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NUMERICAL MODELING OF GROUNDWATER FLOW AND ALLUVIAL FLOODPLAINS NITRATE TRANSPORT GEOECOLOGICAL ASPECTS OF AKTOBE REGION, KAZAKHSTAN

Abstract. Understanding the influence of groundwater contamination in floodplains is critical for developing long-term management plans for subsoil and assessing geo-ecological sustainability. This study aims to create a regional groundwater flow and transport model to evaluate the impact of nitrate groundwater contamination in the Aktobe region alluvial plain in West Kazakhstan. The MODFLOW model was used to construct the groundwater flow model of the local aquifer and simulate regional changes in the water table over time. The calibrated groundwater model yielded a root mean square error of 5.1 m for the entire modeled area. Results of the calibrated model show the extension of a nitrate plume under the current 2023 setting and the long-term 2048 scenario. The model helped clarify the correct location of the intake, considering increased withdrawal rates for the operational period.

Key words: *groundwater, Bestamak site, Middle Quaternary modern alluvial aquifer, water intake, groundwater quality, operational reserves, mathematical model.*

Қазақстанның Ақтөбе облысындағы аллювиалды жайылмаларында жерасты сулары ағынын және нитраттарды тасымалдаудың геоэкологиялық аспектілерін сандық модельдеу

Аңдатпа. Жайылымдардағы жерасты суларының ластануының әсерін түсіну жер қойнауын басқарудың ұзақ мерзімді жоспарларын әзірлеу және олардың геоэкологиялық тұрақтылығын бағалау үшін өте маңызды. Бұл зерттеудің мақсаты жерасты суларының ағыны мен тасымалдауының аймақтық моделін жасау және Ақтөбе облысы, Батыс Қазақстандағы аллювий шөгінділеріндегі жерасты суларының нитраттармен ластануының әсерін бағалау болып табылады. MODFLOW моделі орта төрттік дәуіріндегі заманауи аллювиалды сулы горизонттың жерасты суларының ағынын құру үшін пайдаланылды. Калибрленген жерасты суларының моделі бүкіл модельделген аумақ үшін 5,1 м орташа квадраттық қатені құрады. Үлгіні калибрлеу нәтижелері 2023 жылға және 2048 жылға дейінгі ұзақ мерзімді сценарийге арналған нитрат шлейфінің кеңеюін көрсетеді. Модель пайдалану кезеңінде суға сұраныстың артуын ескере отырып, су алудың дұрыс орнын анықтауға көмектесті.

Түйінді сөздер: *жерасты сулары, Бестамақ учаскесі, орта төрттік заманының қазіргі аллювиалды сулы қабаты, су алу, жерасты суларының сапасы, пайдалану қорлары, математикалық модель.*

Численное моделирование потока подземных вод и геоэкологические аспекты переноса нитратов в аллювиальных поймах Актюбинской области Казахстана

Аннотация. Понимание влияния загрязнения подземных вод в поймах рек имеет решающее значение для разработки долгосрочных планов управления недрами и оценки их геоэколической устойчивости. Целью данного исследования является разработка локальной модели потока и переноса подземных вод и оценки влияния нитратного загрязнения подземных вод аллювиальных отложений в Актюбинской области, Западный Казахстан. Модель MODFLOW была использована для построения потока подземных вод водоносного среднечетвертичного современного аллювиального горизонта. Откалиброванная модель подземных вод дала среднеквадратичную ошибку в 5,1 м для всей моделируемой территории. Результаты калибровки модели показывают расширение нитратного шлейфа на 2023 год и при долгосрочном сценарии до 2048 года. Модель помогла уточнить правильное расположение водозабора, учитывая рост водопотребности на эксплуатационный период.

Ключевые слова: *подземные воды, участок Бестамак, водоносный среднечетвертичный современный аллювиальный горизонт, водозабор, качество подземных вод, эксплуатационные запасы, математическая модель.*

Introduction

Nitrates pose a severe threat to groundwater as a source of drinking water supply, with high concentrations leading to hypoxia and degradation of aquatic ecosystems. It is, therefore, essential to understand the processes that influence the formation, rate of spread, and direction of the plume in the water-rock system. Pressure on surface and groundwater sources is increasing with population growth and water demand, and in terms of availability, groundwater resources, despite their limited replenishment capacity, are subject to overexploitation and increased vulnerability to maintaining quality characteristics within local water abstraction. A number of studies indicate that groundwater may be a source of contaminants in floodplains and coastal zones [1-3]. To successfully conduct and improve such assessments, a better understanding of groundwater seepage and contaminant transport processes in floodplains is needed. The rate and direction of groundwater movement depend on the density and viscosity of the fluid and directly affect the amount and transport of dissolved contaminants in the water [4, 5].

