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Calibration of the Hydraulic Conductivities of the Missão Velha Aquifer using the Iterative Hydraulic Gradient Method

Calibração das Condutividades Hidráulicas do Aquífero Missão Velha usando o Método Iterativo do Gradiente Hidráulico

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Abstract: This paper analyzes the efficiency of the Iterative Hydraulic Gradient Method (HGIM) for calibrating numerical groundwater models through the modeling of the Missão Velha aquifer located in the northern part of the municipality of Brejo Santo-CE. The IHGM converges when the average of the φ angles and/or the RMSEH value reach a predefined minimum value. In the analysis, an RMSEH (root mean square error) of $2.1651x10^{-4}$, was obtained, which resulted in a maximum hydraulic conductivity of $1.01x10^{-5}\ m/s$ and a minimum value of $9.96x10^{-6}\ m/s$. These values are consistent with the expectations for the studied region. The paper concludes that the IHGM proves to be an efficient and reliable method for calibrating hydraulic conductivity in aquifers. Additionally, the UFC-FLOW application proved to be a robust computational tool for modeling underground flow, proving essential in decision-making related to the planning and management of water resources.

Keywords: Calibration; Hydraulic conductivities; Iterative Hydraulic Gradient Method.

Resumo: Este trabalho analisa a eficiência do Método Iterativo do Gradiente Hidráulico (MIGH) para calibração de modelos numéricos de água subterrânea a partir da modelagem do aquífero Missão Velha localizado ao norte do município de Brejo Santo-CE. O MIGH converge quando a média dos ângulos φ e/ou o valor do RMSEH atingem um valor mínimo predefinido. Na análise foi obtido RMSEH (raiz do erro quadrático médio) de $2.1651x10^{-4}$, no qual resultou a condutividade hidráulica máxima de $1.01x10^{-5}\ m/s$ e valor mínimo de $9.96x10^{-6}\ m/s$. Estes valores são consistentes com as expectativas para a região estudada. O trabalho conclui que o MIGH demonstra ser um método eficiente e confiável para calibrar a condutividade hidráulica em aquíferos. Adicionalmente, o aplicativo UFC-FLOW mostrou-se como uma ferramenta computacional robusta para a modelagem de fluxo subterrâneo, provando ser essencial na tomada de decisões relacionadas ao planejamento e gestão de recursos hídricos.

Palavras-chave: Calibração; Condutividade hidráulica; Método Iterativo do Gradiente Hidráulico.

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1. Introduction

Currently, surface water resources are increasingly unsuitable for human consumption, due to the various polluting sources that emit contaminants daily (PEIXOTO, PEREIRA; 2019). As a result, groundwater is an alternative to supply the needs of the population, especially in regions that are difficult to access, in other words, where there is no water network available (FERNANDES, et al. 2020). Furthermore, according to Lopes et al. (2023), the exploitation of groundwater has intensified, largely due to its favorable cost-benefit ratio.

In Brazil, the largest volume of groundwater is destined for public supply, around 61%, with 43% self-supplied by water from deep wells, 12% from springs or sources and 6% from shallow wells, according to the 2000 census (IBGE, 2000).

Given these considerations, it becomes evident the importance of developing methodologies focused on the analysis of groundwater flow. Among the most effective approaches, computational modeling stands out. As outlined by Fetter (2001), hydrogeological mathematical modeling is capable of representing the processes occurring in the aquifer through numerical algorithms. This technique, employing advanced mathematical formulations, serves as a valuable tool in hydrogeological studies.

Works utilizing computational modeling in hydrogeological contexts are widely applied, primarily in aquifer analysis. Engelbrecht and Chag (2015) employed computational modeling to quantify the hydrological balance and understand the dynamics of groundwater flow in the Urucuia Aquifer System (UAS), utilizing the FEFlow computational algorithm (Finite Element Subsurface Flow and Transport Simulation System). Galvão et al (2023) utilized the MODFLOW application (modular three-dimensional finite difference groundwater flow model) to execute the water balance of the Içá-Solimões aquifer, located in the Urucu-AM oil province.

