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Application of Visual MODFLOW to the Analysis of Boundary Conditions for a Phreatic Porous Aquifer Using Limited Available Information: A Case Study

Aplicação do Visual MODFLOW para Análise de Condições de Contorno de um Aquífero Freático Poroso com Base em Informações Limitadas Disponíveis: Um Estudo de Caso

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Abstract

The increasing water demand, especially in developing regions, continuously puts pressure on groundwater resources both quantitatively and qualitatively. Hydrogeological modeling is a tool used in planning and management of groundwater resources. The factors that interfere in groundwater flow dynamics can be determined by developing a conceptual model and they can be validated via a numerical model. The objective of the manuscript is the hydrogeological groundwater flow modeling of the phreatic porous aquifer of the Ribeirão Candidópolis catchment in the Itabira municipality, State of Minas Gerais (Brazil). The software used in this study is GMS: MODFLOW, which enabled a steady state flow regime modeling by means of the Finite Difference Method (FDM) and the parameters calibration from a semi-transient approach. To assess the performance of the model, the Mean Error (ME), the Mean Absolute Error (MAE), and the Root Mean Square Error (RMSE) were calculated. The results proved to be compatible with the values observed in the field. After several adjustments of the boundary conditions, a Normalized Root Mean Square (NRMS) of 9.648% and a correlation coefficient of 0.993 were obtained. Despite the economic importance of the study area, studies made available on groundwater flow behavior are rare. The results obtained via modeling are in accordance with the data observed in the field and consequently our model can be used in the study of water level changes.

Keywords: Groundwater Modeling; Hydrogeology; Itabira-MG

Resumo

O aumento da demanda de água, especialmente em regiões em desenvolvimento, pressiona continuamente os recursos hídricos subterrâneos quantitativamente e qualitativamente. A modelagem hidrogeológica é uma ferramenta utilizada no planejamento e gestão dos recursos hídricos subterrâneos. Os fatores interferentes na dinâmica do fluxo podem ser conhecidos a partir do desenvolvimento de um modelo conceitual e podem ser validados através do modelo numérico. O objetivo do manuscrito é contruir um modelo hidrogeológico de fluxo de água subterrânea para o aquífero poroso freático da bacia do Ribeirão Candidópolis em Itabira, Minas Gerais. A ferramenta utilizada foi o GMS: MODFLOW, software que permitiu uma modelagem do fluxo em regime estacionário através do Método das Diferenças Finitas (MDF) e a calibração dos parâmetros a partir de uma abordagem semitransiente. Para avaliação de desempenho do modelo, o erro médio (Mean Error - ME), o erro absoluto médio (Mean Absolute Error - MAE) e o erro médio da raiz quadrada (Root Mean Square Error - RMSE) foram calculados e os resultados se mostraram compatíveis com os valores observados em campo. Após diversos ajustes das condições de contorno, finalizando com um NRMS de 9,648% e coeficiente de correlação de 0.993. Constatou-se que apesar da importância econômica da região, raros são os estudos sobre águas subterrâneas desenvolvidos e disponibilizados. Os resultados do modelo estão de acordo com os dados observados e, portanto, o modelo pode ser usado para estudar as mudanças do nível de água no aquífero.

Palavras-chave: Modelagem de Água Subterrânea; Hidrogeologia; Itabira-MG

1 Introduction

According to the World Water Assessment Programme report (United Nations Educational Scientific and Cultural Organization 2015), the fresh water demand has been rising and unless the equilibrium between demand and offer is reestablished, the world will face a severe water deficit. Therefore, the possibility of development promoted by such resource contrasts with the challenges

In Earth Sciences, modeling is widely applied to solve problems of groundwater flow, to conceptualize and understand the hydrogeological system behavior, and to predict the consequences of changes in such systems Gonçalves et al. (2005).

The conceptualization of a hydrogeological model offers a general, systematic and consistent view of the system limits and relevant properties and processes occurring in the medium, filling the gaps generated in hydrogeological characterization and groundwater modeling Enemark et al. (2018).

The study area, the geological substrates and the flow regime are the variables that rule a hydrogeological model. The representation of these variables is made conceptually. Before the prediction and the quantification of the physical phenomena, it is necessary to establish a representative model based on the most important information in order to solve hydrogeological problems as demonstrated by several authors such as (McDonald & Harbaugh 1988; White 2003; Galvão 2015; Sobeih et al. 2017; Aghlmand & Abbasi 2019)

Groundwater flow models are guidelines to planning and managing water resources in several regions in Brazil. At present, numerical modeling is considered an important tool for the study of groundwater resources (Santos & Koide 2016). In general a simplified mathematical representation of a groundwater flow system is resolved by a computer program (He et al. 2012). A range of information, such as geological, hydrogeological, hydrological, climatological, and geographical, is required in modeling (Santos & Koide 2016).

The Itabira municipality is inserted in the Peixe River subcatchment that is part of the Piracicaba River basin. Itabira is one of the major Brazilian mining Minas Gerais state that is constantly growing and is consequently dependent on natural resources. Therefore, for a better management and to comply with the present and future demands of water, a proper assessment of the available surface and underground water reserves is necessary. The urban expansion in Itabira affects directly the Ribeirão Candidópolis catchment: its water courses supply 55% of the municipality. This justifies the significance of an adequate management to secure the water availability to the Itabira municipality.

We selected MODFLOW for this study due to its simple methods, modular structure, and separation of packages to solve special hydrogeological problems, MODFLOW has a good response to the simulation and prediction of groundwater flow conditions and interactions between underground and surface waters (Oliveira et al. 2015; GMS 2018).

Searching for an adequate model to project future scenarios of sensible exploitation of groundwater resources in Itabira, this study was designed as a pilot project that aimed at the representation of the groundwater flow behavior in free aquifers of small hydrographic basins. However, small hydrographic basins are devoid of a satisfactory number of data to the construction of a complete conceptual model and a subsequent numerical model. Thus, using limited information, the objective of this study was the construction of a conceptual hydrogeological model for the Ribeirão Candidópolis Basin free aquifer, which is a strategic groundwater source for the Itabira municipality.

2 Methodology and Data

The study area is inserted in the Peixe River basin and stretches out for 33.91 km², representing around 8% of the total area of the Peixe River hydrographic basin. The basin is located in the central portion of the State of Minas Gerais and encompasses the Itabira - Figure 1.

Predominantly trending SW-NE, the water courses of the Ribeirão Candidópolis Basin run ca. 11.17 km until they reach the confluence with the Peixe River. The main water courses of the Ribeirão Candidópolis Basin are: Candidópolis, Contendas, Barreiro, Meio and Vista Alegre.

2.1 Geology Geological Setting

The Ribeirão Candidópolis hydrographic basin is inserted in Archean and Proterozoic units, Jordt-Evangelista et al. (2016) - Figure 2, represented by the Borrachudos Suite, the Guanhães Complex, the Gneissic Amphibolitic Sequence, and the Nova Lima Group. The Borrachudos Suite is composed of Paleoproterozoic intrusive meta-granites and meta-syenogranites (Jordt-Evangelista et al. 2016). The Guanhães Complex encompasses a diversity of rock types, such as tonalitic-trondhjemitic-granodioritic to granitic orthogneisses, amphibolitic gneisses and schists, amphibolites, metapelitic schists, banded gneisses, mafic and ultramafic schists, metagraywackes, amphibolites, and quartzites Jordt-Evangelista et al. (2016). In the northwestern region of the Ribeirão Candidópolis Basin, the Archean Gneissic Amphibolitic Sequence occurs underlying the Guanhães Complex and is represented by an almost rhythmic alternation of granitic gneisses and amphibolites were exhaustively studied in works including Lana et al. (2013).