Recently, numerical models have been increasingly used to determine the extent of groundwater contamination (e.g. nitrogen) at larger scales, to study flow and transport phenomena in aquifer systems, and to evaluate groundwater recharge strategies. In this general context, the objectives of this study are (1) to model groundwater flow in the floodplain of the Ilek River, Aktobe region, to study the hydraulic response of the aquifer to contaminant inputs, and (2) to model particle tracers and simulate nitrate transport in the alluvial aquifer and its impact on the operation of the Bestamak water intake (West Kazakhstan) to predict future concentrations and mass loads of nitrate in groundwater. A conceptual model of groundwater flow and contaminant transport is presented, and a numerical simulation model is used to investigate filtration and migration processes. A modular finite-difference groundwater flow model (MODFLOW) was constructed to simulate three-dimensional regional changes in groundwater levels over time. A modular three-dimensional multi-species transport model (MODPATH) was used to simulate regional changes in the spread of the nitrate plume over time. The results of the groundwater flow and contaminant transport modeling are used to predict the management and sustainable use of the aquifer. In developing the model, several scenarios were considered to determine the optimal location, timing and regime of the intake, with an assessment of the degree of impact on groundwater quality based on the socio-economic needs of the site. This study can help improve water resources management in Western Kazakhstan, both locally and regionally, under water scarcity and climate change conditions, by identifying the optimal operating regime and assessing the degree of impact on the geo-ecological environment.

Materials and Methods

Study area

Administratively, the described territory is a part of the Alga district of Aktobe region. The major industrial centre of the district is Aktobe City; the study area is located 30 km to the south of the city. From the hydrogeological standpoint, the research object is confined to the floodplain terraces of the first and second order of the Ilek River. The area of study is characterised by a high proportion of agricultural land, a well-developed economy, and a growing rate of development (Fig. 1).

Flat terrain and predominantly sandy soils contribute to the rapid infiltration of rainfall to the water table, high water-bearing capacity and migration capacity, and vulnerability of the aquifer due to the lack of reliable overlaying from the surface.

The aquifer is unconfined, and the depth of the water table is defined from 1.6 to 7.0 m in the first floodplain terrace of the Ilek River up to 10.0-17.0 m in the second floodplain terrace. The thickness of the aquifer close to the modern Ilek valley is 12.0-18.5 m. The older «buried» valley increases to 25.0-25.5 m.

