MATHEMATICAL FLOW MODEL OF THE MERICHLERI THERMO-MINERAL FIELD

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ABSTRACT. A generalized conceptual scheme of the thermo-mineral field "Merichleri" is presented that is based on data from its exploitation and on the contemporary ideas for the geological and tectonic characteristics of its imbedding structures. This concept is implemented in the composed three-dimensional model of the flow field in the studied region. The modeled area covers a territory of 4.5 km² and includes the upper part of the thermo-mineral reservoir to a depth of 450 m and its periferial low water-bearing zone. Three hydrogeological units fall within these margins: a volcanogenic fault-fissure drainage complex, a volcanogenic fissure complex, and a low water-bearing fissure complex. By the developed mathematical model are estimated the water balance revenue and expenditure elements and is performed a quantitative assessment of the field water resources. The boundaries of the sanitary protection zone around the existing facility for extraction of thermo-mineral waters are deternined. The computer programs Modflow and Modpath are used for the model development.

Keywords: hydrogeological model, mineral water resources, thermo-mineral field.

МАТЕМАТИЧЕСКИ ФИЛТРАЦИОНЕН МОДЕЛ НА ТЕРМОМИНЕРАЛНО НАХОДИЩЕ "МЕРИЧЛЕРИ" Николай Стоянов¹, Стефан Зейнелов¹

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РЕЗЮМЕ. Представена е обща концептуална схема на термоминерално находище "Меричлери", базирана на данни за неговата експлоатация и на съвременните представи за геолого-тектонския строеж на вместващите го структури. Концепцията е имплементирана в съставения тримерен модел на филтрационното поле в района на находището. Моделната област обхваща горната част термоминералния резервоар до дълбочина 450 m и периферна на него слабо водоносна зона на обща площ 4,5 km². В тези граници попадат три хидрогеоложки единици: вулканогенен разломно-пукнатинен дренажен комплекс, вулканогенен пукнатинен комплекс и пукнатинен слабо водоносен комплекс. С математическия модел са определени приходните и разходните елементи на водния баланс и е направена количествена оценка на водните ресурси на находището. Определени са границите на санитарно-охранителната зона около действащото съоръжение за добив на термоминерални води. При разработването на модела са използвани компютърните програми Modflow и Modpath.

Ключови думи: хидрогеоложки модел, ресурси на минерални води, термоминерално находище

Introduction

The exceptional balneological properties of the water in the Merichleri thermo-mineral field and its close similarity to the water in Karlovi Vari, Chech Republic, have been the main reason for active exploitation and serious scientific research in this water field for the past 100-120 years. The works of various scientific researchers during this period focus on the genesis, the physical and chemical properties, the abstraction and the use of the mineral water (Azmanov, 1940; Shterev, 1964; Petrov, 1964; Petrov et al., 1970; Pencheva et al., 1998). Some unpublished archived materials (reports, statements and notes) contain detailed data from the prospecting of this field, data about the mineral water sources used in the past and information about the only existing borehole C-3x (Geshev and Denkov, 1972; Dobreva, 1997; Neykov, 2017).

The general schemes and estimates presented in referenced sources do not provide satisfactory answers to a number of important questions regarding the properties of the hydrogeological units comprising and bordering the field, the structure of the sub-surface flow, the mineral water balance and resources, the boundaries of the sanitary protection zones (SPZ) surrounding the water sources, etc. Resolving these tasks by conventional or analytical models is not always efficient. Given the high level of heterogeneity of the hydrogeological structure and the more complex boundary conditions prevailing in the Merichleri field, detailed simulation of specific hydrogeological conditions at the required level of precision would require the use of digital 3D models. The limitation of this approach, arising from insufficient volume of data, can be successfully compensated by the use of calibration procedures.

Mathematical digital 3D models have been used to re-create the complex hydrogeological situation in the Merichleri field. These models have determined the flow structure, have produced quantitative balance and resource estimations of the field, and have defined the boundaries of the SPZ around the C-3x borehole. Modflow and Modpath computer software has been applied for this purpose. (McDonald and Harbaugh, 1988; Pollack, 1994.). Scientific publications and archived materials concerning the field have been used as well (Shterev, 1964; Petrov et al., 1970; Stoyanov, 2015; Geshev and Denkov, 1972; Dobreva, 1997; Petrov, 1998; Neykov, 2017).