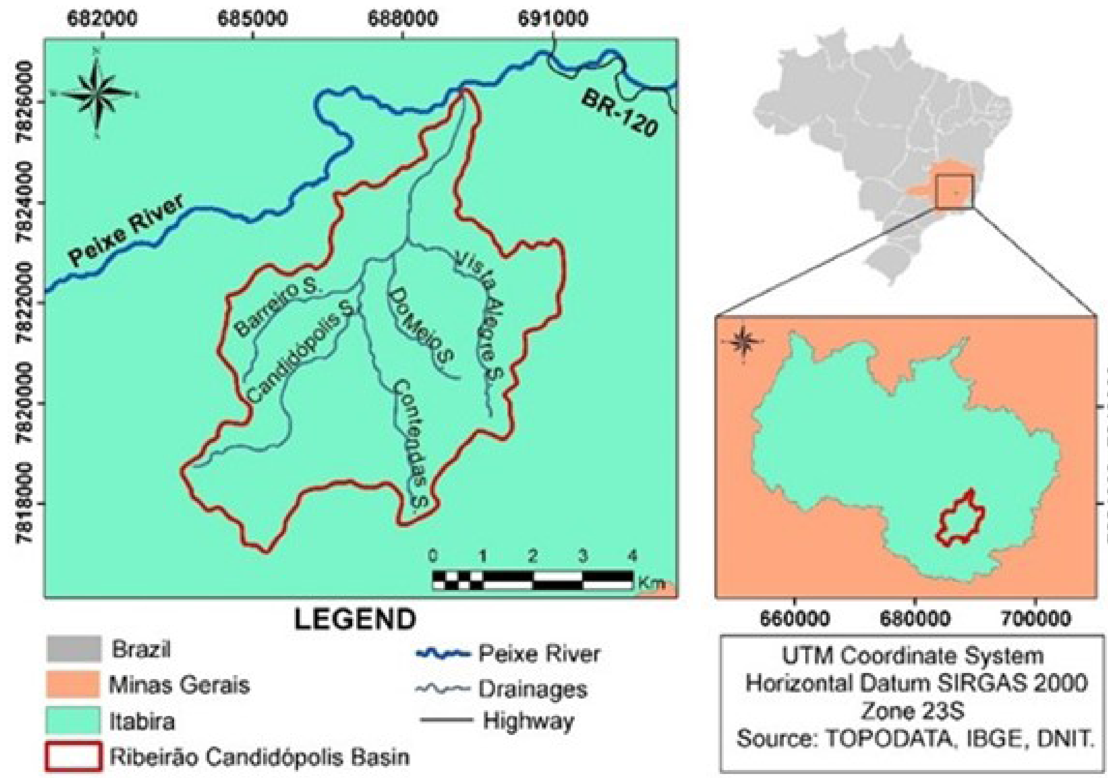

Figure 1 Study area location.

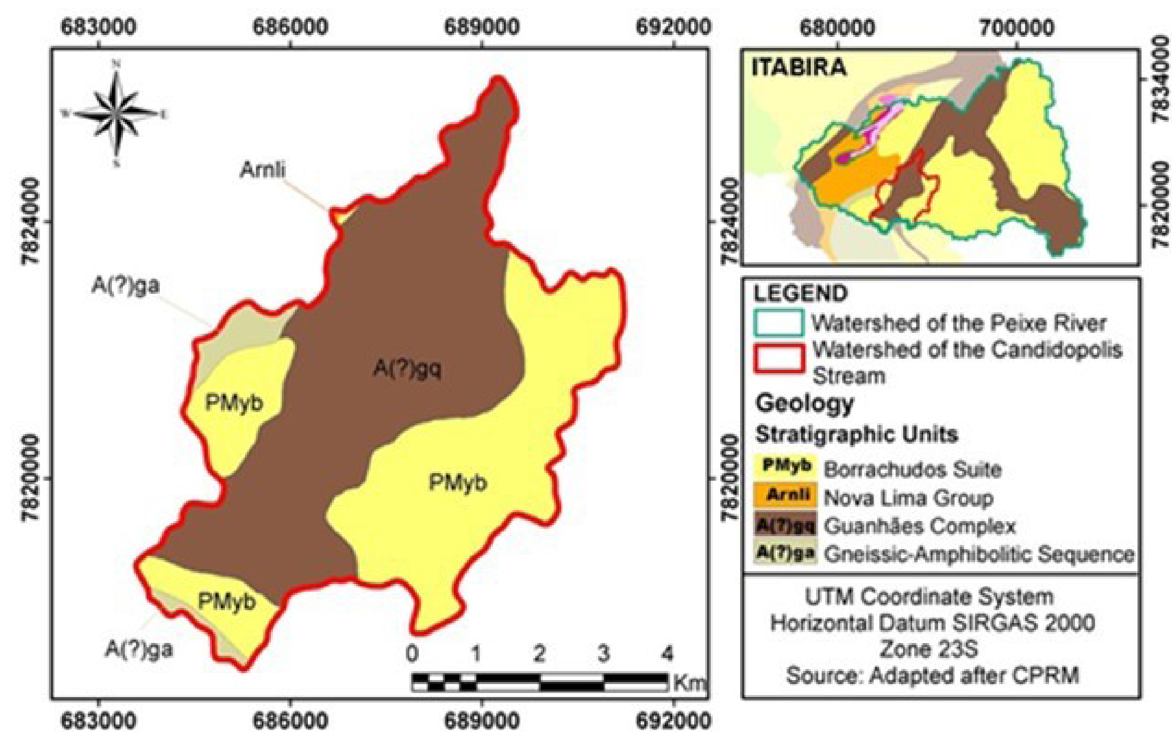

Figure 2 Geological map of the Ribeirão Candidópolis Basin (Modified after Companhia de Pesquisa de Recursos Minerais 2000).

The Nova Lima Group is located in a small area northwest of the basin, and is constituted by schists and phyllites of metasedimentary or metavolcanic origin, among which ferruginous quartzites, iron formations, amphibolites, dolomites, metachert, meta-ultrabasic rocks and rare conglomerates occur.

Table 1 presents the stratigraphic column of the Ribeirão Candidópolis Basin and the respective aquifer systems.

2.2 Hydrogeology

The definition of the hydrogeological units was based on the characteristics of the litho-structural units identified in the study area and on the behavior of the water conducing medium. The hydrogeological units can be characterized as aquifers, aquitards or aquicludes. Two aquifer systems were identified by Gonçalves et al. (2019) in the Peixe River basin: the Nova Lima Aquifer System and the Gneissic-Granitic Aquifer System.

The Nova Lima Aquifer System is composed of schistose rocks that make up the schist aquitard, and the ferruginous quartzitic rocks that make up the iron formation aquifers. These aquifers comprehend fresh schistose rock and interstices of weathered schists. The former is considered a fractured, discontinuous, anisotropic, heterogeneous, usually free, and sometimes confined system. This type of aquifer has reduced groundwater storage and circulation capacity. The latter corresponds to the weathering mantle overlying schistose and pelitic rocks, and is in general characterized by its low permeability and porosity. Natural outlets are isolated or diffuse springs, in swaps along the valleys Gonçalves et al. (2019).

