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Numerical modeling of groundwater flow to delineate spring protection zones. The case of Krokos aquifer, Greece

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ABSTRACT

This study deals with protection of springs, which are fed by aquifers susceptible to contamination by anthropogenic activities. Krokos aquifer, located in Western Macedonia, Greece, whose springs provide water to Krokos town, is used as a case study. In this aquifer, concentrations of nitrates, exceeding the legislation limits, had been occasionally detected. First, some additional water quality measurements have been conducted, covering more than one calendar year, which confirmed rather high concentrations of nitrates, close, but not exceeding the World Health Organization guideline limit of 50 mg/L. Then, numerical simulation of groundwater flow in Krokos aquifer took place. Groundwater modeling system, which allows for construction of a three-dimensional flow model, has been used in this task. First, the boundaries of the aquifer and the respective boundary conditions have been defined, based on available field data. Then, the required hydraulic head and groundwater velocity values have been calculated. Based on them, the spring protection area from pollution sources has been defined, using the particle-tracking package MODPATH. Finally, sensitivity analysis has been conducted to check the influence of some uncertain data to the delineation of the spring protection zone.

Keywords: Spring protection; Hydrochemical analysis; Groundwater flow modeling; Particle tracking; Sensitivity analysis; Krokos aquifer

1. Introduction

Nitrate contamination of groundwater is a severe environmental threat in many areas of the world [1,2]. It may be due to point sources, such as sewage effluents, but it originates mainly from diffuse (non-point) sources related to diverse agricultural practices [3,4]. For this reason, it is widespread in areas of intensive agricultural activities, where the application of artificial fertilizers has severely disturbed nitrogen balance, as the input of nitrogen by far exceeds the yield [5–7]. High mobility of NO_3^- in the environment aggravates the problem.

Possible adverse health effects of high nitrate levels in drinking water that include gastric cancer,

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non-Hodgkin's lymphoma, and methemoglobinemia have been well documented [8–11]. For this reason, the World Health Organization (WHO) [9] promulgated a guideline, setting the maximum for nitrate concentration in drinking water at 50 mg/L. The US drinking water standard, or maximum contaminant level, for nitrate is 44.27 mg/L (10 mg/L as N) [12].

In this study, the aquifer of Krokos, in Western Macedonia, Greece, has been studied. Past water quality measurements in this aquifer revealed that nitrate concentrations have occasionally exceeded the respective WHO concentration limit. The study aims at proposing measures for its sustainable management, focusing on delineation of spring protection zones. Moreover, it aims at investigating the applicability of the proposed methodology.

2. The study area

The semi-confined aquifer of Krokos covers an area of about 3 km^2 and is located between the city of Kozani (capital of West Macedonia Region, Greece) and the town of Krokos, as shown in Fig. 1. The latter is located 5 km south of Kozani and is widely known for the production of Greek Saffron (Crocus). Saffron is a spice derived from the flower of Crocus, an autumn-flowering perennial plant, with vivid crimson stigmas. The dried stigmas are used mainly as a seasoning and coloring agent. Greek red saffron is one of the world's most valuable varieties. Several research studies have hinted that the spice has beneficial properties such as anticarcinogenic, antimutagenic, immunomodulating, and antioxidant [13].

Ground elevation in the study area ranges from 550 to 645 m above sea level. Rainfall is the main source of aquifer's recharge, while it discharges mainly through a number of springs, located in the outskirts of the town of Krokos. Besides their recreational, ecological and cultural value, these springs used to be the main water source for Krokos town and some surrounding villages. Today, they cover local water demands partly only, but their importance is still great.

Agricultural activities are rather intense and major crops grown in the larger area are wheat and saffron. Saffron is grown biologically, but in wheat cultivation fertilizers, insecticides and pesticides are used. The aquifer underlies mainly wheat fields and part of Krokos town, while a small part is covered by a forest (Fig. 1). Therefore, the use of fertilizers, insecticides and pesticides may affect the aquifer, which is rather shallow. Actually, during the last decade, nitrate concentrations in Krokos aquifer exceeded occasionally the recommended limits for drinking water [14].

