

UDC 519.6:626.86

DOI: 10.30838/J.BPSACEA.2312.260324.137.1052

MODELING GROUND WATERS DYNAMICS AND POLLUTION

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Abstract. Problem statement. Large accumulators of liquid waste (e.g., mine water ponds, tailing ponds, etc.) are long-term sources that change the hydrological regime. A negative consequence of this process is flooding of the territory. In addition, the infiltration of contaminated water from such hazardous sources changes the quality of groundwater. Therefore, it is important to analyze the impact of such anthropogenic sources on the process of flooding and deterioration of groundwater quality. To solve this problem, it is very important to use the method of mathematical modeling as an effective mean of researching problems of this class, since the use of physical modeling is practically impossible within the scope of problems of this class. **The purpose of the article.** Development of numerical models for predicting changes in the hydrological regime (flooding of the territory) and groundwater quality under the influence of anthropogenic pollution sources. **Methodology.** To assess the dynamics of changes in the hydrological regime, a two-dimensional equation of filtration of a non-pressure groundwater flow is used. A two-dimensional geomigration equation (planned model) is used to analyze changes in groundwater quality during infiltration of contaminated water from the settling pond. This equation takes into account the convective transfer of contaminants in the filtration flow, dispersion, and the intensity of contaminant infiltration into the groundwater flow. The method of total approximation is used for numerical integration of the filtration equation. For the numerical integration of the geomigration equation, an implicit splitting scheme is used. **Scientific novelty.** Effective numerical models for rapid assessment of changes in groundwater dynamics and quality under the influence of anthropogenic sources that change the hydrological regime are proposed. The constructed numerical models take into account a set of important physical factors that affect the process of geomigration and flooding of the territory, namely: filtration coefficient, variable depth of free-flowing groundwater, dispersion, intensity of the source of impurity emission into the groundwater flow. This makes it possible to obtain a comprehensive assessment of the process of flooding and groundwater pollution. **Practical significance.** A computer code has been created that allows practical usage of the developed numerical models. This code is an effective tool for theoretical study of non-stationary processes of territory flooding and anthropogenic groundwater pollution. **Conclusions.** A numerical model for calculating groundwater dynamics has been developed. The model allows to predict the level of groundwater rise under the influence of a man-made source of wastewater infiltration from a settling pond. A numerical model for calculating the process of geomigration from an anthropogenic source of emissions has been developed. The model makes it possible to predict the dynamics of contamination zone formation in a non-pressure groundwater flow. The developed numerical models take into account the most important parameters that affect the formation of flooding zones and groundwater contamination.

Keywords: *ground waters dynamics; ground waters pollution; territory flooding; mass transfer; mathematical modeling*

МОДЕЛЮВАННЯ ДИНАМІКИ ГРУНТОВИХ ВОД ТА ЇХ ЗАБРУДНЕННЯ

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Анотація. Постановка проблеми. Великі накопичувачі рідких відходів (наприклад, шахтні водойми, хвостосховища тощо) – це довготривалі джерела, що змінюють гідрологічний режим. Негативним наслідком