General information about the Merichleri field

With its genetic features, chemical components and gas content, the Merichleri thermo-mineral field belongs to the group of carbon-acidic nitrous mineral water fields. Initially, the mineral water with TDS of 6.4 g/l had been flowing from the Solentsi natural spring in the Merichlerska river flood plain. 3 km to the south-east of the village of Merichleri. The spring was capped in 1907 and had a flow-rate of approximately 1 l/s at drainage elevation of 150.8 m. Following the Chirpan big earthquake in 1928, the spring dried up, the shocks having opened new underground mineral water discharges along the Merichleri river valley and along the faults running parallel to the Maritsa river, around 20 m below the capped elevation. "Merichleri" type water had surfaced briefly in the Chernokonevo residential area of the town of Dimitrovgrad. Water of similar composition was discovered in 1937, although of lower temperature (20°C), poorer mineral composition (5.1 g/l) and reduced CO₂ content. This water was capped by a 16 m concrete shaft, using a flow-rate of around 0.2 l/s. Two 300 and 220 m long boreholes were drilled in 1958-59 near the old capping structure. The mineral water found there was 33-36°C in temperature and identical in composition to the water in the dried-up spring, and with pumping flow-rate per unit drowdown of 2-4 (I/s)/m. The water entered the boreholes at depths of 40 and 80 m through wide joints, with the water level being established at a depth of 2.5-3.0 m. In the period between 1965 and 1968, the Committee for Geology and Mineral Resources (CGMR) drilled and studied in detail the C-3x exploration borehole - so far the only source for extraction of mineral water from the Merichleri field. This 371 m long borehole runs through wide joints and several fault zones in the 40-70 m and 270-300 m intervals. The static level is established at 5.5 m and the pumping rate per unit drowdown is 5.6 (l/s)/m. TDS of the extracted water is 6.4 g/l, very close in composition to the water that disappeared after the earthquake, but with a higher temperature of 45°C. Its type is sulphate-carbonaceous, sodium, fluorine and boron. The water contains around 500 mg/l of diluted CO2, and 30% of N2 are established in the spontaneous gas. So far, the resource estimates for the field have been based on observations of mineral water rate, chemical composition and temperatures.

The conceptual model

Considering the modern geological and tectonic ideas of the region (Boyanov et al., 1993a,b) and based on the available information about the source of mineral water, the following general concept about the hydrogeological conditions in the thermo-mineral water field has been adopted (Fig. 1).

Main mineral water reservoir

It is assumed that the main reservoir was formed among the very deeply bedded Proterosoic metamorphites, Paleozoic granites and, partially, Mid-Triassic limestones of the Upper Thracian depression rock foundation (Shterev, 1964). The "Merichleri" type of water is regarded as one manifestation of a common mineral basin buried underneath at more than 1,000 m thick Tertiary complex. In chemical composition, in particular, regarding the content of sulphites and chlorides, this water does not correlate to the composition of the hosting rocks, and only the fluorine can be related to the type of the

main collector. Most likely, buried water has penetrated the Pre-Tertiary bedding of ancient Eocene and Pliocene water basins. It is assumed that the water in the ancient basins had been sodium-glauberite in composition, with a very low content of chlorides, subsequently, following geological and tectonic changes and climate alteration, undergoing substantial metamorphosis which has continued during their stay in the main collector. The presence of CO_2 is related to the Oligocene volcanic processes which have also changed the composition of micro-components.





(by the Geological map of Bulgaria M 1:100000. Map of the Chirpan area and map of the Dimitrovgrad area.)

Secondary mineral water reservoir and peripheral zone

According to the accepted assumption, two hydrogeological units can be delineated at a depth of 300-400 m in the accessed and peripheral parts of the mineral water reservoir:

 A volcanogenic fault-fissure drainage complex secondary mineral water reservoir. It is formed in subvolcanogenic Upper-Oligocene bodies latites defined as Meirchleri's latites (mrλPg₃). They are embedded and cut across the terigenic-carbonaceous sediments of the Merichleri limestone Formation (mrPg₃), the Malkotranovo terigenous Formation (mtPg₃), and, also, sediment and pyroclastic materials of the underlying Eocene-Oligocene complexes (Fig. 1). The Merichleri's latites are highly fractured and faulted, with strongly manifested traces of hydrothermal activity. The mineral water from the main reservoir flows toward the surface and circulates mainly through a complex system of sub-meridional and subparallel intersecting fault and downthrow-fault structures. These structures and the fissured volcanogenic bodies are regarded as a secondary reservoir of the Merichleri field. The deeply lying faults and downthrow faults are not only the main path along which the deeply accumulating thermomineral water flows, but are also the main factors determining the quantity and quality of the resources in the field. There are two components in the mineral water flow direction: (a) ascending thermo-mineral flow along faults from the main reservoir toward the surface, and (b) horizontal flow into the secondary reservoir mainly along the fault-downthrow fault sub-meridional structures. In general, the horizontal flow direction is S-SE toward the main regional draining structure - the Maritsa fault zone. The average hydraulic gradient is, approximately, 1.2E-04. Two hydrogeological units of lower order can be differentiated by the flow properties of the media:

- *A tectonic highly conductive zone:* This zone includes the fault-downthrow fault structures.
- *A fractured poor water-bearing zone:* This zone includes the main part of the subvolcanogenic complex outside the the tectonic structures.

