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NUMERICAL MODELING OF GROUNDWATER DYNAMICS AND HEAT AND MASS TRANSFER PROCESSES

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Abstract. ***Problem statement.*** Groundwater is undergoing significant anthropogenic impact in many countries around the world. This impact results in changes in groundwater levels and deterioration of their quality. Protecting groundwater from anthropogenic impact involves solving several important tasks. A significant number of tasks are related to the need to predict the processes of filtration and heat and mass transfer in underground flows. In this regard, it is important to have specialized mathematical models as a modern scientific research tool. It should be noted that the use of physical experiments for problems of this class is significantly limited, due to the high cost of equipment, considerable time spent on setting up and conducting the experiment. ***The purpose of the article***. Development of a set of numerical models for simulation of filtration and heat and mass transfer processes in groundwater. ***Methodology.*** To model the process of non-pressure flow of groundwater, the equation of non-pressure filtration is used. The two-dimensional equation of convective-diffusive movement of a pollutant is used to model the process of mass transfer of an impurity in groundwater. To model the process of heat transfer in groundwater, in the problem of groundwater freezing, a two-dimensional energy equation is used. For numerical integration of modeling equations, finite-difference schemes are used. ***Scientific novelty.*** Numerical models of filtration and heat and mass transfer processes have been developed that allow real-time analysis of changes in groundwater quality and thermal regime. ***Practical significance.*** The developed numerical models make it possible to quickly analyze non-stationary processes of heat and mass transfer in groundwater when developing drainage systems in flooded areas. ***Conclusions.*** Numerical models of filtration and heat and mass transfer in groundwater have been developed. For the practical use of the built models, standard hydrological information is required. The models make it possible to analyze the dynamics of ice formation in groundwater during the implementation of the technology of freezing groundwater flow.

Keywords: *filtration; groundwater; mathematical modeling; heat and mass transfer; groundwater freezing*

ЧИСЕЛЬНЕ МОДЕЛЮВАННЯ ДИНАМІКИ ПІДЗЕМНИХ ВОД ТА ПРОЦЕСІВ ТЕПЛОМАСОПЕРЕНОСУ

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Анотація. ***Постановка проблеми***. Підземні води зазнають значного антропогенного навантаження в багатьох країнах світу. Наслідком такого навантаження є зміна рівня ґрунтових вод, погіршення їх якості. Захист підземних вод від антропогенного навантаження включає рішення декількох важливих задач. Значна кількість задач пов'язана з необхідністю прогнозування процесів фільтрації та тепломасопереносу в підземних потоках. У зв'язку з цим важливо мати спеціалізовані математичні моделі як сучасний інструмент наукового дослідження. Слід зазначити, що використання фізичного експерименту для задач даного класу суттєво обмежено, що пов'язано зі значною вартістю обладнання, значними витратами часу на постановку та проведення експерименту. ***Мета роботи*** – створення комплексу чисельних моделей для моделювання процесів фільтрації та тепломасопереносу в ґрунтових водах. ***Методика***. Для моделювання процесу руху безнапірного потоку підземних вод використовується рівняння безнапірної фільтрації. Для моделювання процесу масоперносу домішки в підземних водах використовується двовимірне рівняння конвективно-дифузійного руху забруднюючої речовини. Для моделювання процесу теплопереносу в підземних водах, в задачі про заморожування підземних вод, використовується двовимірне рівняння енергії. Для числового інтегрування моделюючих рівнянь використовуються кінцево-різницеві схеми. ***Наукова новизна***. Розроблено чисельні моделі процесів фільтрації та тепломасопереносу, що дозволяють в режиме реального часу аналізувати зміну якості та теплового режиму підземних вод. ***Практична значимість***. Розроблені чисельні моделі дають можливість швидко аналізувати нестаціонарні процеси тепломасопереносу в підземних водах при розробці систем дренажу на підтоплених територіях. ***Висновки***. Побудовано чисельні моделі фільтрації та тепломасоперносу в підземних водах. Для практичного використання побудованих моделей потребується стандартна гідрологічна інформація. Моделі дають можливість аналізувати динаміку формування льоду в підземних водах при реалізації технології заморожування потоку підземних вод.

Ключові слова*:* *фільтрація; підземні води; математичне моделювання; тепломасоперенос; заморожування підземних вод*

Problem statement. In many countries of the world, the problem of flooding is very acute. Such flooding has significant negative consequences: groundwater gets into basements and building foundations, it is impossible to carry out agricultural work, and there is a decrease in land fertility [3; 6−7].

