Numerical Modelling Elements as Contribution to Knowledge of the Geohydraulic Model of Sulphurous Groundwater of the Dao River Basin, In Portugal

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Abstract. The Dão River is a tributary river on the right bank of the Mondego River, which is the longest river located exclusively in Portuguese territory. The Dão River Basin, which covers an overall area of 1378 km² and forms an almost ellipsoidal shape contained within a 62 km by 22 km rectangle, is situated in the Central Iberian Zone, the lithology of which consists essentially of elements of a granitic massif dating back to the Hercynian period. The downstream area features schistous rocks (Schist-Greywacke Complex) dating back to the pre-Ordovician period, which are understood to serve as a barrier to the flows that percolate in the granitic massif. Within the Dão River hydrographic basin, the sulphurous groundwater occurs in an upstream to downstream direction, with the following names: Caldas da Cavaca, Sezures, Termas de Alcafache, Termas de Sangemil and Granjal. The sulphurous groundwaters are special because they have applications in thermalism, contributing to the area of public health and tourism, and can also be used while hot for geothermal installations, both in the environmental heating of buildings and the heating of their water supply. They may even be used in electricity production, if collected at temperatures higher than 80ºC. Thus, knowledge of the geohydraulic model of this kind of groundwater is an absolute necessity, in order to make the hydrogeological prospection and collection of this kind of resource more efficient. In an effort to gain the greatest possible knowledge of the geohydraulic model of that groundwater, various studies were carried out to that effect, including geomorphologic, geological, hydrogeological, geochemical and isotopic studies, as well as others, namely numerical models based on finite element software. Thus, in addition to showing the basic elements of some of the aspects used in gaining knowledge of the geohydraulic model of the sulphurous groundwater of the Dão River Basin, this article also presents in particular the contributions obtained from the use of finite elements.

1. Introduction

The Dão River is a tributary river on the right bank of the Mondego River, in the central region of Portugal. The Dão River Basin is almost like an ellipse, where the main axis has an almost NE-SW direction, draining an area of about 1378 km². Under the longitudinal axis of the basin (NE-SW), from upstream to downstream, the following sulphurous groundwaters exist: Caldas da Cavaca, Sezures, Termas de Alcafache, Termas de Sangemil and Granjal. With the exception of Sezures, this sulphurous groundwater arises under an almost NE-SW alignment (figure 1).
Recent studies in the Granjal area have successfully led to new groundwater abstraction of sulphurous water, consisting of a 670.6m deep hole with an allowable flow rate of 13 L/s and a temperature of 22ºC, the main results of which were presented in several scientific papers [2],[3],[4],[5],[6]. In previous studies for locating the hole in Granjal, from the outset it was conceived that the Dão River Fault System, with an overall NE-SW direction and several kilometres of extension on the surface, along almost the entire basin, favoured the percolation of groundwater from great distances [7].

In general, the occurrence of sulphurous groundwater is associated with the proximity of major faults, in addition to being attributed to extensive underground circuits. Therefore, the importance of the definition of the geohydraulic model is evident, not only for locating new abstractions of groundwater, but also for the preservation of the resource and for its correct exploitation in accordance with the fundamental principles of hydrogeology.

It is true that a geohydraulic model is even more representative, let alone the information it synthesizes, but the complexity of geological systems makes it difficult to process all elements, then the technological support tools can be used mainly in the graphical representation of the model.

The methodology of the Finite Element Subsurface Flow (Finite Element Subsurface Flow & Transport Simulation System) software, developed by DHI-WASY [8], was used to represent the conceptual model of the sulphurous groundwater of the Dão River Basin.

2. Geomorphological and geological settings
In terms of relief, in spite of the highest point of the basin under study, 1055 m, being on the western edge of the basin, it is highlighted that the main water line is born NW of the basin, with altitudes of almost 900 m, resulting in a drop of approximately 800 m up to the mouth with the Mondego River. Overall the slopes are gentle to the southwest, around 1% for the water line and about 7% for the average slopes of the basin slopes.
The drainage network consists of rectilinear water lines that adopt preferred directions of NNE-SSW, N-S, NE-SW and NW-SE, coinciding with the main tectonic structures: Régua-Verin Fault, Vilariça Fault and Dão River Fault (figure 1).

