

# Mathematical modeling of pollution of underground aquifers due to mining of minerals

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## Abstract

**Purpose.** The research aims to create a mathematical model of salt contamination spreading through underground aquifers in the event of depressurization of the hydrocarbon production well crater for further assessment of environmental and economic damage from these processes.

**Methods.** To predict the environmental and economic damage from salt contamination, the distribution of concentrations of harmful substances was investigated, taking into account the number of supply sources and their intensity over time, based on situ studies at the Rybalske Oil Field, Okhtyrskyi District of Sumska Oblast in Ukraine, where there were technological failures wells, accompanied by open fountains with the release of large amounts of highly mineralized water and the formation of craters. Mathematical modelling methods were used to process the data from the study of accidental technogenic pollution of underground aquifers.

**Findings.** Based on real data from the study of the processes of potential salt contamination spread in fresh aquifers as a result of accidents at hydrocarbon production facilities, a mathematical model of salt contamination spreading in drinking groundwater in the event of depressurization of an oil field well crater has been developed. Potential economic losses in case of possible groundwater contamination with highly mineralized solution, which can into drinking groundwater aquifers, are substantiated. It has been established that in connection with the occurrence of an emergency situation due to the release of formation water to the surface in the territory of oil and gas fields, the formation of technogenic meromictic reservoirs is possible, which is confirmed by the example of the Rybalske Oil Field. It is proved that the total mineralization of crater water increases linearly with depth of the reservoir occurrence, and a similar dependence is characteristic of the chloride ion content.

**Originality.** For the first time, a multicomponent mathematical model of mineral salt migration processes in underground freshwater aquifers in the case of depressurization of a meromictic reservoir has been developed.

**Practical implications.** The research results obtained using numerical methods make it possible to predict the processes of spreading harmful substances in drinking underground aquifers as a result of emergencies at oil and gas fields, taking into account the number of sources of pollutants penetrating the study area, the heterogeneity of properties of the environment into which the harmful substance enters, and to assess the dynamics of changes in the concentration of these substances and time with further assessment of environmental and economic damage from these processes.

**Keywords:** oil fields, drinking water pollution, mathematical modelling

## 1. Introduction

Despite the intensive development of alternative energy sources [1], hydrocarbons continue to occupy an important place in the overall balance of energy resources [2]. The need for energy resources is constantly growing both in Ukraine [3], and the whole world [4]. Solving the problem of energy security [5] requires a systemic approach. To do this, it is necessary to increase the yield from layers of existing oil and gas fields, to search for and develop new promising fields, and this, in turn, requires an increase in the volume of construction of geological exploration and exploitation wells [6].

It should be noted that at all stages of geological exploration drilling, operational drilling, development of deposits and extraction of hydrocarbons, transportation, processing and storage of petroleum products, a harmful trace of production occurs, which affects climate change [7]. Application of environmentally safe drilling and mining technologies, reclamation of disturbed lands after completion of work, utilization and processing of drilling waste [8]-[10], environmental monitoring at all stages of the life cycle of the well will allow minimizing such a harmful footprint [11], [12].

The rate of consumption of natural resources and mining of minerals in the world is quite high. Identification and assess-

Received: 5 June 2024. Accepted: 14 September 2024. Available online: 30 September 2024

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Mining of Mineral Deposits. ISSN 2415-3443 (Online) | ISSN 2415-3435 (Print)

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ment by the degree of impact on environmental components of the main potential environmental consequences of oil and gas field exploitation in accordance with technological processes and impact media is insufficiently studied problem today [13].

Although the leading countries of the world have chosen the strategy of replacing traditional energy resources with alternative and renewable energy sources, the potential of which (“unconventional” energy resources or renewable energy resources) is many times greater than the volume of world energy consumption, the study of the environmental consequences of long-term, the of the ecological situation development at the fields as a result of accidents is an urgent task today [14], [15].

The oil and gas industry in Ukraine is important for the activities of both households and a society, and it shapes the energy security of a state. At the same time it ranks the first in the negative impact on the environment and affects all its components such as subsoil, soil, atmospheric air, surface and groundwater, and it leads to disturbance in the biological balance of geosystem [16].

As a result, the social tension arises in the society; other industries and agriculture are adversely affected; the economic damage appears along with the environmental deprivation. Exploitation of oil and gas fields is associated with a number of risks, one of which is the disturbance of well integrity and the uncontrolled release of formation waters to the surface [17], [18]. This process poses a serious environmental threat due to environmental pollution and risks to human health [19], [20].

