UNIVERSIDADE DO ALGARVE

Faculdade de Ciências do Mar e do Ambiente

Inverse Calibration of a Groundwater Flow Model for the Almádena-Odeáxere Aquifer System (Algarve – Portugal)

Dissertação para obtenção do Grau de Mestre em Engenharia do Ambiente – Área de Especialização em Modelação Ambiental

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Faro, 2007

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Discussão pública realizada em:
20 de Dezembro de 2007

Título da Dissertação:
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Abstract

The present work consisted on the characterization of the spatial distribution of hydraulic parameters on the Almádena-Odeáxere aquifer system (AO) using the automatic calibration of a finite-element numeric model, in order to improve the simulation accuracy of the aquifer's hydraulic behaviour.

This development has its foundations based on model variants already implemented at the University of Algarve to investigate the hydraulic properties of the AO on the framework of the regional scale groundwater flow studies concerning Algarve aquifers.

The state-of-the-art of the aquifer's hydrogeology was based on previous investigations, taking place on the last years in Algarve, but also on recent fieldwork, namely on the collection of field data from a monitoring network, designed in articulation with the "POCTI/AMB/57432/2004" investigation project, which provided the feedback information needed for the improvement of model variants developed during the course of the present work.

Instead of using a classic, time consuming, trial and error approach for the purpose of determining hydraulic parameters controlling groundwater flow at AO, an automatic inverse calibration algorithm was used, allowing the achievement of parameter distribution values capable of generating realistic hydraulic flow simulations.

The Gauss-Marquardt-Levenberg method of nonlinear parameter estimation, available at the PEST algorithm was assembled to the finite element flow model, which is based in the use of the Galerkin method of weighted residuals.

The results obtained by the use of the inverse method have revealed a good fit between simulated and measured head values, since the correlation coefficient, R, value was higher than 0,9 (0,9967) and the sum-of-squared weighted residuals between model outcomes and corresponding field data (i.e. the objective function, Φ) was only 4,56 m.

The obtained spatial distribution of transmissivity, ranging from 86 m^2/day to 8158 m^2/day on 16 zones, allowed a step further on the reliability of future simulations of spatial distribution and temporal evolution of state variables in natural conditions and considering different scenarios of water use.

Resumo

O trabalho de investigação levado a cabo consistiu na caracterização da distribuição espacial de parâmetros hidráulicos no sistema aquífero de Almádena-Odeáxere, através da calibração automática de um modelo numérico em elementos finitos, com vista a aumentar a fiabilidade das simulações do funcionamento hidráulico do sistema aquífero.

Este trabalho tem como ponto de partida para a execução da referida calibração algumas das variantes do modelo já implementadas na Universidade do Algarve para investigar as propriedades hidráulicas do sistema aquífero de Almádena-Odeáxere no âmbito do estudo do fluxo regional das águas subterrâneas nos aquíferos do Algarve.

Com o intuito de providenciar as bases para a compreensão e desenvolvimento do modelo conceptual deste sistema aquífero, foi inicialmente efectuada uma caracterização do estado actual do conhecimento existente acerca da hidrogeologia, baseada nas investigações levadas a cabo nos últimos anos no Algarve. Para além disso, foram também tidos em conta, dados de campo recolhidos recentemente, por meio da utilização de uma rede de monitorização, desenvolvida em articulação com o projecto de investigação POCTI/AMB/57432/2004, intitulado “Modelação de Escoamento Subterrâneo e Optimização de Redes de Monitorização à Escala Regional em Aquíferos Costeiros - O caso do Algarve”. O acesso à rede de monitorização implementada foi indispensável, uma vez que forneceu a informação adicional necessária para o desenvolvimento das variantes do modelo desenvolvidas durante o curso do presente trabalho.

Após a caracterização efectuada, e mediante a execução de um cálculo de balanço hídrico que teve em consideração os valores disponíveis de precipitação, estimativas de recarga e de evolução do consumo de água no sistema aquífero de Almádena-Odeáxere, para o período compreendido entre 1989 e 2005, pôde-se estimar, que para os anos de 1994 e 1998 este poderá ter estado em défice hídrico. Relativamente aos últimos anos (a partir do ano 2000), verificou-se que as extracções no sistema aquífero foram gradualmente diminuindo e este poderá encontrar-se actualmente sub-explorado.

Relativamente ao balanço efectuado, é importante referir que, pelo facto de se ter considerado um valor de taxa de recarga (40,2 %) situado perto do intervalo inferior dos valores de recarga conhecidos (que variam de 40 % a 60 %), certamente se contribuiu para uma subvalorização da quantidade de água disponível no sistema aquífero, na avaliação efectuada.

Constatou-se que, até á presente data, só se encontravam disponíveis, em trabalhos anteriores, estimativas de valores de transmissividade obtidos através de ensaios de bombagem ou do uso do caudal específico (método de Logan). Uma vez que estes métodos apenas permitem determinar os valores de transmissividade á escala da captação, as anteriores simulações á

escala regional no sistema aquífero de Amádena-Odeáxere, apenas contemplavam um valor único de transmissividade (valor médio) aplicado em toda a sua área.

O desenvolvimento destas simulações iniciais permitiu obter as primeiras estimativas acerca da distribuição de variáveis de estado no sistema aquífero de Amádena-Odeáxere. No entanto (e apesar de existir inclusivamente uma versão do modelo que permitiu estudar o impacte causado pela captação de água em furos destinados á rega, no padrão regional de escoamento do sistema aquífero) quando confrontadas com dados reais obtidos no terreno, estas simulações revelaram ser incapazes de reproduzir a distribuição espacial dos valores de piezomentria medidos.

Foi portanto assumido que a determinação da distribuição espacial dos parâmetros hidráulicos que controlam o fluxo da água subterrânea no sistema aquífero deveria ser a maior dificuldade a superar no decurso do presente trabalho. De facto, o cumprimento desta tarefa, afigura-se hoje em dia, como um dos maiores desafios na calibração de modelos numéricos em elementos finitos.

O uso de uma abordagem clássica de tentativa e erro para levar a cabo este processo, normalmente envolve o desperdício de tempo precioso até se conseguir obter um valor de distribuição capaz de gerar simulações de fluxo hidráulico realistas. Alternativamente, foi utilizado um algoritmo de calibração inversa que permitiu uma análise mais rápida e fiável á variação da distribuição dos parâmetros no espaço.

Foi utilizado o método de Gauss-Marquardt-Levenberg para estimação de parâmetros não-lineares, disponível no algoritmo PEST. O algoritmo foi acoplado a um modelo em elementos finitos, que se baseia no método Galerkin de resíduos ponderados.

Os resultados obtidos através do uso do método inverso revelaram um bom ajuste entre valores simulados e valores obtidos no terreno, uma vez que o coeficiente de correlação, R, revelou-se mais elevado que 0,9 (0,9967) e a soma do quadrado dos resíduos ponderados entre resultados do modelo e dados obtidos em pontos de observação no terreno (isto é, a função objectivo, Φ) foi apenas de 4,56 m.

A distribuição espacial de transmissividade obtida variou entre 86 m^2/dia e 8158 m^2/dia em 16 zonas. Estes resultados foram convertidos em valores de condutividade hidráulica (através da sua divisão pela espessura aproximada do sistema aquífero (1000 m) e constatou-se, através de uma análise estatística que estes revelam ser mais elevados que os obtidos por autores anteriores, através de ensaios de bombagem. A diferença verificada deve-se ao facto de a condutividade hidráulica variar com o efeito de escala, particularmente no caso de aquíferos cársicos, como é o caso do sistema aquífero de Almádena-Odeáxere.