The Borrachudos Suite, the Guanhães Complex and the Gneissic Amphibolitic Sequence constitute the Gneissic-Granitic Aquifer System, which is characterized by fractured aquifer zones throughout its extension. This system is composed of granites, gneisses, migmatites, granitoids, and intrusive basic and metabasic rocks Gonçalves et al. (2019). It occupies 99% of the study area and is discontinuous, anisotropic, heterogeneous, fractured, and free to semi-confined by the weathered rock. It presents double porosity, with groundwater circulation and storage in discontinuities caused by rock fracturing (fracture porosity) and in the interstices of the weathering mantle (interstitial porosity). In this aquifer system the fracture porosity yields higher permeability, and the interstitial porosity higher groundwater storage capacity. Due to the local rainfall indices and the presence of a thick regolith, underground recharge is potentialized. In an adjacent hydrographic basin, the transmissivity values obtained from 11 wells drilled in this aquifer system varied from 0.10 to 12.00 m^2/day, with a mean value of 3.99 m^2/day and median value of 2.20 m^2/day; the conductivity values varied from 0.01 to 0.04 m/day, with a mean value of 0.02 m/day Gonçalves et al. (2019).

The Gneissic-Granitic Aquifer System is composed of a porous zone in the weathering mantle and a fractured medium. This characteristic causes groundwater to flow through preferential paths, making the understanding of the flow behavior difficult.

To determine the flow behavior, the water level elevations at the springs were used. Thus, our model reproduces the static flow condition of the study area, thus avoiding the interference of pumping wells that may have been allocated but not identified in the study area.

The terrain topography was used as a guide to the water flow direction in sites lacking of information. Table 2 presents the characteristics of the points used to generate the potentiometric map.

Table 1 Stratigraphic column of the study area.

Lithostratigraphic unit	Lithology	Aquifer systems
Borrachudos Suite	Meta-granites, Meta-syenogranites	Gneissic-Granitic Aquifer System
Undivided Nova Lima Group	Schists, Phyllites	Nova Lima Aquifer System
Guanhães Complex	Banded gneisses, Amphibolites, Schists, Quartzites	Gneissic-Granitic Aquifer System
	Granitic gneisses, Amphibolites	Gneissic-Granitic Aquifer System

Table 2 Characteristics of the springs of the Ribeirão Candidópolis Basin.

Main water courses	Spring altitude (m)	Length (Km)	Drainage area (km²)	Lithology
Córrego do Meio	788	3.19	3.00	Borrachudos Suite
Córrego do Barreiro	826	3.47	3.94	Borrachudos Suite
Córrego Vista Alegre	860	4.86	6.67	Borrachudos Suite
Ribeirão Candidópolis	872	5.6	7.71	Borrachudos Suite
Córrego Contendas	945	4.39	7.18	Borrachudos Suite

The natural aquifer recharge is predominantly pluvial and takes place throughout the terrain surface, representing the effective rainfall contribution that infiltrates to the subsurface Ayvaz & Elçi (2014). From rainfall data the recharge rate was calculated for hydrogeological units of the study area. In terms of discharge, the springs of the main water courses were considered.

Figure 3 shows the potentiometric map constructed manually and that was vectorized by means of the ArcGIS software, according to topographic criteria and the elevation of the water level. Figure 4 shows the 3D geometric configuration of the water flow in the study area.

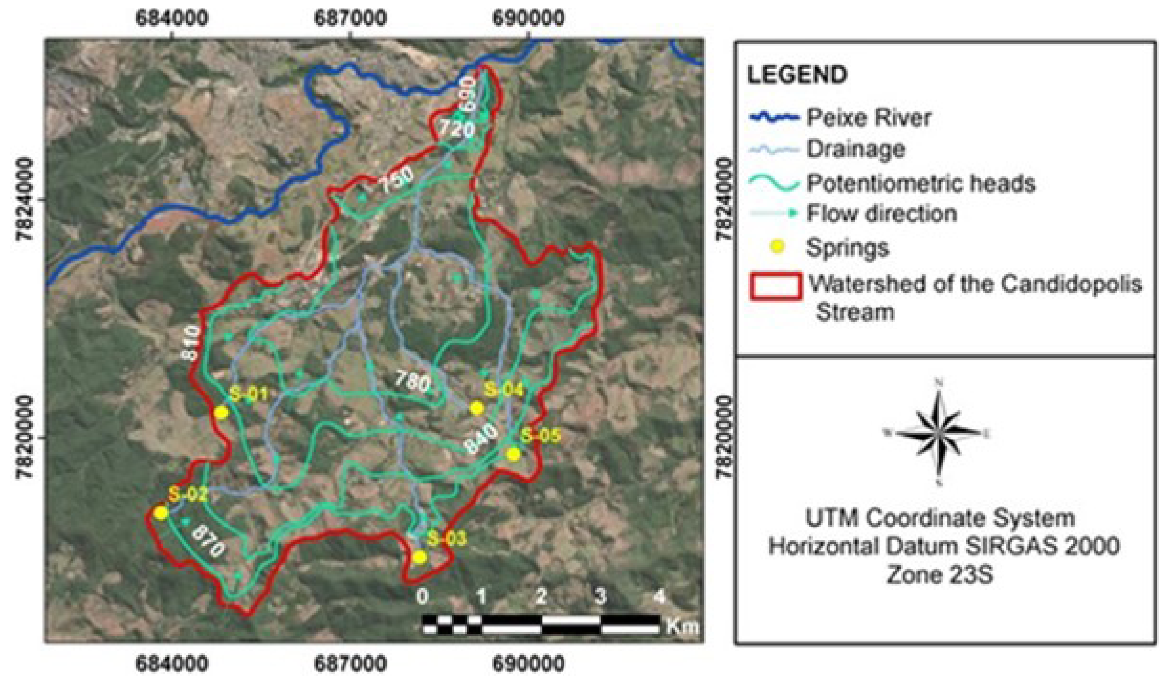

Figure 3 Potentiometric map (Modified after Google Earth 2020).

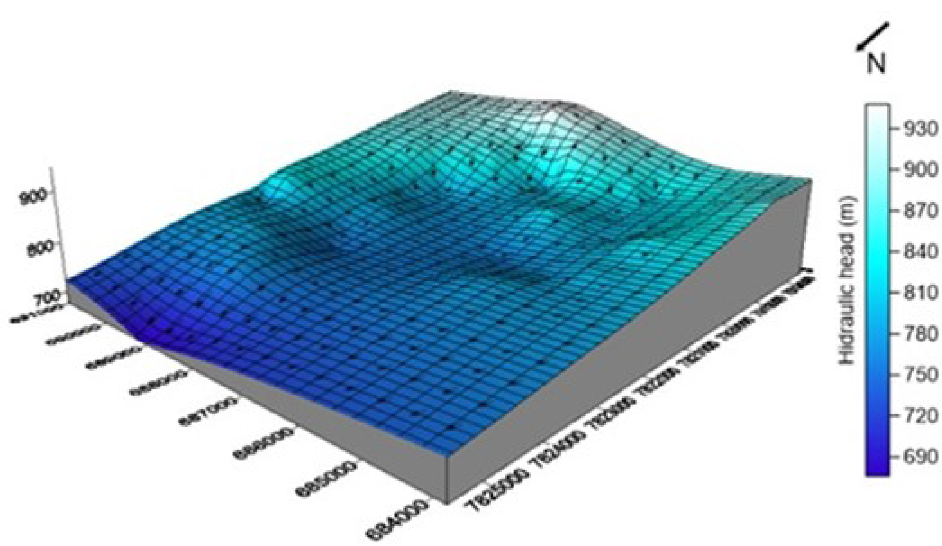

Figure 4 3D geometric configuration of the water flow in the study area.