The secondary reservoir is recharged by the ascending thermo-mineral flow from the main reservoir and by a lateral flow along a fault from the north. The adjoining low waterbearing complex of shallow cold water supplied from the Merichlerska river plain and from precipitation provides a very limited level of recharging. The average precipitation total - 606 mm in the Dimitrovgrad gauging station (Koleva and Peneva, 1990) and the water permeability of the surface layer lead to the assumption that the average recharge rate (W) in the tectonic highly conductive zone is around 2.0E-04 m/d, and around 1.0E-04 m/d in the fractured poor waterbearing zone. The main part of the water accumulated in the secondary reservoir leaves the field, draining underground toward the Maritsa fault zone and, partially, toward some of the neighbouring water-bearing complexes. Another smaller portion of the mineral water is abstracted from the C-3x mineral water borehole.

· A fractured poor water-bearing complex - peripheral zone. This zone includes the sediments of the Merichleri limestone Formation (mrPg₃) and the Malkotranovo terigenous Formation (mtPg₃) in the upper part of the cross section, and is assumed to comprise rocks of varying composition and genesis at depth. In an upward direction, the section includes Upper Eocene and Lower Oligocene rock complexes, attributed by stratigraphic study to the Marllimestones Formation (5Pg2³) – organogenic and sandy limestones and marls; the formation of the first mediumacidic volcanism (Pg_{2^3}) – tuffs, tuffites and latites, and the formation of the first acidic voclanism (Pg₃) - tuffs, tuffites, tuff-sandstones, sandstones, siltstones and limestones. These rocks are fractured and secondarily altered at varying degrees. As a whole, the water bearing capacity of this rock complex is very low. The water in the areas close to the surface is cold and fresh, while at depth and near the secondary reservoir, it has a higher temperature and altered chemical composition. This zone is recharged by fresh cold water from the Palaeogene karst aquifer, by water from the

Merichlerska river flood plain, by precipitation, and by water from the secondary reservoir. The lower permeability of the layer close to the surface leads to the assumption of a lower recharge rate W - approximately 5.0E-05 m/d. The peripheral zone is drained by the fault-downthrow fault structures which control the groundwater flows, to the south, toward the Palaeogene karst aquifer.

Boundary hydrogeological units

Looked at in plan, the field borders on two high-order hydrogeological units: A Palaeogene karst aquifer (on the western and southern borders) and a Palaeogene-Neogene complex of low water-bearing capacity (on the northern and eastern boundaries).

- *The Palaeogene karst aquifer.* This aquifer was formed within highly fractured and karsted carbonaceous sediments of the Marl-limestones Formation (5Pg₂³) and the formation of the first acidic voclanism (Pg₃). It marks the western and southern boundaries of the field. This aquifer is among the highest ranking and economically most important fresh-water bearing reservoirs in the Dimitrovgrad and Chirpan areas. Its average transmissivity is approximately 500 m²/d and the hydraulic conductivity most frequently is between 5 and 8 m/d. Generally, the groundwater flow direction is S-SW, and the average hydraulic gradient is 5.0E-4.
- The Palaeogene-Neogene complex of low water-bearing capacity. This complex was formed among the Oligocene-Miocene sediments of the Maritsa Formation (mPg₃-N₁). The section is represented by thick layers of clay, thin layers and lenses of sandy clays and clayey sands, coal slates and coals with a total thickness of around 350-400 m and more. Generally, the permeability of this sediment complex is very low and it acts as a virtually water-tight lateral boundary around the field on the north and east.

