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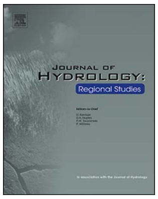

Comparative analysis of different boundary conditions and their influence on numerical hydrogeological modeling of Palmital watershed, southeast Brazil

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ABSTRACT

Study region: The study is based on field data of a shallow phreatic aquifer occurring at a small watershed in Viçosa, Minas Gerais, Brazil.

Study focus: The present study aims to evaluate numerical hydrological models generated using different boundary conditions as field data did not allowed a proper definition of the most adequate boundary condition to simulate the field characteristics observed within the study area. Data field was used to build a conceptual model and to determine initial and some of the boundary conditions of model mesh. Three numerical hydrogeological models were generated on Visual Modflow®. Once created, the models were calibrated using the WinPEST®. GHB, River and Stream boundary conditions resulted on a calibrated standard Root Mean Square (RMS) varying from 7.3% to 13.02% and showed high correlation coefficients, varying from 94% to 97%. Using another set of hydraulic head field data, these models were later validated.

New hydrological insights for the region: Results show that, for all three boundary conditions, the normalized RMS obtained in calibration was similar to that obtained in validation, confirming its validity. The Rivers boundary condition have presented the most representative values for normalized RMS, absolute average error and correlation coefficient, and are the most indicated boundary conditions for areas with similar physical characteristics to the area under study.

Introduction

Brazil has more than 113,000 km^3 of groundwater in its territory and around one third of total Brazilian territory—approximately 3,000,000 km^2, is considered to be in recharge zones (CREA-MG, 2013). The use of groundwater is rapidly increasing in the country due to an increase in consumption and degradation of superficial water bodies (Cabral et al., 2006). There is an estimate that at least 416,000 wells are currently operating in the country, and every year 10,800 new wells are being installed (Hirata et al., 2010). Given the relevance of aquifers for the Brazilian economy, their use should follow a good management program including actions to promote sustainable use and prevent their contamination and allow maintenance of groundwater quality and quantity for its multiple uses.

Despite being low storage aquifers, superficial unconfined aquifers are an important source of water for rural populations because there is no water supply for these areas in Brazil. Even with their importance, there are not many studies regarding aquifers in Brazil.

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Only in recent year has attention been given to these issues, especially in developing countries, because these aquifers comprise an important source of water for the rural areas (Appiah-Adjei et al., 2013; El Samanoudy et al., 2013; Flores-Marquez et al., 2008).

In Brazil, there is also an urgent need for promoting studies involving distribution and forms of occurrence of groundwater on different geological environments. This includes the following: comprehension of superficial and groundwater relationship, its vulnerabilities and storage capacities, recharge areas, flow identification, groundwater quality, and water table monitoring (Krebs and Possa, 2008; Soares, 2010).

These studies should address environmental management perspectives and also allow the creation of hydrogeological models (Marthers et al., 2012). Once calibrated, these models could be used as a tool to predict changes in those aquifers and on water storage and supply as a response to the introduction of new pumping wells, or for analysis of underground contaminant movement. Aigler and Ge (2013) have modeled Fraser River watershed, in order to simulate groundwater flow and to examine the simulated localized depression resulting from a proposed increase in groundwater withdrawal, in an approach similar to the one used in this study.

Xi et al. (2010) studied a superficial aquifer at Ejina Basin, North China, simulating groundwater level variations, both spatial and temporal, using MODFLOW, and have reached good calibrated results that matched well with the observed data.

Carrol et. al (2009), studying the Death Valley Regional Flow System using MODFLOW, pointed out that its most significant limitation was that the model was built using the confined layer assumption to improve numeric stability, considering that the saturated thickness remains constant throughout the entire simulation. They considered that this approach allows unrealistic estimates of drawdown to occur in transient simulations.

In Brazil, Filho and Cota (2002) performed a sensitivity analysis for conductivity through a simulation of a hypothetical superficial, homogeneous and isotropic aquifer involving a GHB (General Head boundary) contour condition and aquifer drawdown by pumping. These authors also presented a comparative analysis of mathematical features of MODFLOW packages or modules, which are forms of implementation of boundary conditions (GHB, River, Drain and Evapotranspiration-EVT). The results contributed to a greater understanding of the operation of these mathematical routines, helping thus the hydrogeologists to develop models that best represent these characteristics.