There is a whole series of subjective and objective reasons that can become factors of the release of formation waters to the surface of oil and gas fields. In order to achieve the maximum mechanical speed of drilling, operators can apply forced drilling modes and make mistakes when compiling the layout of the drill string lower part [21], [22]. Being forced to save money on equipment rental, drilling customers often ignore the use of telemetry and anti-vibration equipment [23], [24]. All this can lead to emergency situations, in particular, depressurization of the well and release of formation waters to the surface [25]. The probability of damage to the oil and gas well integrity is significantly influenced by the correct centering of the casing string, which can be considered a preventive measure to guarantee the long-term well integrity [26], [27]. A centered casing allows for high-quality cementing of the annular space and reliable formation isolation, while ensuring uniform distribution of stresses from formation pressure and minimizing the risk of column collapse [28], [29]. Errors in the perforation of the well, for example, getting into watered intervals, can lead to excessive inflow of formation waters [30]-[32]. Aging and degradation of the pipe column material [33], failure of threaded connections and corrosion of casing strings can also cause failure of reservoir isolation [34], [35]. Here, special attention should be paid to the features of the deformation behavior of pipe steels during long-term operation in corrosive environments [36], [37], as well as the formation of microcracks and structural changes in the metal of threaded joints [38], [39]. It should also be noted that, under certain geological conditions, formation waters can be under significant reservoir pressure, and when the pressure decreases during the production process, they can break out to the surface. Watering of macro-heterogeneous gas reservoirs and opening

of gas condensate formations in conditions of geological uncertainty can significantly increase the probability of breaking the isolation of productive horizons [40], [41]. In addition, faults and fissures in rocks, natural seismic activity can create ways for formation water to reach the surface [42], [43].

A few years ago, the technological accidents in the wells No.5 and No.111 occurred at the Rybalske Oil Field, Okhtyrskyi District of Sumska Oblast in Ukraine, which were accompanied by open fountains with the removal of a large amount of highly mineralized waters and the formation of craters. However, a considerable amount of the formation water was concentrated in the well crater No. 5. In the case of depressurization of the well crater No. 5 at the Rybalske Oil Field, highly mineralized water can reach the underground aquifers.

The purpose of this research is to mathematically model the spread of salt contamination in underground aquifers due to anthropogenic activity. The case of depressurization of the crater of a well used for mining is considered, with subsequent assessment of environmental and economic losses from the emergency situation.

## 2. Methods

Systems analysis was applied during the planning and execution of experimental studies. Standard methods of determining the physical-chemical composition of surface, underground, formation waters, the content of macroinones of salts and petroleum products in the soil were used, namely: chromatographic analysis, potentiometric titration, flame photometric spectral analysis, gravimetric analysis, electrometry, infrared photometric analysis. Processing of the obtained results of experimental studies was carried out by means of pairwise and multivariate correlation-regression analysis.

The surveys of surface and groundwater at the field were conducted by the Northeast Scientific Centre “Intellect-Service” [44], [45] and subsequently supplemented by the Scientific Research and Design Institute of PJSC “Ukrnafta” and other research organizations [46], [47]. Based on the results of the research, the ecological state of the underground aquifers of the Rybalske Field has been determined.

The research results of physical-chemical properties of water in the well crater No. 6 of the Kehychivske Gas Condensate Field are presented in the paper [48]. The investigations have shown that the mineralization of water on the surface and at the bottom of the crater is 10 times different. In addition, the groundwater was surveyed from observation wells and mine wells in the crater area. According to the research results, it has been found that there is no impact of the crater on the groundwater of the surrounding territories.

The environmental pollution caused by the operation of oil and gas complexes can be considered from the economic point of view as a loss defined in value terms [49]-[51]. The environmental and economic losses allow for an economic assessment of environmental losses as a result of environmental pollution in monetary terms, caused by the activities of oil and gas complexes [52]. Two types of losses are taken into account. Firstly, the direct losses of natural resources and the losses caused by the deterioration of the environment quality, which are manifested in health deterioration and reduction in life expectancy of the population. Secondly, costs in value terms that are incurred to eliminate the harmful effects [53].

In Ukraine, the amount of economic losses caused by contamination of surface water bodies by petroleum products as a result of oil and gas well activities was determined in accordance with the "Methodology for Calculating the Reimbursement of Losses Caused to the State as a Result of Violation of the Legislation on the Protection and Rational Usage of Water Resources" [54]. The amount of damage is calculated in two stages. The total mass of oil discharged into the water body ( $M_n$ ) was determined by the following Formula (1):

$$M_n = \frac{M_p}{(1 - \varepsilon)}, \quad (1)$$

where:

$M_p$  – the mass of oil film, t;

$\varepsilon$  – the oil fraction dissolved and emulsified in water (for water bodies  $\varepsilon = 0.15$ ).

The mass of the oil film ( $M_p$ ) was determined by the following Formula (2):

$$M_p = M_{pm} \cdot S \cdot 10^{-6}, \quad (2)$$

where:

$M_p$  – the mass of oil film, t;

$M_{pm}$  – the oil specific gravity per 1 m<sup>2</sup> of water surface, g/m<sup>2</sup> (determined according to the Appendix 1 of [54]).

The reimbursement of losses caused to the water bodies as a result of contamination of the substance in the pure state in the composition of products or raw materials (in this case, petroleum products) was calculated by the following Formula (3):

$$Z = K_c \cdot K_{cat} \cdot K_p \cdot K_z \cdot \left[ (M_{i1} \cdot \gamma_{i1}) \cdot (M_{i2} \cdot \gamma_{i2}) + \dots \right], \quad (3)$$

where:

$K_c$  – the coefficient that takes into account the increase in damage to the aquatic ecosystem by unauthorized or emergency discharge ( $K_c = 1.5$ );

$K_{cat}$  – the coefficient that takes into account the category of water body, determined in accordance with the Appendix 2 of "Methodology..." [54];

$K_p$  – the regional coefficient of scarcity of surface water resources, determined in accordance with the Appendix 3 of "Methodology..." [54];

$k_z$  – the affection coefficient of aquatic ecosystem ( $k_z = 1.5$ );

$m$  – the amount of pollutants in the return water;

$M_i$  – the mass of the excess discharge of the  $i$ -contaminant into a water body with the return water, t;

$\gamma_i$  – the specific economic loss from the water contamination in the current year (USD/t).