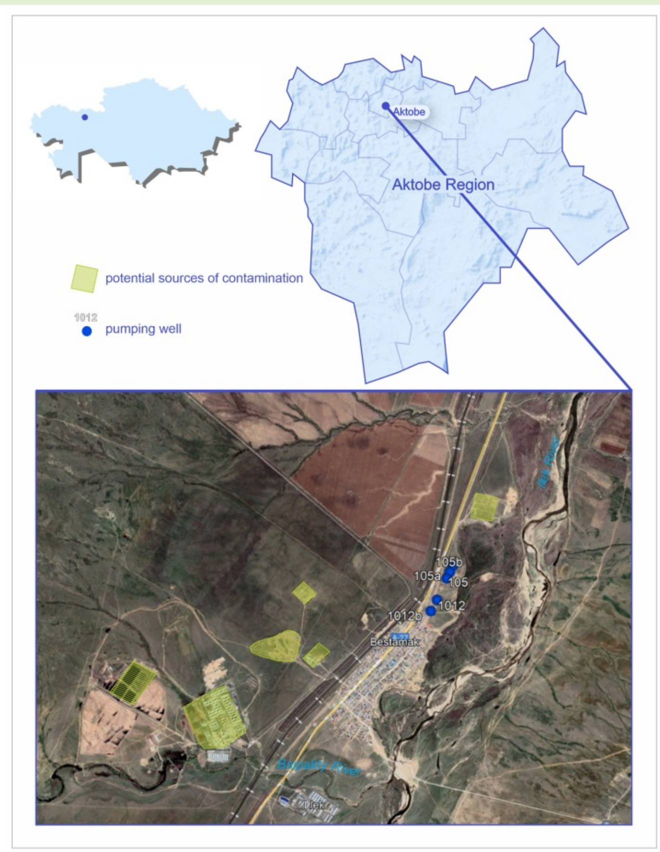


Figure 1. Study area location. Living filter, potential sources outline and well location overlaid on the satellite image.
Сурет 1. Зерттеу объектісі. Спутниктен түсірілген суретте елді мекендер, ластау көздері және ұңғымалардың орналасуы көрсетілген.
Рис. 1. Расположение объекта исследований. Населенные пункты, потенциальные источники и расположение скважин наложены на космоснимок.

The study area includes the Bestamak water intake, which consists of a production well and a reserve well for municipal water. To ensure the continued operation of the water intake, given the increase in water consumption of up to 1200 m^3/day, it is crucial to assess the potential impact of identified sources of contamination.

One such source is a filtration field of a settlement located 2.0 km southwest of the Bestamak water intake. Also identified is a field of a closed pig farm located 4.4 km southwest of the existing Bestamak water intake and a poultry farm located 3.6 km south-southeast of the existing water intake.

The analysis of previously conducted works within the study area showed that well flow rates vary from 0.01 to 9.0 L/sec with a drawdown from 4.8 to 4.43 m, respectively. Specific yield varies from 0.002 to 2.03 L/sec.

Regarding quality, the groundwater at the site is fresh, with salinity ranging from 0.3 to 0.7 g/L. The chemical composition combines sodium-calcium, sodium hydrocarbonate sulfate, or calcium-sulfate predominance. The groundwater is neutral, with total hardness between 3.1 and 6.8 mmol/L and pH between 7.1 and 8.0. Among the anions, hydrocarbonates predominate with contents ranging from 85.4 to 292.8 mg/L (0.02-44.9%) and sulfate with contents ranging from 43.6 to 411.5 mg/L (9.38-42.7%). The chloride content varies from 45.6 to 197.6 mg/L (8.7-23.6%) and increases with salinity.

The cation composition is dominated by sodium, with contents ranging from 20.2 to 219.3 mg/L (3.17-26.9%), magnesium 6-54 mg/L (0.74-8.16%), and calcium – 0.12-120 mg/L (0.014-15.2%).

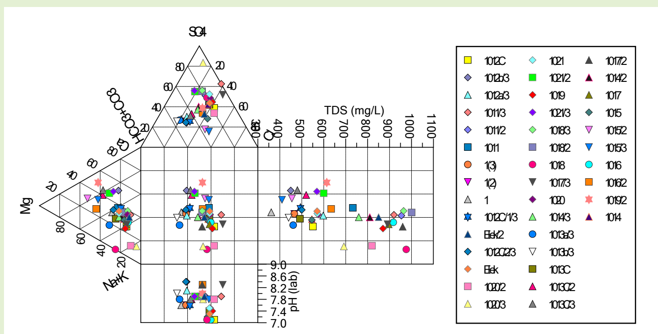


Figure 2. Groundwater quality of the research object.
Сурет 2. Зерттеу объектісіндегі жерасты суларының сапасы.
Рис. 2. Качество подземных вод объекта исследований.

The nitrate content in groundwater samples does not exceed the standard (MAC – 45 mg/L), ranging from 0.32 to 28.16 mg/L. Nitrate concentration in the storage ponds is defined as 230-480mg/L. Fluorine content in water varies between 0.14-0.18 mg/L (MAC – 1.5 mg/L). Fluorine in water is of natural origin. Boron content in the water varies within 0.1-0.148 mg/L, and does not exceed the norm (MAC – 0.5 mg/L).

Outline of the numerical modelling concept

The modeling approach was based on the combined application of different modules simulating water flow and mass transport and its turnover in soil and groundwater, assuming interconnection with surface water. The models were coupled, using results from the preceding model as input for the subsequent model.