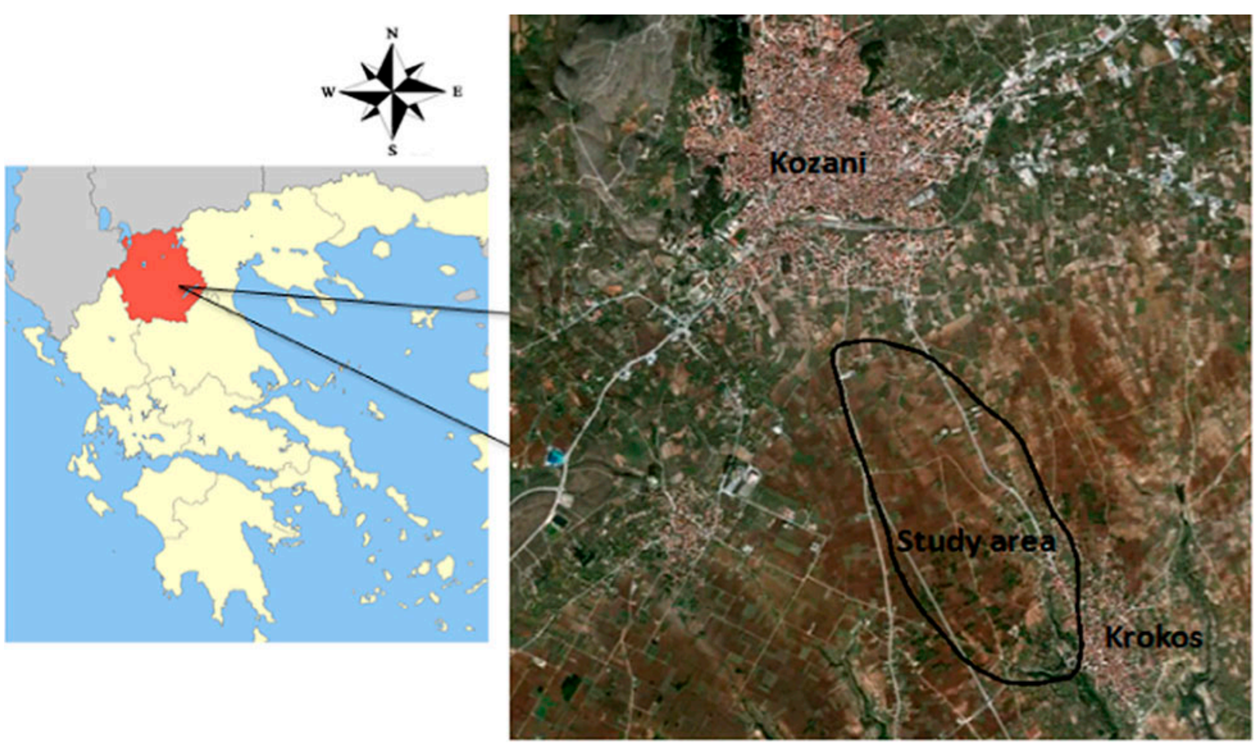

Fig. 1. Greece, West Macedonia, Kozani County, Krokos aquifer.
Source: Google, Map data: Digital Globe, Google Earth (2013).

According to local authorities, though, other sources, such as urban wastewaters and seepage of absorbent cesspools, contributed to ground water deterioration, until some years ago. Due to such water quality concerns, two wells, which have been drilled in the aquifer, are rarely used, and for irrigation purposes only. So, quantitatively, the aquifer is mildly developed.

3. Steps of the study

The study of Krokos aquifer includes the following steps: (a) literature review regarding hydrogeologic, hydrologic, and hydraulic features of the groundwater system; (b) field research on land use to determine groundwater pollution sources; (c) laboratory measurements of nitrate concentrations and other significant parameters; (d) numerical simulation of groundwater flow, using the groundwater modeling system, which supports the MODFLOW code; (e) delineation of springs' protection zone using the MODPATH package; and (f) sensitivity analysis of the results to the location of aquifer's boundaries and to the type of boundary conditions.

3.1. Sampling and chemical analysis

Protection of Krokos aquifer springs aims at providing water of good quality to the residents of the area. During the last few years, water supply authorities use to mix water from Krokos springs with water pumped from a nearby deeper aquifer. For this reason, in the framework of our study, samples from three different sites have been collected: (a) Krokos springs waters; (b) water reservoir supplied by the deeper aquifer; and (c) a typical end user outlet. Six sets of water samples have been collected during the period May 2013–November 2014. Collection of the 3 samples of each set has been always achieved in less than 30 min.