To maximize the efficiency of computational models in hydrogeology, it is necessary for the modeling to describe the geological and hydrological reality, involving initial and boundary conditions that depict groundwater flow. Furthermore, the calibration process must ensure that the model not only reproduces but also reliably predicts the aquifer behavior. This situation includes adjusting variables and parameters according to empirical observations and collected data, so the model can provide accurate results. Among the calibration methods, there is the Hydraulic Gradient Iterative Method.

The Hydraulic Gradient Iterative Method (HGIM) is an implicit method that was initially developed by Guo and Zhang (2000) for the calibration of hydraulic transmissivity in underground aquifers. The method has been applied in several studies, such as Mclaughlin and Townley (1996), Guo and Zhang (2000), Schuster and Araújo (2004), and Tavares (2010). According to Schuster and Araújo (2004), one of the advantages of HGIM is its ability to transform the multidimensional optimization procedure into multiple one-dimensional procedures, resulting in a significant reduction in computational time, as well as resolving convergence issues and the improper positioning of the linear system.

In this context, the main objective of this study is to assess the effectiveness of the Hydraulic Gradient Iterative Method (HGIM) in calibrating the hydraulic conductivity of the Missão Velha Aquifer System, located north of the municipality of Brejo Santos, Ceará, using the UFC-Flow software. Additionally, based on the results, it was possible to analyze the current situation of groundwater flow in the region.

2. Study area

The study area is located north of the municipality of Brejo Santo, which is situated in the southern region of the state of Ceará, as shown in Figure 1.

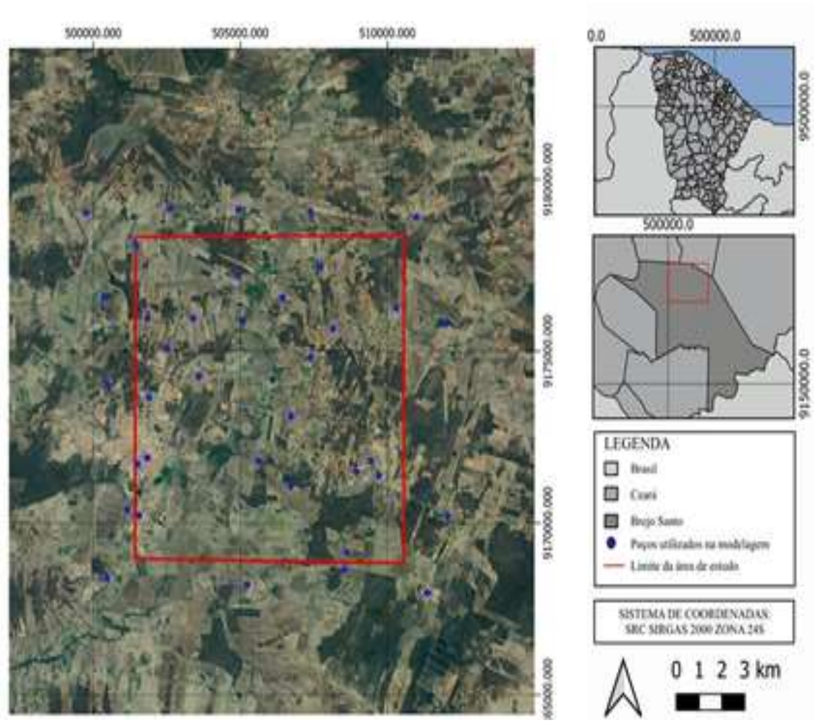

Figure 1 – Mapa de localização
Source: Authors (2023)

According to the Institute of Research and Economic Strategy of Ceará (IPECE, 2023), the municipality has a semi-arid hot tropical climate, with temperatures ranging between 24°C and 26°C. Additionally, the average annual rainfall is 895.8 mm, with the rainy season concentrated between January and April.