A obtenção destes dados, permite a melhoria da fiabilidade de simulações futuras da distribuição espacial e evolução temporal de variáveis de estado, quer em condições naturais, quer considerando diferentes cenários de utilização do recurso água.

Para além do valor intrínseco da informação hidrogeológica obtida acerca do sistema aquífero de Almádena-Odeáxere, espera-se que o presente trabalho possa contribuir para difusão desta abordagem de calibração, que até ao presente se encontra insuficientemente divulgada e aplicada fora dos círculos académicos.

O presente trabalho abre, para além disso, a possibilidade de num futuro próximo, a gestão das reservas de água subterrânea do sistema aquífero de Almádena-Odeáxere poder vir a ser efectuada utilizando este tipo de modelos, uma vez que o modelo numérico calibrado se apresenta agora mais fiável e passível de poder ser utilizado (assumidas as suas limitações) no desenvolvimento de cenários de funcionamento hidráulico do sistema aquífero mediante a pressuposição de diferentes regimes de exploração ou de alterações climatéricas, com todas as vantagens que daí advêm no que diz respeito á utilização racional dos recursos hídricos da região.

Acknowledgements

I would like to thank, first of all, the support given by Professor José Paulo Monteiro and his availability to supervise the elaboration of the present thesis. His advices on the technical and scientific aspects of this work were crucial for its progress.

It is also important to point out that the logistic and financial support made available by the investigation project: “POCTI/AMB/57432/2004” - “Groundwater Flow Modelling and Optimisation of Groundwater Monitoring Networks at the Regional Scale in Coastal Aquifers – The Algarve Case Study”, funded by the FCT (Science and Technology Foundation) was essential for the fast and effective development of the thesis.

I am grateful for the cooperation of Eng. Ricardo Martins during the fieldwork taken place on the Almádena-Odeáxere region.

I thank the support of the Lagos Municipality, which authorized the placement of water level probes within the municipality’s boreholes; in particular the help given by Eng. Catela. For the same reason I thank the support of the Vila do Bispo Municipality, in particular Eng. Xavier, and all the private owners of boreholes that contributed for the aquifer’s monitoring activities.

And last but not the least, the help of my wife Paula was crucial in helping me to go further and motivating me when my morale was low.

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1. Introduction

1.1. Scope

The present work was developed in articulation with the work activities of the investigation project: “POCTI/AMB/57432/2004: Groundwater Flow Modelling and Optimisation of Groundwater Monitoring Networks at the Regional Scale in Coastal Aquifers – The Algarve Case Study”.

The referred investigation project, among other objectives, put into practice the installation of *in situ* Piezometers in the Almádena-Odeáxere aquifer system (hereafter referred as AO), as well as in other aquifer systems, for real-time monitoring of hydraulic heads, water temperature and electric conductivity in pilot areas in order to analyse the reliability associated with the present and future schemes of long-term groundwater monitoring at the regional scale. Apart from this, regional finite element flow models were developed in the context of the referred project as well as in the context of past investigations carried out by the project’s investigation team to study the regional pattern of groundwater flow in Algarve.

Coincidently, because the author of this thesis is collaborating with the team carrying out the execution of the above mentioned investigation project, an important confluence of efforts was made available. Therefore, relevant fieldwork as well as computer calculations and analysis were herein carried out taking advantage of the work efforts achieved by the referred project.

The use of numeric models to represent the hydraulic behaviour of aquifer systems is nowadays one of the most advanced methodologies for understanding events controlling water flow and contaminant transport on the subsoil. These can, by consequence constitute important tools for water management.

Moreover, these can accomplish several tasks: testing and improving different conceptual models, assess hydraulic parameters and, in what concerns directly to practical water management issues, predict the aquifer’s chance of response to certain water use scenarios and climate conditions.

The determination of hydraulic parameters controlling groundwater flow is one of the greatest challenges on the calibration of finite-element numeric models. With the objective to introduce the proposed theme, a general description of the type of methodologies currently available to automatically calibrate models, as well as some remarks on the hydrogeologic characteristics of the AO will be discussed on this section.

1.2. General framework for the use of automatic model calibration methods

The initiative to determine the flow domain's transmissivity distribution from head measurements at boreholes is as old as groundwater modelling. It is, on the other hand, one of the most challenging tasks still to achieve in this field (Carrera *et al.*, 2005).

Bennett & Meyer (1952) were the first to determine aquifer properties from head measurments. The work of Stallman (1956) was the first documented attempt to achieve this goal using informatics support. Interpolating the values from head measurements at the nodes of a finite difference network and assuming that the recharge and storage coefficients were known, Stallman (1956) was able to simulate the transmissivity distribution on the network area.

This initial experiment early revealed some difficulties related to the implementation a resolution of the "inverse problem". First, Stallman (1956) noticed that solutions tended to be unstable. To overcome this instability he assumed transmissivity as constant in vast aquifer areas (zones) and used the least square method to estimate the values of parameters (T) at those areas.

The author also observed that these zones shouldn't be too big, because otherwise important information about the parameter's spatial variation could be lost, what in turn could disclose an obstacle to obtaining a satisfactory estimate between measured and simulated values.

Later on, Neuman (1973) classified the methods to determine parameter values in two groups:

- "Direct", when it is assumed that transmissivity parameters are unknown and hydraulic parameters are known in the context of the Cauchy formulation. This way, mass balance at the nodes is linear for transmissivities and the problem can be solved "directly", without the use of iterations. This method is relatively simple to understand, since it consists on simply substituting heads, assumed to be known, into the flow equation, which leads to a first order partial differential equation in transmissivity and has been widely used after Nelson (1960, 1961).

- "Indirect", which consists on acknowledging that measurements contain errors and finding the hydraulic properties suitable to minimize these errors. That is, parameters are found by minimizing an objective function (Carrera *et al.*, 2005). In this case, the problem is not linear for parameters and should be solved iteratively at repeated simulations. Therefore, at its essence, the indirect method consists of an automatic version of the manual trial and error calibration, which may become a huge computational task.

According to Poeter & Hill (1997) the concept of nonlinearity is sometimes confusing for groundwater hydrologists because they are used to thinking of the ground-water flow equation as linear when applied to confined layers, a characteristic which allows application of the principle of superposition. That is, however, linearity of the differential equation that relates hydraulic head to space and time given fixed parameters values, not linearity of hydraulic head with respect to parameters.

Neuman (1973) early stated that the indirect method produces better solutions than the direct method. This happens because the use of the least squares method on residuals always contributes to filtrate part of the "noise" on the piezometric information used on the process of calibration, unlike the case of direct methods.

1.3. Remarks on the karstic character of AO and the used modelling approach

Application of numerical models in karst aquifers is often problematic, since Karst aquifers are generally highly heterogeneous. These are dominated by secondary (fracture) or tertiary (conduit) porosity and may exhibit a hierarchical permeability structure or flow paths. They are, therefore, likely to have a turbulent flow component, which may be problematic in the sense that most numerical models are based on Darcy's law, which assumes laminar flow (Scanlon *et. al.*, 2003).

As stated by Quinlan *et al.* (1996): "Although modeling of karstic processes is often possible and numerical flow models can sometimes simulate hydraulic heads, groundwater fluxes, and spring discharge, they often fail to correctly predict such fundamental information as flow direction, destination, and velocity." Therefore, when discussing the relevance of numerical modeling in a karst aquifer, it is crucial to identify what type of model (i.e. flow model or transport model) is being proposed (Scanlon *et al.*, 2003).