Chemical analyses were conducted at the Laboratory of Environmental Engineering and Planning, at the Civil Engineering Department of the Aristotle University of Thessaloniki, Greece. They included measurements of pH, electrical conductivity (EC), NO_3^-, and PO_4^{2-}, in order to check for pollution caused by sources related to agricultural activities. Moreover, measurements of Cr_6^+ were conducted, too, since important chromite ores and ore-processing facilities exist near the study area [15]. Chromium (Cr) is a heavy metal that naturally occurs in the Earth's crust, either in the trivalent (Cr_3^+) or hexavalent (Cr_6^+) form. The main environmental threat is posed by the presence of the highly toxic Cr_6^+ form in soil and groundwater. It occurs under oxidizing and alkaline conditions [16,17], and its geogenic or anthropogenic origin may not be easily defined [18–20].

3.2. Numerical simulation of groundwater flow and advective mass transport

Decisions regarding aquifer management and protection, and water decontamination, require knowledge of the features of the respective groundwater flows. In most cases, numerical simulation of flow and mass transport phenomena is required. In the Krokos aquifer case, the MODFLOW package [21] has been used. It produces three-dimensional, cell-centered, saturated flow models, using implicit finite-difference schemes.

First, data on the geology, the hydrogeology and the hydrology of the study area, as well as on the geometry of the aquifer boundaries, have been collected, mainly from existing studies and documents [14,22] provided by local water authorities. The aquifer consists mainly of marly chalks. Some layers of sand appear, too. Its overall behavior is that of a porous medium, due to the degree of karstification of the marly chalk. The respective hydraulic conductivity K ranges between 5 and 10 m/d, while its average width is 10 m.

To proceed with the numerical simulation, aquifer boundary and the respective boundary conditions had to be defined. Its shape is shown in Fig. 2. Based on available geological data [14,22], it has been considered as impervious, except for a small part, where a known hydraulic head value has been assigned, as required by the numerical modeling process. The locations and flow rates of the natural springs were also included in the model, while the two irrigation wells were ignored, as they are used sporadically only, in order to meet small fields' irrigation needs. For the numerical solution, a square grid was created, consisting of a single layer and including 1,132 active cells, with dimensions 66 × 38 m each. The grid's orientation was parallel to the major dimension of the flow field (Fig. 2(A)). Recharge due to rainfall (equal to 0.98 mm/d) [14] and a hydraulic conductivity value (equal to 7.5 m/d) were assigned to all active grid elements. Moreover, the aquifer has been considered as homogenous and isotropic.

Finally, the MODPATH package [23], a three-dimensional particle-tracking model, which cooperates with MODFLOW, has been used. As mentioned above, based on field research and on Corine Land Cover (a web-map of the European environmental landscape based on interpretation of satellite images),