Computer simulations of groundwater flow systems numerically evaluate the mathematical equation governing the flow of fluids through porous media. To determine a unique solution, it is necessary to specify boundary conditions around the flow domain for head or its derivatives in a so-called boundary-value problem (Collins, 1961). Not only the location of these boundaries is important but, their numerical representation is also critical. This is because many physical features (that are hydrologic boundaries) can be mathematically represented in more than one way, and determining the best mathematical representation usually depends upon the objectives of the study and can affect the ability of a model to make accurate forecasts (Reilly, 2001).

Determining of contour (boundary) conditions for hydrogeological mathematical simulations is an essential step of numerical modeling, but it is not trivial, as it depends on a detailed knowledge of the simulated system and on some mathematical specificities of the chosen model (Filho and Cota, 2002). As no sufficient knowledge was available for a proper selection of boundaries conditions that could represent the characteristics of the drainage system existing in the study area, the authors have developed a study focusing on an evaluation of the effects of the use of three different (GHB, River and Stream) contour conditions on numerical hydrogeological simulations of an unconfined (phreatic) aquifer occurring in a rural watershed of Southeast Brazil, and to and to define the most suitable boundary condition to the model. This study was part of a major study involving hydrogeological modeling of Palmital watershed, and the effect of increased groundwater withdrawal by new pumping wells in terms of both its quantity and its quality.

The study area is a small watershed (125.6 ha) located in the rural area of Viçosa, a small city in the Southeast state of Minas Gerais, Brazil (Fig. 1). It is located between UTM plane coordinates (23S Zone, SAD69 Datum): 723,100 m and 724,400 m East and 7,695,900 m and 7,697,400 m North. Palmital watershed belongs to the Rio Doce Federal Watershed and it is an important fountainhead for Viçosa (Fernandes, 1996). The Rio Doce watershed is of great interest for hydrological studies because it presents a wide range of economic activities that are influenced by water availability, such as agriculture, agro-industry, mining, steel, pulp and dairy products. It must be pointed out that besides the Palmital watershed being small, its characteristics (geology, pedology, vegetation, soil uses, topography, and climate) are representative of an extent region of Southeast Brazil region.

2. Methods

All field data was obtained from the work developed by Carvalho (2013) and Andrade (2010). The following sections detail some of the methods used. Additional information can be found in Carvalho (2013) and Carvalho et al. (2014).

2.1. Conceptual and numerical model construction

Data collected in the field by Carvalho (2013) and Andrade (2010) have allowed the definition of geology, pedology, land use, and topography, and were used to determine the hydrogeological conceptual model for the watershed under study.

All data was converted from the conceptual model to numerical model through Visual Mod Flow Pro 2009.1® software using finite differences method. In addition, data from the register of all springs found in the watershed, SPT and auger boreholes, five monitoring wells, and water level monitoring during one hydrological year on each of the five wells and slug tests have been used.

2.1.1. Model mesh definition

The watershed was divided into 25 m^2 cells and the area outside its limits was not modeled and was considered as inactive cells.

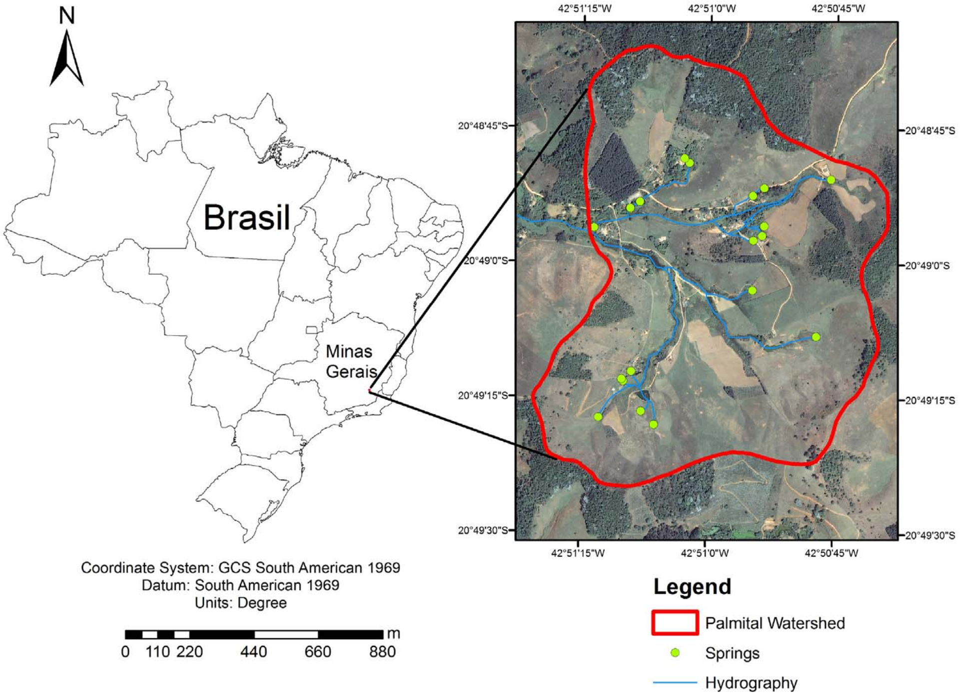

Fig. 1. Location of study area.