In addition, lowering the groundwater level is necessary during the construction of a number of structures [1]. Therefore, considerable attention is paid to this problem. Nowadays, various methods of lowering the groundwater level are used. Often, drill bits are used to solve this problem [1]. The method of freezing a groundwater area with subsequent pumping of water from this area is also widely used.

For this purpose, special equipment is used (Fig. 1) and wells that provide a constant mode of refrigerant supply to the flow where cooling is carried out (Fig. 2) [5; 10; 14].

A particularly important problem in this area is the development of calculation methods for analyzing the effectiveness of various engineering technologies for lowering groundwater levels.

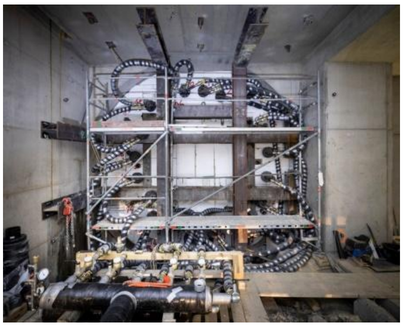

Fig. 1. Special equipment for refrigerant supply to groundwater (https://cutt.ly/3eHG9as9)

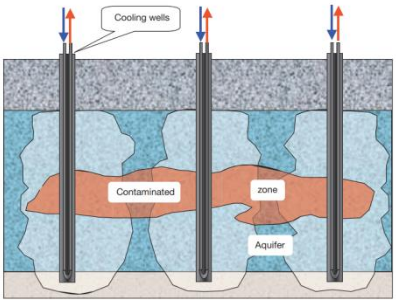

Fig. 2. Wells with refrigerant in the ground water [15]

The most widely used empirical and analytical calculation methods for problems of this class make it possible to predict the processes of geomigration, heat transfer and groundwater dynamics during the operation of drainage systems, etc. However, the use of such methods allows obtaining information only for “simplified” scenarios. High requirements for forecast data require the creation of more advanced mathematical models for solving complex problems in the field of groundwater dynamics and heat and mass transfer processes in them. An alternative is to use numerical models [2; 8–9; 13]. However, the problem of developing fast-calculating numerical models for analyzing complex processes of groundwater dynamics and heat and mass transfer processes in them will remain relevant.

The purpose of the article. Development of a set of mathematical models for calculating groundwater filtration and heat and mass transfer processes in terms of solving engineering problems of groundwater protection.

Methodology. To calculate the dynamics of groundwater and the processes of heat and mass transfer in them, the fundamental equations of the mechanics of the whole medium are used.

Modeling of the filtration process. The Boussinesq's equation is used to describe the motion of the free-flowing groundwater:

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

where h is the depth of a non-pressure groundwater flow; k is the aquifer filtration coefficient; μ is the saturation deficit (water yield); h_m is the average depth of the groundwater flow.

When using equation (1), the water resistance is assumed to be horizontal.

The components of the groundwater flow velocity vector are calculated on the basis of Darcy's law:

$$u = -k \frac{\partial h}{\partial x}; \quad v = -k \frac{\partial h}{\partial y}. \tag{2}$$

The boundary conditions for the modeling equation (1) are discussed in [3].

It should be noted that for real problems of groundwater dynamics, the solution of the filtration equation (1) can be found only by using numerical methods. The numerical solution of this equation is discussed below.

Modeling the process of geomigration. A significant number of problems in the field of groundwater dynamics are related to the analysis of the movement of impurities in these waters. Contaminants can enter the groundwater flow during the filtration of contaminated water from storage tanks, during accidental spills, etc. Therefore, there is often a problem of determining the size and intensity of contamination zones in groundwater that form over time. To study the processes of contaminant movement in groundwater, we use the mass transfer equation averaged over the depth of the flow [2]:

$$\frac{\partial S}{\partial t} + \frac{\partial uS}{\partial x} + \frac{\partial vS}{\partial y} = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial S}{\partial x} \right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial S}{\partial y} \right) +$$

$$+\sum_{i=1}^{n} Q_{Si}(t)\,\delta(x - x_i)\,\delta(y - y_i), \tag{3}$$

where u, v are components of the groundwater flow velocity; S is the concentration of an impurity in the groundwater flow; Q is the intensity of the impurity emission into the groundwater flow; μ_x, μ_y are dispersion coefficients; t is 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 are the Cartesian coordinates of the emission source.

The setting of boundary conditions for equation (3) is discussed in [2].