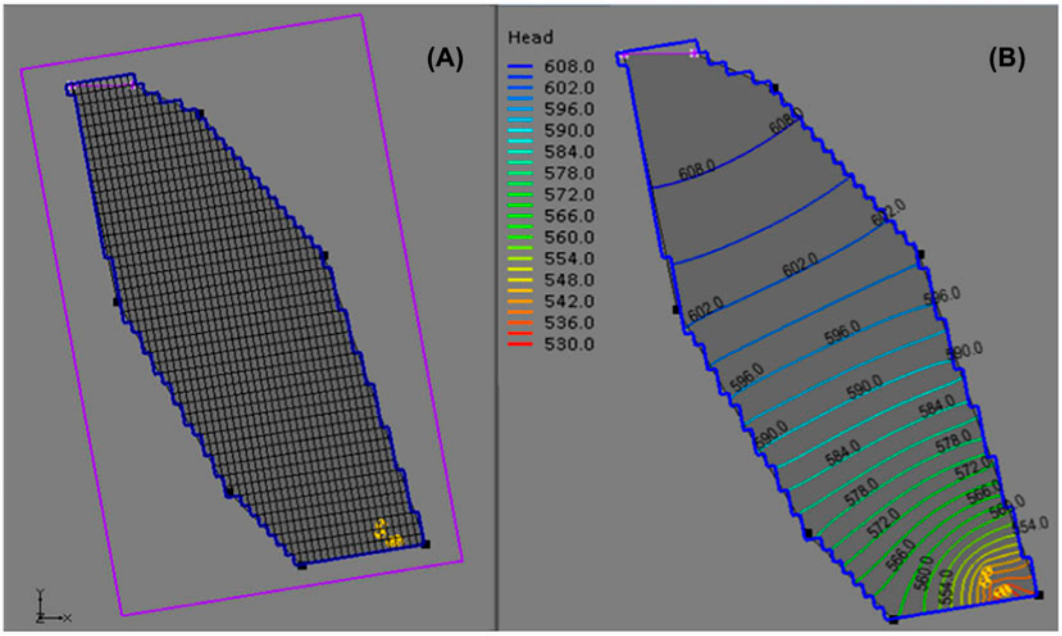

Fig. 2. Grid map (A) and the distribution of groundwater piezometric head (B).

it was concluded that only diffuse pollution sources exist in the wider study area. Then, using a methodology well known from well protection studies [24,25], the MODPATH package has been applied to determine advective transport paths in order to delineate spring protection areas. A backward in time scheme was used to track particles from the springs back to the origins of pollution, using the "travel time" criterion. It was assumed that pollutants remain active at most for one year, so a 365 d limit to backward particle tracking was set.

3.3. Sensitivity to boundary conditions

Sensitivity analysis is the study of a system response to disturbances [26] and is now recognized as an integral part of the modeling process [27]. It is particularly useful when there is uncertainty, regarding assumptions or parameter values, which have been used in the mathematical and/or the numerical model. In the simulation of Krokos aquifer, the main source of uncertainty is the length of the constant head boundary. Actually, this boundary type has been introduced for computational reasons only. In the reference case, it has been set at 336.13 m. To check its effect on the results, a substantially larger and a substantially smaller value have been used, namely 458 and 163.7 m, respectively.

Moreover, the influence of the constant head value has been checked, which has been set at 610 m in the reference case. A 10 m larger value and a 10 m lower value have been used in the sensitivity analysis.

4. Results and discussion

4.1. Summary of laboratory water analyses

As mentioned in the previous section, laboratory analyses of water samples included determination of physicochemical properties (pH, EC), major ions (NO_3^-, PO_4^{2-}), and the trace element Cr^{6+}. Nitrate concentrations in the spring water varied from 30.7 to 46 mg/L, indicating a significant nitrate contamination in Krokos aquifer that exceeds the maximum desired level and approaches the EC drinking water limit of 50 mg/L [28]. Actually, springs offer a way to assess groundwater quality, because their discharge integrates, both spatially and temporally, groundwater from large parts of an aquifer [29,30]. The pollutant mass migrates with the groundwater flow and manifests itself at springs areas. In the case of Krokos aquifer, increased nitrate content can be attributed to anthropogenic factors, most probably irrational agricultural practices, such as excessive use of chemical fertilizers, insecticides, and pesticides.

Nitrate concentrations in the water reservoir, which is being fed by a deeper aquifer, ranged from 6.5 to 8.5 mg/L and at the typical user outlet between 8.0 and 21.7 mg/L. Tables 1–3 summarize the results of the water analyses. The results of our study indicate that

Table 1
Results of laboratory analyses for NO_3^-

	NO_3^- (mg/L)		
	Spring waters	Water reservoir	Typical user outlet
28/05/2013	46	6.5	18
24/07/2013	31.2	7.1	8
16/09/2013	42	7.72	8.42
30/09/2013	34	6.52	11.34
27/08/2014	30.7	8.3	16.01
18/11/2014	38.6	8.5	21.7

Table 2
Results of laboratory analyses for Cr_6^+ and PO_4^{2-}

	Cr_6^+ (mg/L)			PO_4^{2-} (mg/L)		
	Spring waters	Water reservoir	Typical user outlet	Spring waters	Water reservoir	Typical user outlet
24/07/2013	<a	<a	<a	0.16	<a	<a
16/09/2013	<a	<a	<a	0.01	0.052	0.038
30/09/2013	<a	<a	<a	0.025	0.057	0.04
27/08/2014	<a	<a	<a	0.019	0.043	0.024
18/11/2014	<a	<a	<a	<a	0.045	0.015

a—Below the detection limit (PO_4^{2-} = 0.01, Cr_6^+ = 0.02 mg/L).