The modeled domain was separated into two layers: the superior one, representing mature residual soil (with no sign of geological structure and original mineralogy); and the lower one, representing the young residual soil (with preserved geological structure and mineralogy). The superior layer had a thickness of 5 m, while the lower had a thickness equal to 25 m. Also, into the superior layer, an alluvium layer was modeled along the main water channels.

2.1.2. *Simulation conditions*

Models were simulated on steady-state condition in which the model considers that no significant changes on hydraulic heads occur during time.

2.1.3. *Boundary conditions*

External boundary conditions were based on topographic divides considered to be coincident to groundwater divides, as the aquifer is porous and there are no pumping wells close to these divides. This approach has resulted in minimal errors.

Internal boundary conditions corresponding to superficial water channels also must be considered because they influence the underground dynamics, and must have its location and behavior described and considered by the model. Three different types of internal boundary conditions representing existing water channels in the watershed were considered, tested and analyzed in this paper: *Stream*, *River*, and *General Head Boundary (GHB)*.

In mathematical terms, boundary hydrogeological conditions are represented by three different types: type 1–boundary with specified head (Dirichlet conditions); type 2–boundary with specified flow (Neumann conditions); and type 3–boundary with head dependent flow (Cauchy or mixed conditions).

GHB boundary condition (type 3) represents the most general boundary condition available on MODFLOW (Filho and Cota, 2002). The other boundary conditions were developed from this and represent simulation of particular phenomena. On this condition, there is no limit for the validity of equations used for calculation of water discharge.

River condition (type 3) simulates the water flow between aquifer and superficial water on the model cells for which this condition was selected. If the head in the aquifer is above the head in the river, water will flow from the aquifer to the river. If the opposite occurs, water will then flow from the river to the aquifer. The difference between GHD and River conditions is that the last one presents a validity limit for the general equation for discharge calculus, whenever the aquifer head in a cell becomes lower than the elevation of the riverbed.

Stream condition (type 3) is similar to the River condition in terms of how the amount of water is added to or removed from the groundwater system. Nevertheless, water that is removed from the groundwater system then is routed downstream where it can re-enter the groundwater system again.

All used tools considers conductance as one of its parameters. This property can be calculated through Eq. (1).

$$C = \frac{K \times L \times W}{M} \tag{1}$$

Where:

C = conductance at water channel bed ($L^2\,T^{-1}$)
K = hydraulic conductivity at water channel bed ($L\,T^{-1}$)
L = cell width where the drain was installed (L)
W = width of water channel (L)
M = thickness of drainage layer (L)

Hydraulic conductivity (*K*) of alluvium layer was calculated by Carvalho (2013) and is equal to 0.000022 cm s^{-1}. Width *L* and *W* were defined as 5.0 m each one. The thickness (*M*) adopted as being equal to 1.0 m resulting in a conductance of 4752 m^2/day, which was rounded to 4700 m^2/day and used as input data for the models. Another necessary part of the input data is the hydraulic head, which is considered to be equivalent to the highest terrain elevation for each stretch. For *River* and *Stream* boundary conditions, it was considered that the water level at water channels was equal to terrain level, and that the river presents a water depth equal to 30 cm on all channel extension, which is in accordance to field observations. Water **channel** bed level was obtained from subtraction of water depth from the terrain level, as no direct measure of this was available.

For *Stream* condition, it is also necessary to obtain the average watershed flow. Carvalho (2013) has measured the flow on an area of 22.8 ha located inside the study, from March 2012 to September 2012 and has found it to be equal to 146.8 m^3/day. For the calculation of average watershed flow, the drainage area ratio method was used. As being an interpolation method, there is no need to define homogeneous hydrological regions (Chaves et al., 2002). Using the proposed method for total drainage area of the watershed under study (125.6 ha), an average flow equal to 808.8 m^3/day was found.