In fractured systems, as in karst systems, the concept of a representative elementary volume is used where the size of the area of interest, or the cell in a model, becomes large enough to approximate equivalent porous media (Pankow *et al.*, 1986; Neuman, 1987). Although accurate simulation of transport processes is still problematic, one may be able to model hydraulic heads, flow volumetrics, and general flow directions as supported by the characterization of the aquifer (Huntoon, 1994). On the present work, the calibration of a regional-scale flow model is proposed for AO, thus being much more likely to be successful than intermediate or local-scale models.

The fact that regional piezometry at AO is characterized by low gradients (large flat areas) denotes the existence of a conduit network controlling flow at the regional scale. In these conditions, discrete-continuum models are mode adequate to deal with karst fractures, as described in (Monteiro, 2001). However, even with the above limitations, useful single continuum numerical flow models can be developed in karst aquifers, as long as their limitations are appreciated and respected. These models have proved adequate for simulating regional groundwater flow (Ryder, 1985, Kuniansky, 1993, Teutsch, 1993, Angelini & Dragoni, 1997, Keeler & Zhang, 1997, Greene *et al.*, 1999, Larocque *et al.*, 1999 *in* Scanlon *et al.*, 2003).

Previous studies related with the characterization of AO (Reis, 1993, Almeida *et al.*, 2000), have based their assumptions uniquely on the existing transmissivity values, achieved by means of the use of pumping tests at borehole scale. These values (which range from 25 to 8784 m^2/day) may at best perhaps cover (linearly) the aquifer's maximum thickness, i.e., 1000 meters, which can be observed on **Section 2.2**.

Being AO a karst aquifer, denoting more or less independent dissolution channels in different sectors of the aquifer system, it is very likely borehole results were collected away from their reach. Therefore, it is expected, that transmissivity values determined at regional scale are higher than values obtained at borehole scale.

1.4. Objectives

The present work aims at articulating specifically designed monitoring networks (which are part of the undergoing “POCTI/AMB/57432/2004” investigation project referred on beginning of the introduction), put in place to allow the interactive calibration and validation of the AO groundwater flow model, with the particular objective of improving the characterization of the spatial distribution of hydraulic parameters controlling groundwater flow on this aquifer system.

In order to fulfil the proposed objectives, the spatial distribution of transmissivity values will be calibrated for the AO groundwater flow model, using available head values, through the use an automated inverse calibration algorithm, based on the non-linear least squares regression method.

It s expected that this method should allow a significant increase on the reliability of the simulation of spatial distribution and temporal evolution of state variables (hydraulic head and natural outflow) at the AO. This quality increment can be crucial for simulations focusing on different water withdrawal scenarios, namely in what accounts for the trustworthiness of water balance calculations made for this aquifer system.

2. Characterization of the case study

2.1. Location

The AO is located in Portugal, Algarve region, on the “Ribeiras do Barlavento” hydrografic basin, west of the Arade River, and is integrated on the Lagos and Vila do Bispo municipalities. It has an area of 63,5 km^2 spreading between Odeáxere (East) and Almádena (West) (Almeida *et al*., 2000) (**Figure 1**).

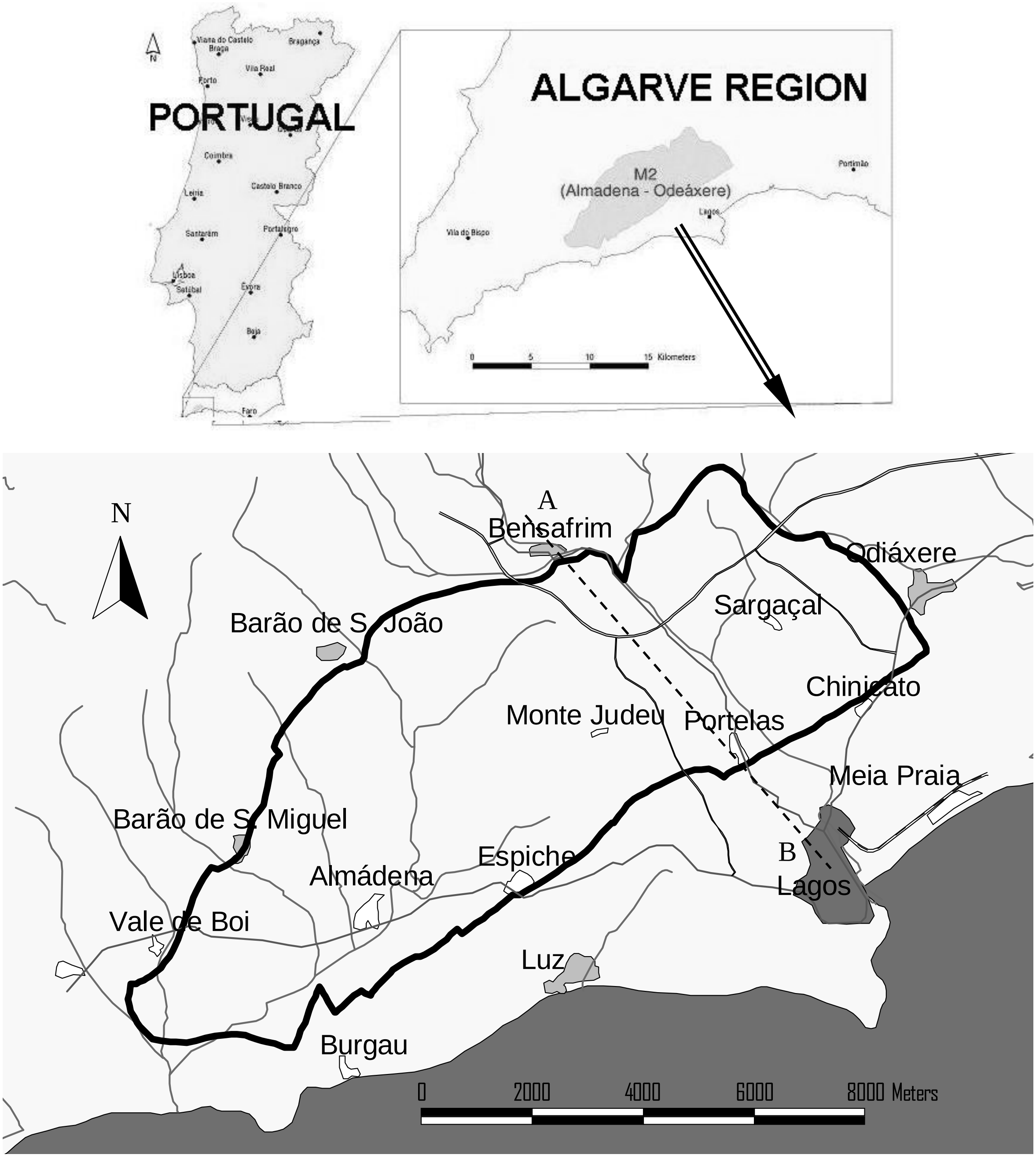

Figure 1 – Location of the Almádena-Odeáxere aquifer system, hydrologic network, main populated places and roads on the AO vicinities.

In the past, AO was used as the main water source for the Lagos and Vila do Bispo municipalities' public supply system. Water withdrawals from AO diminished when Algarve's multi-municipal supply system began its activity on late 1999. There is, however, a strong possibility that some of the existent boreholes could be used, in the future, in an integrated public supply management, as happened recently during the 2004/2005 drought period.

