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Modeling of Filtration and Geomigration Under Anthropogenic Impact on Groundwater

Purpose. One of the most widespread methods of liquid waste disposal is the use of settling ponds. Wastewater in such lagoons eventually infiltrates into the aeration zone and reaches groundwater. Thus, a chemical contamination area is formed both in the aeration zone and in groundwater. When reengineering sedimentation ponds (for example, when increasing the height of the dam), there is an increase in the pressure in the structure, which will affect the intensity of infiltration of wastewater from the pond into the aeration zone), it is necessary to determine the change in the intensity of environmental pollution in advance. To solve such a forecasting problem, it is necessary to use specialized mathematical models. The aim of the study is to develop numerical models for assessing the dynamics of aeration zone pollution during the infiltration of liquid waste from a sedimentation pond. **Methodology.** The Laplace equation for the head is used to solve the filtration problem. The process of mass transfer of impurities in the aeration zone is modeled using the mass transfer equation, which takes into account the convective-dispersive transfer of impurities. The numerical integration of the modeling equations is carried out using finite-difference schemes. **Findings.** Numerical models of filtration and mass transfer are considered, which allow to estimate the dynamics of changes in the contamination area in the aeration zone during the infiltration of liquid wastewater from a sedimentation pond. **Originality.** The construction of mathematical models for analyzing the infiltration of liquid wastewater from a sedimentation pond is considered. Numerical models take into account the convective-dispersion process of impurity propagation in the aeration area. **Practical value.** The considered numerical models can be used to assess the environmental impact of sedimentation ponds used for the accumulation of liquid waste.

Keywords: geomigration; filtration; mass transfer; sedimentation pond; mathematical modeling

Introduction

Settling ponds containing liquid waste have a significant negative impact on the subsoil and groundwater. This is due to the filtration of liquid waste through the aeration zone into groundwater. As a result, a halo of heavily contaminated groundwater is formed in the area of influence of the settling pond. Over time, this contamination zone migrates and reaches water sources and surface water bodies. Thus, the disposal of liquid waste by discharging it into sedimentation ponds requires a scientific justification for such waste management and determination of the extent of groundwater contamination.

Fig. 1. Settling pond (https://cutt.ly/8rTpoWyJ)

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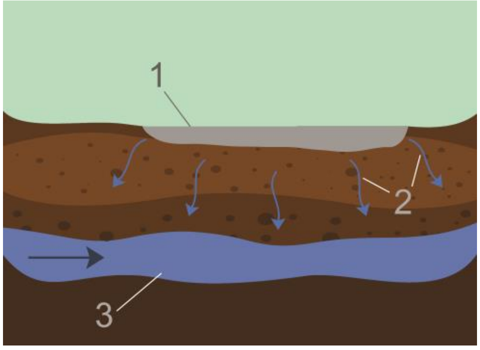

Fig. 2. Groundwater contamination due to wastewater infiltration:
1 – settling pond; *2* – filtration; *3* – ground water

The analysis of literature sources has shown that the following methods are used to study the processes of filtration and geomigration under the influence of anthropogenic factors:

1. *Physical experiment* (Fig. 3). The purpose of the physical experiment is to determine the hydrodynamic and physicochemical parameters of migration [7, 8].

Fig. 3. Preparation of equipment in the field [5]

These parameters are used to predict the hydrogeological situation.

Field measurements are used to monitor groundwater near large sources of pollution, but this requires a significant number of observation wells (Fig. 4).

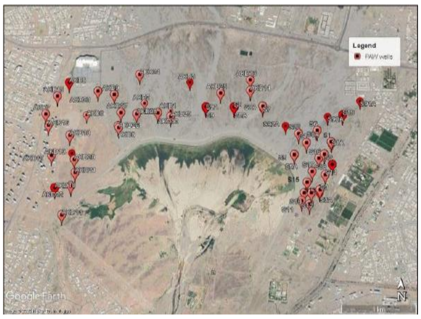

Fig. 4. Wells in the study area [8]

2. *Mathematical modeling* makes it possible to quickly obtain predictive data on changes in groundwater dynamics and the level of their pollution under various types of anthropogenic load. For theoretical problem solving, it is used:

– *empirical models* based on the processing of field observations and physical experiment results [3];

– *analytical models* are computational relationships that are an exact solution to the filtration or mass transfer equations [3];

– *numerical models* are built by applying various approximate (numerical) methods for solving boundary value problems of filtration and geomigration [1, 2, 4–12]. A significant number of numerical models are implemented in the form of commercial software products (e.g., MODFLOW, COMSOL [6, 10, 11]).