Modeling the process of heat transfer in groundwater. To model the process of freezing groundwater and calculate the dynamics of changes in its temperature, we use the following heat transfer equation:

$$\frac{\partial T}{\partial t}+\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y}=$$

$$\frac{\partial}{\partial x}\left(a_x\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(a_y\frac{\partial T}{\partial y}\right), \qquad (4)$$

where u, v are the components of the groundwater flow velocity; T is the temperature in the flow; a_x, a_y are the thermal conductivity coefficients; t is time.

To model the hydrodynamics of groundwater flow in problems of its freezing, we propose to use the velocity potential equation:

$$\frac{\partial^2 P}{\partial x^2}+\frac{\partial^2 P}{\partial x^2}=0, \qquad (5)$$

where P is the velocity potential.

If the velocity potential field is defined, then the components of the flow velocity vector are defined as follows:

$$u=\frac{\partial P}{\partial x};\ v=\frac{\partial P}{\partial y}. \qquad (6)$$

Solving equation (5) and determining the components of the groundwater flow velocity vector based on dependencies (6) make it possible to determine the groundwater flow rate during the formation of a cooling zone (ice) near wells that use a special solution for cooling water.

Numerical models. For the numerical integration of the considered modeling equations, we use a rectangular difference grid.

When constructing numerical models, their parameters on the difference grid are determined as follows:

1) the depth of the underground flow is determined at the centers of the difference cells;

2) the concentration of the impurity is determined at the centers of rectangular difference cells;

3) the components of the filtration flow rate are determined on the sides of the difference cells;

4) the temperature of the water flow is determined in the centers of rectangular difference cells.

We form the appearance of the computational domain using markers. The markers determine the position of wells, rivers (groundwater discharge zone), liquid waste storage facilities, etc.

To construct a numerical model of the filtration flow, we reduce equation (1) to the following form:

$$\mu\frac{\partial h}{\partial t}=kh_m\left(\frac{\partial h^2}{\partial x^2}+\frac{\partial h^2}{\partial y^2}\right); \qquad (7)$$

$$\mu\frac{\partial h}{\partial t}=W. \qquad (8)$$

To numerically solve equation (7), we use a difference scheme of total approximation:

− the first step of splitting:

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

− the 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 $a=\frac{kh_m}{\mu}$.

To numerically solve the geomigration equation (3), we decompose it as follows [1]:

$$\frac{\partial S}{\partial t}+\frac{\partial uS}{\partial x}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial S}{\partial x}\right), \qquad (9)$$

$$\frac{\partial S}{\partial t}+\frac{\partial vS}{\partial y}=\frac{\partial}{\partial y}\left(\mu_y\frac{\partial S}{\partial y}\right), \qquad (10)$$

$$\frac{\partial S}{\partial t}=\sum_{i=1}^{n}Q_{Si}(t)\,\delta(x-x_i)(y-y_i). \qquad (11)$$

To numerically solve equation (9), we apply a two-step splitting scheme [2]:

– in the first step:

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

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

– in the second step:

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

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

where $u^{+} = \frac{u + |u|}{2}$; $u^{-} = \frac{u - |u|}{2}$.

To numerically solve equation (10), we apply the following two-step splitting scheme [2]:

– in the first step:

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

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

– in the second step:

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

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

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

To numerically integrate equation (11), we use the Euler method.

It should be noted that the solution of the flow freezing problem is one of the most difficult problems of groundwater dynamics. This is due to the fact that it is necessary to search for a solution (temperature field, groundwater flow velocity) in a region whose appearance changes over time due to the appearance of a freezing zone, i. e., a zone where there is no fluid movement. Thus, a zone appears in the flow that is impermeable and changes its size and shape over time.

When solving problems related to the process of freezing a groundwater flow, the first step is to numerically integrate the Laplace equation using an explicit formula. To do this, we perform the following approximation of the derivatives:

$$\frac{\partial^2 P}{\partial x^2} = \frac{P_{i+1,j} - 2P_{i,j} + P_{i-1,j}}{\Delta x^2};$$

$$\frac{\partial^2 P}{\partial y^2} = \frac{P_{i,j+1} - 2P_{i,j} + P_{i,j-1}}{\Delta y^2},$$

where Δx, Δy is the step of the difference grid in the direction of the *OX*, *OY* axes, respectively.