цього процесу стає підтоплення території. Крім того, проникнення забрудненої води з таких небезпечних джерел змінює якість ґрунтових вод. Тому актуальним бачиться аналіз впливу таких антропогенних джерел на процес підтоплення та погіршення якості підземних вод. Для розв'язання цієї задачі дуже важливе застосування методу математичного моделювання як ефективного засобу дослідження задач цього класу, оскільки застосування фізичного моделювання в рамках задач цього класу практично неможливе. **Мета роботи** – розроблення чисельних моделей для прогнозування зміни гідрологічного режиму (підтоплення території) та якості підземних вод за впливу джерел антропогенного забруднення. **Методика.** Для оцінення динаміки змін гідрологічного режиму використовується двовимірне рівняння фільтрації безнапірного стоку підземних вод. Двовимірне рівняння геоміграції (планова модель) використовується для аналізу змін якості ґрунтових вод під час інфільтрації забрудненої води з відстійника. Це рівняння враховує конвективний перенос забруднень у фільтраційному потоці, дисперсію та інтенсивність інфільтрації забруднювачів у потік ґрунтових вод. Для числового інтегрування рівняння фільтрації застосовується метод повної апроксимації. Для чисельного інтегрування рівняння геоміграції використовується неявна схема розщеплення. **Наукова новизна.** Запропоновано ефективні числові моделі для експрес-оцінки змін динаміки та якості підземних вод за впливу антропогенних джерел, що змінюють гідрологічний режим. Побудовані чисельні моделі враховують комплекс важливих фізичних факторів, що впливають на процес геоміграції та затоплення території, а саме: коефіцієнт фільтрації, змінну глибину залягання безнапірних підземних вод, дисперсність, інтенсивність джерела викиду домішок у підземні води, потік. Це дає можливість отримати комплексну оцінку процесу підтоплення та забруднення підземних вод. **Практична значимість.** Створено комп'ютерний код, який дозволяє практично використовувати розроблені числові моделі. Цей код – ефективний інструмент для теоретичного дослідження нестационарних процесів підтоплення території та антропогенного забруднення підземних вод. **Висновки.** Розроблено чисельну модель для розрахунку динаміки підземних вод. Модель дозволяє прогнозувати рівень підняття ґрунтових вод за впливу техногенного джерела інфільтрації стічних вод із відстійника. Розроблено числову модель для розрахунку процесу геоміграції від антропогенного джерела викидів. Модель дає змогу прогнозувати динаміку формування зони забруднення в безнапірному стоці ґрунтових вод. Розроблені числові моделі враховують найважливіші параметри, що впливають на формування зон затоплення та забруднення ґрунтових вод.

Ключові слова: динаміка підземних вод; забруднення підземних вод; затоплення території; масоперенос; математичне моделювання

Problem statement. Problem of ground waters rise, pollution and its management attracts attention among the world [1; 3; 8; 9].

Many engineering projects, especially large-scale ones, involve excavation work on aquifers. For all such excavations, an appropriate groundwater and surface water management and control system(s) must be planned before the start of each project. In practice, this can only be done with information about the soil conditions and groundwater that may be encountered based on site investigation data. Groundwater control (as well as surface water runoff) is generally considered by the client, engineer, and architect to be a “temporary work”, the contractor's responsibility, and is almost always of little or no interest to them. In many cases, this philosophy proves to be short-sighted and ultimately results in significant financial, time and reputational losses for the client.

Sometimes, as the work progresses, the actual soil and groundwater conditions may differ from those expected. If this occurs, all

stakeholders should be prepared to consider changing operations and construction methods as the work progresses and more information becomes available. This will provide the best assurance that the project will be completed safely, economically, and within the realistic timeframe and cost of the program.

It is particularly important to note that the rise in groundwater levels is occurring in areas where there is a change in the hydrogeological regime, for example, due to the construction of wastewater storage ponds from various enterprises (Fig. 1).



Fig. 1. Settling pond

https://www.pseau.org/outils/ouvrages/irc_university_of_leeds_waste_stabilization_ponds_2004.pdf

Infiltration of wastewater from ponds leads not only to a rise in the water table (the process of flooding the territory begins), but also to a deterioration in groundwater quality. The situation can be aggravated by the fact that, in addition to deteriorating groundwater quality, wastewater entering the underground stream from storage facilities can be aggressive and, over time, affect the stability of the foundations of structures, underground utilities, etc. In this regard, an important task arises of predicting changes in groundwater dynamics and quality under the influence of man-made, long-term sources of pollution.

It should be emphasized that currently, empirical and analytical models are used to solve problems of this class, which make it possible to determine the dynamics of groundwater and the impact of drainage systems on its change [2; 3–6; 9; 10]. Such models are effective in engineering practice, but they provide predictive data only for “simplified” scenarios. Due to the increasing level of requirements for predictive results, there is an increasing need to use numerical models to solve problems of this class. Therefore, the development of numerical multifactor models that allow solving applied problems at a new level remains an urgent problem.

The purpose of the article. Development of a numerical model for analyzing changes in groundwater dynamics and quality under the influence of anthropogenic sources of pollution.