Composing of the 3D flow model

The 3D flow model (FM3D) is a three-dimensional simulation of the flow structure in the Merichleri field accounting for specific hydrogeological conditions and for all external impacts, including the impact of the C-3x borehole. The general ideas and input parameters used in the making up of the model are as follows:

- FM3D was developed using Modflow software in accordance with the conceptual model.
- The model area covers the exploited part of the mineral water field, with a total area of 4.5 km². A non-uniform orthogonal network was used to establish the spatial discretisation. This network is denser around the C-3x borehole where the gradients are the highest.
- FM3D includes three model layers ML-1, ML-2 and ML-3 (Fig. 2). Each model layer delineates 3 model zones which are used for a comparatively accurate determination of the spatial boundaries of the hydrogeological units identified in the field (Fig. 3). The hydraulic conductivity (k) and active porosity (n₀) values set for each model zone are presented in Table 2.
- The regional flow was modelled for an Order III boundary condition using the *General Head Boundary* (GHB) scheme for the outer boundaries of the model. The conductance along the boundaries has been calculated based on the depth and hydraulic conductivity for the zone to which the

respective model cell belongs. The boundary hydraulic head were set in the following manner: (1) The general direction of the horizontal flow is to the south-west toward the Maritsa Fault zone, with an average gradient of around 1.2E-04; (2) Some of the groundwater flow is oriented toward the large fault-downthrow fault zones in the south-eastern part of the model area.

- Recharging through infiltration was set as a constant value in all cells of the first model layer W = $4x10^{-5}$ m/d. The boundary condition *Recharge* is used for this. The flow rate values in the three model zones are as follows: MZ-1.1 W_{1.1} = 2.0E-04 m/d; MZ-1.2 W_{1.2} = 1.0E-04 m/d; MZ-1.3 W_{1.3} = 5.0E-05 m/d.
- The ascending flow from the main reservoir was set at the bottom of the ML-3 layer, within the MZ-3.3 model zone, with an Order II boundary condition following the *Specified Flow*

Table 1.

Hydrogeological units, model laye	ers and model zones
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scheme. The initially set flow value was adjusted during model calibration.

• The C-3x borehole was simulated as a three-dimensional object with the relevant coordinates and structural features (diameter, depth, position of the water intake, etc.) The model was set with a constant pumping rate of Q = 5 l/s, using an Order II boundary condition following the *Specified Flow* scheme.

The FM3D model was calibrated using the following: (1) data about the static water levels in exploration boreholes and in the C-3x borehole; (2) pumping tests data. The calibration procedure involved varying of the initial conditions and flow velocities for each model zone, and, also, the hydraulic head and transmissivity along the outer boundaries.

Hydrogeol	ogical unit	Coological unit	Lithological characteristics	Geological	Model	Model
1st rank	2nd rank			index	layer	zone
Volcanogenic fault- fissure drainage	Tectonic highly conductive zone	Mairshlari's latitas	amphibole-biotin-pyroxenes	mr)Da	ML-1	MZ-1.1 MZ-2.1 MZ-3.1
complex (secondary reservoir) Fractured poor water- bearing zone		latites	TITAF 93	ML-2 ML-3	MZ-1.2 MZ-2.2 MZ-3.2	
Fractured poor water- bearing complex (peripheral zone)	-	Meirchleri limestone Formation, Malkotranovo terrigenous Formation, Upper Eocene and Lower Oligocene rock complexes *	limestones, marls, sandstones, conglomerates, tuffs, tuffites, siltstones, tuff-sandstones	mrPg3 mtPg3 Pg2 ³ - Pg3	ML-1 ML-2 ML-3	MZ-1.3 MZ-2.3 MZ-3.3

* *Note*: Upper Eocene and Lower Oligocene rock complexes of the peripheral zone includes deep parts of the Marl-limestones Formation (5Pg₂³), formation of the first medium-acidic volcanism (Pg₂³) and formation of the first acidic volcanism (Pg₃).



Table 2. Hydraulic conductivity (k) and active porosity (n_0) of the model layers and zones

Hydrogeological unit	Model zone	k, m/d	n ₀ , -
Tectonic highly conductive zone (secondary reservoir)	MZ-1.1 MZ-2.1 MZ-3.1	3.3E00	8.0E-03
Fractured poor water-bearing zone (secondary reservoir)	MZ-1.2 MZ-2.2 MZ-3.2	7.5E-01	7.0E-03
Fractured poor water-bearing complex (peripheral zone)	MZ-1.3 MZ-2.3 MZ-3.3	4.5E-01	5.0E-03

Note: The values of k and n_0 are determined using literature data based on the type of litological kinds and a performed qualitative analysis of the character, size and filling of the fissures in the rock mass, as well as the characteristics of the products of the weathering processes and the secondary change (Spitz and Moreno, 1996; Stoyanov, 2015).