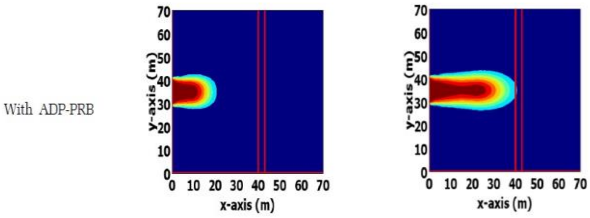

Fig. 5. Groundwater contamination area modeled using COMSOL code [12]

The use of numerical modeling to solve geomigration problems is a major trend in solving geomigration problems.

Purpose

The aim of the article is to develop fast numerical models for analyzing the dynamics of groundwater contamination during the infiltration of contaminated water from a sedimentation pond into an aquifer.

Methodology

The paper deals with the problem of wastewater filtration from a settling pond through an aeration zone. It is assumed that a stable hydraulic connection has been established between the water in the pond and groundwater.

To solve the problem of wastewater filtration through the aeration zone, the following filtration equation is used:

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$$\frac{\partial^2 H}{\partial^2 x}+\frac{\partial^2 H}{\partial^2 y}=0, \qquad (1)$$

where H is the hydraulic head.

The components of the groundwater flow rate are determined on the basis of Darcy's law:

$$\frac{\partial^2 H}{\partial^2 x}+\frac{\partial^2 H}{\partial^2 y}=0,$$

where k is the filtration coefficient.

At t = 0 the groundwater level in the study area and the water level in the settling pond are set.

The boundary condition $\frac{\partial H}{\partial n}=0$ is implemented on the sides of the computational domain, where n is a unit vector of the external normal to the boundary.

To build a numerical model of the process, the filtration equation (1) is used:

$$\frac{\partial H}{\partial t}=\frac{\partial^2 H}{\partial^2 x}+\frac{\partial^2 H}{\partial^2 y}, \qquad (2)$$

where t – a fictitious time.

The two-stage difference splitting scheme for (2) is written as follows (conditional approximation scheme):

$$\frac{H_{i,j}^{n+\frac{1}{2}}-H_{i,j}^{n}}{\Delta t}=$$

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

$$\frac{H_{i,j}^{n+1}-H_{i,j}^{n+\frac{1}{2}}}{\Delta t}=$$

$$=\left[\frac{H_{i+1,j}^{n+1}-P_{i,j}^{n+1}}{\Delta x^2}\right]+\left[\frac{H_{i,j+1}^{n+1}-H_{i,j}^{n+1}}{\Delta y^2}\right]. \qquad (3)$$

At each stage, the value of the velocity potential is determined by an explicit formula.

Also, for the numerical integration of equation (20), another splitting scheme is used. At the first stage, the geometric splitting of equation (2) is performed:

$$\frac{\partial H}{\partial t}=\frac{\partial^2 H}{\partial x^2},\ \frac{\partial H}{\partial t}=\frac{\partial^2 H}{\partial y^2}.$$

Next, the following dependence is used to determine the unknown value of the head based on the first equation from this system:

$$H_{i,j}^{n+1}=H_{i,j}^{n}+\Delta t\frac{H_{i+1,j}^{n}-H_{i,j}^{n}}{\Delta x^2}+\Delta t\frac{-H_{i,j}^{n}+H_{i-1,j}^{n}}{\Delta x^2}.$$