As can be seen, the calculation of losses involves a preliminary calculation of oil mass released into water bodies as a result of oil and gas field exploitation. Since there is no primary data on the exact amount of oil, the oil mass is calculated using the Delphi method (expert evaluation method) based on laboratory and instrumental control results. The basis for the calculation of oil mass using the Delphi method is a visual assessment of oil film thickness according to its external features.

As for the discharge of harmful substances into the aquatic environment, they are also considerable, since the oil and gas industry uses water in large quantities. Water is necessary for both basic water-consuming technological processes and for auxiliary and household needs. Oil-field waters are

highly mineralized by nature and contain a high concentration of heavy metals. As a result, salt contamination of underground aquifers may occur [55].

To predict the ecological and economic losses caused by salt contamination, it is first necessary to investigate the processes of spreading harmful substances, taking into account the number of inflow sources in the study area and their intensity over time [56].

### 3. Results and discussion

The diffusion process models are used to describe the process of salt contamination spreading in the aquifer. The occurrence of the first one from the aquifer surface was found at a depth of 0.5-7.8 m with the crater depth of 9 m.

To study the diffusion of harmful substances, the models of diffusion processes are constructed and the diffusion equation is used, which in an arbitrary coordinate system is written in the following form:

$$\frac{\partial}{\partial t} c(\vec{r}, t) = (\nabla, D \nabla c(\vec{r}, t)) + f(\vec{r}, t), \quad (4)$$

where:

$\nabla$  – the covariant differentiation operator which in an arbitrary curvilinear coordinate system is written in the following form:

$$\nabla_i w^k = \frac{\partial w^k}{\partial \eta^i} + \sum_{j=1}^3 w^j \Gamma_{ij}^k, \quad (5)$$

where:

$w^k$  – the contravariant component of the vector;

$\Gamma_{ij}^k$  – the Christoffel symbols of the second kind which for an arbitrary curvilinear coordinate system are defined by Formula:

$$\Gamma_{ij}^k = \frac{1}{2} \sum_{s=1}^3 g^{ks} \left( \frac{\partial g_{js}}{\partial \eta^i} + \frac{\partial g_{is}}{\partial \eta^j} - \frac{\partial g_{ji}}{\partial \eta^s} \right), \quad (6)$$

where:

$g_{ij}$  – the components of the metric tensor of an arbitrary coordinate system ( $\eta^1, \eta^2, \eta^3$ );

$\vec{r}$  – the radius vector of the point of the study area;

$\nabla, D \nabla c(\vec{r}; t)$  – the operator of the dot product of the corresponding vectors;

$f(\vec{r}; t)$  – the function that describes the sources of harmful substances in the area and their intensity;

$D = D(\vec{r}; c; t)$  – diffusion coefficient at point  $\vec{r}$  and time  $t$ .

It should be noted that the Dependences (5) and (6) differ depending on the coordinate system: e.g., in a rectilinear Cartesian coordinate system, Dependence (5) means finding an ordinary partial derivative, and  $\Gamma_{ij}^k = 0$  in (6).

For a known cylindrical coordinate system:

$$\begin{cases} g_{11} = g_{33} = 1; g_{22} = r^2; \\ g^{21} = g^{22} = 1; g^{22} = \frac{1}{r^2}. \end{cases} \quad (7)$$

The calculations (5) and (6) are performed on the basis of (7). The choice of the model of diffusion processes is conditioned by the fact that when using different types of filtration processes it is necessary to set the pressure gradient in the area, which is very difficult to determine in the conditions of real areas and the objects under the study.

Without violating the generalization of the model, in order to simplify the computational schemes and algorithms, we consider the diffusion processes in Cartesian rectangular coordinate system (it is considered that any area in which the process is studied can be placed in a rectangular region  $V = \{(x; y); 0 \leq x \leq L_1; 0 \leq y \leq L_2\}$ ). In this case, the Equation (4) can be written as:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( a(x; y; t) \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( a(x; y; t) \frac{\partial c}{\partial y} \right), \quad (8)$$

where:

$c$  – the substance concentration at the point  $(x; y)$  at the time  $t$ ;

$a(x, y, t)$  – the diffusion coefficient at each point of the study area  $V$ .