The geological framework of the study area is shown in figure 2. In the local areas of study there is outcrops of Tardi-post-D3 granitoids (biotitic granites and associated basic rocks in the downstream zone, and biotitic-muscovite granites in the upstream zone).

Possibly the Fault of the River Dão determines the direction of the flows that infiltrate the zones to the west of the Fault, and at the same time it functions as the preferential path, next to itself, of these same flows, from NE to SW, to the Santa Comba Dão and, in particular, in granitoid / shale contact areas (figure 2).

It is also worth mentioning the phylonean structures, which have a similar orientation to that of the Dão River and which promote underground circulation in that direction, especially driving which part of the water infiltrated in zones more to the West of the basin, flows into the surroundings of the Granjal.

Thus, the existence of quartz veins combined with elements of the granite massif, sometimes altered and very fractured, that in association with gentle slopes and dense vegetation cover, promote the process of infiltration and subsequent deep circulation.
3. Hydrogeological and environmental aspects

The main climatic elements for the Dão River basin are shown in figure 3; it is worth noting that in the intermediate zone of the basin (western zone) the most significant precipitations occur, being in this zone that the upper altitudes occur (the upstream slope of Serra do Caramulo), being configured as an important geostructural element in the refilling of the aquifer systems.

![Figure 3. Framing in map of the average daily air temperature and the total annual rainfall of the Dão River basin [10]](image)

For the detailed characterisation of the hydrological resources of the Dão River basin, a survey was made of water sources with perennial flow, with groundwater circulation in each village (villages, towns and cities), with 146 water points being charted (including the sulphurous groundwater). In this study, rainwater was collected in various areas of the basin (upstream, intermediate and downstream) to determine the physicochemical and radiological quality of these waters before entering the underground system.

The various sulphurous groundwater that exist along the basin are waters that percolate essentially into granite rocks and into the draining zones, correspond to semi-confined to confined aquifers, of the fissural type, with their groundwater having pH values between 8.0 and 9.5 and electrical conductivity higher than 350 μS/cm, with high physicochemical stability. Table 1 summarises the physicochemical parameters of the sulphurous groundwater under study [2].

Of the non-sulphurous groundwater of the basin, 141 water points were mapped, being careful to select those whose resource is used in standpipes with perennial flow. For each point, an expedited analysis was made using a portable measuring instrument (multiparameter meter), recording the temperature, pH, electrical conductivity (C), among other parameters.

About rainwater, considering that there is published data for the upstream zone [1], chemical and radiological analysis was carried out for the Tondela (intermediate zone) and the Granjal (downstream zone) samples.

4. Hydrogeochemistry elements

For all groundwater, in the treatment of their pH and electrical conductivity results of each basin water point, in order to know the various hydrochemical trends, contour maps of these parameters were made (figure 4), using the ArcMap software [11].

Figure 4a highlights the contribution zones of the sulphur waters, with the highest pH values, followed by some water points of groundwater circulation. On the other hand, Figure 4b shows that...
the sulphuric groundwater corresponds to singular zones, and the water of Granjal has the highest electrical conductivity (C= 634 µS/cm).