Table 3
Results of laboratory analyses for pH and EC

	pH			EC (μS/cm)		
	Spring waters	Water reservoir	Typical user outlet	Spring waters	Water reservoir	Typical user outlet
16/09/2013	7.27	8.06	7.93	860	562	562
30/09/2013	7.4	7.9	7.9	835	586	610
27/08/2014	7.2	7.7	7.55	820	550	625
18/11/2014	7.17	8.1	7.66	823	546	614

Table 4
Maximum desirable and permissible limits for potable water

	Max level	
	Desirable	Permissible
pH	6.5–9.5	–
EC (μS/cm)	400	2,500
NO_3^- (mg/L)	25	50
PO_4^{2-} (mg/L)	0.4	5
Cr_6^+ (mg/L)	–	0.05

the water supplied to the consumers meet all the quality criteria for potable water, shown in Table 4. It is worth mentioning that Cr_6^+ concentrations were below detection limits, despite the comparatively small distance of Krokos aquifer from known chromite deposits, which could result in ground water contamination.

4.2. Groundwater flow modeling

The aquifer's boundaries were efficiently simulated using the "conceptual model" option of the MODFLOW code, which is flexible regarding the shape of boundaries. The first output is the groundwater head contour map (Fig. 2(B)). Groundwater head levels tend to be higher in the northern part of the aquifer compared to its southern part, where the springs are located. Moreover, the piezometric contours are denser in the southern part, indicating higher groundwater velocities. Fig. 3(A) presents the direction of the flow velocity vector at each grid cell. It is clear that water is moving toward the springs' area.

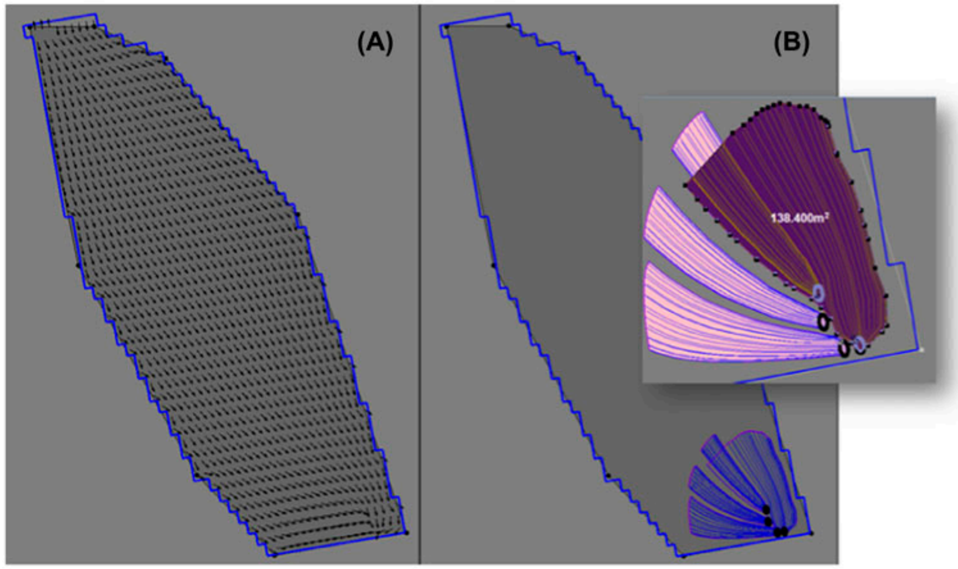

Fig. 3. Direction of groundwater flow (A) and particle path lines used to delineate spring protection zones (B).

Table 5
Flow budget of the aquifer system

	Inflow (m^3/d)	Outflow (m^3/d)	Inflow (%)	Outflow (%)
Boundaries	7.605	−0.581	0.27	0.02
Springs	0.0	−2,750.0	0.0	99.98
Recharge	2,742.98	0.0	99.72	0.0
Total source/sink	2,750.582	2,750.581	100	100

Note: The plus and minus sign indicate the inputs and outputs of the aquifer system, respectively.