Taking these approximations into account, the Laplace equation can be written as follows:

$$\frac{P_{i+1,j} - 2P_{i,j} + P_{i-1,j}}{\Delta x^2} + \frac{P_{i,j+1} - 2P_{i,j} + P_{i,j-1}}{\Delta y^2} = 0.$$

The value of the velocity potential is determined as follows:

$$P_{i,j} = \left[\frac{P_{i+1,j} + P_{i-1,j}}{\Delta x^2} + \frac{P_{i,j+1} + P_{i,j-1}}{\Delta y^2} \right] \Big/ Z,$$

where $Z = \left(\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2} \right)$.

The splitting of equation (4) has the form [5]:

$$\frac{\partial T}{\partial t} + \frac{\partial uT}{\partial x} = \frac{\partial}{\partial x}\left(a_x \frac{\partial T}{\partial x} \right), \tag{12}$$

$$\frac{\partial T}{\partial t} + \frac{\partial vT}{\partial y} = \frac{\partial}{\partial y}\left(a_y \frac{\partial T}{\partial y} \right). \tag{13}$$

To numerically solve equation (12), we apply a two-step splitting scheme [2]:

– in the first step:

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

$$+\Delta t a_x \frac{-T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{2\Delta x^2} + \Delta t a_x \frac{-T_{i,j}^{n} + T_{i+1,j}^{n}}{2\Delta x^2};$$

− in the second step:

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

$$+\Delta t a_x \frac{-T_{i,j}^{n+\frac{1}{2}} + T_{i-1,j}^{n+\frac{1}{2}}}{2\Delta x^2} + \Delta t a_x \frac{-T_{i,j}^{n+1} + T_{i+1,j}^{n+1}}{2\Delta x^2},$$

where $u^{+} = \frac{u + |u|}{2}$; $u^{-} = \frac{u - |u|}{2}$.

To numerically solve equation (13), we apply the following two-step splitting scheme [2]:

− in the first step:

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

$$+\Delta t a_y \frac{-T_{i,j}^{n+\frac{1}{2}} + T_{i,j-1}^{n+\frac{1}{2}}}{2\Delta y^2} + \Delta t a_y \frac{-T_{i,j}^{n} + T_{i,j+1}^{n}}{2\Delta y^2};$$

− in the second step:

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

$$+\Delta t a_y \frac{-T_{i,j}^{n+\frac{1}{2}} + T_{i,j-1}^{n+\frac{1}{2}}}{2\Delta y^2} + \Delta t a_y \frac{-T_{i,j}^{n+1} + T_{i,j+1}^{n+1}}{2\Delta y^2},$$

where $u^{+} = \frac{u + |u|}{2}$; $u^{-} = \frac{u - |u|}{2}$.

The algorithm for solving problems of this class is as follows:

1. Form a view of the computational domain.
2. Enter information about the physical parameters of the problem.
3. Set the position of the wells used to freeze the underground flow.
4. Solve the Laplace equation for the velocity potential.
5. Determine the components of the flow velocity vector.
6. Calculate the temperature field in the flow.
7. Determine the region where the flow temperature is 0, i. e., water freezing has occurred.

The appearance of ice in the flow changes the geometry of the computational domain, since there is no longer any water movement in the area where there is ice. Therefore, it is necessary to solve the problem of groundwater dynamics again and determine the groundwater flow velocity field again, and then solve the heat transfer problem. That is, the process is repeated starting from step 4.

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 − a file of initial data (entering information on the size of the calculated area, the location of the pollution source, the concentration of impurities in the underground flow, the position of wells, etc);

2) Wa1 − a SUBROUTINE-type subroutine for calculating the dynamics of groundwater depth change over time;

3) Wa2 − SUBROUTINE subroutine for calculating the components of the filtration flow rate;

4) Wa3 − SUBROUTINE subroutine for calculating the change in the concentration of impurities in groundwater over time;

5) WaT3 − SUBROUTINE subprogram for calculating the change in temperature concentration in groundwater over time;

6) WaTV2 − a SUBROUTINE subroutine for calculating the components of the flow velocity used in solving the heat transfer problem;

7) WaTR2 − a SUBROUTINE subroutine for solving the velocity potential equation.

Results. A computational experiment was conducted to verify the stability of the calculation of the developed numerical models for simulating the process of groundwater freezing. Two wells were considered (Fig. 3, marker 4), where a constant temperature of 0 °C was maintained. The ambient temperature was 20 °C. It was necessary to determine the dynamics of the freezing zone formation. It was assumed that in the difference cell where the temperature became 0 °C, ice formed and this zone ceased to be a flow zone.

Figures 3–7 show the freezing area which was formed in the groundwaters flow during time. Time in these figures is dimensionless. These figures show the change in the shape of the freezing zone in the flow.