The Brejo Santo area is part of the Chapada do Araripe relief. Thus, the region has a maximum altitude of 1001 meters, with minimum and average altitudes of 344 meters and 515 meters, respectively. Additionally, the region is included in the Salgado basin, with the drainage network consisting of streams such as Oitis, Bálsamo, Jenipapeiro, Porcos, and Cana Brava.

Two distinct hydrogeological domains are highlighted: sedimentary rocks and alluvial deposits. It is worth noting that sedimentary rocks, according to CPRM (1998), are characterized by having primary porosity and, in sandy terms, high permeability, resulting in geological units with excellent water storage and supply conditions. This underscores the fact that 98% of the urban population is supplied with groundwater from natural sources, with a supply of 6m³/h.

Furthermore, CPRM (1998) highlights the area as part of the Missão Velha formation, where the Report on the Hydrogeological Characterization of the Sedimentary System of the Crato-Juazeiro Graben, in the Cariri Valley (CE) (SRH, 2005), indicates that the hydraulic conductivity of this formation ranges from 1.65x10-5 to 6.00x10-5 m/s.

3. Methodology

The UFC-FLOW was developed by the Computational Hydraulics Laboratory, part of the Department of Hydraulic and Environmental Engineering at the Federal University of Ceará.

The latest version of UFC-FLOW features a graphical interface that simplifies interaction with the MODFLOW (modular three-dimensional finite difference groundwater flow model) program. For the calibration process, the application utilizes the HGIM.

The Hydraulic Gradient Iterative Method, as per Guo and Zhang (1990, 1994) and Schuster and Araújo (2004), focuses on minimizing the difference between the observed hydraulic gradient (∇h_obs) and the calculated hydraulic gradient (∇h_calc). It employs a Lagrangian function (L), which integrates the governing equation, and a Lagrange multiplier (λ) to optimize the process. The expression for the Lagrangian function is given by Equation 1.

$$L = \int_R \{(\nabla h^{calc} - \nabla h^{obs}) \cdot (\nabla h^{calc} - \nabla h^{obs}) + \lambda[-\nabla(T\nabla h^{calc}) + q]\}\, dx\, dy \quad (1)$$

Where:

$\lambda = \lambda(x, y)$ is a Lagrange multiplier in space;
$-\nabla\left(T\nabla h^{calc}\right) + q$ is the governing equation.

In the case of groundwater flow, the governing equation is given by Equation 2 for unconfined aquifers considering anisotropy and two-dimensional flow, and Equation 3 for confined aquifers, anisotropic with three-dimensional flow.

$$\frac{\partial L}{\partial T_i} = -\frac{2}{T_i}\int_{r_i} \nabla h_i^{calc} \cdot \left(\nabla h_i^{calc} - \nabla h_i^{obs}\right) dxdy \qquad i = 1, 2, ..., N \quad (2)$$

Onde:

r_i is a small subdomain of the domain R;
T_i is the mean transmissivity in the subdomain r_i.
N is the total number of subdomains in R.

$$\frac{\partial F_{obj}}{\partial K_i} = -\frac{1}{2K_i}\int_{r_i}\left[\nabla\left(h_i^{calc}\right)^2 - \nabla\left(h_i^{obs}\right)^2\right] \cdot \left(\nabla h_i^{calc}\right)^2 dxdy = 0 \quad (3)$$

K_i is the hydraulic conductivity [L/T]

The numerical procedure involves expressing the equation in finite differences and performing an iterative process, starting with an initial estimate and adjusting the value of the hydrodynamic parameter at each iteration until convergence criteria are met. Parameter adjustment can be performed using the method of deep descent, originally represented in Equation 4.

$$K_i^{j+1} = K_i^j - \lambda\left(\frac{\partial F_{obj}}{\partial K_i}\right)^j \quad (4)$$

Where:
λ is the step length factor;
i is the cell index;
j is the iteration index.