Next, the MODPATH package has been applied to delineate the protection zone of each spring (Fig. 3(B)). The total area that should be protected is approximately equal to 267,692.12 m^2. This approach is a good tool for sustainable water quality management [31]. It can also provide guidelines for future planning of agricultural activities.

The flow budget (Table 5) shows a balance between water inflows and outflows, with no change in aquifer storage. This is consistent with the steady state modeling conditions. The two last columns give the different water budget terms as percentages of the total inputs or outputs. As mentioned before and as demonstrated below, groundwater inflow occurs mostly from recharge (99.72%).

4.3. Sensitivity analysis of groundwater flow model results to field boundary conditions

As mentioned in Section 3.3, the length of the constant head boundary and the respective hydraulic head value are the main sources of uncertainty. The influence of the constant hydraulic head value has been studied first. Results are shown diagrammatically in Figs. 4 and 5 for a 10 m larger and a 10 m lower value. The total area of the spring protection zones is 267,692.12 m^2 in both cases, namely identical to that of the reference case. Moreover, their shape is similar. These results were expected and indicate that the numerical simulation of the flow field is consistent.

Then, the influence of the length of the constant head boundary has been studied. Its reduction from to 163.7 m has led to the results, shown in Fig. 6(A). The total area of the spring protection zones is equal to 267,692.83 (Fig. 6(B)), namely practically identical to that of the reference case. Moreover, their shape is also similar.

Finally, the length of the constant head boundary has been increased to 458 m. Results are shown in Fig. 7. The total area of the spring protection zones is 264,034.88 m^2, again quite close to that of the reference case, and with a similar shape.

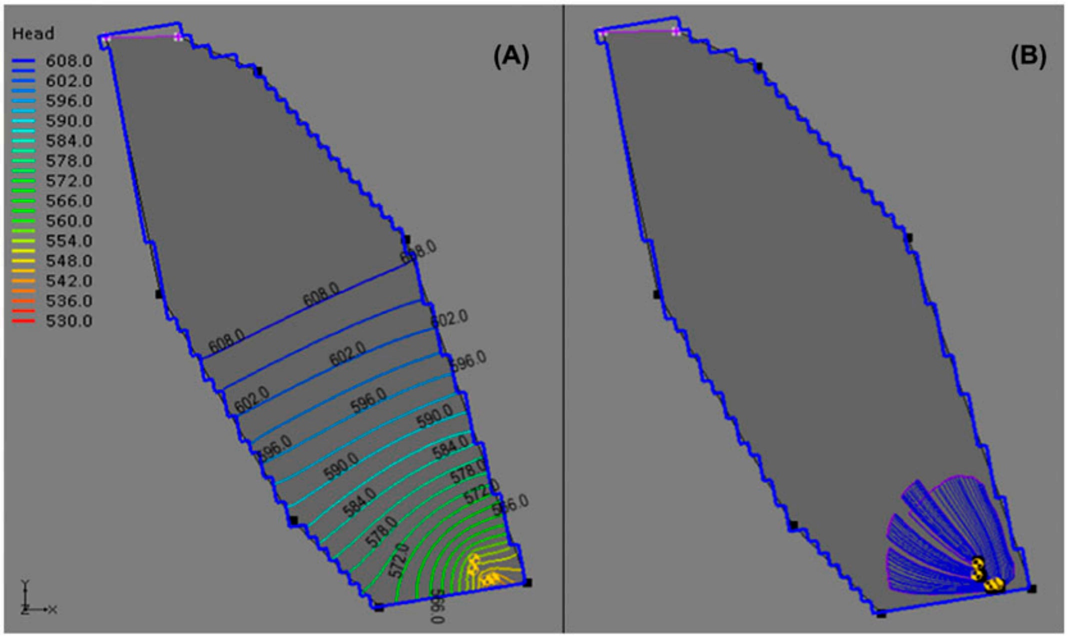

Fig. 4. Distribution of groundwater piezometric head (A) and particle path lines (B) for constant head value 10 m larger than the reference case.