To determine the unknown value of the head based on the second equation, the following relationship is used:

$$H_{i,j}^{n+1}=H_{i,j}^{n}+\Delta t\frac{H_{i,j+1}^{n}-H_{ij}^{n}}{\Delta y^2}+\Delta t\frac{-H_{i,j}^{n}+H_{i,j-1}^{n}}{\Delta y^2}.$$

The values of the components of the filtration flow velocity vector are calculated as follows:

$$u_{ij}=-k\frac{H_{ij}-H_{i-1,j}}{\Delta x},v_{ij}=-k\frac{H_{ij}-H_{i,j-1}}{\Delta y}.$$

The calculation based on the considered dependencies ends when the condition is fulfilled:

$$\left|H_{ij}^{n+1}-H_{ij}^{n}\right|\le\varepsilon,$$

where ε – a small number; n – an iteration number.

The values of the components of the filtration flow velocity vector are used to solve the problem of mass transfer of an impurity from the pond to groundwater. The following equation is used to model the mass transfer process:

$$n\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}+$$

$$+\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right) \qquad (4)$$

where C – impurity concentration; μ_x, μ_y – dispersion coefficients; n – porosity; u, v – components of the filtration flow velocity vector; t – time.

Boundary conditions for equation (4):

1) at the entrance to the computational domain:

$$C=C_{(in)},$$

where $C_{(in)}$ – known concentration of the impurity, i.e., the concentration of the impurity in the settling pond;

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2) at the outlet of the calculation area:

$$C(i+1, j)=C(i, j),$$

where $C(i+1, j)$ is the concentration of the impurity in the last computational cell; $C(i, j)$ is the concentration of the impurity in the previous computational cell.

3) on the sides of the computational domain:

$$\frac{\partial C}{\partial n}=0,$$

where n – the unit normal to the solid surface.

For equation (4), the initial condition is set: at $t = 0$ $C = C_{(0)}$, $C_{(0)}$ – impurity concentration in the pond.

To numerically solve equation (4), the following splitting is performed:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}=0. \qquad (5)$$

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right). \qquad (6)$$

The following dependencies are used for the numerical integration of equation (5):

$$\frac{\partial uC}{\partial x}=\frac{\partial u^+C}{\partial x}+\frac{\partial u^-C}{\partial x},$$

$$\frac{\partial vC}{\partial y}=\frac{\partial v^+C}{\partial y}+\frac{\partial v^-C}{\partial y},$$

$$u^+=\frac{u+|u|}{2}, u^-=\frac{u-|u|}{2},$$

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

$$\frac{\partial u^+C}{\partial x}\approx\frac{u^+_{i+1,j}C^{n+1}_{i,j}-u^+_{i,j}C^{n+1}_{i-1,j}}{\Delta x}=L^+_xC^{n+1},$$

$$\frac{\partial u^-C}{\partial x}\approx\frac{u^-_{i+1,j}C^{n+1}_{i+1,j}-u^-_{i,j}C^{n+1}_{i,j}}{\Delta x}=L^-_xC^{n+1},$$

$$\frac{\partial v^+C}{\partial y}\approx\frac{v^+_{i,j+1}C^{n+1}{}_{i,j}-v^+_{i,j}C^{n+1}{}_{i,j-1}}{\Delta y}=L^+_yC^{n+1},$$

$$\frac{\partial v^-C}{\partial y}\approx\frac{v^-_{i,j+1}C^{n+1}{}_{i,j+1}-v^-_{i,j}C^{n+1}{}_{i,j}}{\Delta y}=L^-_yC^{n+1}.$$

The variable-triangular splitting scheme for equation (5) is written as follows:

– first step:

$$\frac{C^k_{i,j}-C^n_{i,j}}{\Delta t}+L^+{}_xC^k+L^+{}_yC^k=0; \qquad (7)$$

– second step:

$$\frac{C^{n+1}_{i,j}-C^k_{i,j}}{\Delta t}+L^-{}_xC^{n+1}+L^-{}_yC^{n+1}=0. \qquad (8)$$

The unknown value of C in each equation is determined by the «running calculation» formula.