2.3 The Conceptual Hydrogeological Model

The first and most important step in modeling is the structure of the groundwater flow system conceptual model, which represents a simplified version of the real aquifer system, presented by Guiguer & Franz (1996). Due to the complexity of the hydrogeological system and insufficient data, the conceptual model and its structure were applied in function of the available data - Figure 5. To establish a conceptual groundwater model for the study area, many challenges exist, including: a) Insufficient knowledge and information on the physical properties of soils and rocks, once they are the main groundwater reservoirs in the study area; b) Lack of statistical data and consolidated information on local pluviometric and fluviometric parameters that would aid the calculation of the water balance; c) Lack of tubular wells or observation piezometers to collect information on the aquifer hydrodynamic parameters; d) Lack of enough information on the hydraulic links between surface waters (for example, rivers and lakes) and groundwater resources; e) Lack of enough information to calculate the use of water resources in farming and industrial activities and local public supply.

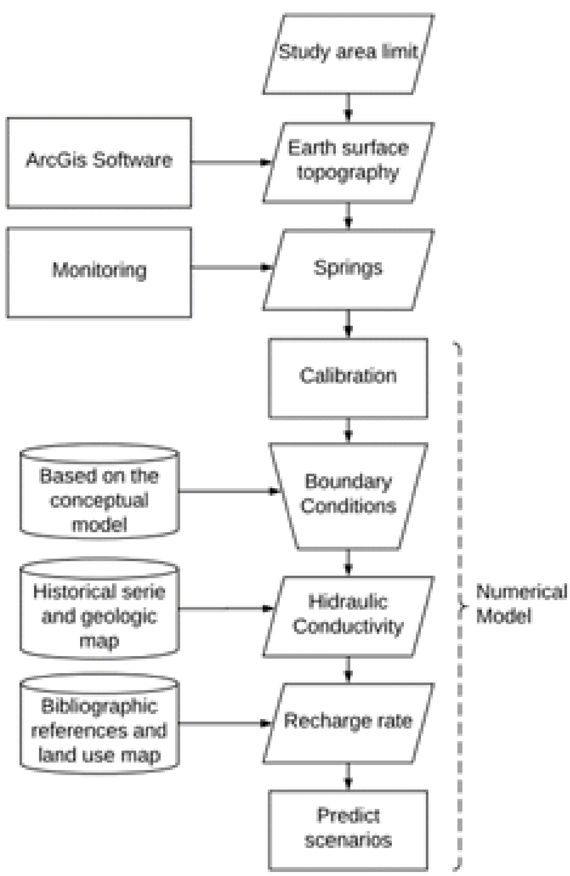

Figure 5 Flowchart of the building the conceptual model of aquifer.

For the preparation of the conceptual hydrogeological model (CHM), the hydro-stratigraphic units, the hydrodynamic variables and the flow conditions (recharge and discharge) were identified and determined in accordance with the objectives to be achieved, (Reilly & Harbaugh 2004; Khadri & Pande 2016). The most representative lithostratigraphic units of the study area were identified from information compiled from the regional geology literature, logs of drillings, excavated wells, geologic maps, and hydrogeological data Rapantova, Tylcer & Vojtek (2017). The adopted model was calibrated on the basis of hydraulic conductivity values, observed water levels, drain conductance, and assuming the flow to be permanent, that is, disregarding the variation of the water level with time (Owen, Jones & Holland 1996).

All the parameters used in the model were adjusted to reduce the great number of required data in face of the small number of available information. The results show that the model thus prepared is reliable and can be used in the investigations of the Ribeirão Candidópolis catchment aquifers and for predictions of boundary conditions for the aquifers in different scenarios.

Geographic criteria were taken into account when defining the area to be modeled, i.e., the contour of the Ribeirão Candidópolis hydrographic basin itself. From the adjusted and georeferenced digital elevation model, the limits of the study area, the main drainage network, the geometry and the aquifers dimensions were obtained - Figure 6.

The topographic highs act as watersheds and therefore the external areas close to this contour were considered as having null flow, thus limiting the study to the behavior within the Ribeirão Candidópolis Basin. The springs were considered the aquifer discharge points and points of reference of the local water level, because when it comes to drilled wells no information is available regarding pumping tests and geologic descriptions Fiorillo, Pagnozzi & Ventafridda (2014). The pieces of software used for the statistical data treatment and the generation of thematic maps and numerical flow model were: Excel 2016, ArcGis 10.5, Surfer 13 and Visual MODFLOW 2011.1.

The water recharge of the basin aquifers results from the infiltration of rain water to the aquifers and contributions from other aquifers.

The water table configuration varies seasonally because the groundwater recharge, which is understood as the accumulation of water in the upper surface of the saturated zone, is related to the variation in the amount and temporal distribution of rainfall Kushwaha, Pandit & Goyal (2009).

The recharge rate was obtained by the water balance method, proposed by Thornthwaite (1948) and calculated according to Equation 1.

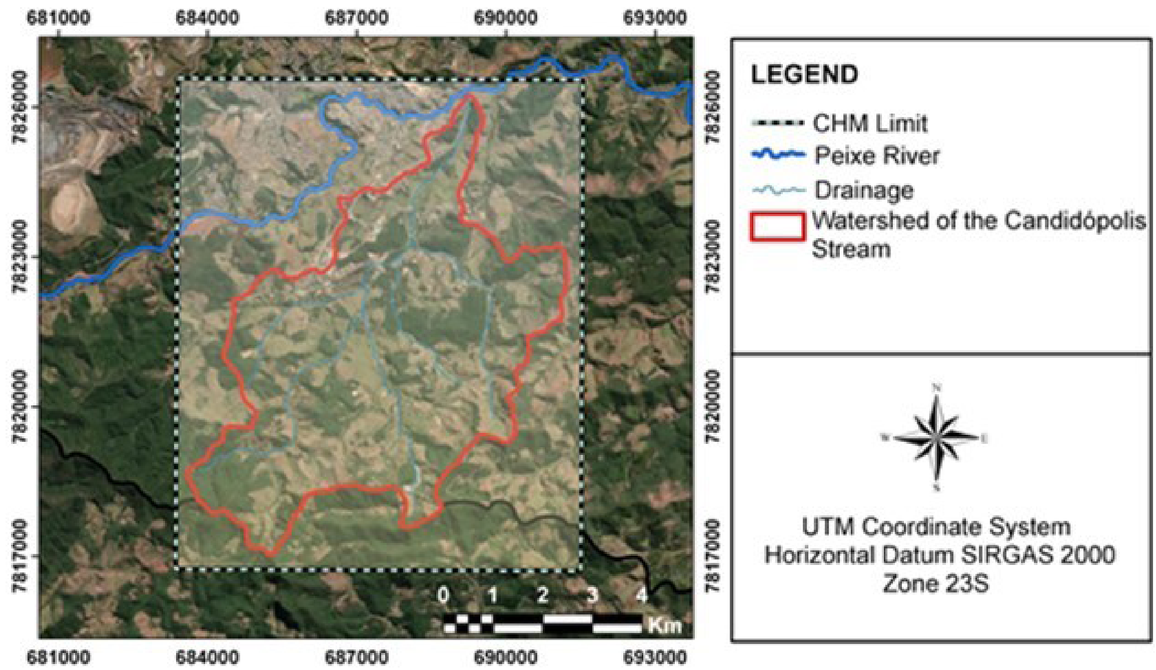

Figure 6 Projection of the limits of the conceptual model (Modified after Google Earth 2020).

$$R = P - D - Evap + \Delta V \quad (1)$$

where:

- R is the mean monthly recharge, in mm;
- P is the mean monthly rainfall, in mm;
- D is the mean monthly discharge, in mm;
- Evap is the mean monthly evapotranspiration, in mm;
- ΔV is the mean monthly variation of water stored in the soil, in mm.