Flow processes were simulated using MODFLOW [6], a combination of the MODPATH, a particle-tracking post-processing model by USGS [7] and the mass transport model MT3DMS [8]. MODFLOW and its associated post-processors, such as MODPATH, MT3DMS, PEST, and others, are currently the most widely used software modules for solving problems related to groundwater movement modelling [9]. This software package has been developed for over 30 years and is considered the most reliable and extensively tested. MODFLOW and its related modules are a world standard for solving groundwater dynamics and mass transport [10]. The USGS MODFLOW model was used for the groundwater flow model simulations of the alluvial floodplains in the Ilek River. The partial differential solution in MODFLOW is expressed in Equation (1):

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+ \\ +\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+W=S_s\frac{\partial h}{\partial t} \qquad (1)$$

where ***W*** is the model sources and sinks (recharge, pumping, discharge to river, discharge from streams); ***Kii*** is the hydraulic conductivity in the ***x, y,*** and ***z*** direction; ***H*** is the potentiometric head; ***T*** is the time; and ***Ss*** is the specific storage.

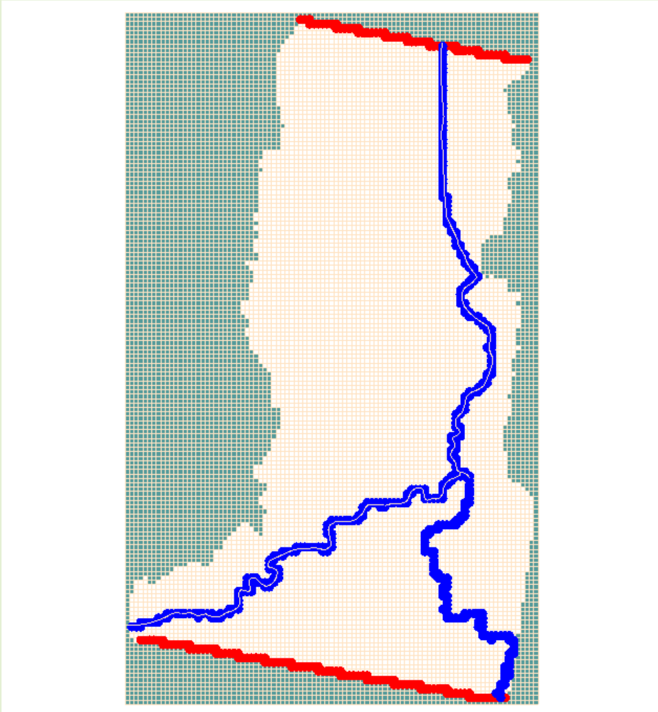
The solution to Equation (1) involves using the finite difference method to divide the entire model area into conditional blocks. In the centre of each block, an equation of this type is solved for seven unknowns, including the block's six sides and the central resultant.

The model grid was initially created with a rectangular grid of 100×100 m grid cells in the ***X*** and ***Y*** directions. For this purpose, the contour of the model area is approximated by a complex shape within a rectangle of 8552×14480 m; the sides coincide with the schematic boundaries (Fig. 3). The model area is divided into 29016 blocks (156×93 by coordinate axes).

Absolute ground surface markers were set from the space image produced by the SRTM satellite radar topographic survey with a cell size of 90×90 m high accuracy. Absolute surface elevations of the layers were set according to the data of geological and technical borehole sections according to their coordinates with further automatic interpolation using the Kriking method built into the Visual MODFLOW software package and the creation of model layers.

The dimensions of the filtration area in the plan were determined taking into account the natural boundaries of the alluvial aquifer on the sides of the Ilek River valley, as well as the technically feasible removal of the filtration area boundaries up and down the river valley from the groundwater intake of the Bestamak site. At the same time, the latter boundaries were chosen so that the area of influence of the water intake did not extend beyond them.