For the numerical integration of (6), we use the total approximation scheme:

$$\frac{C^{n+\frac{1}{2}}_{i,j}-C^n_{i,j}}{\Delta t}=$$

$$=\left[\mu_x\frac{-C^{n+\frac{1}{2}}_{i,j}+C^{n+\frac{1}{2}}_{i-1,j}}{\Delta x^2}\right]+\left[\mu_y\frac{-C^{n+\frac{1}{2}}_{i,j}+C^{n+\frac{1}{2}}_{i,j-1}}{\Delta y^2}\right],$$

$$\frac{C^{n+1}_{i,j}-C^{n+\frac{1}{2}}_{i,j}}{\Delta t}=$$

$$=\left[\mu_x\frac{C^{n+1}_{i+1,j}-C^{n+1}_{i,j}}{\Delta x^2}\right]+\left[\mu_y\frac{C^{n+1}_{i,j+1}-C^{n+1}_{i,j}}{\Delta y^2}\right],$$

were it is assumed that $\Delta t=\frac{\Delta t}{n}$.

The unknown value of the impurity concentration is determined from these dependencies by an explicit formula.

Another splitting scheme is also used for the numerical integration of equation (4):

– first step (k = 1/4):

$$\frac{C^{n+k}_{ij}-C^n_{ij}}{\Delta t}+\frac{1}{2}(L^+_xC^k+L^+_yC^k)=$$

$$=\frac{1}{4}(M^+_{xx}C^k+M^-_{xx}C^k+M^+_{yy}C^n+M^-_{yy}C^n);$$

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– second step (k = n+1/2; c = n+1/4):

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^- C^k + L_y^- C^k) =$$

$$= \frac{1}{4}(M_{xx}^- C^k + M_{xx}^+ C^c + M_{yy}^- C^k + M_{yy}^+ C^c);$$

– third step (k = n+3/4; c = n+1/2):

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^+ C^k + L_y^- C^k) =$$

$$= \frac{1}{4}(M_{xx}^- C^c + M_{xx}^+ C^k + M_{yy}^- C^k + M_{yy}^+ C^c);$$

– fourth step (k = n+1; c = n+3/4):

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^- C^k + L_y^+ C^k) =$$

$$= \frac{1}{4}(M_{xx}^- C^k + M_{xx}^+ C^c + M_{yy}^- C^c + M_{yy}^+ C^k).$$

At each splitting step, the unknown value of the impurity concentration is determined using an explicit formula.

Findings

The considered numerical models were used to simulate the infiltration of wastewater from the pond. It is assumed that the wastewater contains chlorides, the concentration of which in the pond is $C_0 = 1$ (in a dimensionless form). The calculation was performed with the following data:

1. The head at the beginning of the calculation area h = 0.2 (in dimensionless form).

4. The head at the end of the calculation area h = 0.02 (in dimensionless form).

3. The filtration coefficient in the aeration zone is 2 m/day.

4. Porosity 0.2.

5. Background concentration of impurities in the aeration zone C = 0.

6. Length of the computational domain $L_x = 1$ (dimensionless value)

7. Width of the computational domain $L_y = 0.5$ (dimensionless value)

The following figures show the dynamics of the development of pollution areas in the aeration area for different moments of time. The concentration and time values are given in a dimensionless form.

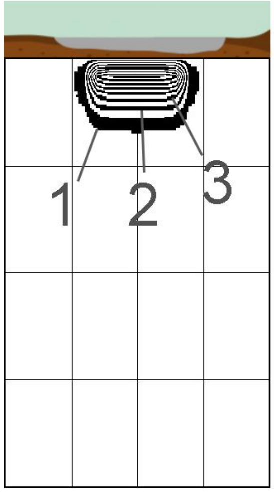

Fig. 6. Contamination area in the aeration zone, t = 0.03:
1 – C = 0.12; *2* – C = 0.23; *3* – C = 0.34