The above equation has limitations once the local geologic package is not taken into account. It is thus considered that for a conceptual model of a fractured medium the checking of infiltration rates is complex, making the assertiveness of the recharge rate difficult.

The primary partial differential equation that defines the three-dimensional movement of groundwater in MODFLOW is defined by Harbaugh (2005) (Equation 2).

$$\frac{\partial}{\partial x}\left(k_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_{yy}\frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_{zz}\frac{\partial h}{\partial z}\right) + W = S_s\left(\frac{\partial h}{\partial t}\right) \quad (2)$$

where:

- k_{xx}, k_{yy}, k_{zz} are the hydraulic conductivity values (L/T);
- *h* is the hydraulic head (L);
- *W* represents the water sources or sinks for system (T^{-1});
- S_s is the specific storage of the material (L^{-1});
- *t* is time (T).

Equation 2 is solved in order to determine the value of the hydraulic head of an aquifer system in each node. It is known that the numerical model has defined functions for certain points of the model. The discretization of the points is random, both in position and quantity. Each chosen point is called node. Each node represents a limited portion of the aquifer to be modeled, so that the parameters attributed to the node are considered constant for the region it represents, Feitosa & Filho (2008). Guiguer & Franz (1996) explains that the terms on the left side of Equation 2 represent the amount of water that enters and leaves the control volume, and the terms on the right side indicates the variation of the water store in the volume element. For a permanent regime flow, i.e., considering the aquifer in static mode, storage is considered null Harbaugh (2005).

In the net, the nodes can be positioned in the center or at the corners of the cells. In practice, the centered net in the middle of the cell is usually chosen, displaying a better physical concept when it comes to quantifying the mean characteristics of each cell, Feitosa & Filho (2008).

In each node, each derivative of the mathematical function is approximated by an algebraic expression with reference to the neighboring nodes. Equation 3 is used to represent the variation in each axis of the Cartesian plane by means of the central difference, that is, using a point in the middle of the interval ahead and another derive the hydraulic head: in the middle of the interval behind, Feitosa & Filho (2008).

$$\frac{\partial}{\partial x} \approx \frac{h_{i,j+1/2} - h_{i,j+1/2}}{\Delta x} \quad (3)$$

After developing the equation, the second derivative will be based on Equation 4 and Equation 5.

$$\frac{\partial_2 h}{\partial x^2} \approx \frac{1}{\Delta x}\left(\frac{h_{i,j+1/2} - h_{i,j+1/2}}{\Delta x}\right) \quad (4)$$

$$\frac{\partial_2 h}{\partial x^2} \approx \left(\frac{h_{i,j+1} - 2h_{i,j} - h_{i,j-1}}{(\Delta x)^2}\right) \quad (5)$$

Analogously we develop the differential equation for axis y. Thus, an algebraic equation is obtained for a homogeneous, isotropic, permanent two-dimensional problem with no recharge (Equation 6).

$$\left(\frac{h_{i,j+1} - 2h_{i,j} - h_{i,j-1}}{(\Delta x)^2}\right) + \left(\frac{h_{i,j+1} - 2h_{i,j} - h_{i,j-1}}{(\Delta y)^2}\right) = 0 \quad (6)$$

Because of the lack of wells with recorded historical pumping series or aquifer tests that could attest deviations from the original flow direction, it is assumed that the groundwater flow is uniform, with no drawdown cones, which can be corroborated by the 3D flow model, presented by (Poeter & Anderson 2005; Pholkern et al. 2019). The flow inflections take a radial form to the outlet of the main sub-basins of the Ribeirão Candidópolis and follow northwards, towards the Peixe River. Then, the water drains south-eastwards, leaving the study area. Because it is a fissural aquifer and therefore anisotropic, there may be no hydraulic connections that lead to the direct recharge of the fractures aquifer zones located at greater depths (Roy et al. 2015; Qiu et al. 2015; Meredith & Blais 2019). The equipotential lines were generated every 30 m, being the less spaced lines concentrated in the high parts of the basin. The highest hydraulic gradient exceeds 100 m, between NAS-01 and NAS-05. In general, the drawdown of the local water level is observed, but not local interferences resulting from mining in the northern and northwestern parts of the study area (Jingli et al. 2013; Bushira, Hernanez & Sheng 2017; Chakraborty, Maity & Das 2019).

In the vertical direction (axis Z), the depth of the model is 100 m divided in ten 10 m-thick layers. The layers were defined from the topographic surface. This interval was chosen after the analysis of the available geological sections. For the purpose of the research, the cells external to the geographic limit of the Ribeirão Candidópolis Basin were inactivated. Figure 7A, B, C shows an image of the study area and vicinities with colors indicating the active and inactive regions.

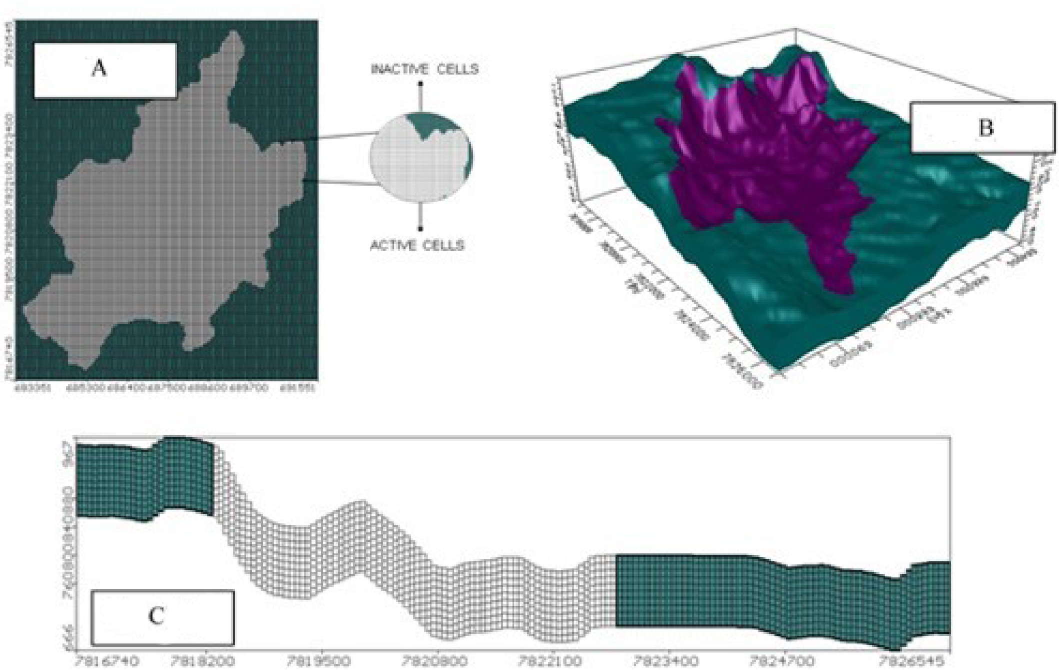

Figura 7 A. Plan view of the mesh configuration adopted in the numerical model; B. Column 60 view of the mesh configuration adopted in the numerical model; C. Inactive (green) and active (purple) cells – 3-D view with 5x vertical magnification.