2.1.4. Recharge

Through the water table fluctuation (WTF) method (Carvalho et al., 2014), it was possible to calculate the recharge for all the monitoring wells. Based on the results, an average value equal to 271 mm·y^{-1}, was found.

2.1.5. Hydrogeological parameters

For all boundary conditions, the hydraulic conductivity used was obtained from Carvalho (2013). Hydraulic conductivity was calculated from the average data obtained from slug tests and from EnviroBase® software databank. Different hydraulic conductivity values were considered to vary with depth (It was inputted according to the depth in which the property was calculated). Conductivity for *x* and *y* axes were considered to be equal, while conductivity for *z* axis was considered 10 times lower than for the one for other two axes.

The modeled area was separated into two layers. The upper layer represents the mature residual soil (Fig. 2) which was divided by using a pedological classification, as they present different hydrogeological properties. The second layer represents the young residual soil.

Hydraulic Conductivity values used as input data on all contour conditions analysis are shown on Table 1.

2.1.6. Model calibration and validation

Models were calibrated using a statistical calibration evaluation as suggested by Wels et al., 2012, using the following criteria: average residual error, absolute average error, root mean square error (RMS), and the normalized root mean square error (normalized RMS).

Calibration was carried out based on the average of water level measurements on all five wells during a hydrological year and also in the location of five springs (Fig. 3a) occurring in the area. Hydraulic head on all these 10 points served as a reference to compare heads calculated by the model on all these points. Models were considered well calibrated when a normalized RMS value lower than 10% was found.

Model validation was based on nine springs (Fig. 3b) that were different from those used for calibration. These springs were as reference hydraulic heads to confirm input data obtained throughout calibration process. So the data from the model were compared to hydraulic heads on those nine points.

3. Results and discussion

Hydraulic conductivity values obtained after calibration of River, GHB, and Stream boundary conditions are shown on Table 2. The geographical coordinates of the wells and springs allocated in the models, as well as their pressure heads for calibration and validation are presented in Table 3; and the final values of statistical analysis carried out during calibration process are shown on Table 4.

All boundary conditions have presented low normalized RMS. GHB and River conditions have presented values lower than 10%, respectively, 8.41, and 7.29%. The highest normalized RMS was obtained for Stream condition and was equal to 13.02%, resulting in a model considered not well calibrated, according to the criteria adopted in this paper. High correlation coefficients have also been found for all conditions, the lowest equal to 93% (Stream), and the highest equal to 98.5% (River). The reason for the higher normalized RMS value (superior to 10%) found for stream condition is related to the fact that average watershed discharge was obtained throughout regionalization procedure, which may not correspond to the actual value found in field.

Even though the boundary conditions adopted have different validation limits, they are mathematically similar and follow the same equation when the validity limits are not achieved. Furthermore, they are highly topographically dependent, the more pronounced the relief is, the better the results obtained are. This is why the results were so similar.