The western boundary was drawn along the surface outcrops of Triassic terrigenous sediments of the Kurailinsky Formation, which are represented by clays and are water-bearing. Accordingly, along the bed of the Ilek River, the boundary is set with a variable head, type III, which varies depending on the gradient

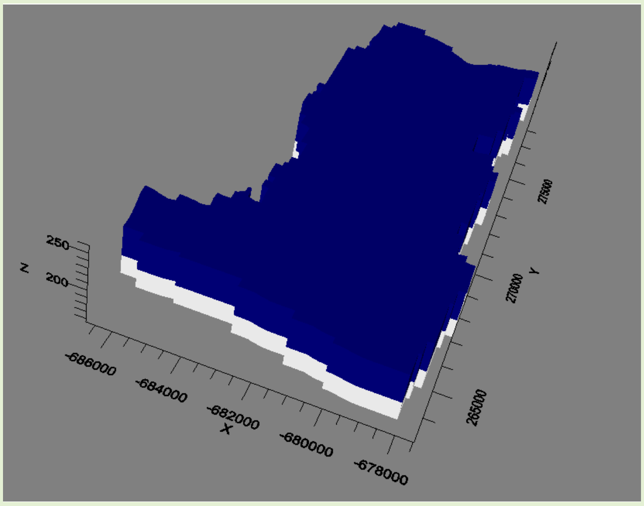


Green colour means inactive model cells, red is – the «CONSTANT HEAD» boundary, and blue is – a «RIVER» type boundary corresponding to the contours of the Ilek and Baipakty rivers.

Figure 3. Schematical map of the study area boundary conditions assignment.
Сурет 3. Схематикалық карта зерттеу аймағының шектеулі шарттарының ерекшеліктері.
Рис. 3. Схематическая карта задания граничных условий участка исследований.

of the channel from 230.0 m at the head of the river according to the water level measurements at the gauging stations to 218.0 m downstream. On the Baipakty River, a type III variable level boundary with interpolation of the level according to the results of measurements from 226.5 m at the junction with the Ilek River bed to 228.9 m at the western boundary of the model area is set. The northern boundary of the model filtration area is set along the isohypses line with the absolute level mark of 214.0 m. The southern boundary is set along the isohypses with a level mark of 230.0 m. The schematisation of the hydrogeological section was made considering the actual natural conditions of the water-bearing alluvial horizon ***(aQ_{II-IV})***. The aquifer is underlain mainly by clays of terrigenous aquitard ***(T_3kr)***. An initial filtration coefficient of 29.1 m/day was set for the productive aquifer, which was further refined during the calibration of the filtration parameters. For water-bearing sediments, the filtration coefficient is set at $k = 1\text{-}10^{-10}$ m/day (Fig. 4).

The assumed value of gravity water yield for the productive aquifer (layer 1) is ***m = 0.2,*** based on experimental pumping data. The recharge value for the upper layer of the model area is set at 250 mm/year, according to observations by RGP «Kazgidromet» [11] at Aktobe station for the minimal residual value.



The white colour represents the lower water-impermeable layer with a given filtration coefficient equal to ***k*** *=* ***1 – 10****$^{-10}$ m/day; the blue represents the productive aquifer.*

Figure 4. Hydrogeological cross-section schematisation and filtration parameter fields.
Сурет 4. Гидрогеологиялық қиманың және сүзу параметрлері өрістерінің схемасы.
Рис. 4. Схематизация гидрогеологического разреза и полей фильтрационных параметров.

Transport modelling concept

MODPATH is referred to as a particle tracking post-processor model for MODFLOW. MODPATH uses the heads and fluxes calculated by MODFLOW and derives a pathline that an imaginary packet of water will follow. The MODPATH module uses a semi-analytical particle tracking scheme that uses an analytical expression to calculate particle trajectories based on the head data in each finite-difference grid cell during the simulation. The results of solving the equation show the groundwater flow direction and magnitude in each cell.

MODPATH calculates particle pathlines by solving Eq.2 to determine their direction:

$$d = \frac{\bar{v}(\Delta t)}{n_{eff}}, \quad (2)$$

where v – represents the average filtration rate, calculated by the MODFLOW module for the centre of each block; Δt – change over time (10,000 days); n_{eff} – effective porosity (0.35 according to the data of earlier works).

Our study measures nitrate concentration in ponds rather than separating based on crop cover, as crop cover and application rates vary yearly. The objective is to focus on areas with higher concentrations. Therefore, we do not assume crop areas are a source of pollution in this case, as previous nitrate measurements have shown no excess nitrate accumulation in the soil.