2.4 Recharge

The recharge zones were defined based on the areas that were modified as a result of soil use and occupation. It was possible to identify and define sites of more or less recharge by the analysis of satellite images.

Recharge is lower in urbanized areas because of soil impermeabilization. Infiltration rates are the highest in areas covered with vegetation, agricultural areas, swamps and those cited in (Xue et al. 2018; Hashemi, Berndtsson & Kompani-Zare 2012; Chatterjee et al. 2018).

Regarding the numerical model, recharge is attributed to the first layer, thus the first cell of each column of the model being considered active. Figure 8 shows recharge zone 1, which corresponds to natural areas of the basin, and recharge zone 2, where urbanization prevails (Sadeghi-Tabas et al. 2017; Karimi et al. 2019).

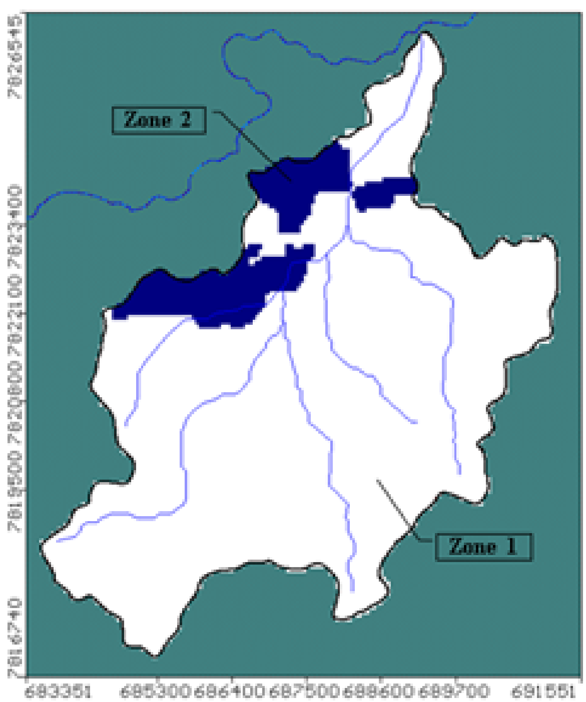

Figure 8 Recharge zones classified in the model-Zone 1: Natural (white) and Zone 2: Anthropized (blue).

Using pluviometric data of complete hydrological years, a pluri-annual mean rainfall of 1300 mm/year was obtained for the study area. Differentiated infiltration conditions were firstly infered, adhering a rainfall percentage for the two different zones. According to Carvalho et al. (2016) the recharge value that best fits the numerical model was defined in the calibration. The persistent change of the recharge percentages was necessary in order to better approximate the real water level conditions of the Ribeirão Candidópolis Basin.

2.5 Drains

The drains were designed in order to simulate the removal of water from the aquifers. Such resource was attributed to all water courses with conductance values of the order of 5 m²/day, as suggested by the calibration of model, once recent monitoring data are not available. Conductance is a parameter associated with the hydraulic conductivity in the vicinity of the drain, which in turn depends on the characteristics of the geological materials and empty spaces between them, Filho & Cota (2002). Conductance is the facility or difficulty of water flowing through the cells, and is expressed in m²/day (He et al. 2013; Nan et al. 2018).

2.6 Hydrogeological Units (Properties)

From the available data, the lithostratigraphic units were discretized in weathering mantle and fresh rock. The hydrogeological units were thus defined, by applying secondary data, define the range of hydraulic conductivity valuesIt was possible to establish with the available data the mean thickness of 30 m for the weathering mantle that overlies the crystalline rocks of the Borrachudos Suite, Guanhães Complex and the Gneissic Amphibolitic Sequence, Figure 9.

The springs used in the model are located in the Borrachudos Suite, unit that encompasses variably fractured coarse-grained granites and gneisses. The lack of more precise geological sections prevents the detailing of the numerical model layers and consequently calibration.

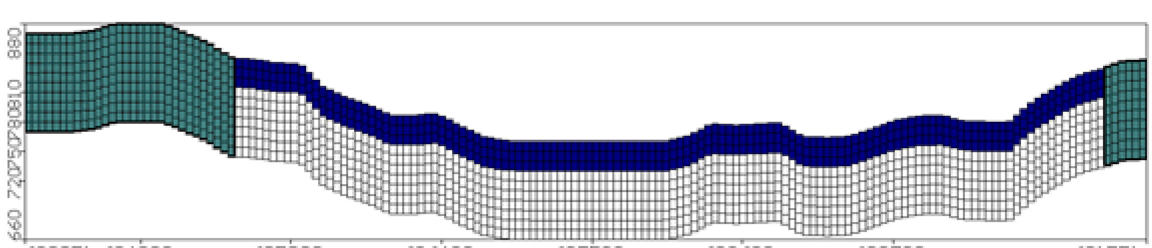

Figure 9 Conductivity weighing method in the weathering mantle (blue) and fresh rock (white) – Line 68 with 10x vertical magnification.

Kx, Ky, Kz values for the hydraulic conductivity were defined according to the Darcy Law. Some aquifers present vertical anisotropy, i.e., the K values for each axis can be different. Thus, a premise of no anisotropy was adopted for the model, i.e., the hydraulic conductivity does not vary along each of the directions. A hydraulic conductivity of 0.001 m/day was used for fresh rock and of 0.02 m/day for the more porous layers of the weathering mantle. The values were modified in the calibration and satisfactory results were obtained from retro-analysis. Storage was not considered, once it is a permanent flow regime modeling. The variation of water level with time was not considered either El-Zehairy, Lubczynski & Gurwin (2018).

2.7 Water Level Monitoring Instruments

The springs were considered in the model as water level observation points, because they represent the static level of the local free aquifer Arnold et al. (1995). The seasonal climatic dynamics was taken into account, especially in the alterations of flow rate and water level in the springs used in the model. For the research purposes, the main springs of the hydrographic basin were used, as shown in Table 3.

Table 3 Input of water level elevation (head) in the numerical model.

Code	UTM Coordinates		Head
	X	Y	
NAS-01	689126	7820501	788
NAS-02	684829	7820425	826
NAS-03	686181	7818937	817
NAS-04	683812	7818739	872
NAS-05	688170	7817995	945

2.8 Balance Zones

The available flow rate data is insufficient to represent the water behavior in the study area, which makes the calibration of the flow rates impossible. The balance zones are located in the first layer of the model and their layout coincides with the drains so as to calculate the flow rate of each portion. Figure 10 lists the water courses to which this property was attributed, which can also be seen.