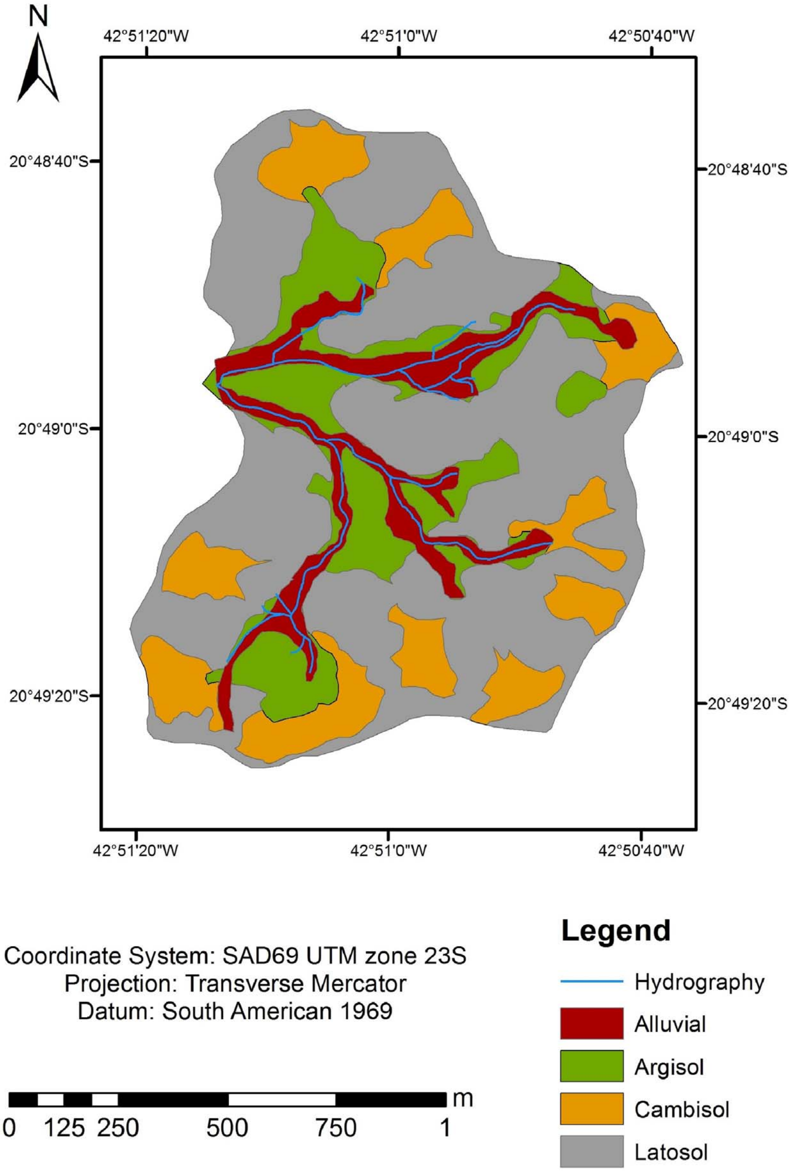

Fig. 2. Soil classes present on layer 1.

By using another group of hydraulic heads obtained from field mapping and composed by nine springs, the models were then submitted to validation (Table 3). Values obtained during calibration process were compared to those obtained during validation and the results are presented in Table 4. The same pattern observed during calibration was observed in the validation process, with River

Table 1
Hydraulic conductivity (*K*) values used as input data on *River*, *GHB*, and *Stream* boundary conditions model for *x*, *y*, and *z* axes.

Layer 1	*Kx* (cm s^{-1})	*Ky* (cm s^{-1})	*Kz* (cm s^{-1})
Alluvium	2,48E-05	2,56E-05	2,28E-05
Argisols	4,55E-05	4,29E-05	3,40E-06
Cambisols	1,41E-04	1,35E-04	4,02E-07
Latosols	2,10E-05	2,03E-05	1,87E-06
Layer 2	*Kx* (cm s^{-1})	*Ky* (cm s^{-1})	*Kz* (cm s^{-1})
Argisols	1,57E-04	1,89E-04	1,80E-04
Cambisols	4,10E-05	6,07E-05	1,56E-06
Latosols	3,45E-05	3,56E-05	3,05E-03

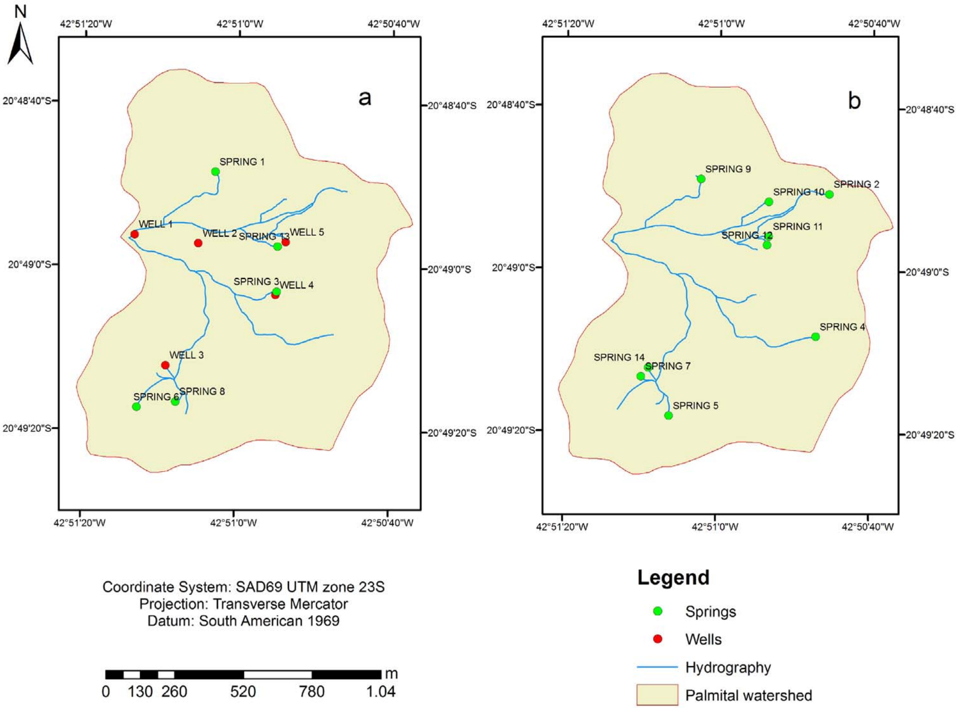

Fig. 3. (a) Wells and springs used to calibrate hydrological model using all contour conditions; (b) Springs used to validate hydrogeological model for all contour conditions.

condition presenting lower RMS values then the other boundary conditions.