In this case, the harmful substance enters the area across its boundary, therefore,  $f(x, y, t) = 0$ , and the sources of harmful substances are described in the boundary conditions. Assuming that  $a(x, y, t) = \text{const} = a^2$ , then the Equation (8) is written in the following form:

$$\frac{\partial c}{\partial t} = a^2 \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right). \quad (9)$$

It is considered that at the initial time the salt concentration in the fresh aquifer is given by:

$$c(x, y, t)|_{t=0} = c_0(x, y). \quad (10)$$

The salt concentration on the boundary of the study area is given by the ratios:

$$\begin{cases} c|_{x=0} = c_1(y, t); \\ c|_{x=L_1} = c_2(y, t); \\ c|_{y=0} = c_3(x, t); \\ c|_{y=L_2} = c_4(x, t). \end{cases} \quad (11)$$

For the Equations (8) and (9) with the initial (10) and the boundary Conditions (11), there are analytical solutions based on the fundamental results [57]. In particular, for the Equation (8), provided that  $a(x, y, t) = \text{const} = a^2$  with the initial Conditions (10) by the Fourier method, we obtain for the rectangle  $(0; L_1) \times (0; L_2)$ :

$$C(x, y, t) = \frac{4}{L_1 \cdot L_2} \sum_{k,j=1}^{\infty} a_{kj} \cdot e^{-\pi^2 a^2 \left( \frac{k^2}{L_1^2} + \frac{j^2}{L_2^2} \right) t} \sin \frac{k\pi x}{L_1} \sin \frac{j\pi y}{L_2}, \quad (12)$$

where:

$$a_{kj} = \int_0^{L_1} \int_0^{L_2} C_0(x; y) \cdot \sin \frac{k\pi x}{L_1} \cdot \sin \frac{j\pi y}{L_2} dx dy. \quad (13)$$

$$a_{kj} = \int_{x_0-\delta}^{x_0} dx \int_0^{\frac{y_0}{\delta} x - \frac{(x_0-\delta)}{\delta} y_0} \left( -\frac{D_1}{C} - \frac{A}{C} - \frac{B}{C} y \right) \sin \frac{\pi k x}{L_1} \sin \frac{\pi j y}{L_2} dy + \int_{K_0}^{x_0+\delta} dx \int_0^{\frac{y_0}{\delta} x - \frac{(x_0-\delta)}{\delta} y_0} \left( \frac{A}{C} x - \frac{B}{C} y + \frac{D_2}{C} \right) \sin \frac{\pi k x}{L_1} \sin \frac{\pi j y}{L_2} dy. \quad (16)$$

The solution can be analytically obtained.

To determine (16), the following integrals should be calculated:

$$\int_{x_1}^{x_2} dx \int_0^{mx+n} x \sin px \sin qy dy;$$

The function  $C(x, y, t)$  is a multiple Dirichlet series on the complex variables  $t, x, y$ , so it is an analytic multivariate function for which it is possible to study its local properties, boundary behaviour, and value distribution by analogy to [58], [59].

In this case, the boundary Conditions (11) are replaced by the initial distribution of salts in the study area. It should be noted that the coefficient  $a_{kj}$  is calculated accurately only in some cases. In those cases when the analytic form of the function  $C_0(x; y)$  does not allow calculating the coefficients accurately (13), the numerical integration formulas are used. When modelling the boundary Conditions (11), the following formulas are used:

$$C_0(x; y) = \sum_{i=1}^n \frac{C_i}{K_i [(x-x_i)^2 + (y-y_i)^2 + 1]}, \quad (14)$$

which specifies  $n$  contamination sources concentrated at the points  $(x_i; y_i)$  with the intensities  $C_i$  and the diffusion coefficient  $K_i$ , or in the form:

$$C_0(x; y) = \sum_{i=1}^n \left[ \frac{C_{ix}}{K_i (x-x_0)^2 + 1} \cdot \frac{C_{yi}}{K_i (y-y_0)^2 + 1} \right], \quad (15)$$

which allows obtaining the simple analytical dependences – in this case the double integrals (13) are replaced by two ordinary Riemann integrals. The application of (14) or (15) requires using the numerical integration packages.

In the special case where in a rectangular region the initial concentration distribution on the region boundary is given as shown in Figure 1, this concentration distribution  $C(x; y) = z$  is a piecewise linear function. The coordinates of the corresponding points in Figure 1 are given as follows:

$P(x_0; 0; z_0)$ ;  $K(x_0-\delta; 0; 0)$ ;  
 $A(x_0; 0; 0)$ ;  $O(x_0; y_0; 0)$ ;  
 $K_1(x_0 + \delta; 0; 0)$ .

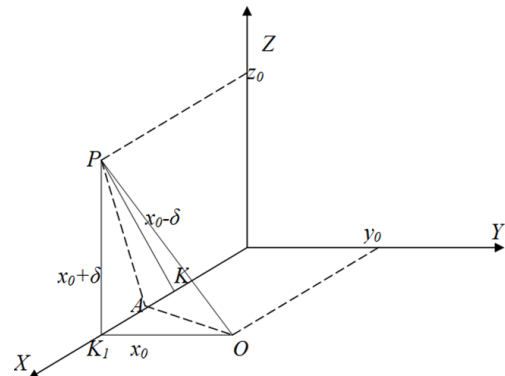


Figure 1. Initial distribution of salt concentration

For the coefficients  $a_{kj}$  (13), the following form of representation is obtained:

$$\int_{x_1}^{x_2} dx \int_0^{mx+n} y \sin px \sin qy dy;$$

In addition, the value in (13) is denoted by:  $A = x_0 y_0$ ;  $B = \delta z_0$ ;  
 $C = \delta y_0$ ;  $D_1 = -x_0 y_0 \delta_0 - \delta y_0 z_0$ ;  $D_2 = -x_0 y_0 \delta z_0 + \delta y_0 z_0$ .