In the adaptation by Schuster and Araújo (2004), Equation (4) was replaced by Equation (5) with the constraints expressed in Equation (6).

$$K_i^{j+1} = K_i^j \frac{\left|\nabla h_i^{calc^j}\right|}{\left|\nabla h_i^{obs^j}\right|} \quad (5)$$

$$K_i^{min} < K_i < K_i^{max} \quad (6)$$

During each step of the iterative process, the angle φ, which is formed between the vectors of the observed and calculated hydraulic gradient, is determined, as described in Equation (7). Simultaneously, the root mean square error (RMSEH) is also calculated, as indicated by Equation (8). The iterative cycle is completed when the average of the angles φ and/or the value of the RMSEH reach a predefined minimum value.

$$\phi_j = \text{acos}\frac{\nabla h_j^{i\,obs} \cdot \nabla h_j^{i\,calc}}{\left|\nabla h_j{}^{obs}\right|\left|\nabla h_j{}^{calc}\right|} \quad (7)$$

$$RMSEH = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(h^{obs} - h^{calc}\right)_i^2} \quad (8)$$

N is the quantity of observed points or the number of active cells.

3.1 Data acquisition

The well data to be used in the modeling were obtained from the shapefile (.shp) file obtained from the Integrated Groundwater Monitoring Network (RIMAS) for a better delineation of the study area (Figure 2) and for obtaining data through the attribute table. For pumping wells, UTM coordinates and discharge were considered; for monitoring wells, UTM coordinates, discharge, static water level, and dynamic water level were considered; finally, for auxiliary wells, UTM coordinates and dynamic water level were considered. The discharge data used in this study were obtained from pumping tests conducted in wells during the period between 1979 and 2015.

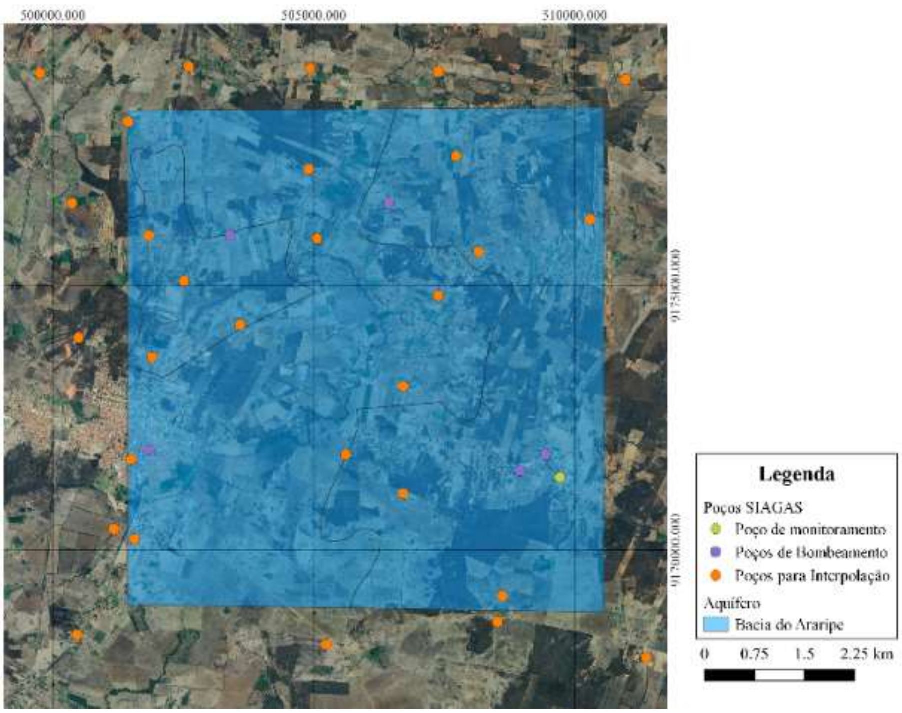

Figure 2 – QGIS
Source: Authors (2023)

Subsequently, the topographic elevations were obtained using the UFC-FLOW application. It is worth noting that the bottom elevation was generated according to Equation 9.

$$C_{f,i} = C_{t,i} - p \quad (9)$$

Where:

$C_{f,i}$ is the elevation of the bottom;
$C_{t,i}$ is the elevation of surface;
p is the depth.