It can be observed that for all boundary conditions, both normalized RMS and the correlation coefficient values obtained at validation are very similar to those obtained at calibration.

Table 2
Hydraulic conductivity (*K*) values for calibrated model for all three boundary conditions in three (*x*, *y*, and *z*) axes.

Contour condition	Results			
GHB	**Layer 1**	***Kx*** **(cm s^{-1})**	***Ky*** **(cm s^{-1})**	***Kz*** **(cm s^{-1})**
	Alluvium	3,61E-05	2,56E-05	2,34E-05
	Argisols	1,37E-05	4,28E-05	3,37E-05
	Cambisols	1,45E-04	1,35E-04	4,36E-07
	Latosols	1,28E-05	2,03E-05	7,47E-06
	Layer 2	***Kx*** **(cm s^{-1})**	***Ky*** **(cm s^{-1})**	***Kz*** **(cm s^{-1})**
	Argisols	1,21E-04	1,88E-04	3,13E-04
	Cambisols	6,71E-05	6,07E-05	3,67E-05
	Latosols	3,91E-05	3,56E-05	3,34E-04
River	**Layer 1**	***Kx*** **(cm s^{-1})**	***Ky*** **(cm s^{-1})**	***Kz*** **(cm s^{-1})**
	Alluvium	2,56E-06	2,56E-05	1,68E-04
	Argisols	4,28E-05	4,28E-05	4,38E-06
	Cambisols	1,97E-05	1,34E-04	9,96E-08
	Latosols	2,03E-5	2,03E-05	1,92E-06
	Layer 2	***Kx*** **(cm s^{-1})**	***Ky*** **(cm s^{-1})**	***Kz*** **(cm s^{-1})**
	Argisols	1,61E-04	1,88E-04	2,52E-04
	Cambisols	1,14E-05	6,07E-04	4,51E-06
	Latosols	2,18E-05	3,56E-05	4,26E-02
Stream	**Layer 1**	***Kx*** **(cm s^{-1})**	***Ky*** **(cm s^{-1})**	***Kz*** **(cm s^{-1})**
	Alluvium	2,87E-04	2,56E-05	5,70E-06
	Argisols	4,28E-05	4,28E-05	4,38E-06
	Cambisols	1,58E-05	1,34E-04	3,76E-07
	Latosols	2,03E-05	2,03E-05	1,92E-06
	Layer 2	***Kx*** **(cm s^{-1})**	***Ky*** **(cm s^{-1})**	***Kz*** **(cm s^{-1})**
	Argisols	1,88E-04	1,88E-04	1,55E-04
	Cambisols	6,07E-05	6,07E-05	3,67E-06
	Latosols	3,56E-05	3,55E-05	3,05E-04

GHB: General Head Boundary.

Table 3
Geographical coordinates and hydraulic heads of wells and springs used in the calibration and validation of models GHB, River and Stream.

Calibration			
Point	Longitude UTM-E	Latitude UTM-N	Hidraulic Head (m)
Spring 1	723667	7696998	740,32
Spring 3	723895	7696087	742,65
Spring 6	723368	7696115	760,75
Spring 8	723511	7696131	752,49
Spring 13	723932	7696733	746,24
Well 1	723352	7696763	722,82
Well 2	723592	7696762	727,19
Well 3	723525	7696325	736,16
Well 4	723816	7696488	732,50
Well 5	723945	7696773	743,10
Validation			
Point	Longitude UTM-E	Latitude UTM-N	Hidraulic Head (m)
Spring 2	724165	7696925	769,10
Spring 4	724114	7696385	764,67
Spring 5	723557	7696087	742,65
Spring 7	723446	7696242	745,56
Spring 9	723679	7696984	739,66
Spring 10	723899	7696868	744,57
Spring 11	723899	7696717	731,28
Spring 12	723935	7696765	745,44
Spring 14	723479	7696271	744,85
Spring 2	724165	7696925	769,10

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These results demonstrate the validity of the hydrogeological numerical model and, more important, shows, for the physical characteristics of the watershed under study, that the use of GHB and River conditions no significant change could be noted on the results from the hydrogeological numerical model. Based on these outcomes, both GHB and River boundary conditions could be used as they have resulted in similar RMS values. As GHB is simpler, processing time for this condition is lower than for River and so, time spent on running the model would also been lower.