The following is obtained:

$$\int_{x_1}^{x_2} dx \int_0^{mx+n} x \sin px \sin qy dy = \left\{ -\frac{1}{2q} \left( -\frac{1}{p+mq} x \cos[(p+ym)x+qm] + \frac{1}{(p+qm)^2} \sin[(p+qm)x+qm] \right) - \right. \\ \left. -\frac{1}{p-qm} x \cos[(p-qm)x-qm] + \frac{1}{(p-qm)^2} \sin[(p+qm)x+qm] + \frac{1}{q} \left( -\frac{1}{p} x \cos px + \frac{1}{p^2} \sin px \right) \right\} \Big|_{x_1}^{x_2}; \quad (17)$$

$$\int_{x_1}^{x_2} dx \int_0^{mx+n} y \sin px \sin qy dy = -\frac{1}{2q} \left( -\frac{m}{p+mq} x \cos[(p+qm)x+qn] + \frac{m}{(p+mq)^2} \sin[(p+qm)x+qn] \right) \Big|_{x_1}^{x_2} + \\ + \left( \frac{n}{2w} \frac{1}{p+qm} \cos[(p+qm)x+qn] \right) \Big|_{x_1}^{x_2} - \frac{1}{2q} \left( -\frac{m}{p-qm} x \cos[(p-qm)x-qn] + \frac{m}{(p-mq)^2} \sin[(p-mq)x-qn] \right) \Big|_{x_1}^{x_2} + \\ + \cos[(p+mq)x+qn] \Big|_{x_1}^{x_2} - \frac{1}{2q^2} \frac{1}{(p-mq)} \cos[(p-mq)x-qn] \Big|_{x_1}^{x_2}; \quad (18)$$

$$\int_{x_1}^{x_2} dx \int_0^{mx+n} \sin px \sin qy dy = \frac{1}{2q} \frac{\cos[(p+mq)x+qn]}{p+mq} \Big|_{x_1}^{x_2} + \frac{1}{2q} \frac{\cos[(p-mq)x-qn]}{p-mq} - \frac{1}{qp} \cos px \Big|_{x_1}^{x_2}. \quad (19)$$

The recent results indicate that obtaining analytical formulas is associated with performing cumbersome calculations, so it is advisable in the future to pay attention to the methods of numerical solution of the problem.

When numerically solving Equations (8) or (9) with the initial (10) and boundary Conditions (11), we use method of variable directions [17]-[19], which allows writing the system of difference equations for the specified equations (e.g., for the Equation (9):

$$\begin{cases} \frac{2(\tilde{c}_{k,m} - c_{k,m}^n)}{\tau} = a^2 \frac{\tilde{c}_{k+1,m} - 2\tilde{c}_{k,m} + \tilde{c}_{k-1,m}}{h_x^2} + a^2 \frac{c_{k+1,m}^n - 2c_{k,m}^n + c_{k-1,m}^n}{h_y^2} + f_{k,m}^n; \\ \frac{2(c_{k,m}^{n+1} - \tilde{c}_{k,m})}{\tau} = a^2 \frac{\tilde{c}_{k+1,m} - 2\tilde{c}_{k,m} + \tilde{c}_{k-1,m}}{h_x^2} + a^2 \frac{c_{k+1,m}^{n+1} - 2c_{k,m}^{n+1} + c_{k-1,m}^{n+1}}{h_y^2} + f_{k,m}^n. \end{cases} \quad (20)$$

The difference scheme in the first group of Equations (20) is explicit in the  $y$  coordinate, while in the second group, it is explicit in the  $x$  coordinate. In the final step of the calculation procedure, a system of linear algebraic equations with a tridiagonal matrix is calculated.

When studying the stability of difference schemes, the spectral stability characteristic is used to establish stability conditions:

$$\lambda_1 = \frac{1 - \frac{2\tau}{h_y^2} \sin^2 \frac{\phi}{2}}{1 + \frac{2\tau}{h_x^2} \sin^2 \frac{\psi}{2}}; \quad (21)$$

$$\lambda_2 = \frac{1 - \frac{2\tau}{h_x^2} \sin^2 \frac{\psi}{2}}{1 + \frac{2\tau}{h_y^2} \sin^2 \frac{\phi}{2}}. \quad (22)$$

The condition of stability is as follows:

$$|\lambda^*| = |\lambda_1 \cdot \lambda_2| \leq 1, \quad (23)$$

which is performed for any values  $\tau$ ;  $h_x$ ;  $h_y$ ;  $\sin^2 \phi / 2$ ;  $\sin^2 \psi / 2$ , taking into account that these values in the module are much smaller than 1. Therefore, the difference schemes are absolutely stable and, thus, the specified values are selected only, if the required level of calculation accuracy is fulfilled.