3.2 Development of the conceptual model, application of boundary conditions, and initial conditions

In the UFC-FLOW application, the conceptual model was discretized into a 40x40 grid. Applying the simplification that the medium is homogeneous and isotropic, only one layer was considered, thus characterizing a three-dimensional conceptual model with 40 rows, 40 columns, and 1 layer.

For the simulation, a constant head boundary condition was considered at the edges of the grid in the study area, and an active cell condition was considered in the rest of the grid (Figure 3). It is worth noting that inactive cells were not inserted since impermeable areas or crystalline formations were not identified in the area.

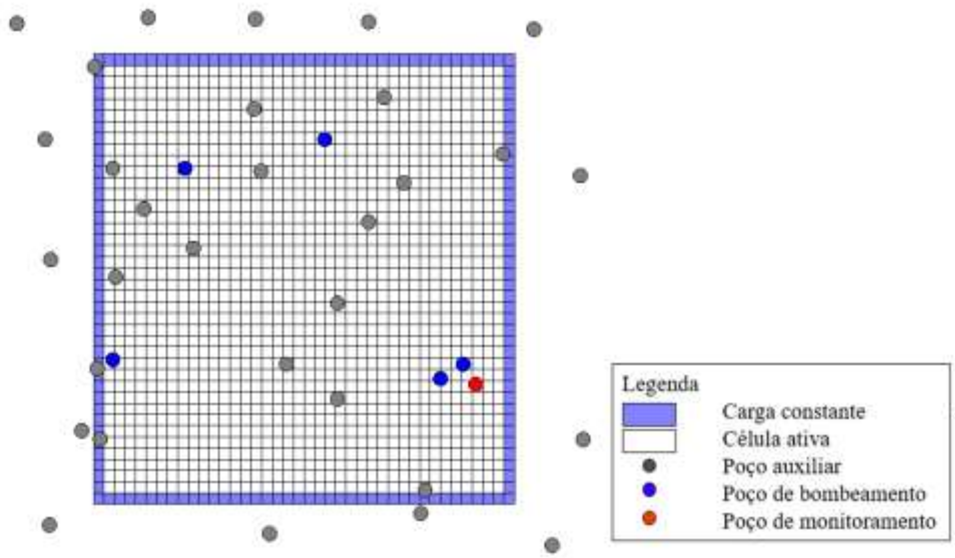

Figure 3 – Boundary conditions
Source: Authors (2023)

Also in figure 3, the inserted wells can be observed. Furthermore, the initial value of the horizontal hydraulic conductivity was based on the range reported by (SRH, 2005), with a value of $1x10^{-5} m/s adopted.$

3.3 Analysis of model accuracy

To evaluate the accuracy of the model and, consequently, the use of HGIM in the calibration process, the coefficient of determination (Equation 10) was used, analyzing the correlation between the observed head and the calculated head.

$$r = \frac{\left[\sum_i (X_{m,i} - \bar{X}_m)(X_{s,i} - \bar{X}_s)\right]}{\sqrt{\sum_i (X_{m,i} - \bar{X}_m) \sum_i (X_{s,i} - \bar{X}_s)}} \quad (10)$$

Dancey and Reidy (2005) point to a slightly different classification: r = 0.10 to 0.30 (weak); r = 0.40 to 0.60 (moderate); r = 0.70 to 1 (strong).