**Table 1. Physico-chemical analysis from sulphurous groundwaters water**

|                        | C. Cavaca (spring) | Sezures (spring) | T. Alcafache (*)(spring) | C. Sangemil (*)(spring) | Granjal (hole) |
|------------------------|--------------------|------------------|---------------------------|--------------------------|---------------|
| Temperature (°C)       | 29.6               | 15.7             | 50.9                      | 49.5                     | 22.7          |
| pH                     | 8.28               | 8.17             | 8.44                      | 8.11                     | 9.07          |
| Electrical Conductivity (µS/cm) | 357            | 542               | 458                       | 528                      | 634           |
| Alkalinity (mL/L)      | 27.5               | 45.0             | 30.0                      | 30.7                     | 32.7          |
| Hardness water (p.p.10⁵CaCO₃) | 1.5           | 1.4               | 1.2                       | 1.4                      | 0.60          |
| Silica (mg/L de SiO₂)  | 57.2               | 40.0             | 57.7                      | 89.8                     | 45.5          |
| Sulphuration (mL/L de I₂ 0,01N) | 4.0            | <0.25             | 2.5                       | 19.85                    | 51.8          |
| Dry residue 180°C (mg/L) | 261.0           | 381.0             | 311.0                     | 390.0                    | 429.9         |
| Total mineralization (mg/L) | 336.7           | 518.0             | 392.0                     | 475.0                    | 499.3         |
| Anions (mg/L)          |                    |                  |                           |                          |               |
| F⁻                     | 14.0               | 15.9             | 18.1                      | 16.6                     | 29.0          |
| Cl⁻                    | 20.2               | 39.1             | 35.9                      | 54.0                     | 76.0          |
| HCO₃⁻                  | 154.0              | 275.0            | 163.0                     | 179.0                    | 168.1         |
| HS⁻                    | -                  | 0                | -                         | -                        | 7.7           |
| SO₄²⁻                  | 1.9                | <1.0             | 2.7                       | 4.4                      | 9.6           |
| NO₃⁻                   | <0.12              | 0.42             | 0.27                      | 0.33                     | 0.20          |
| Cations (mg/L)         |                    |                  |                           |                          |               |
| Li⁺                    | 0.43               | 0.64             | 0.75                      | 1.5                      | 0.39          |
| Na⁺                    | 79.4               | 140.0            | 99.8                      | 116.0                    | 155.7         |
| K⁺                     | 2.7                | 2.9              | 2.7                       | 4.5                      | 2.9           |
| Mg²⁺                   | 0.09               | 0.44             | 0.15                      | 0.13                     | 0.04          |
| Ca²⁺                   | 5.9                | 4.8              | 4.3                       | 5.2                      | 2.3           |
| NH₄⁺                   | <0.10              | <0.10            | 0.32                      | 0.29                     |               |

(*) Adapted by [2].

**Figure 4.** Map of pH and electrical conductivity (C) from in situ records in groundwater of the basin under study.

The rainwater samples presented pH and conductivity values of 5.2 on a scale of 9.
For the hydrochemical profiles of the main groundwaters of the basin, the waters referenced in Table 2 were projected in the Piper Diagrams (figure 5).

**Table 2.** Basic parameters of the main waters of the Dão River basin.

| Watershed area | Rainwater     | Sulphurous groundwater | Sulphurous groundwater |
|----------------|---------------|-------------------------|------------------------|
| Upstream       | (sem dados)   | Cavaca - CVC-FR         | Cavaca: CVC            |
| Middle         | Tondela: PVHQ | -Fail-FAI               | Sezures: SGM-FR        |
|                |               | -Caramulo: CRM          |                        |
|                | Granjal: PGRQ | -Fonte da Bica: BBQ     | Granjal: GRJ           |
| Downstream     |               | -Fonte Loreto: CVQ,     |                        |
|                |               |                        |                        |

**Figure 5.** Piper classification of some of the waters of the Dão River basin.

The analysis of Figure 5 shows the similarity between sulfuric groundwater, especially in the cationic component (Ca, Mg, Na e K), while the non-sulfurous groundwater presents greater diversification in its chemical composition. For the rainwater, the cationic proximity of the non-sulfurous groundwater is highlighted, whereas in the anionic component (Cl, SO₄, CO₃ e HCO₃) the projection of the results resembles the projection of some sulfurous groundwater.

5. Elements of numerical modelling

In the first phase of the conceptual simulation, it was considered that the medium under study is of the saturated type, considering only the groundwater flow along the basin equivalent to a groundwater circulation, although the circuit in the sulphur water aquifer system in the drainage zones is of the semi-confined type. This perspective allowed us to infer the general notion about the overall lines of the model to be developed.

Prior to the simulation of the model, it was necessary to characterise the basin of the Dão River defining the limits (figure 6a), as well as to quantify the hydrostatic levels of the basin (figure 6b), storage coefficient, aquifer refill, among others. The initial hydrological conditions for optimisation of the model correspond to the extrapolation of the piezometric levels at the points under study in the
basin (all water points), applying the cubic "Akim inter/extrapolation" extrapolation method to the surrounding points [8].

After the inclusion of data in the system, the first simulation of the model in the software for the saturated medium is started, based on the flow in the basin only in transient conditions, in an unconfined aquifer, with horizontal projection for 365 days, resulting in the projection of figure 7.