The pluviometric data from the Nova Era municipality station (Code 01943100) were selected for recording complete a hydrological dataset under the ANA responsibility,

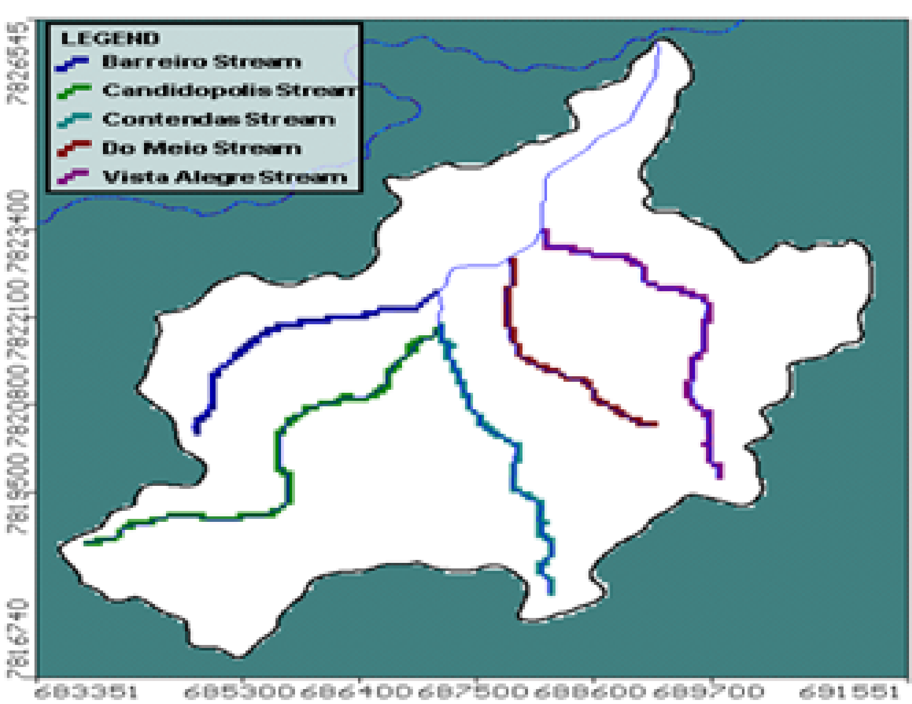

Figure 10 Balance zones in the Visual MODFLOW.

encompassing a monitoring interval from January 2003 to June 2019: Mean, maximum and minimum rainfall values for the Nova Era station. Figure 11A: Accumulated Rainfall per hydrological year. The time interval represented in the graph starts in the rainy period (October) and ends in the dry period (mid-August), highlighting a maximum value of 1976.9 mm, mean value of 1299.9 mm, and minimum value of 974.6 mm. The rainiest trimester is December, January and February, when the rainfall reaches a total mean of 479 mm. The driest trimester is June, July and August, marked by a rainless period. Figure 11B shows 16 years variation.

3 Results

The recharge values for the Ribeirão Candidópolis Basin, Table 4, were obtained according to rainfall indices and soil use and occupation. The boundary conditions were recalculated and inserted several times, after the analysis of the results obtained in the Calculated vs. Observed calibration graph. For balance zones 1 and 2 recharge values were respectively 10% and 5% of the pluri-annual recharge. These values are valid since recharge in the anthropized zone is naturally lower due to the low infiltration rate, and in the less urbanized areas, because there is no soil sealing or other factors that slow the flow of water into the aquifer.

The hydraulic conductivity values used in the simulation of the recharge of the aquifer system are in accordance with those recommended in the literature for the rock types of the study area. Considering the anisotropy of the Gneissic-Granitic Aquifer System, the same values of hydraulic conductivity (Kx, Ky and Kz) were inserted. Table 5 presents the values obtained after calibration.

For the proposed model, the calibration of the water level values was performed with the springs of the local water courses, namely Córrego Barreiro, Córrego Contendas, Córrego do Meio, Córrego Vista Alegre and Ribeirão Candidópolis. Table 6 presents the water level values after calibration. The graph in Figure 12 shows the calibration line generated by Visual MODFLOW. The absolute residual mean (Abs. Residual Mean) indicates the magnitude of the residual data, i.e., the difference between the observed and calculated maximum and minimum water level values are within the confidence interval established by the software, (Gurwin & Lubczynski 2005; Lutz et al. 2007; Aghlmand & Abbasi 2019).

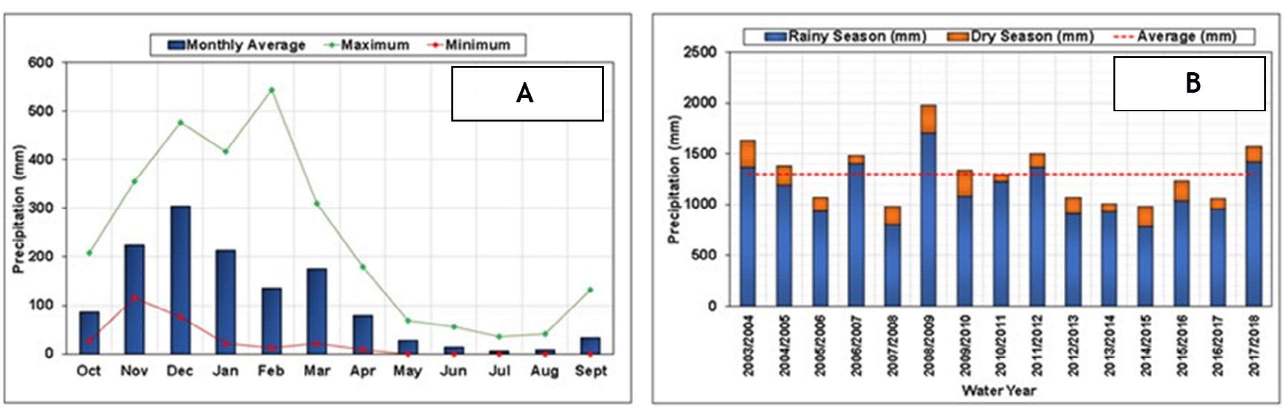

Figure 11 A. Mean, maximum and minimum rainfall values for the Nova Era station; B. Accumulated Rainfall per hydrological year.

Table 4 Recharge values after calibration.

Balance Zones	Use and occupation	Recharge (mm/year)
1	Natural	130
2	Urban	65

Table 5 Hydraulic conductivity values after calibration.

Balance Zones	Hydrogeological unit	Hydraulic conductivity (m/day)		
		Kx	Ky	Kz
1	Fresh rock	0.01	0.01	0.01
2	Weathering mantle	0.2	0.2	0.2

Table 6 Water level values of the springs after calibration.

Springs	Observed head (Obs) (m)	Calculated head (Cal) (m)	Difference (Obs - Cal)
NAS-01	826	839.04	-13.04
NAS-02	872	881.59	-9.59
NAS-03	945	957.88	-12.88
NAS-04	788	810.65	-22.65
NAS-05	860	875.06	-15.06

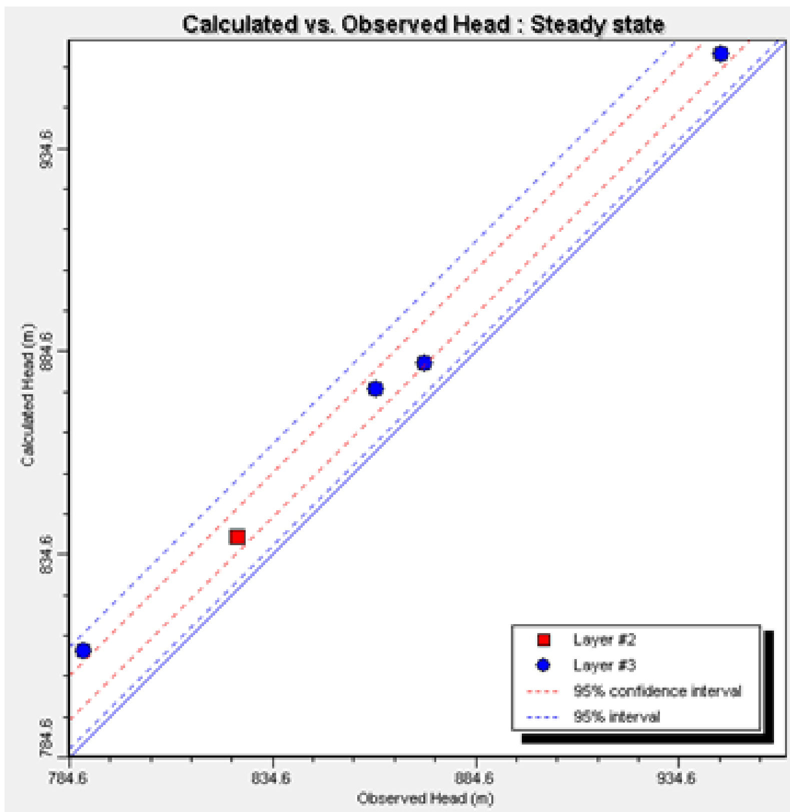

Figure 12 Calibration criterion and graph with the reference points used in this study.