3.1. Hydrogeological model

Results from hydrogeological numerical model shows that groundwater flow follows the terrain topography, moving from the highest places to the bottom of the watershed. Figs. 7 and 8 show the equipotential lines and the vectors representing the magnitude and the groundwater flow direction as calculated by the model.

Black lines represent the equipotential lines of hydraulic heads calculated by the software for every 5 m. Flow vectors are represented by three colors:

- Red − characterize the group of cells that contribute to water infiltration into aquifer (recharge);
- Blue − characterize the group of cells that receive water from the aquifer (discharge); and
- Green − characterize groups of cells that only conduct water from one region to other inside the aquifer.

Groundwater flow's highest velocities occur at areas with high elevation and are illustrated by larger arrows, close to the springs. However, lowest velocities occur at lower areas or far from the drainage system and are represented by small arrows. This occurs due to higher hydraulic gradient in the superior portions of watershed (higher slopes) when compared to the ones occurring in the lowered terrain portions.

Table 4
Results of calibration and validation processes for each contour condition on the numerical hydrological model.

Condition	*GHB*		*River*		*Stream*	
	C	*V*	*C*	*V*	*C*	*V*
Average error (m)	1.25	0.08	0.42	−0.52	2.43	−0.08
Absolute average error (m)	2.29	1.96	2.15	1.67	4.06	3.19
RMS (m)	3.16	2.78	2.74	2.20	4.88	4.08
Normalized RMS (%)	8.41	9.44	7.29	7.48	13.02	13.86
Correlation coefficient	0.96	0.96	0.97	0.98	0.94	0.93

GHB: General Head Boundary.

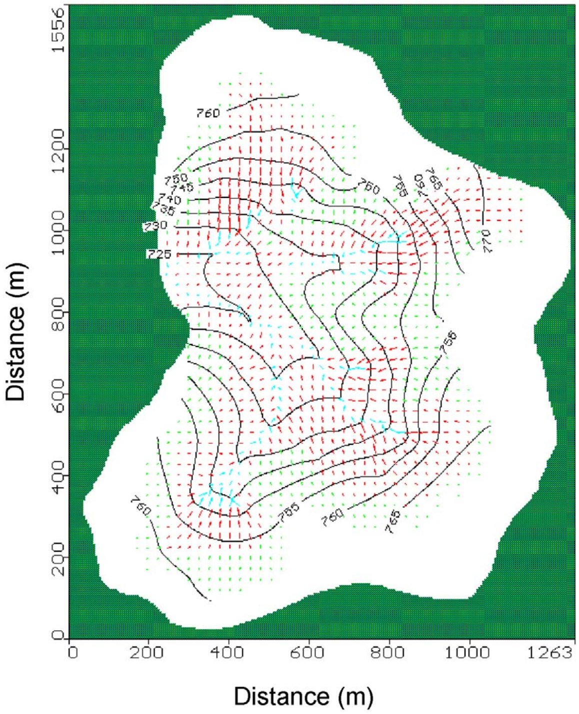

Fig. 4. Equipotential lines and vectors indicating flow direction and magnitude of underground flow at watershed as calculated by the model using *GHB* contour condition.

Comparison of maps presented in Figs. 4–6 show that all boundary conditions applied have resulted in similar underground flow magnitudes. But, despite that, some important differences can be noted.

One important change observed from Figs. 4–6 is related to the fact that for Stream condition the model has resulted in a largest discharge (drained) area with a higher density of the cells composed by blue vectors, located along river valleys; while GHB and River