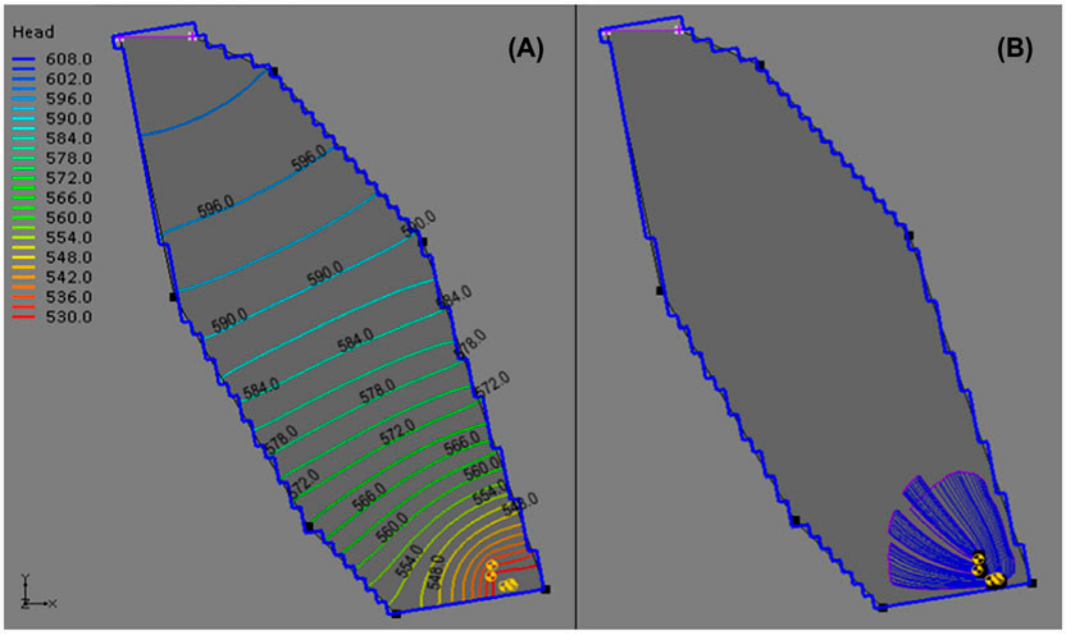

Fig. 5. Distribution of groundwater piezometric head (A) and particle path lines (B) for constant head value 10 m lower than the reference case.

The aforementioned results are due to the fact that in all three cases inflows and outflows from the constant head boundary are very close to zero and they do not interfere with the spring capture zones.

Based on this analysis, we have concluded that our results on the spring protection zones are reasonably safe.

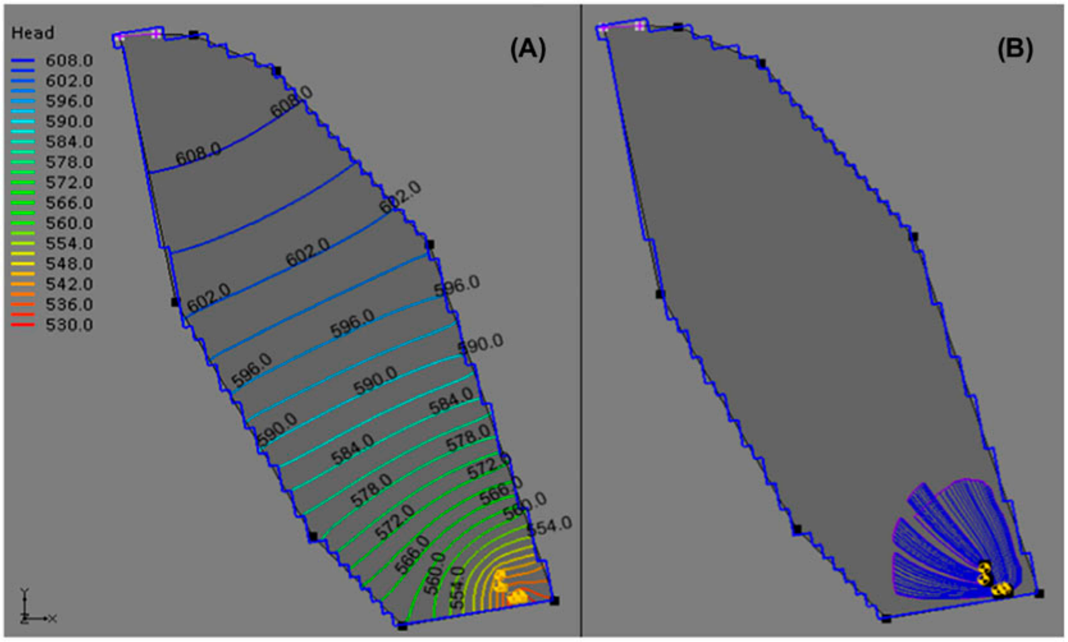

Fig. 6. Distribution of groundwater piezometric head (A) and particle path lines (B) for constant head boundary length smaller than that of the reference case.