Methodology. The process of groundwater rise under the influence of a settling pond with contaminated wastewater is considered. The groundwater dynamics is described by the following equation (generalized Boussinesq equation):

$$\mu \frac{\partial h}{\partial t} = kh_m \left(\frac{\partial h^2}{\partial x^2} + \frac{\partial h^2}{\partial y^2} \right) + W, \quad (1)$$

where h – depth of underground flow; k – filtration coefficient; μ – lack of saturation; W – infiltration rate; h_m – average depth of underground flow.

When using equation (1), an aquitard is assumed to be horizontal.

The components of the underground flow velocity vector are determined on the basis of Darcy's law:

$$u = -k \frac{\partial h}{\partial x}, v = -k \frac{\partial h}{\partial y}. \quad (2)$$

The setting of boundary conditions for equation (1) is discussed in [3].

Since the wastewater in settling ponds is contaminated, the infiltration of this wastewater into groundwater leads to its gradual contamination. Therefore, when analyzing the environmental impact of settling ponds, it is necessary to analyze the process of mass transfer of contaminants in groundwater. Over time, these impurities will reach water intakes from groundwater sources, which will have a negative impact on public health.

The geomigration equation averaged over the depth of the groundwater flow is used to predict groundwater contamination [3–5]:

$$\begin{aligned} n \frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} + \frac{\partial vS}{\partial y} = \\ = \frac{\partial}{\partial x} \left(\mu_x \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_y \frac{\partial S}{\partial y} \right) + \\ + \sum_{i=1}^n Q_{Si}(t) \delta(x-x_i) \delta(y-y_i), \end{aligned} \quad (3)$$

where u, v – components of the underground flow rate; S – concentration of impurities in the underground flow; Q – intensity of impurity emission into the underground stream; μ_x, μ_y – dispersion coefficients; n is porosity coefficient; t – time.

The position of the emission source (sedimentation pond) is modeled using the Dirac delta function $\delta(x-x_i)(y-y_i)$, where x_i, y_i – Cartesian coordinates of the emission source.

The formulation of boundary conditions for equation (3) is discussed in [4; 5].

Numerical model. For the numerical integration of modeling equations (1), (3), a rectangular difference grid is used. The value of the depth of the underground flow and the concentration of the impurity is determined in the middle of the rectangular difference cells. The components of the filtration flow rate are determined on the sides of the difference cells. Markers are used to build the view of the

computational domain, specify the position of the pollution source, the location of the river, etc.

To build a numerical model of the filtration flow, equation (1) is reduced to the form:

$$\mu \frac{\partial h}{\partial t} = kh_m \left(\frac{\partial h^2}{\partial x^2} + \frac{\partial h^2}{\partial y^2} \right), \quad (4)$$

$$\mu \frac{\partial h}{\partial t} = W. \quad (5)$$

For numerical solution of equation (4), a difference scheme of total approximation was used:

- first step of splitting:

$$\frac{h_{i,j}^{n+\frac{1}{2}} - h_{i,j}^n}{\Delta t} = \left[a \frac{-h_{i,j}^{n+\frac{1}{2}} + h_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} \right] + \left[a \frac{-h_{i,j}^{n+\frac{1}{2}} + h_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2} \right],$$

- second step of splitting:

$$\frac{h_{i,j}^{n+1} - h_{i,j}^{n+\frac{1}{2}}}{\Delta t} = \left[a \frac{h_{i+1,j}^{n+1} - h_{i,j}^{n+1}}{\Delta x^2} \right] + \left[a \frac{h_{i,j+1}^{n+1} - h_{i,j}^{n+1}}{\Delta y^2} \right],$$

where $a = \frac{kh_m}{\mu}$.

For numerical integration Eq. (5) Euler method was used.

For numerical solution of the geomigration equation (3), it was split as follows [1]:

$$n \frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} = \frac{\partial}{\partial x} \left(\mu_x \frac{\partial S}{\partial x} \right), \quad (6)$$

$$n \frac{\partial S}{\partial t} + \frac{\partial vS}{\partial y} = \frac{\partial}{\partial y} \left(\mu_y \frac{\partial S}{\partial y} \right), \quad (7)$$

$$n \frac{\partial S}{\partial t} = \sum_{i=1}^n Q_{Si}(t) \delta(x - x_i)(y - y_i). \quad (8)$$

A two-step splitting scheme was used for numerical solution of equation (6) [1]:

- first step of splitting:

$$S_{i,j}^{n+\frac{1}{2}} = S_{i,j}^n - \Delta t \frac{u_{i+1,j}^+ S_{i,j}^{n+\frac{1}{2}} - u_{i,j}^+ S_{i-1,j}^{n+\frac{1}{2}}}{\Delta x} + \Delta t \mu_x \frac{-S_{i,j}^{n+\frac{1}{2}} + S_{i-1,j}^{n+\frac{1}{2}}}{2\Delta x^2} + \Delta t \mu_x \frac{-S_{i,j}^n + S_{i+1,j}^n}{2\Delta x^2};$$

- second step of splitting:

$$S_{i,j}^{n+1} = S_{i,j}^{n+\frac{1}{2}} - \Delta t \frac{u_{i+1,j}^- S_{i+1,j}^{n+1} - u_{i,j}^- S_{i,j}^{n+1}}{\Delta x} + \Delta t \mu_x \frac{-S_{i,j}^{n+\frac{1}{2}} + S_{i-1,j}^{n+\frac{1}{2}}}{2\Delta x^2} + \Delta t \mu_x \frac{-S_{i,j}^{n+1} + S_{i+1,j}^{n+1}}{2\Delta x^2},$$

where $u^+ = \frac{u + |u|}{2}$, $u^- = \frac{u - |u|}{2}$. Here and further

the following designation was used: $Vt = \frac{Vt}{n}$.

The following two-step splitting scheme was used for numerical solution of equation (7) [1]:

- first step of splitting:

$$S_{i,j}^{n+\frac{1}{2}} = S_{i,j}^n - \Delta t \frac{v_{i,j+1}^+ S_{i,j}^{n+\frac{1}{2}} - v_{i,j}^+ S_{i,j-1}^{n+\frac{1}{2}}}{\Delta y} + \Delta t \mu_y \frac{-S_{i,j}^{n+\frac{1}{2}} + S_{i,j-1}^{n+\frac{1}{2}}}{2\Delta y^2} + \Delta t \mu_y \frac{-S_{i,j}^n + S_{i,j+1}^n}{2\Delta y^2},$$

- second step of splitting:

$$S_{i,j}^{n+1} = S_{i,j}^{n+\frac{1}{2}} - \Delta t \frac{v_{i,j+1}^- S_{i,j+1}^{n+1} - v_{i,j}^- S_{i,j}^{n+1}}{\Delta y} + \Delta t \mu_y \frac{-S_{i,j}^{n+\frac{1}{2}} + S_{i,j-1}^{n+\frac{1}{2}}}{2\Delta y^2} + \Delta t \mu_y \frac{-S_{i,j}^{n+1} + S_{i,j+1}^{n+1}}{2\Delta y^2},$$

where $v^+ = \frac{v + |v|}{2}$, $v^- = \frac{v - |v|}{2}$.

For numerical integration of equation (8), the Euler method is used.

The computer code WatGE-2 was created on the basis of the developed numerical models. The programming language is FORTRAN. The computer code includes:

1. Wa.DAT – initial data file (entering information about the size of the calculation area, the location of the pollution source, the concentration of the impurity in the wastewater in the lagoon, etc.);

2. Wa1 is a subroutine for calculating the dynamics of groundwater depth change over time;

3. Wa2 is a subroutine for calculating the components of the filtration flow rate;

4. Wa3 – a subroutine for calculating the change in the concentration of an impurity in groundwater over time.

The proposed numerical model can be used for solving the following problems:

1. Modeling ground waters dynamics due to different factors.

2. Modeling dynamics of ground waters pollution near storages with wastes.

3. Modeling ground waters pollution after accident spillages.

4. Modeling ground waters dynamics due to drainage systems.

Results. Below there are the results of model problem solving. The following problem was considered: there is a contamination zone in ground waters which was formed after the accident spilling (Fig. 2). The underground water layer had the following parameters: 15 m was the depth of underground flow at the upper boundary of the calculation region (boundary $x = 0$) and at the low boundary the depth of underground flow was 11 m; $k = 4$ m/day; $\mu = 0.2$; $W = 0.001$ m/s; $\mu_x = 0.1u$; $\mu_y = 0.1v$; $S = 100$ (dimensionless concentration).

