partial v_i}{\partial x_j} \right] - \frac{\mu}{K} v_i + \rho g_i, \tag{2}
\]

where \( m, K \) - porosity and permeability of a porous medium, respectively; \( \rho \) - fluid density, \( v_i \) - velocity vector components \((i=1,2,3)\), \( \mu \) - dynamic fluid viscosity. The density was considered to depend
on the water salinity according to a linear law \( \rho = \rho_0 + 0.702 s \) kg/m\(^3\), where \( \rho_0 = 1000.196 \) kg/m\(^3\) – density of pure water and \( s \) – mass concentration of salts dissolved in water measured in g/l.

The impurity transfer equation has the form:

\[
\frac{\partial}{\partial t} (m \rho c) + \nabla \cdot (\rho \vec{v} c) = -\nabla \cdot \vec{J}.
\] (3)

Here \( \vec{J} \) – diffusion impurity flux, determined by the expression

\[
\vec{J} = -\rho D_n \nabla c,
\] (4)

where \( D_n \) – coefficient of molecular diffusion.

The no-slip and impermeability conditions for the substance were set on the solid walls of the computational domain. On the free surface of the liquid, the conditions were set both on the non-deformable and free from tangential stresses boundary (equality to zero of the normal components of the velocity and tangential stresses) and the condition for the absence of a substance flux. At the boundaries of the computational domain, which are a continuation of the porous medium, “soft” boundary conditions are set - equality to zero of the derivatives along the normal to the boundary. Based on the data of field measurements, it was assumed that the characteristic concentration of ammonium ion in the groundwater near the storage facility is at least ~ 10 g/l. This condition was set at the input boundary of the computational domain.

3. Results of numerical simulation of contaminants dynamics in a porous medium

Modeling was carried out with averaging over the width of the lake containing pollutants. A vertical section was considered in the middle of the Bobrovoe 1 lake, which is a rectangular area 1900 m long and 12 m deep (Figure 1).

![Figure 1. Vertical section from Bobrovoe 1 Lake to the Vyatka River.](image)

The process of filtration of water containing ammonium nitrogen was considered. At the entrance to the computational domain, a constant flow rate of 1e-07 m/s was set in an aquifer 7 m thick and \( 10^{-13} \) m\(^2\) permeability, and \( 10^{-8} \) m/s in a layer above the aquifer with a thickness of 5 m and a permeability of \( 10^{-14} \) m\(^2\). The porosity of rocks was considered to be 0.2. An impermeable clay layer is located below the aquifer; therefore, the lower boundary of the computational domain is considered to be solid impermeable. At the initial time, the concentration was set to zero in the entire computational domain.

Figure 2 shows the dynamics of the spread of pollution through Bobrovoe 1 Lake. The concentration fields for different points in time are shown in a vertical section in the middle of the lake. The concentration front spreads in the aquifer. When the concentration front reaches the lake boundary, intense movement occurs in the reservoir. The flow arises due to the concentration-convective transport, while the impurity mixes and the concentration of ammonium nitrogen increases in a few months. Thus, the lake becomes a source of pollution. Due to filtration from the storage, the concentration front moves at a speed of 1e-07 m/s, i.e. in three months, pollution spreads to 1 meter. However, in the presence of lakes with non-isolated shores, the impurity spreads from the lake, while simultaneously accumulating in it.
Figure 2. Time evolution of the ammonium nitrogen concentration field in the vertical section in the middle of Bobrovoe 1. The scale is presented in g/l.

Thus, for six months from the moment when the concentration front reaches the lake, the pollution spreads to 15 meters, while the concentration value is 4 g/l (Figure 2). From the data obtained, the increase in the amount of ammonium nitrogen in lakes over 100 years was estimated, 5 x 10^3 tons.

The case is also considered when in the initial state there was a linear distribution of impurities from 12 g/l to 0 g/l at a distance of 400 meters (Fig. 3).