**Figure 6.** Definition of the initial parameters for the Feflow simulator application: a) finite element mesh for the 2D underground flow model of the Dão River Basin; b) distribution of hydrostatic levels in the Dão River Basin, based on registered water points.

**Figure 7.** Result of the initial simulation of the underground flow of the Dão River Basin: a) general aspect of the basin, with the sources of sulphurous groundwater; b) Detailed views of the flow in the intermediate (downstream-b1) and downstream (b2)
From the analysis of figure 7 the contribution of the terrain morphology and the system of discontinuities is evident, reflected in the flow model. The direction flow is perceptible in the details of figure 7 (with the approximation of the visualisation of the simulated model-figure 7a and figure 7b).

In the initial simulation it was also intended to visualise the flow lines associated with the abstractions of sulphurous water: Cavaca, Sezures, Alcafache, Sangemil and Granjal with artesian flow, simultaneously, of 0.2 L/s, 0.04 L/s, 1.4 L/s, 0.2 L/s e 1.4 L/s, respectively. The flow lines of the sulphur waters present a tendency in the NE-SW direction (in figure 8), although for the waters of Granjal and Sangemil the flow projection also appears with a NS component, possibly resulting from the contribution of flows to from higher levels (Serra do Caramulo).

![Figure 8](image_url)

**Figure 8.** Graphical result of the flow lines for the sulphurous springs in the initial simulation

The flow of deep circulation groundwater is the result of several components, were made several simulations using the various software tools. In case the model is considered a confined aquifer, with preferably horizontal circulation, the map in figure 9a is obtained, which highlights the substantial reduction of the visualisation/projection of the flow lines. For the same situation, but preferably with vertical circulation, the simulator presents the flow lines of the abstractions of the sulphurous waters of figure 9 b.

From the various tests reproduced in Figures 8 and 9 it is possible to emphasise that regardless of the form of the circulation component (vertical, horizontal) the flow lines have a tendency in the NE direction, although, in some projections, the flow is concentric around the collection, showing that in general terms, each collection will also have a component resulting from the "local" circulation.

6. Conclusions

The numerical modelling for the groundwater of the Dão River Basin, with the objective of knowing the geohydraulic model of the 5 deep-water sulphurous systems (Cavaca, Sezures, Alcafache, Sangemil and Granjal) either in terms of the in global terms the model, either in terms of each one of the sectors or possible relations between them.

From the simulations admitting, it is especially directed so that the flows have a preferred direction from NE to SW, with the particularity of the Cavaca, Sangemil and Granjal poles, particularly in
upstream zones, having a significant component of N to S, demonstrating the refilling from zones of higher altitudes.

**Figure 9.** Graphic result of the flow lines for the sulphurous springs considering the model as a confined aquifer: a) preferably horizontal circulation; b) considering the circulation preferably vertical.

From simulations allowing confined aquifer systems, as in fact is close to reality in the proximity of the abstractions of sulphurous groundwater, the preferred directions of the flow lines are lost significantly, leading to drainage coming from several directions around the collection, especially at the poles of Alcafache and Sangemil.

Evidence relaunched by numerical methods demonstrates that Sezures water has a zone of "influence" entirely in the easternmost part of the "Dão River rift" system”.

It is also worth noting the influence of the proximity of the Serra do Caramulo in the most western zone of the Basin, as demonstrated in the various simulations, especially in the Sangemil and Granjal centres, which point to contributions in the refilling from the slopes of that mountain range.

The overall direction of the various simulations is also emphasised in the sense that there is no dependence between the various poles. If there are some refill contributions, from upstream to downstream of the overall basin (from NE to SW), as some studies on groundwater chemical aspects suggest, in these numerical models this is not perceptible.

Although the numerical modelling has contributed to the modelling of the geohydraulic system of the sulphurous waters of the Dão River, it is understood that this is a basic tool that can complement or be complemented by several other classic approaches: the application of geochemical methods, geothermal methods, as well as methods with the analysis of the isotopic component of water, among others. These studies were applied in this study, with interesting contributions to the refinement of the presented models, and are expected to be presented in other future scientific articles.
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