4. Results and discussions

After the calibration process, where the RMSEH was $2.1651x10^{-4}$, 40x40 matrices of hydraulic head and horizontal hydraulic conductivity were generated. The hydraulic head matrix allowed for the application of Equation 10. A correlation coefficient of 0.70 was obtained. This value is particularly significant because, according to Dancey and Reidy (2005), it indicates a strong positive correlation between the variables studied. This suggests that as the observed hydraulic head varies, either increasing or decreasing, the program adjusts its calculations of hydraulic head correspondingly, maintaining a high level of correlation. This strong agreement validates the accuracy and reliability of HGIM in the calibration process.

Analysis of the horizontal hydraulic conductivity matrix revealed a calculated mean of $1.00x10^{-5} m/s$. This value is significant because it provides a measure of the ease with which water can move through the aquifer substrate. In addition to the average, a maximum value of $1.01x10^{-5} m/s$ was observed, which is considerably lower than the maximum reference value established at $6.00x10^{-5}m/s$. Similarly, the minimum recorded value was $9{,}96x10^{-6}\ m/s$, which also falls below the previously defined maximum reference value of $1.65\ x10^{-5}m/s$. These results indicate that the conceptual model adopted for the study area, along with the simplifications applied, such as the consideration of an isotropic medium and steady-state regime, adequately reflects the real conditions of the Missão Velha aquifer, suggesting that the applied boundary conditions and simplifications are representative of the studied aquifer system, thus allowing for an efficient calibration of the model.

The UFC-FLOW software allows users to generate contour lines representing hydraulic head, as illustrated in Figure 4. These contour lines are continuous lines that connect points of equal hydraulic head value within a flow field, providing a clear and detailed visualization of how hydraulic head is distributed across the studied field.

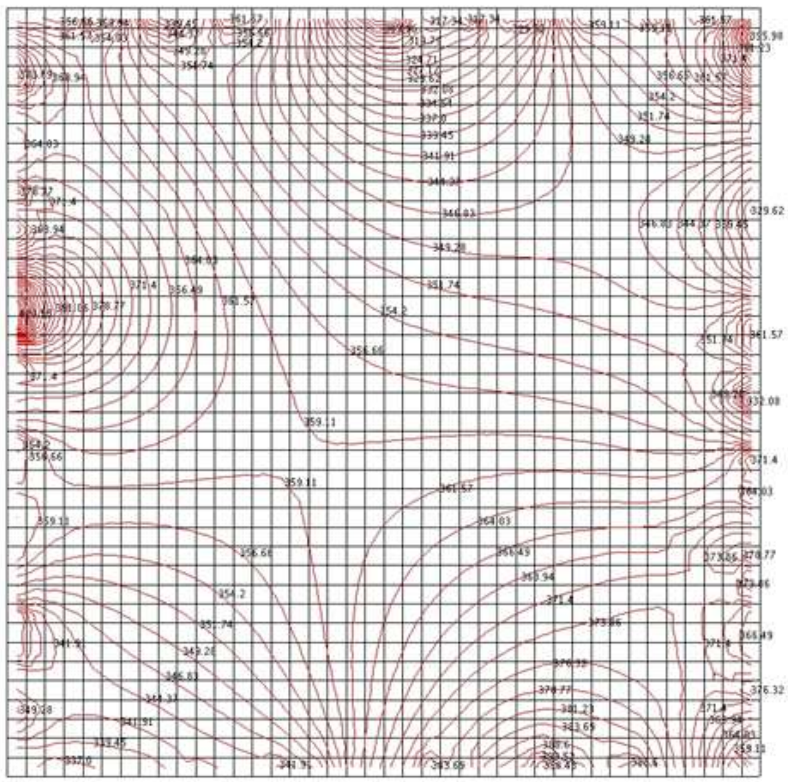

Figure 4 – Hydraulic head contour lines
Source: Authors (2023)

A detailed analysis of the hydraulic head contour lines in the studied region reveals a distinct pattern at the eastern and western edges, where the contour lines are closer together. This proximity between the contour lines suggests a steeper hydraulic gradient in these areas, implying faster groundwater movement through the subsurface. In contrast, in the central region, a different pattern is observed: the contour lines are more spaced apart, indicating a smoother hydraulic gradient. This greater spacing between the contour lines in the central part suggests that groundwater flow is slower in this area.