2.2. Geologic Setting

The AO is considered to be a free to confined karstic system and develops in carbonate Lias-Dogger outcrops, limestone, dolomitic limestone and dolomite rock, which show, in some places, a well developed karst (Almeida *et al.*, 2000). The Lias-Dogger outcrops have thicknesses non inferior to 60 m (Rocha *et al.*, 1979), reaching up to 1000 m as can be seen on the geologic cross section shown on **Figure 2** (Reis, 1993).

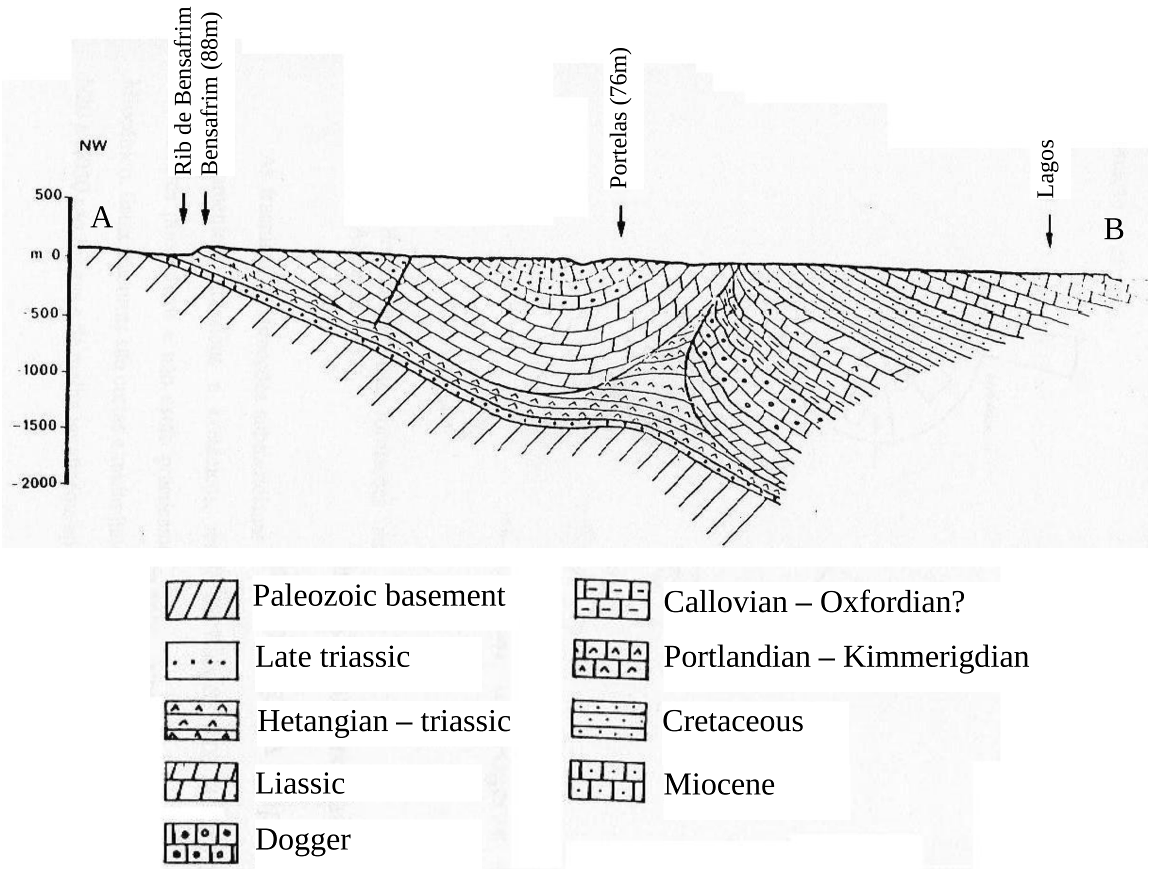

Figure 2 – Geologic cross section between Bensafrim and Lagos (signalled as a dashed line on **Figure 1**. Adapted from Reis (1993).

The lithologies supporting the AO, according to the previously referred authors, as well as the AO geometric limits, as defined by Almeida *et al*. (2000), are represented on **Figure 3**.

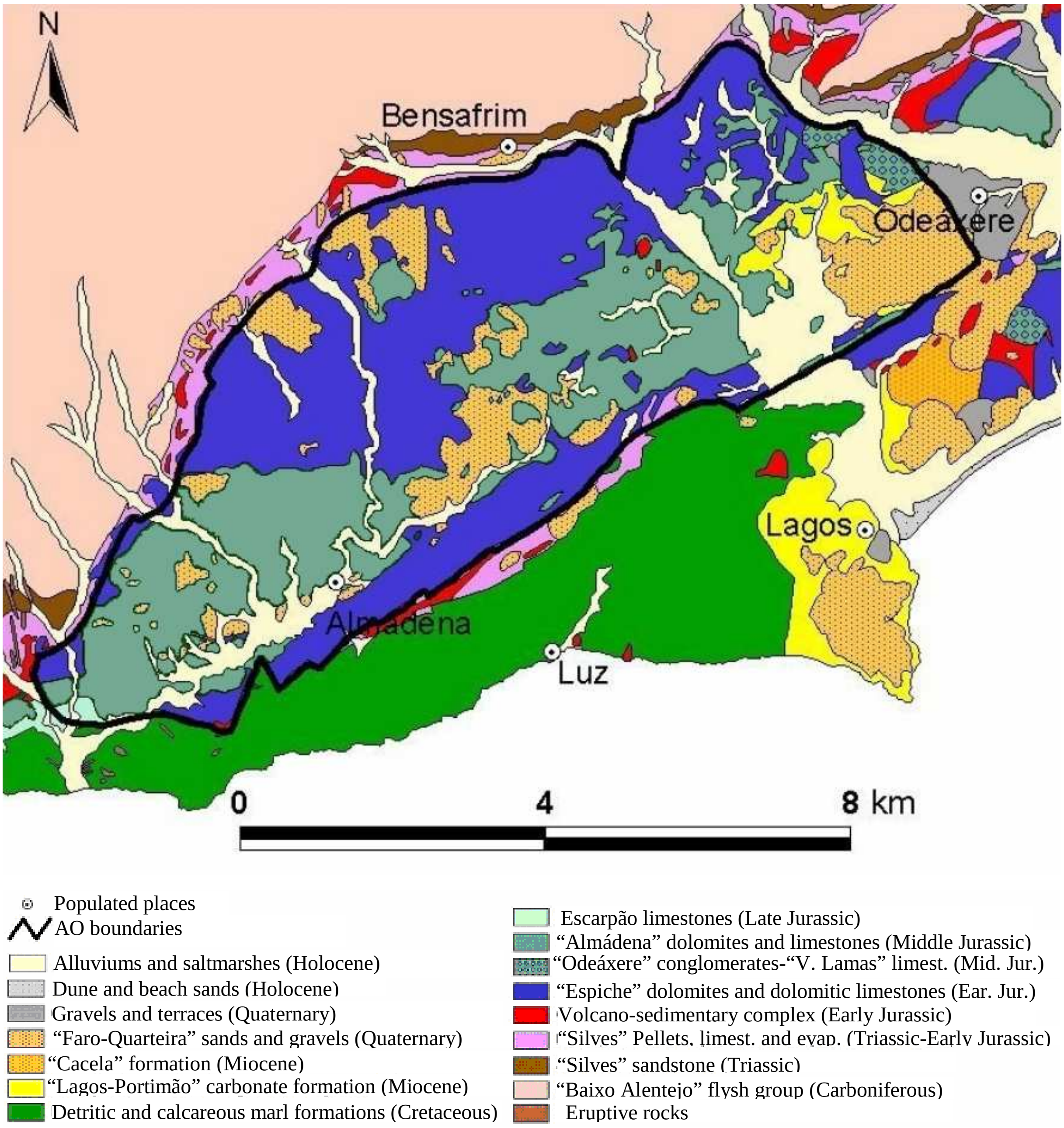

Figure 3 – Lithologies supporting the AO and geometric limits. Adapted from: Almeida *et al.* (2000).