The System (20) is implemented by solving two systems with a triangular matrix using the sweep method, the first of which has the form:

$$-\frac{\tau a_{k,m}^2}{2h_x^2} \tilde{c}_{k+1,m} + \left( 1 + \frac{\tau a^2}{h_x^2} \right) \tilde{c}_{k,m} - \frac{\tau a_{k,m}^2}{2h_x^2} \tilde{c}_{k-1,m} = c_{k,m}^n + \frac{\tau a_{k,m}^2}{2h_y^2} \cdot (c_{k,m+1}^n - 2c_{k,m}^n + c_{k,m-1}^n); \quad (24)$$

$$\tilde{c}_{1,m} = c_1; \tilde{c}_{k,m} = c_1; m = 1, \dots, M,$$

where the unknown values are  $\tilde{c}_{k,m}$ , and the system:

$$-\frac{\tau a_{k,m}^2}{2h_y^2} c_{k,m-1}^{n+1} + \left(1 + \frac{\tau a_{k,m}^2}{h_y^2}\right) c_{k,m}^{n+1} - \frac{\tau a_{k,m}^2}{2h_y^2} c_{k,m+1}^{n+1} = \tilde{c}_{k,m}^n + \frac{\tau a_{n,m}^2}{2h_x^2} \cdot (\tilde{c}_{k+1,m} - 2\tilde{c}_{k,m} + \tilde{c}_{k-1,m}); \quad (25)$$

$$\tilde{c}_{k,1}^{n+1} = c_1; \tilde{c}_{k,M}^{n+1} = c_2; k = 1, \dots, K,$$

where the unknown values are  $\tilde{c}_{k,1}^{n+1}$ .

It should be noted that in Systems (24) and (25), the value  $a_{k,m}$  is determined at each point of the computational grid. This means that it is possible to simulate the diffusion process for a heterogenetic medium with different values of this coefficient for different areas of the studied field. All the proposed numerical algorithms and forms for setting the boundary conditions have been implemented in the form of software products, the numerous model or test calculations have been performed. For modelling boundary conditions, the following is used:

$$C(x, 0, t) = \sum_{i=1}^N \frac{C_i}{(x - x_i)^2 + (t - t_0)^2 K_i}; \quad (26)$$

$$C(0, y, t) = \sum_{j=1}^K \frac{C_j}{(y - y_j)^2 + (t - t_0)^2 K_j}, \quad (27)$$

which allows simulating both the location of the leak and its intensity over time (changing this intensity).

Figure 2 shows the concentration distribution along the cross sections perpendicular to the axis  $O_y$ . In the calculations it was specified that  $a^2 = \text{const}$ , so the pressure boundary Conditions (14) and (15) give a symmetric distribution of salt concentration in the study area. Figure 3 shows the salt concentration distribution for different locations of inflow sources – one of them is on the left boundary of the study area, the other – on the right. The intensity of the leaks is different.

Figure 4 presents the calculation results using schemes (14), (15), provided that  $a^2 \neq \text{const}$ ,  $a^2 = a^2(x, y, t)$ . The concentration distribution is revealed to be asymmetric due to the inhomogeneity of the medium into which the salts enter.

Figure 5 shows how the concentration of harmful substances changes over time with the same diffusion coefficient values. The model Dependences (16), (17) were used in this case.

The hydrocarbon content, high total mineralization of formation water and especially increased chloride ion content are the factors that negatively affect surface and groundwater and are the main criteria for assessing their pollution.

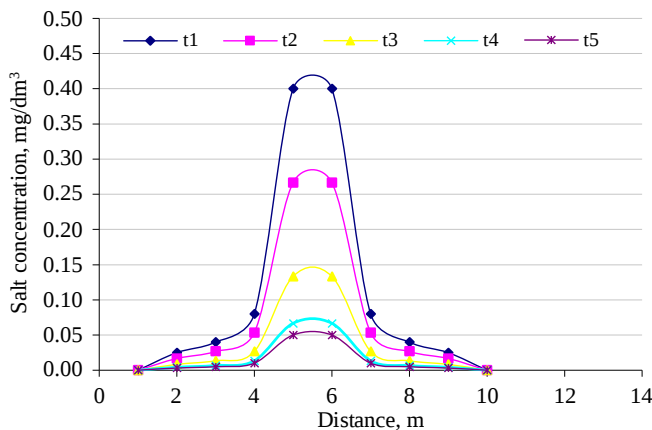


Figure 2. Distribution of concentration along the cross-sections at the location of the inflow source on the line  $y = 0$ : t1-t5 – time frames from 1 to 5 days at regular intervals

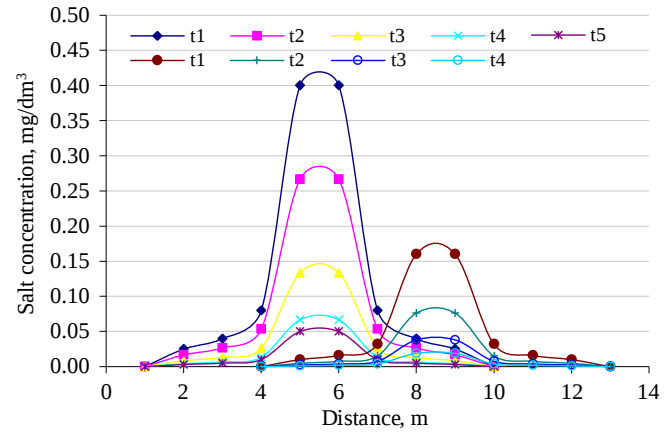


Figure 3. Distribution of salt concentration at two inflow sources, one of them is on the line  $y = 0$ , second is on the line  $y = L2$ : t1-t5 – time frames from 1 to 5 days at regular intervals