These observations about the velocity and direction of groundwater flow are not only based on the analysis of hydraulic head contour lines; this situation can also be observed through the flow vectors presented in Figure 5. The flow vectors, which represent the direction and magnitude of groundwater movement, provide an additional visual representation that confirms the existence of faster groundwater flow at the eastern and western edges of the studied region, and slower flow in the central area.

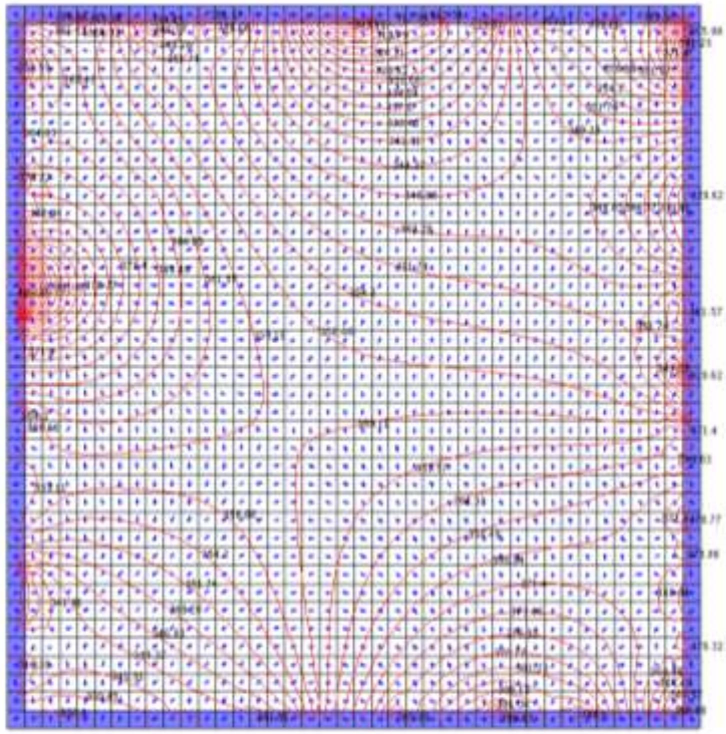

Figure 5 – Contour lines and vectors of groundwater flow
Source: Authors (2023)

5. Final considerations

The obtained results indicate that the HGIM proved to be an effective technique in the calibration of the hydraulic conductivity of aquifers, enabling reliable outcomes that can be confidently used for decision-making and water resources management. The method achieved a low RMSEH value, which evidences high precision in calibration and the suitability of the conceptual modeling in representing the physical reality of the analyzed aquifer.

Moreover, the UFC-FLOW software proved to be an efficient tool for the effective management of groundwater resources. Through the contour lines provided by the program, it is possible not only to observe the distribution of the hydraulic head but also to identify the head gradients, that is, the variations in the intensity of the hydraulic head throughout the field. Furthermore, the flow vectors offer a more complete and detailed understanding of the hydraulic behavior of the region, facilitating the identification of areas with different underground flow dynamics.

The exposed methodology provides fundamental guidance for the planning and management of water resources. With a deeper and more accurate understanding of aquifer behavior, managers can develop more effective strategies to mitigate critical problems, such as groundwater contamination and aquifer depletion, which are imminent challenges in the face of increasing demands for fresh water and climate change. Moreover, the ability to predict and model aquifer behavior accurately is indispensable for sustainable development, ensuring that the use of groundwater resources is done in a way that preserves their availability and quality for future generations. Additionally, it is highlighted the need to implement the methodology in regions that present a range of hydraulic conductivity values different from those used in this study, to evaluate the capacity of the UFC-FLOW software to deal with different levels of hydraulic conductivity.