Fig. 3. Model zones and boundary conditions in model layers ML-1, ML-2 and ML-3

Table 3.	
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Boundary conditions				
Boundary	Туре	Part	Length, m	Average conductance Cav, m ² /d
North – simulate a flow coming at through faults from the Paleogene karst aquifer	GHB	GHB-L1	1310	100
West – simulate an Inflow from the Paleogene karst aquifer	GHB	GHB-L2	1965	50
South – simulate a flow draining from the field into the Paleogene karst aquifer	GHB	GHB-L3	2919	20
South-East – simulate a flow from the field draining at depth through faults	GHB	GHB-L4	1005	500
Note: In addition another external boundary condition is set: Recharge from precipitation and from the river flood plain in all cells of the model laye ML-1				

Table 4.

Water balance of the volcanogenic fault-fissure drainage complex - secondary mineral water reservoir

flow in, Q _i ⁱⁿ , L/S flow out, Q _i ^{out} , L/S				
THE THERMO-MINERAL FLOW ASCENDING FROM THE	17.25	DRAINING TO THE ADJACENT AQUIFERS AND AT	10.25	
MAIN RESERVOIR	17.25	DEPTH THROUGH FAULTS	10.25	
INFLOW FROM THE FRACTURED POOR WATER-	5.27	DRAINING TO THE FRACTURED POOR WATER-BEARING	5 20	
BEARING COMPLEX (PERIPHERAL ZONE)	5.27	COMPLEX (PERIPHERAL ZONE)	0.29	
INFLOW FROM THE ADJACENT AQUIFERS	3.85	PUMPING RATE OF THE C-3X MINERAL WATER	5.0	
Recharge from precipitation and from the river flood plain	2.18	BOREHOLE	5.0	
Total flow in:	28.55	Total flow out:	28.54	
Difference 0.04.0/				

Difference 0.04 %



Fig. 4. Flow structure in model layers ML-1, ML-2 and ML-3



Fig.5. Boundaries of SOZ around the C-3x borehole in the Merichleri thermo-mineral field

Model solution results

Flow structure

FM3D was used to produce a mathematical simulation of the flow structure. The resulting solution for the distribution of hydraulic heads in the three model layers is presented in

Figure 4. This flow structure illustrates the hydrodynamic situation of the field during uninterrupted operation of the C-3x borehole.

Water balance. Mineral water resources

Table 4 presents a summary of the FM3D generated quantitative estimates for the water-balance elements in the field. The results allow the following important conclusions about the water resources in the Merichleri field:

- The mineral water resources of the volcanogenic faultfractured draining complex, which is the secondary reservoir, are 28.55 l/s.
- Approximately 60% of the resource is formed by the ascending thermo-mineral flow from the main reservoir. Another 18% enter via the peripheral zone around the secondary reservoir. The remaining 22% are from adjacent aquifers, from precipitation and from the river flood plain.
- The regional resources of the field, assumed as equal to the thermo-mineral flow ascending from the main reservoir, are 17.25 l/s.
- Mineral water is extracted via the C-3x borehole at a constant pumping rate of 5 l/s and with an operational drawdown of 1.85 m. This mode of operation is optimal and ensures that the composition and temperature of the extracted water are preserved. The remaining resources in the field drain (disperse) at depth through various faults into adjacent aquifers and into the peripheral zone.

Models to determine the SPZ boundaries

The boundaries of sanitary protection zone (SPZ) - Subzone II and Subzone III around the C-3x mineral water borehole have been determined using Modpath software. This software created two migration models, MP3D-1 and MP3D-2, based on the FM3D generated model solution of the flow structure. The porosity n₀ values assumed for the modelled areas of both models were based on reference data (Spitz and Moreno, 1996), in accordance with the lithological features and the secondary alterations comprising the hydrogeological units (Table 2). MP3D-1 was used to determine the boundaries of Subzone II over a calculation period of 400 days, and MP3D-2 was used to determine the boundaries of Subzone III over a

calculation period of 25 years. These periods are consistent with Bulgaria's current regulatory documents. The boundaries of subzones are presented in Figure 5a and Figure 5b.

Conclusion

The elaborated 3D model has successfully determined the complex structure of the flow area and has generated a quantitative estimate of the water balance and of the resources in the Merichleri thermo-mineral field, and, also, the optimal abstraction parameters and the sanitary protection zone boundaries. The model estimations allow for a better understanding of the mineral water formation and movement mechanisms, and produce new data about the mineral water resources. The results are also of high practical importance for the efficient operation of the Merichleri field. This model is a universal facility and can be used to predict higher abstraction rates of mineral water by means of new boreholes or by increased flow-rate at the C-3x borehole, without changing the composition or temperature of the extracted water or without disturbance to the ecological balance. The research approach presented here would be useful for resolving of similar tasks of hydrogeological nature.

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