The model's nitrate application rate is directly proportional to the total amount of nitrate applied to the ponds in the form of wastewater effluent. Background nitrate values were used to simulate nitrate dynamics in the aquifer, and mass loading from rainwater was considered. Simulations were conducted for 15 and 25 years to reflect concentrations in 2008 and predicted concentrations for 2048.

Results and discussion

Results for the groundwater modelling portion of our analysis compared with the previous fieldwork monitoring results. The model assumes that diffuse flow is the dominant flow regime in the overall geologic unit, although there may be areas of turbulent conduit flow within the river. Anisotropy was set to a constant 10:1 ratio between the horizontal and vertical in each geologic layer using established measures. The hydraulic heads from 5 wells [11] taken in 2008 were used for calibration. Based on modelling experience, it is assumed that normalised root mean square error (from now on RMSE) with heads should not exceed 15-30% of the calculated values. The steady-state calibration solution was repeated until the modelled and measured levels in the observation wells coincided satisfactorily, estimated at 5.94%.

The RMSE was computed for steady state and transient models using Equation (3) based on the observed well values from the fall of 2008:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(hcal_i - hm_i)^2}{n}}, \quad (3)$$

where $hcal_i$ is the calculated head at a node, hm_i is the measured head at a node, n is the number of comparison points, and i is the subscript defining comparison point between 1and n.

The adequacy of the mathematical model to the natural conditions can also be substantiated through transient model calibration. To specify the capacitive parameters of the model, Eq.1 is solved to determine the adequacy of coincidence or to obtain groundwater level reductions in the productive aquifer at the site of the operating water intake. After confirming that the mathematical model aligns with the hydrogeological conditions through steady-state calibration for 2008, the operation process of the Bestamak water intake from 2008 to 2022 was replicated. The initial state of the groundwater level was determined by conducting non-stationary calibration. Repeating the water intake operation on the developed model enables the selection of a depression funnel formation process that resembles the one observed in natural conditions. This also prepares the hydrodynamic basis of the model, which can be used for solving forecasting scenarios.

Figure 5 shows a graph of the convergence of modelled and actual measured groundwater levels for the present period, assuming the water intake operation. The evaluation was carried out on 12 control measurements, demonstrating a high convergence of values. The correlation coefficient was 0.99, and the normalised mean square error was estimated to be 6.21%.

The analysis of the steady-state and transient calibrations results shows a relatively high convergence with the natural conditions. It confirms the possibility of using the developed model for solving prediction problems and mass transfer.

The necessity to set forecast migration problems is determined by potential sources of anthropogenic pollution within the Bestamak water intake, including filtration fields, poultry farms and others.

The solution of migration is realised on the basis of a developed hydrodynamic mathematical model – the filtration mathematical model modelled particle transport of a conservative pollutant by groundwater flow. The MODPATH module of the Visual MOFLOW Flex software package was used for the solution. The software's technical capabilities enable a comprehensive forecast of the simultaneous transport of pollutant particles from all sources.

The text presents trajectories of pollutant particles' movement at different times, indicating areas with potential sources of pollution. Figure 6 displays the predicted trajectories of particles from potential sources of pollution for a forecast period of 10000 days in a section.

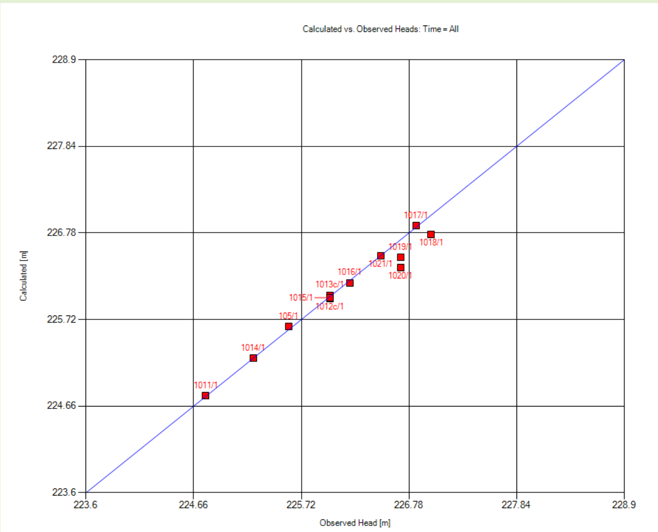


Figure 5. Graph of modelled and measured values non-stationary calibration.
Сурет 5. Стационарлық емес калибрлеу нәтижелері бойынша үлгі және өлшенетін шамалардың жинақтылық графигі.
Рис. 5. График сходимости модельных и фактических значений по результатам нестационарной калибровки.