As can be observed on **Figure 3**, Jurassic outcrops are abundant throughout the aquifer area, except for the SE edge and a few areas in the central section.

2.3. Precipitation

Yearly average precipitation values were obtained at SNIRH (National Service of Information on Water Resources) (SNIRH, 2007a) for the Lagos gauge, which is the closest gauge to AO (**Figure 4**), considering the 1959/60-2005/2006 hydrologic years period. Some of these values were replaced (1959/60-1984/85 period) by the precipitation values obtained by Reis (1993) for the same gauge, which were corrected using a multivariate regression model and were therefore considered to be more reliable for the observation of the variation of precipitation along the selected period.

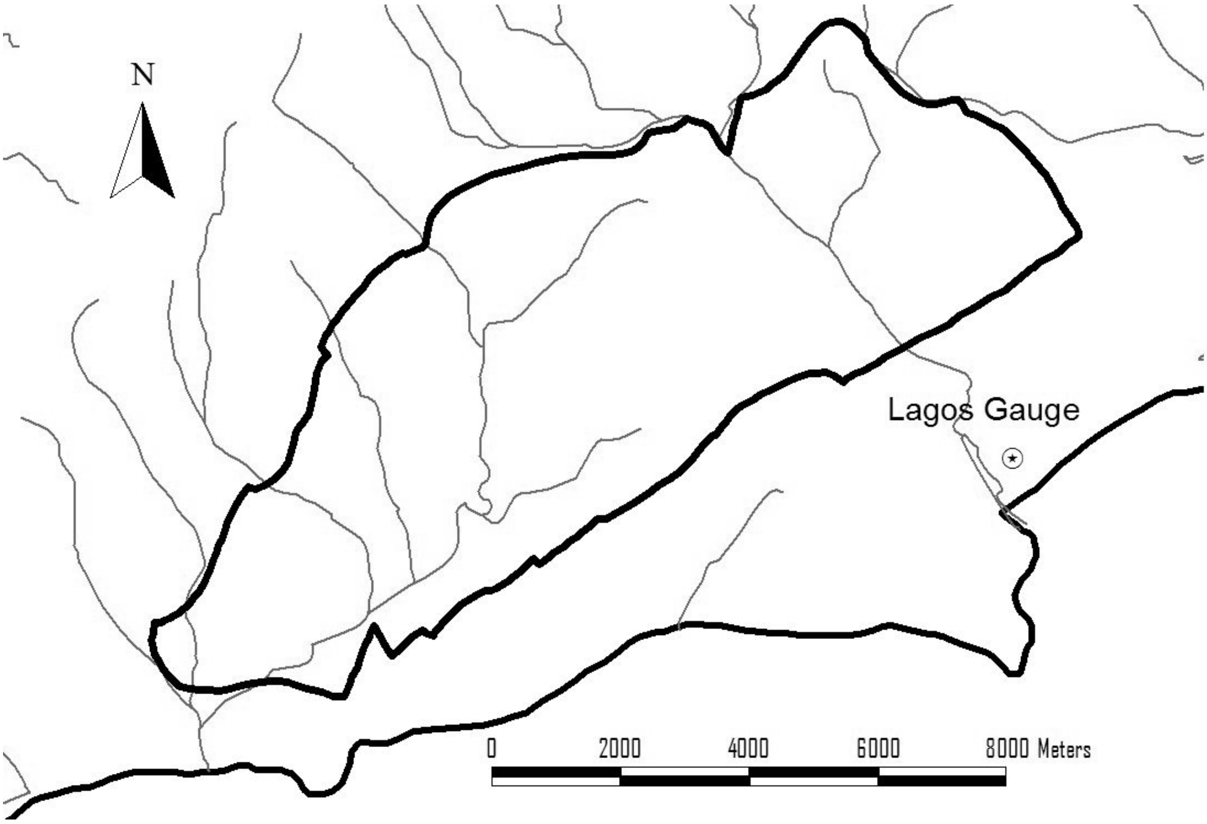

Figure 4 –Location of the Lagos gauge and hydrologic network.

These values ranged from 203,8 mm (in 2004/05) to 1035,9 mm (in 1989/90) as can be seen on **Figure 5**. The precipitation data reveals the existence of dry years intercalated with wet years, abruptly in an irregular patter occurring with 2 to 5 years lapses.

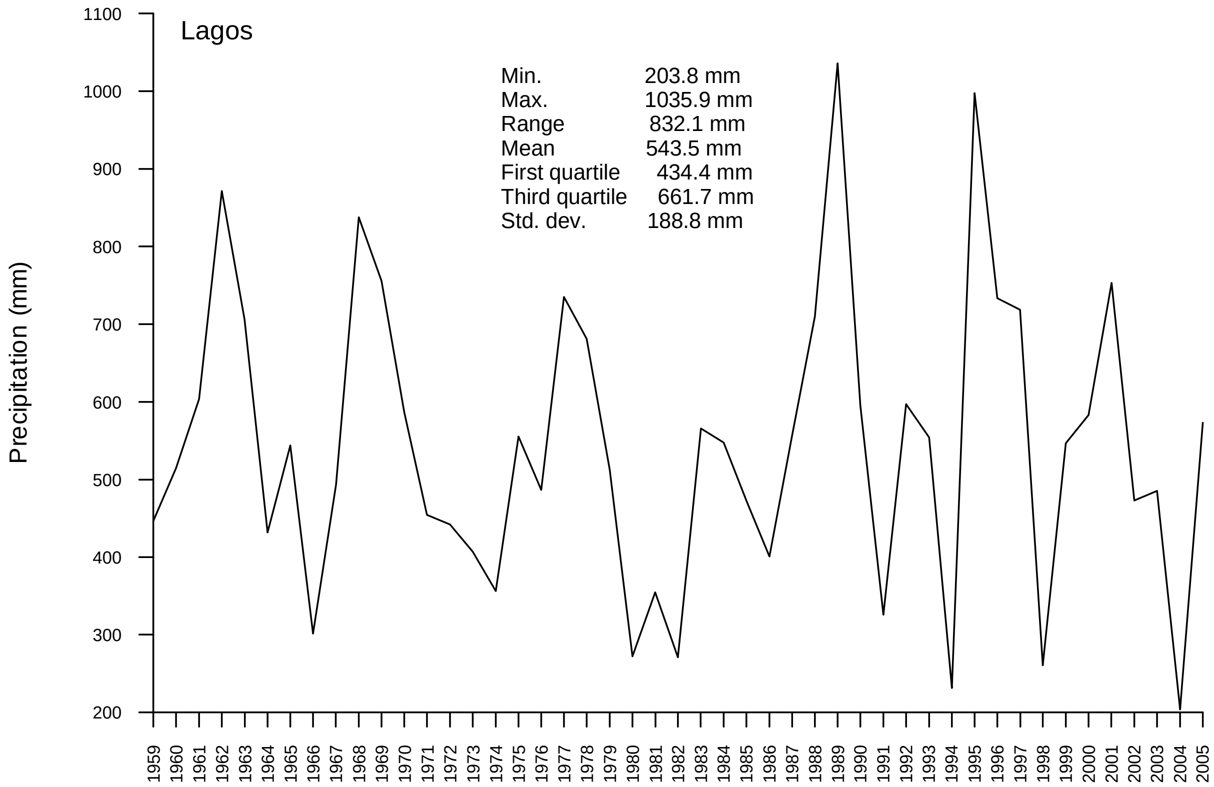

Figure 5 – Yearly average precipitation at the Lagos gauge, for the 1959/60 – 2005/06 precipitation series. Source SNIRH (2007a).