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References

CORREA, M.R; LOULA, A.F.D; GARCIA, E.L.M. Implicit Alternating Direction Finite Difference Methods for Groundwater Modeling. *Brazilian Society of Applied and Computational Mathematics*, vol. 5, No. 1 (2004), pages 65-76.

DANCEY, Christine & REIDY, John. (2005), Statistics Without Maths for Psychology: Using SPSS for Windows. *Artmed*, Porto Alegre.

ENGELBRECHT, Bruno Zanon; CHANG, Hung Kiang. Numerical simulation of water flow in the Urucuia aquifer system in the Corrente hydrogeological basin (BA), *Groundwater* (2015) 29(2): 244-256.

FERNANDES, G. D. et al., Estimation of Natural Vulnerability to Aquifer Contamination on a Municipal Scale: Case Study in Panambi/RS *Northeast Geosciences Journal*, Caicó, vol.6, no.2, (Jul-Dec) pages 126-132, 2020.

FETTER, C.W. Applied Hydrogeology. Upper Saddle River, N.J: Prentice Hall, 2001.

GALVÃO, Paulo; DEMÉTRIO, José Geilson Alves; SOUZA, Eliene Lopes de; BAESSA, Marcus Martins. Numerical Modeling of the Içá-Solimões Aquifer System for Water Availability and Demand Purposes in the Urucu Oil Province, Amazonas, Brazil, *Groundwater*, vol. 37, no. 3, e-30216, 2023.

Geological Survey Company (CPRM). *Diagnosis of the Municipality of Brejo Santo. Fortaleza*: CPRM, 2005. Available at: https://rigeo.cprm.gov.br/jspui/bitstream/doc/15853/1/Rel_Brejo%20Santo.pdf. Accessed on: November 2, 2023. Fortaleza, 1998.

GUO, X; ZHANG, C.-M. Hydraulic gradient comparison method to estimate aquifer hydraulic parameters under steady-state conditions. *Ground Water*. vol. 38, no. 6, pages 815-826, 2000.

Institute for Economic and Strategic Research of Ceará (IPECE). *Socioeconomic Profile of the Municipality of Brejo Santo - 2017*. Fortaleza: IPECE, 2023. Available at: http://ipecedata.ipece.ce.gov.br/ipece-data-web/module/municipal-profile.xhtml. Accessed on: December 15, 2023.

LOPES, M. C.; VIEIRA, V. C.; MORGADO, L. G. M.; TAVARES, P. R. L. Qualitative characterization of groundwater in the Saco Lobo microbasin through the relative quality index (RQI). *Latin American Economic Observatory Journal*, Curitiba-PR, vol.21, no.10, pages 16079-16093. 2023.

MCLAUGHIN, D; TOWNLEY, L. R. A reassessment of the groundwater inverse problem. *Water Resources Research*. vol. 32, no. 5, pages 1131-1161, 1996.

PEIXOTO, F. S.; PEREIRA, T. C. Supply and quality of groundwater in the Municipality of Serra do Mel –RN/Brazil. *Northeast Geosciences Journal*, Vol. 5, No. 1(2019).

SCHUSTER, H. M. D.; ARAÚJO, H. D. B. An alternative formulation of the iterative hydraulic gradient method in the calibration procedure of hydrodynamic parameters of the aquifer system. *Brazilian Journal of Water Resources*, vol. 9, no. 2, pages 31-37, 2004.

Secretary of Water Resources (SRH). *Hydrogeological characterization of the sedimentary system of the Crato-Juazeiro Graben, in the Cariri valley (CE)*. Fortaleza, 2005.

TAVARES, P. R. L. *Computational modeling and calibration of horizontal hydraulic conductivity in an aquifer of the Araripe Sedimentary Basin using the iterative hydraulic gradient method*. Fortaleza: Federal University of Ceará, 2010.