Considering the results thus obtained, the values validate and indicate a good calibration of the model.

Even if calibration was satisfactory, this research can be refined by improving the monitoring net and more detailed geologic studies.

The results show that the spring head values correlate with the observed values, yielding a NRMS of 9.648% and a correlation coefficient of 0.993. The Normalized Root Mean Square (NRMS) is the error magnitude (RMS) divided by the maximum difference between the observed values, which should be less than 10% of this difference to be considered.

The best approximation was obtained at NAS-02, with a 9.59 m difference between the observed and calculated head values.

The most discrepant value, 22.65 m, was obtained at NAS-04. In this case, lower recharge values were tested, but the values established initially corresponded best to the calibration for this point. An explanation for the discrepancy is an existing lake in the vicinity, which may affect the hydraulic behavior of this spring.

Figures 13A, B present the potentiometric maps drawn with the results obtained with the numerical model, enabling the comparison between the flow equipotential lines and vectors generated automatically and manually for the conceptual model. It is possible to note not only a quantitative difference in the distribution of the hydraulic head, but also a qualitative difference, related to regions where monitoring data are lacking, (McDonald & Harbaugh

1988; Katpatal Pophare & Lamsoge 2014; Jalut, Abbas & Mohammad 2018).

There are similarities between the shapes of the equipotential lines of the conceptual model and the levels of the piezometric surface resulting from the numerical model. The sites where the shape of the contours of the numerical model differs from those of the conceptual model are those where measured water levels are lacking. It is worth stressing out that in the conceptual model the equipotential lines are more precise, once all springs were taken into account.

The flow rates of the water courses were also used to calibrate the model. The flow rates of the Ribeirão Candidópolis and Córrego Vista Alegre were considered in this study, because monitoring data are available.

The flow rates of the water courses of the Ribeirão Candidópolis catchment are low, when compared to those of adjacent basins. Thus, the initial conductance suggested in the final calibration for the drain boundary conditions was 5m²/day.

Considering the operation of the model from the flow rates of the water courses, it is assumed that only the underground discharge of the base flow in the drought period should be used.

Thus, the calculated flow rates must be smaller than the mean flow rates along the whole period. Table 7 lists the flow rates calculated in the balance zones.

The model considers the long period average flows, in other words, the average annual flows, thus contemplating the dry and rainy periods. Since the software is programmed to work with the base flow, it is correct to consider the average flows to the drought conditions. This way, the flows that will be calculated by the software will be smaller than the long period average flows. Despite considering only the flow rates of the driest months (June, July and August), the final mean calculated from the observed value is still high. This can be related to the drain conductance used. To answer more accurately what interferes with the evidenced peaks, it is necessary to perform field measurements and then a new calibration in the model.

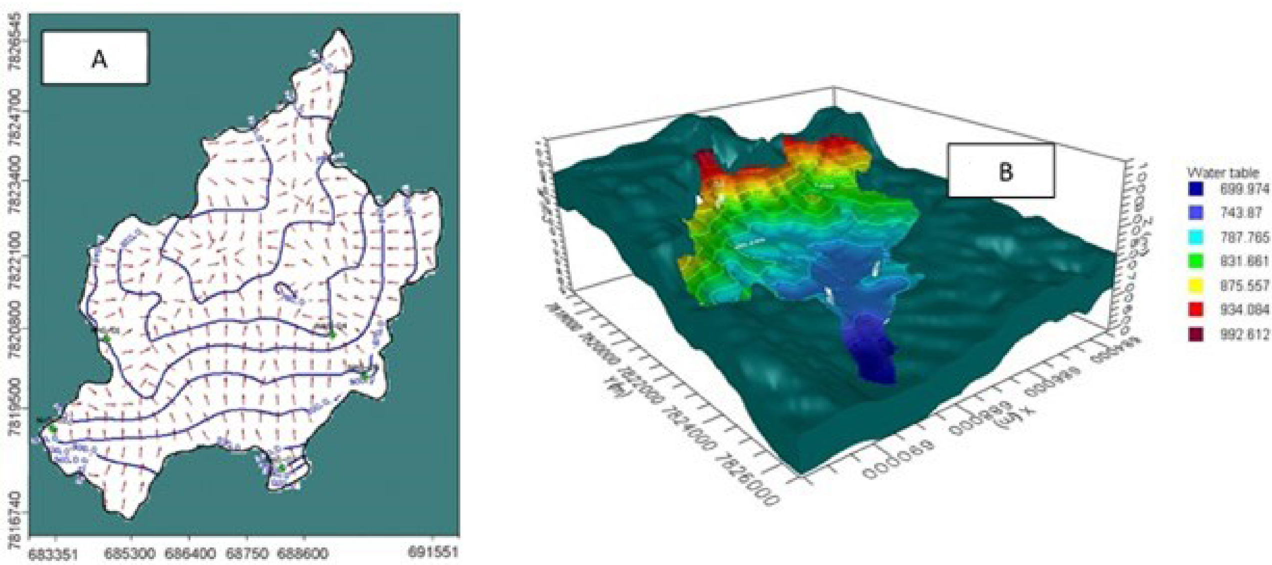

Figure 13 A. Equipotential lines and vectors indicating the groundwater flow direction in the sub-basin; B. 3D Potentiometric map generated by Visual MODFLOW.

Table 7 Flow rates calculated in the balance zones and observed in the field

Balance zones	Location	Observed flow rate (m³/h)	Calculated flow rate (m³/h)
1	Total area	-	-
2	Córrego Barreiro	64	56.2
3	Ribeirão Candidópolis	936	148.7
4	Córrego Contendas	65	56.4
5	Córrego do Meio	118	92.0
6	Córrego Vista Alegre	216	103.2

4 Conclusions

A model in Modlflow can be developed based on the following aspects: conceptualization of hydrogeological units or aquifer systems; estimation of water inflows and outflows, such as hydraulic loading and streamflow; and on hydrodynamic parameters, such as recharge and hydraulic conductivity. Model calibration is linked to the quality and quantity of field data, making a network of monitoring wells, rain gauges, spillways, and geological tests essential to ensure that the representation of the area occurs reliably. This implies investments in research and equipment when there is no secondary database available for consultation and application.

To assess the effectiveness and efficiency of the model adopted here, assessment indices, such as the mean error, mean absolute error and root mean square error, were calculated. According to these indices, the performance of the model is promising.

The semi-transient calibration of the model and the steady state flow regime approach were used in this study, being applicable to other regions with similar problems.

The coupled use of Visual MODFLOW and ArcGIS made possible the simulation of the groundwater flow in the study area in a consistent way.

The results of the study can improve the management of the groundwater resources and contribute to the sustainable development of this vital water source.

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