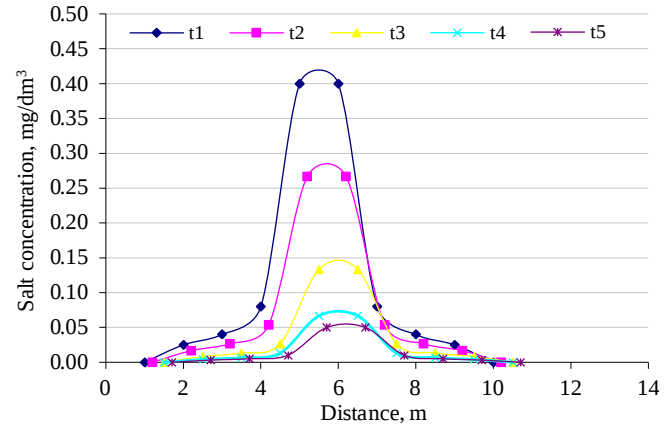


Figure 4. Influence of inhomogeneity of the medium properties on the concentration distribution; t1-t5 – time frames from 1 to 5 days at regular intervals

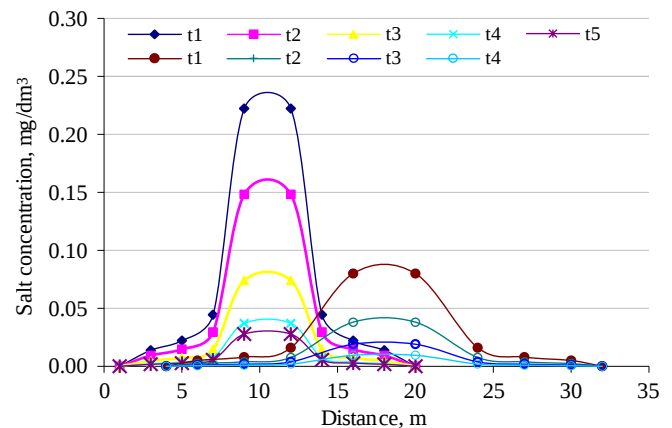


Figure 5. Changing of salt concentration in the study area over time: t1-t5 – time frames from 1 to 5 days at regular intervals

This approach to establishing the negative impact of formation water on surface and groundwater is correct in most cases, but this method allows establishing negative environmental changes at a late stage, when this impact is significant and significantly changes the physical-chemical properties of

water. In this regard, we have proposed a methodology for determining the impact of associated formation water on surface and groundwater, which enables to establish the impact at a stage when pollution is minimal, mineralization of surface and groundwater is not yet high, i.e. the impact of formation water is insignificant or classified as absent.

Thus, we have established that the formation of technogenic meromictic reservoirs is possible as a result of an emergency situation, due to the ingress of formation water to the surface in the territory of oil and gas fields. This is confirmed by the crater of well No. 5 at the Rybalske Oil Field. Undoubtedly, the formation of such reservoirs poses a direct potential threat to freshwater aquifers and surface water bodies located gipsometrically below the crater. The proposed mathematical model allows predicting the potential contamination of vital drinking aquifers in specific hydrogeological conditions of mineral deposits under conditions of technogenic accidents. This makes it possible to refine emergency response plans and develop measures to ensure a reliable level of environmental safety of enterprises and territories.

Prevention and rapid elimination of emergencies is an important task for ensuring environmental safety at mining enterprises and territories of mineral deposits. For example, for the conditions of the studied Rybalske Oil Field, based on the drainless nature of the reservoirs, we propose to eliminate salinity by continuously taking highly mineralized water from the bottom of the reservoir. This water can be used in the reservoir pressure maintenance systems used at the field. In the process of water withdrawal, highly mineralized water will be gradually replaced by fresh water from surface runoff. Thus, over time, the salinity of the crater water will decrease until safe water salinity concentrations are reached.

Formation waters that come to the surface of an oil and gas field have increased mineralization and density compared to fresh water, so there is always a risk of technogenic reservoirs [60], [61]. When in contact with atmospheric air, formation water cools and degasses, resulting in density stratification. To assess the safety consequences of such processes, methods are being developed for assessing the state of hydroecosystems and the level of hydroecological risks at the pre-project stages of implementation of technogenic objects [62] and in the process of developing river basin management strategies [63]. However, this study differs in that it is the first to develop a multicomponent mathematical model of mineral salt migration processes in underground freshwater aquifers in the case of depressurization of a meromictic reservoir.

Groundwater management, including artificial recharge, as proposed by [64], plays an important role in ensuring the sustainability of water resources for future generations. The purpose of the study was to identify suitable sites for artificial groundwater recharge in the state of Jammu in India. The authors used geospatial methods and groundwater modelling. Their approaches can be adapted to the conditions of mineral mining and complement the model we have developed. Artificial recharge can prevent critical groundwater loss in emergency situations.