Recently, new average precipitation values were calculated by Nicolau (2002) for Portugal. These values were obtained using an orthogonal grid with a resolution of 1 km × 1 km and calculated by Kriging, using elevation as an external drift, as this method proofs to be the better-suited option from among different auxiliary variables and resolutions for the characterization of the physiographic factors affecting the spatial distribution of rainfall in Portugal.

The average precipitation occurring in the area of the AO, considering the 1959/60-1990/91 period used by Nicolau (2002) is 650 mm/year and its distribution pattern along AO can be observed on **Figure 6**.

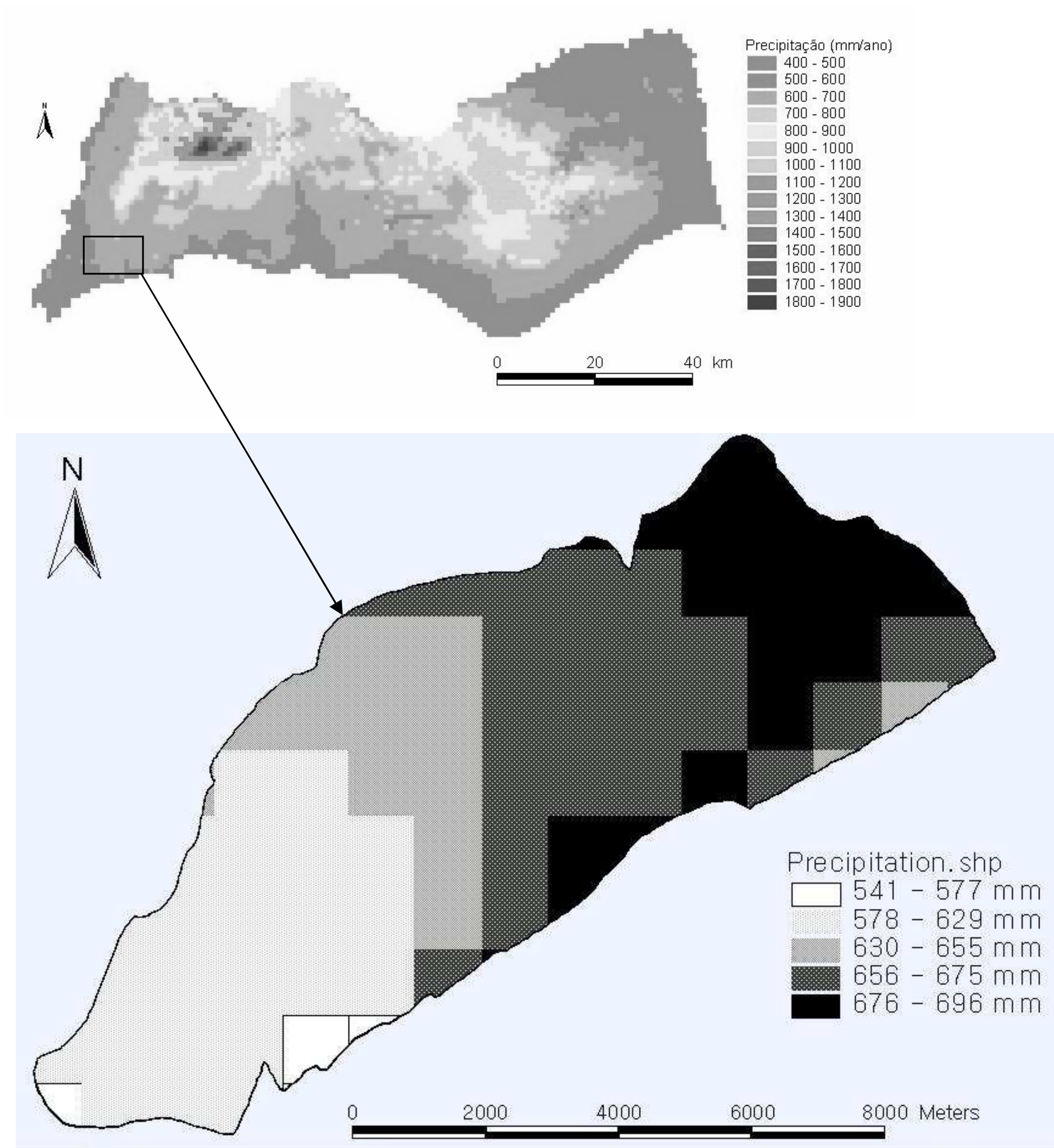

Figure 6–Average annual precipitation. Values extracted from the available data on orthogonal networks for the 1959/1960 – 1990/1991 precipitation series (Nicolau, 2002).

Since these values were considered to be the better suited to characterize the spatial distribution of precipitation on AO, they were later used on the most up-to-date recharge calculations which are presented on the following section.

2.4. Water Budget

2.4.1 Recharge

Recharge at the AO occurs mainly through 2 sources: indirect infiltration from the water flowing on the creeks crossing the system (being the Bensafrim and Odeáxere creeks the most relevant); direct infiltration over the outcrops (Reis, 1993).

The conceptual recharge model used on the flow model adopted on the present work (which does not consider indirect infiltration) considers a recharge rate of 40.3 % of the average precipitation (649 mm/year), occurring on the 63,5 km^2 of the aquifer system, while using the precipitation data made available by Nicolau (2002), which was referred on **Section 2.3.**.

This conceptual recharge model was proposed by Vieira & Monteiro (2003) and Monteiro *et al.* (2003). The recharge rate was obtained from a weighted average having into account the presence of sub-areas where recharge classes range between 5 % and 50 %, depending on the outcropping geologic structures. The recharge value of 40,3 % for all aquifer area is almost the same as the one obtained by Almeida (1985) for Central Algarve aquifers and Reis (1993), for Algarve aquifers Western of the Arade River, which is 40 %. Almeida *et al.* (2000) has later pointed out that recharge rates should stand between 40 % and 60 % for AO. Therefore, the recharge value considered on the conceptual recharge model, which is used on the flow model adopted on the present work, may be considered somewhat conservative.

It is important to point out that these authors defined recharge rates as a percentage of deep infiltration of precipitation according to both the existence of carbonate outcrops and the existence of sectors where carbonate outcrops are covered by different types of sedimentary deposits.

The Kessler (1965) method was applied by these authors in order to quantify recharge in the areas where carbonate outcrops exist. This method was originally developed to estimate recharge in karstic regions in Hungary, taking water consumption by vegetation into consideration. Moreover, Almeida (1985) applied this method in different karstic aquifers in Mediterranean environments showing good correlation with values estimated using other mass balance calculations. The same author calculated the average fraction of precipitation supplying deep recharge on central Algarve aquifers, obtaining values slightly higher than 60%.

Reis (1993), considered precipitation occurring on the 1959/60-1984/85 series (hydrologic years) for the Lagos gauge (**Figure 5**) and calculated for each year the values of the average fraction of precipitation supplying deep recharge in the nearby area of AO. These values ranged from 25,7 % to 83,4 % and average recharge is 62,7 % (**Figure 7**).