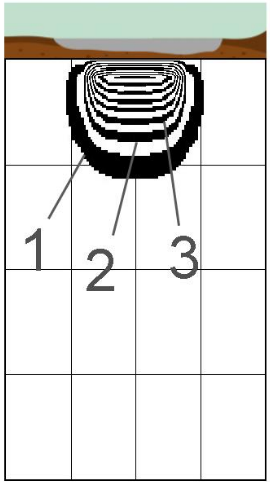

Fig. 7. Area of contamination in the aeration zone, t = 0.05:
1 – C = 0.14; *2* – C=0.24; *3* – C = 0.35

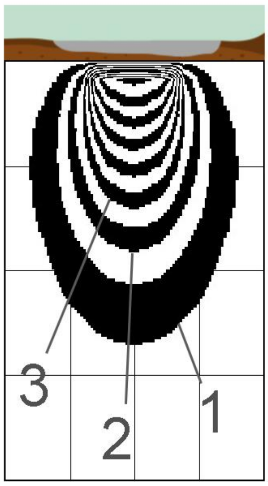

Fig. 8. Pollution area in the aeration zone, t = 0.09:
1 – C = 0.13; *2* – C = 0.23; *3* – C = 0.34

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The analysis of the data shown in Figs. 4-6 shows that the contamination area significantly increases in width, which is due to the dispersion process. The contamination area looks like a «tongue».

Thus, the considered numerical model makes it possible to determine the size, shape, and intensity of the contamination areas in the aeration zone.

Originality and practical value

Numerical models of infiltration of wastewater from a sedimentation pond through the aeration zone into the groundwater flow are considered. The models are based on the use of the splitting method for the filtration and mass transfer equations. The calculation of unknown parameters is based on explicit difference dependencies, which makes it possible to implement numerical models in a simple programmatic manner.

The considered numerical models can be used for rapid assessment of the impact of wastewater settling ponds on groundwater pollution.

Conclusions

1. The development of a numerical model for solving the problem of filtration of wastewater from a sedimentation pond is considered.
2. The development of numerical models for calculating the process of mass transfer of impurities in the filtration flow is considered.
3. The results of a computational experiment to determine the dynamics of groundwater pollution during the infiltration of wastewater from a sedimentation pond are presented.

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Моделювання фільтрації та геоміграції при техногенному впливі на ґрунтові води

Мета. Одним з широко розповсюджених методів утилізації рідинних відходів є використання ставків-відстійників. Стічні води в таких відстійниках з часом інфільтруються в зону аерації та досягають ґрунтових вод. Таким чином, формується область хімічного забруднення як в зоні аерації, так і в ґрунтових водах. При реінжинірингу ставків-відстійників (наприклад, при нарощуванні висоти дамби) має місце збільшення напору в споруді, що вплине на інтенсивність інфільтрації стоків зі ставка в зону аерації) потрібно заздалегідь визначати зміну інтенсивності забруднення довкілля. Для рішення такої прогнозної задачі необхідним є використання спеціалізованих математичних моделей. Метою роботи є розробка чисельних моделей для оцінювання динаміки забруднення зони аерації при інфільтрації рідинних відходів зі ставка-відстійника. **Методика.** Для рішення задачі фільтрації використовується рівняння Лапласа для напору. Процес масопереносу домішки в зоні аерації моделюється з використанням рівняння масопереносу, що враховує конвективно-дисперсійний перенос домішки. Чисельне інтегрування моделюючих рівнянь здійснюється за допомогою кінцево-різницевих схем. **Результати.** Розглянуто чисельні моделі фільтрації та масопереносу, що дозволяють оцінювати динаміку зміни області забруднення в зоні аерації при інфільтрації рідинних стоків зі ставка-відстійника. **Наукова новизна.** Розглянуто побудову математичних моделей для аналізу інфільтрації рідинних стоків зі ставка-відстійника. Чисельні моделі враховують конвективно-дисперсійний процес поширення домішки в області аерації. **Практична значимість.** Розглянуті чисельні моделі можуть бути використані для оцінювання впливу на довкілля ставків-відстійників, що використовуються для накопичування рідинних відходів.

Ключові слова: геоміграція; фільтрація; масоперенос; ставок-відстійник; математичне моделювання

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