An important aspect is the monitoring of water quality in drinking aquifers during the mining of mineral sites, which is based on measurements at specific points with a limited number of wells. This situation leads to uncertainty in estimating the distribution of real hydrochemical parameters due to limited data availability. An important scientific task is to

reduce uncertainty to obtain accurate and reliable monitoring results. In [65], the authors used geostatistical kriging and a differential evolution algorithm to optimize the design of a groundwater monitoring network in the Namoi region of Australia. The authors propose the integration of geostatistical methods for interpolation of parameters. The research is quite interesting, but foreign practice often includes complex methods that require significant financial, human and information resources, online availability of the results of state environmental monitoring programs, which is unavailable or rather limited in modern Ukrainian realities.

#### 4. Conclusions

The most significant negative impacts during oil and gas field development are uncontrolled release of reservoir fluids and salinization of groundwater as a result of formation water entering drinking underground aquifers. It has been determined that as a result of emergency situations associated with the release of formation water to the surface in the territory of oil and gas fields, the formation of technogenic meromictic reservoirs is possible. This is confirmed by the crater of well No. 5 at the Rybalske Oil Field. The total mineralization of crater water increases linearly with the depth of the reservoir, and a similar dependence is characteristic of the chloride ion content.

To predict the ecological and economic losses from salt contamination, the concentration distribution of harmful substances was studied, taking into account the number of inflow sources in the study area and their intensity over time.

The mathematical model for salt distribution in the aquifers in the case of crater depressurization has been developed. The analytical methods for determining the concentration of harmful substances should only be used in certain cases, when the initial conditions are modelled by simple analytical relations – e.g., by linear functions. The numerical methods make it possible to model the processes of spreading the harmful substances, taking into account the number of inflow sources in the study area, the inhomogeneity of the medium properties into which the harmful substance enters, and to assess the dynamics of changes in concentration of these substances over time.

#### Author contributions

Conceptualization: AP, OM; Data curation: LA, SS; Formal analysis: AP, LA; Funding acquisition: AP, SS, DH; Investigation: AP; Methodology: AP, OM; Project administration: OM, LA; Resources: AP, SS; Software: OM, DH; Supervision: LA; Validation: OM, LA; Visualization: SS, DH; Writing – original draft: AP, OM; Writing – review & editing: LA, SS, DH. All authors have read and agreed to the published version of the manuscript.

#### Funding

This research received no external funding.

#### Acknowledgements

The authors would like to express their gratitude to the staff of PJSC “Ukrnafta” for cooperation.

#### Conflicts of interests

The authors declare no conflict of interest.

## Data availability statement

The original contributions presented in the study are included in the article, further inquiries can be directed to the corresponding author.

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## Математичне моделювання забруднення підземних водоносних горизонтів внаслідок видобутку корисних копалин

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**Мета.** Створення математичної моделі розповсюдження соляного забруднення підземними водоносними горизонтами у разі розгерметизації кратера свердловини видобутку вуглеводнів для подальшої оцінки екологічних та економічних збитків від цих процесів.

**Методика.** Для прогнозування еколого-економічних збитків від соляного забруднення було досліджено розподіл концентрацій шкідливих речовин з урахуванням кількості джерел надходження та їх інтенсивності в часі на основі даних польових досліджень на Рибальському нафтовому родовищі Охтирського району Сумської області в Україні, де сталася технологічна збої на свердловинах, які супроводжувалися відкритими фонтанами з виносом великої кількості високомінералізованих вод та утворенням кратерів. Для обробки даних досліджень аварійного техногенного забруднення підземних водоносних горизонтів застосовано методи математичного моделювання.

**Результати.** У статті на основі реальних даних результатів дослідження процесів потенційного поширення соляного забруднення у прісних водоносних горизонтах внаслідок аварій на промислах видобування вуглеводневої сировини розроблено математичну модель розподілу солей у питних підземних водах у разі розгерметизації кратера свердловини нафтового родовища. Обґрунтовано потенційні економічні втрати при можливому забрудненні ґрунтових вод високо мінералізованим розчином, що може потрапити в питні підземні водоносні горизонти. Встановлено, що у зв'язку з виникненням надзвичайної ситуації внаслідок виходу

пластової води на поверхню на території нафтогазоносних покладів можливе утворення техногенних мероміктичних колекторів, що підтверджено на прикладі Рибальського нафтового родовища. Доведено, що загальна мінералізація води кратера лінійно зростає з глибиною водойми, подібна залежність характерна і для вмісту хлорид-іонів.

**Наукова новизна.** Вперше розроблено багатокомпонентну математичну модель процесів міграції мінеральних солей у підземних прісних водоносних горизонтах у випадку розгерметизації мероміктичної водойми.

**Практична значимість.** Отримані результати досліджень за допомогою чисельних методів дозволяють прогнозувати процеси розповсюдження шкідливих речовин в питних підземних водоносних горизонтах внаслідок аварійних ситуацій на нафтогазових промислах, враховуючи кількість джерел надходження забруднювачів в зону дослідження, неоднорідність властивостей середовища, в яке потрапляє шкідлива речовина, та оцінити динаміку зміни концентрації цих речовин у часі з подальшою оцінкою екологічних та економічних збитків від цих процесів.

**Ключові слова:** нафтопромисли, забруднення питних вод, математичне моделювання

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