Figure 3. Initial distribution of concentration, t=0.
It is shown that with a constant supply of an impurity with a concentration of 10 g/l, the amount of an impurity in the lake does not change and is 10 g/l. The front of concentration spreads over 2 years 9 months to 210 meters (Figure 4). The rate of propagation of an impurity is not constant and increases over time, until the concentration of impurities in the reservoir stops changing.

![Figure 4](image)

**Figure 4.** Concentration distribution after t = 1029 days (2 years 9 months).

At a distance of 0.5 km, pollution will spread from the lake in seven years (Figure 5). At a distance of 300 meters, a maximum impurity concentration of 10 g/l is detected. It will take six months for the impurity to spread in a porous medium in groundwater by 0.5 m.

![Figure 5](image)

**Figure 5.** Concentration distribution after t = 2878 days (7 years 10 months).

4. **Conclusion**

The formation of the hydrochemical regime of water bodies and adjacent territories with a significant role of density stratification effects due to the heterogeneity of the distribution of mineralization fields has been studied. When the concentration of a heavy solute is large than one ppm under terrestrial conditions, these effects have a great influence on the nature of the flow. Numerical modeling of the formation of diffuse pollution of theVyatka River during the washing of floodplain water bodies (quarries, lakes) in the region of the Kirovo-Chepetsk industrial complex has been carried out. The assessment of the scale and intensity of the intake of nitrogen-containing compounds was performed. The process of water filtration with ammonium nitrogen content in the geological environment was considered. The concentration front from solid waste storages during precipitation spreads in the aquifer with a constant flow rate of $10^{-7}$ m$^3$/sec with a thickness of 7 m and a permeability of $10^{-13}$ m$^2$. When the concentration front reaches the boundary of the lake, intense movement occurs in the reservoir. The flow arises due to the concentration-convective transfer, while the impurity mixes and the concentration of ammonium nitrogen increases in a few months. The lake becomes a source of pollution. Due to filtration from the storage, the concentration front moves at a speed of $10^{-7}$ m/s, i.e. in six months, pollution spreads to 1.5 m. However, in the presence of lakes with uninsulated shores, the impurity spreads from the lake, simultaneously accumulating in it. So, for six months from the moment the concentration front reaches the lake, the pollution spreads by 15 m. The rate of spread of pollution increases by an order of magnitude.
Acknowledgments
The study was carried out with the financial support of the Russian Foundation for Basic Research (project No. 19-41-590013).

References

[1] Yasinskii S V, Venitsianov E V, Vishnevskaya I A 2019 Water Resources (Institute of Water Problems, Russian Academy of Science, Moscow, Russia) 46(2) 266–277
[2] Lyubimova T P, Lepikhin A P, Parshakova Y N, Tsiberkin K B Journal of Applied Mechanics and Technical Physics 57(7) pp 1208–1216
[3] Franz T J, Rowe R K 1993 Int. J. Numer. Anal. Met. 17 435–455
[4] Bear J 2010 Cheng A H D Modeling groundwater flow and contaminant transport (Amsterdam: Springer) 834 p
[5] Anderson M P 1992 Applied groundwater modeling: simulation of flow and advective transport (New-York: Academic Press) 381 p
[6] Berkowitz B, Dror I and Yaron B 2008 Contaminant geochemistry (Berlin: Springer) 412 p
[7] Polubarinova-Kochina P Ya 1962 Theory of ground water movement (Princeton: Princeton University Press) 613 p
[8] Bear J, Cheng A H D 2010 Modeling groundwater flow and contaminant transport (Amsterdam: Springer) 834 p
[9] Anderson M P 1992 Applied groundwater modeling: simulation of flow and advective transport (New-York: Academic Press) 381 p
[10] Lepikhin A P, Lyubimova T P, Parshakova Ya N, Tiunov A A 2012 Journal of Mining Science 48(2) 390–397
[11] Nield D A, Bejan A 2013 Convection in porous media (Berlin: Springer) 778 p
[12] Lyubimova T, Zubova N Transport in Porous Media 127(3) 559–572