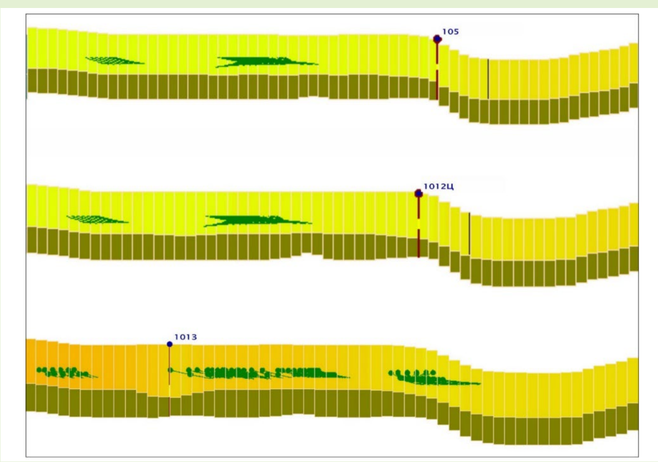


Figure 6. Particulate matter trace profiles by wells.
Сурет 6. Ұңғымалар бойынша ластаушы бөлшектердің профильдерін қадағалау.
Рис. 6. Профили трассировки загрязняющих частиц по скважинам.

The model successfully carried out predictive migration analysis. Based on the results defined at well No. 1013C, pollutants are expected to be pulled up from the filtration fields due to the stated design of water withdrawal. As a preventive measure, it is recommended that this well be excluded from the general scheme of water intake and that the load be redistributed to water intakes of other sites with the possibility of their expansion.

The model includes a degree of uncertainty due to the lack of screened elevations for each monitoring well. When a screen elevation is not assigned to a well, MODFLOW assumes that the well intersects the top of the water table. This can skew the accuracy of nitrate concentration in deep-screened wells. Although the well reflects the potentiometric head, the water from within the well may be much more profound. Nitrate is often used as a conservative tracer in groundwater due to its unhindered flow. Nitrate concentrations will likely be highest closest to the potentiometric surface, as horizontal flow transports more nitrate than vertical flow. This difference in velocity is also evident in cross-sections of the model, where nitrate concentrations decrease significantly with depth.

Conclusion

This study presents a framework for modelling the impact of treated wastewater and its large-scale use in irrigating agricultural and forested lands. The framework includes a regional groundwater flow model and an assessment of groundwater nitrate contamination in an alluvial landscape. The study utilised MODFLOW and MODPATH models to simulate groundwater flow and contaminant transport in the aquifer, which was consistent with previous models. The 12 wells within the model area had a normalised standard deviation of 0.14 m for their water level values. The RMSE for the entire model was 6.21%.

Nitrate concentrations in groundwater were highly variable across the watershed and seasons but correlated with field study. The 2023 nitrate model was compared to measured nitrate concentrations in groundwater wells. The observed and modelled nitrate concentrations in the aquifer differed due to the heterogeneity of the subsurface environment caused by the unpredictable terrain with lenses of clays present, leading to non-uniform flow and nitrate transport. Nitrate concentrations were simulated for 2048 under a specific land-use scenario involving nitrogen fertiliser application and irrigation with treated wastewater. The nitrate concentrations modelled in 2048 were similar to those in the 2023 model. This demonstrates that if the total nitrogen contribution to the aquifer remains at the wastewater threshold, the concentrations within the groundwater should closely reflect current values, assuming no significant change in the volumetric rate of effluent application.

The results of the 2048 model demonstrate the sustainability of wastewater use. This information is helpful to local governments and policymakers when formulating long-term management and sustainable development plans. Wastewater can be used to optimise agricultural management practices and reduce groundwater contamination from nitrate. The developed modelling framework can simulate nitrate concentrations' spatial and temporal variability in aquifers found in alluvial fans. These aquifers are characterised by high permeability materials and high conductivity solution conduits, making water resources vulnerable to non-point source pollution. The framework can be applied to similar aquifers with comparable characteristics.

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