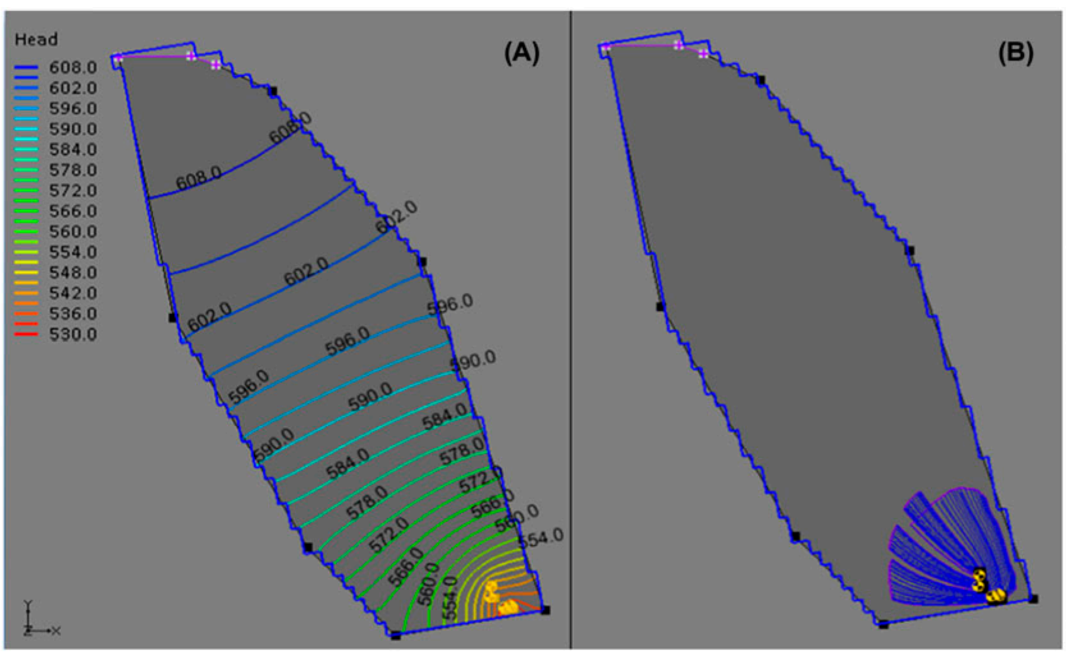

Fig. 7. Distribution of groundwater piezometric head (A) and particle path lines (B) for constant head boundary length larger than that of the reference case.

5. Conclusions

In this study, protection of springs which are fed by aquifers susceptible to contamination by anthropogenic activities has been studied. Krokos aquifer, located in an area of rather intense agricultural activity of Greece, has served as case study. Laboratory measurements revealed increased NO_3^- water content, which can be attributed to intrusion of agrochemicals. The rest of the measured parameters, namely pH, EC, PO_4^{2-}, and Cr^{6+} exhibited values well within acceptable limits. Nevertheless, careful planning of spring protection zones by means of numerical simulation of groundwater flow is necessary.

The MODFLOW package has been used as computational tool. It resulted in hydraulic head contour map and in water velocity calculations, which can be considered as reasonable. Moreover, use of the particle-tracking package MODPATH allowed for delineation of spring protection zones.

The accuracy of the numerical results depends on that of field data. Field data allowed us to consider a homogeneous, isotropic, constant width aquifer. To increase confidence on the final results, we have proceeded to sensitivity analysis of certain assumptions, regarding aquifer boundaries. It has been proved that the main outcome of our study, namely the area and the shape of the spring protection zones, is not affected by reasonable changes to the length of the constant head boundary and of the respective hydraulic head value.

Hopefully, the results obtained in the framework of this study, are useful for planning future agricultural activities. Moreover, the procedure that has been followed can serve as an example for spring protection studies.

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