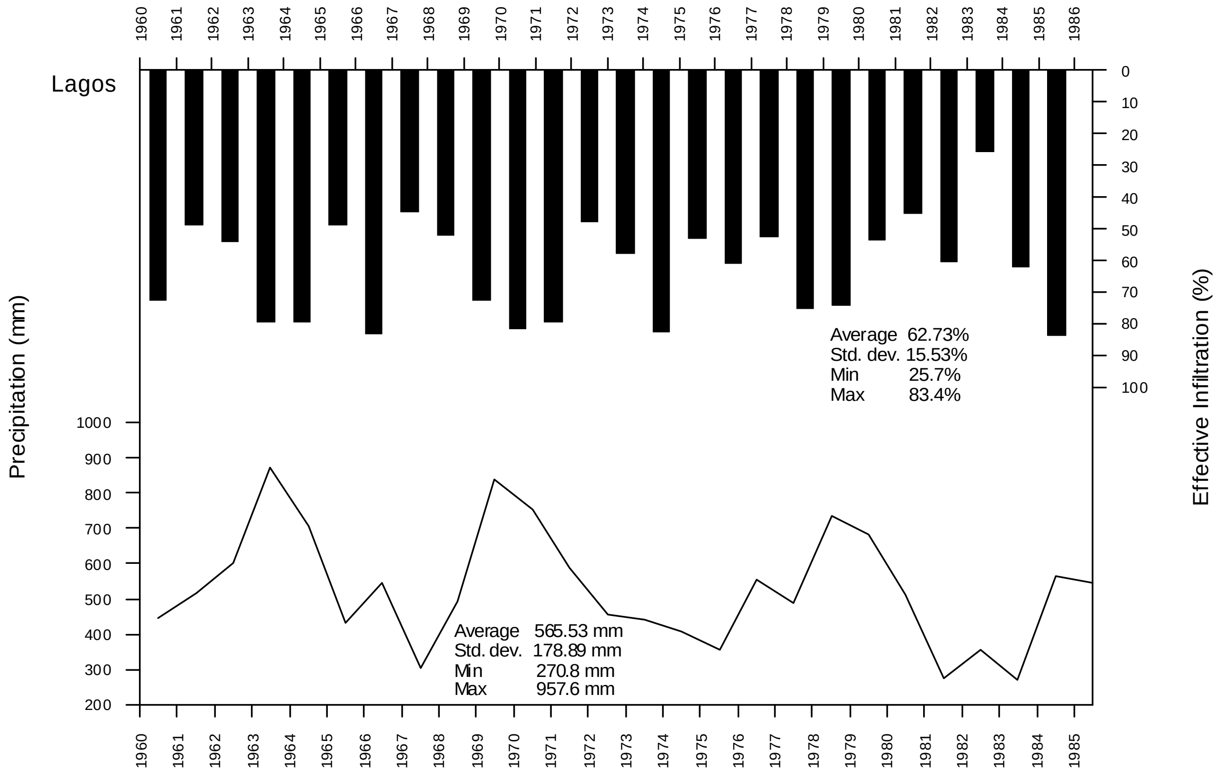

Figure 7 – Recharge calculated applying the Kessler (1965) method using the 1959/60-1984/85 precipitation series for the Lagos gauge.

For the sectors where carbonate rocks are covered by different types of sedimentary deposits, recharge rates were estimated on previous works with basis on the convergence of calculated values of potential and actual evapotranspiration, using methods that consider the transient mass balance of water storage in the soil for different values of field capacity. These techniques were actually extensively applied in the southern area of Portugal and showed a good adaptation of the particular climatic conditions of the region (Almeida, 1985; Andrade 1989). Almeida (1985) which used the Turc (1955), Thornthwaite (1948) and Coutagne (1954) methods, points out a value of 38,5 % for the value of precipitation feeding the aquifers of Central Algarve (although not for AO).

Using the Penman (1948) and Tornthwaite (1948) methods, Reis (1993) has implicitly obtained recharge rates ranging from 13 % to 32 % for the area of influence of the Lagos gauge, considering an average precipitation of 565,5 mm and a gauge area of influence of 35,3 km^2 (containing 14 km^2 of sediment-covered carbonate rocks).

If a recharge rate value of 40 % (Reis, 1993; Almeida, 1985) should be considered for the whole area of the aquifer, an average recharge of 13,8 hm^3/year is to be expected. According to the research work carried out by Almeida *et al.* (2000), considering the aquifer system's area, the mean renewable resources should stand between 16 and 24 hm^3/year.

The calculation of these first recharge estimates considered precipitation values with low spatial resolution because they relied either on the isoiethal or on the Thiessen polygons method. Vieira & Monteiro (2003), on the other hand took into consideration precipitation values available on the orthogonal networks made available by the work of Nicolau (2002), as well as the fraction of precipitation assumed to occur for each one of the outcroping on the aquifer area. Hence the calculated recharge for AO, according to this method, corresponded to 16,6 hm^3/year, which stands inside the series of recharge values proposed on previous works.

In conclusion, it seems acceptable to consider the recharge rate value of 40,3 % for the whole area of the aquifer, as is proposed on the conceptual recharge model used on the flow model, which is adopted on the present work.

2.4.2 Natural Discharge Areas

The only known flow values concerning springs in the AO area are mentioned by Reis (1993) that suggested that 2,6 hm^3/year (300 m^3/h) should be the drained volume in springs near the Bensafrim creek, south of Sargaçal, on February, 1992.

The most important natural discharge areas (**Figure 8**) exist near the Bensafrim creek, which consists of the main draining axis of the aquifer system. There are exsurgencies in the left bank as well as in the right bank of this creek. One other area which has diffuse discharge is at the SW limit of the AO (Boca do Rio), supplying wetlands (Almeida *et al.*, 2000).

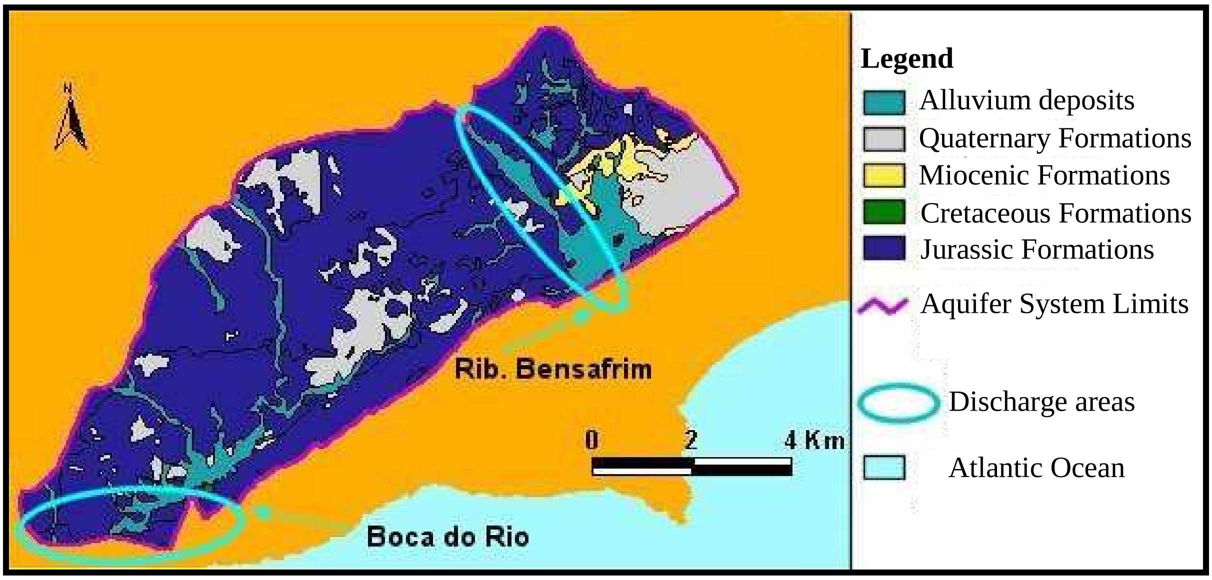

Figure 8 – Geologic setting and position of the main discharge zones of AO. Adapted from Vieira & Monteiro (2003).