Dynamics of pollutant zone moving is shown in Figures 2–4. Time is dimensionless. Every number in these Figures show the dimensionless concentration as the percentage from the maximum concentration C_{max} at this time step.

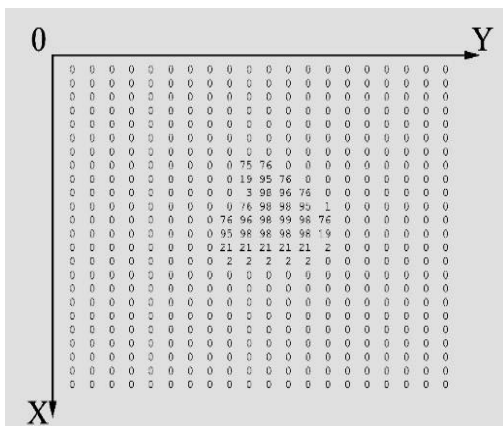


Fig. 2. Contamination area $C_{max} = 98$, $t = 0.15$

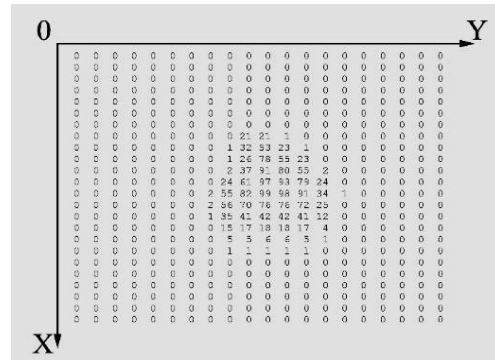


Fig. 3. Contamination area $C_{max} = 84$, $t = 0.22$

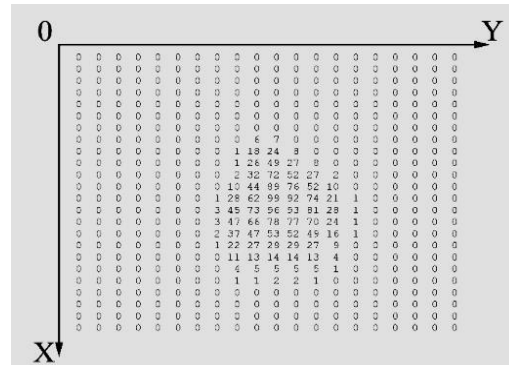


Fig. 4. Contamination area $C_{max} = 72$, $t = 0.22$

As can be seen from Figures 2–4 the contaminated zone slowly enlarges. It moves to the low boundary of the calculation region. Diffusion and convection cause decrease of impurity concentration in ground waters. It should be noted that the calculation time for each variant of the problem was 3 seconds. Thus, the built numerical models allow us to quickly analyze changes in the hydrogeological regime and groundwater pollution. This is very useful when performing serial calculations in practice.

Scientific novelty and practical value.

Effective numerical models for quick assessment of changes in groundwater dynamics and quality under the influence of anthropogenic sources that change the hydrological regime are proposed. The constructed numerical models take into account a set of important physical factors that affect the process of geomigration and flooding of the territory, namely: filtration coefficient, variable depth of free-flowing groundwater, dispersion, intensity of the source of impurity emission into the groundwater flow. This makes it possible to obtain a comprehensive assessment of the process of groundwater flooding and

contamination. A computer code has been created that allows for the practical use of the developed models.

Conclusions. 1. A numerical model for calculating groundwater dynamics was developed. The model makes it possible to predict the level of groundwater rise under the influence of a man-made source of wastewater infiltration from a pond - a sedimentation tank.

2. A numerical model for calculating the process of geomigration from an anthropogenic source of emissions was developed. The model makes it possible to predict the dynamics of the

formation of a contamination zone in a non-pressure groundwater flow.

3. The constructed numerical models take into account the most important parameters affecting the formation of flooding zones and groundwater contamination.

4. The results of the computational experiment show that the constructed mathematical models make it possible to quickly obtain predictive data for analyzing the impact of anthropogenic sources on changes in groundwater quality and their regime.

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Надійшла до редакції: 01.03.2024.