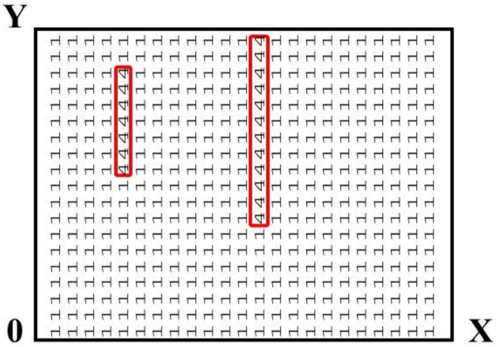

Fig. 3. Scheme of the computational domain:
4 – position of the well supplying the freezing agent

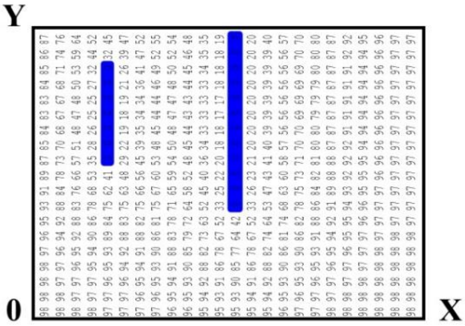

Fig. 4. Freezing area for time t = 0.7

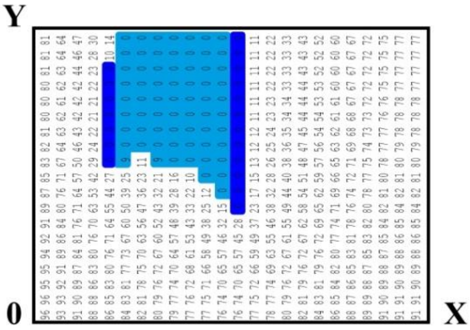

Fig. 5. Freezing area for time t = 2.1

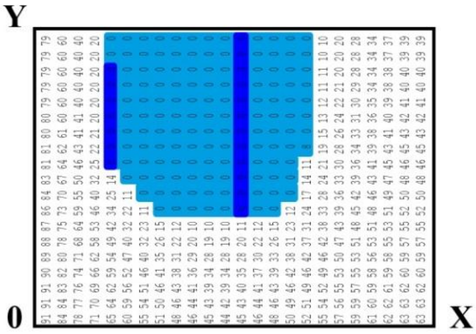

Fig. 6. Freezing area for time t = 4.9

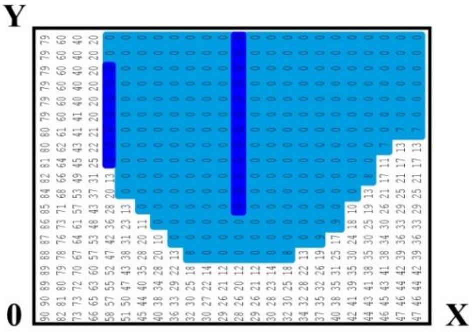

Fig. 7. Freezing area for time t = 6.3

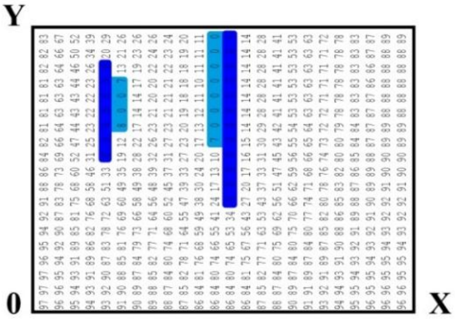

Fig. 8. Freezing area for time t = 1.4

As can be seen from the figures above, the developed numerical model allows us to determine dimensions of freezing zone and shape of the cooling zone during freezing operation.

Note that the calculation time for each variant of the problem is 8 s.

Scientific novelty and practical value. Effective mathematical models for predicting the level of chemical contamination of groundwater, groundwater dynamics, and thermal regime in groundwater are proposed.

The constructed mathematical models make it possible to determine the dynamics of changes in the temperature regime of groundwater during the operation of wells used for freezing individual sections of groundwater.

The developed computer program allows for a comprehensive assessment of groundwater conditions.

Conclusions

1. A set of mathematical models has been developed to calculate the process of filtration of unconfined groundwater and its chemical contamination.
2. An experiment was carried out to confirm the adequacy of the constructed numerical model of filtration of the free-flowing groundwater flow.
3. An effective mathematical model was constructed that allows determining the temperature fields in groundwater during the operation of wells used to freeze individual sections of the flow.
4. The results of computer modeling indicate the effectiveness of the developed mathematical models.

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