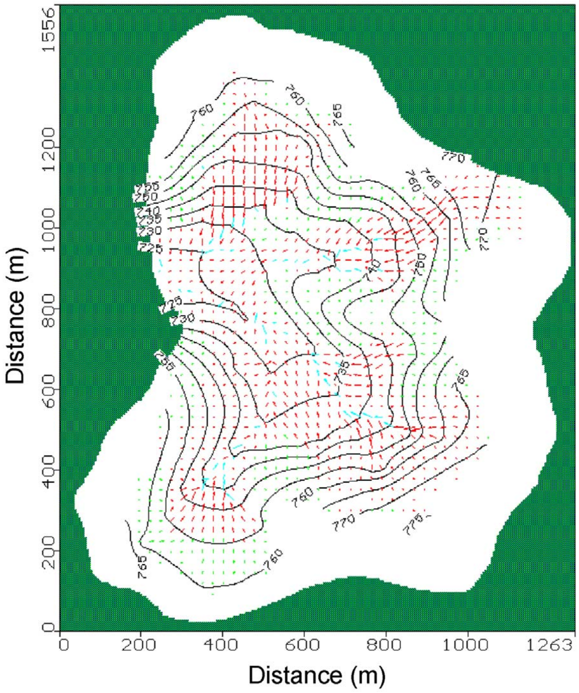

Fig. 5. Equipotential lines and vectors indicating flow direction and magnitude of underground flow at watershed calculated by the model using *River* contour condition.

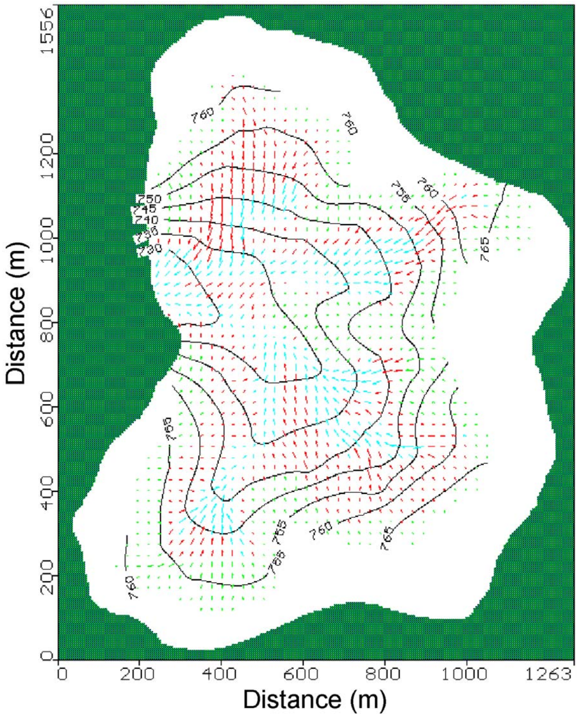

Fig. 6. Equipotential lines and vectors indicating flow direction and magnitude of underground flow at watershed calculated by the model using *Stream* contour condition.

has presented a lower drainage area, as a response of the different limits for the equation used by each condition to calculate water discharge/recharge. Water that was removed from the groundwater system on Stream condition did not re-enter the groundwater system again, at least in the physical limits of Palmital watershed, as only blue flow vectors occurs downstream. This behavior is quite different for GHB and River, as it can be noted that the upstream blue flow vectors are followed by red flow vectors downstream, for both conditions. This means that by using Stream condition, water is withdrawn by the drainage system from aquifer, while on GHB and River part of this water recharge the aquifer on the lower portions of the watershed.

For the recharge areas, a noticeable difference can be observed from GHB and River to Stream condition. The recharge area for the first two are considerably higher, and again, this can be explained by its differences in the equations used by each condition, This difference is attributed to the fact that Stream condition uses the stream discharge as an input data and this discharge is then added or deducted to the head, increasing the water flux in the areas near the water bodies.

The comparison between equipotential lines from three boundary conditions shows that River condition resulted in a higher hydraulic gradient (45 m slope/1000 m distance) and that Stream condition resulted a lower hydraulic gradient (35 m slope/1000 m distance).

4. Conclusions

The study was based in the assumption that, for the physical characteristics of the watershed under study, and based on the fact that information that is necessary to define a proper hydraulic boundary condition cannot always be available, as it depends on a detailed knowledge of the simulated system, it may be necessary to evaluate which boundary condition can better fit the hydrogeological model.

Numerical hydrogeology models output maps obtained from the studied watershed by using three different boundary conditions have led to similar results in relation to magnitude and directions of water flow for GHB and River conditions.

Stream condition has led to a higher normalized RMS value so indicating that the model is not as precise that the ones from GHB and River condition. Another important difference is that the Stream condition results in withdraw of water from aquifer along major drainages of the area, while for GHB and River condition shows some re-recharge on lower portion of the watershed, which is more connected with data collected on observation of the wells located on theses areas.

Based on this, the authors suggest that for watersheds with similar characteristics located on the same region, that the use of Stream boundary condition should be used only if there is available knowledge regarding effluent and influent behavior of the drainage system.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ejrh.2017.05.006.

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