2.4.3 Evolution of Water Use

According to Almeida *et al.* (2000) the system's productivity, obtained from a statistical analysis (performed on 11 boreholes) ranges from 0,3 to 50 l/s, with an average of 8 l/s. The main boreholes used for public water supply at AO and respective withdrawal capacity (values acknowledged by the year 2005) according to Nunes *et al.* (2006) are shown on **Table 1**. The location of these boreholes is presented on **Figure 9**.

Table 1 – Main boreholes extracting water for public supply at the AO. Source: Nunes *et al*. (2006).

CCDR Code	Reference	COORD_M	COORD_P	Withdrawal capacity (l/s)	Service Provider
602/9	FD3-Almádena	144060	14700	25	Águas do Algarve S.A.
602/112	JK8-Almádena	143370	15370	60	Águas do Algarve S.A.
602/10	LF11-Almádena	143870	14710	25	Águas do Algarve S.A.
602/78	LF5-Portelas	151350	18200	22	CM Lagos
602/12	LF0-Almádena	142664	14298	12	CM Vila do Bispo
602/35	LF1-Almádena	142567	14416	20	CM Vila do Bispo

Figure 9 – Position of the main boreholes extracting water for public supply at the AO. Three Águas do Algarve, S.A. boreholes (black dots), two Vila do Bispo's Municipality boreholes (light grey triangles) and one Lagos' Municipality borehole (black cross.)

According to Reis (1993), the sum of withdrawals made by the Vila do Bispo Municipality at AO, in 1989, stands in the region of 0,41 hm^3/year and the sum of withdrawals for the Lagos Municipality at AO, in 1990, are roughly 3,6 hm^3/year. Furthermore, Almeida *et al.* (2000) mentions that by 1993, withdrawals for public supply occurring at AO were approximately 3,8 hm^3 and reached 4 hm^3/year in 2000.

Withdrawals for irrigation and private supply in 2000 have the value of 1,3 hm^3/year, according to an inventory of DRAOT Algarve which covers approximately half of the known boreholes. It is natural that, therefore, total withdrawals should double that value for this year, reaching 2,6 hm^3/year (Almeida *et al*., 2000).

Considering the mean annual precipitation, for data collected at the Lagos gauge from 1989 to 2005 (civil years), the aquifer area (63,5 km^2) and a recharge rate of 40,3 %, assumed on the conceptual recharge model used on the adopted flow model, the water budget of AO is shown on **Table 1,** were an estimation of pumping/recharge ratio for the aquifer is presented.

On this estimation, it is assumed that total withdrawals for public supply considered for the years of 1989 and 1990 correspond to the sum of withdrawals carried out by the Lagos and

Vila do Bispo municipalities occurring in 1990 and 1989 respectively (Reis, 1993). Total withdrawals occurring on 1993 and 2000 (Almeida *et al.*, 2000) are extrapolated from 1991 to 1992, and 1994 to 1999 respectively. Values from 2001 onward correspond to withdrawal values available at Nunes *et al*. (2006) for the AO.

It is also assumed that withdrawals for irrigation and private supply from 1989 to 2005 have a constant value of 2,6 hm^3/year ($2{,}6\times10^6$ m^3/year). The term "withdrawals" on **Table 2** thus comprises the sum of withdrawals for public water supply and withdrawals for irrigation and private supply.

Table 2 – Water budget and estimation of the pumping/recharge ratio for AO, considering the average annual precipitation occurring in the Lagos gauge from 1989 to 2005. The aquifer area is 63.5 km^2. Years having a hydraulic deficit are highlighted. Recharge is considered to be 40.3 % of precipitation.

Year	Precipitation (mm)	Recharge (m^3/year $\times10^6$)	Withrawals (m^3/year $\times10^6$)	Pumping/recharge ratio (%)
1989	1097,7	28,02	6,6	23,66
1990	553,9	14,14	6,6	46,88
1991	436,5	11,14	9,4	84,36
1992	422	10,77	9,4	87,26
1993	638,4	16,30	9,4	57,68
1994	317	8,09	9,6	118,63
1995	498,8	12,73	9,6	75,40
1996	1016,6	25,95	9,6	36,99
1997	787,9	20,11	9,6	47,73
1998	354,6	9,05	9,6	106,06
1999	399,2	10,19	9,6	94,21
2000	611,2	15,60	9,6	61,53
2001	720	18,38	9,6	52,23
2002	590,9	15,08	3,0	19,60
2003	602,4	15,38	2,9	19,14
2004	254,8	6,50	2,6	40,24
2005	361,5	9,23	3,2	34,18

The data presented on **Table 2** indicates that, there is a possibility that hydraulic deficit has occurred for the years of 1994 and 1998 given the relation between water inflow and outflow on the aquifer system. From the year 2000 onwards, the pumping/recharge ratio has diminished gradually, mainly because the public water supply at the Lagos and Vila do Bispo Municipalities has changed its origin from groundwater (withdrawing water from AO, and having the municipalities as service providers) to surface water (withdrawing water from the Bravura dam, N of Sargaçal, and having the Águas do Algarve S.A. company as service provider).

During 2004 and 2005 a severe drought has affected Portugal. Along with lower values of precipitation, the public water supply from the Bravura dam has diminished, forcing an increase on the use of boreholes at AO, which explains the higher pumping/recharge ratio.

Considering the current water use, there is a high chance that AO is being underexploited, since withdrawals for irrigation must have also shifted its source of water from groundwater to surface water (in fact withdrawals for 2000 onwards, shown on the water budget, are probably lower at AO because of this fact).

It must be taken in consideration that the recharge value (40,3 %) adopted for the water budget calculations may be considered somewhat conservative, bearing in mind that recharge values referred on previous works (**Section 2.4.1**) range from 40 % up to 60 % which means not only the estimated hydraulic deficit on 1994 and 1998 has a high chance of not ever having occurred, but also that the aquifer's available water reserves may be underestimated on this analysis.

2.5. Piezometric data

2.5.1. Analysis of Historical data

Historical information on piezometric levels (acquired form March 1978 to February 2007) was gathered from data made available at two sources: the SNIRH website (SNIRH, 2007b) and at the Lagos Municipality (Environment and Water resources Department). This data was collected manually on 19 observation points. The observation points' CCDR ("Comissão de Cooordenação e Desenvolvimento Regional") reference, borehole reference, coordinates (Portuguese Military Coordinates, Lisbon Datum) and statistical data are presented on **Table 3.**

Table 3 – Observation points composing the historical data network.

CCDR Ref.	Borehole Ref.	X Coordinate	Y Coordinate	Max.	Min.	Mean	Range
593/5	-	149150	22050	22,73	18,48	19,79	4,25
594/400	-	152345	20470	4,10	1,77	3,15	2,33
602/32	LF9	142640	14260	7,68	1,56	5,64	6,12
602/36	LF10	142500	14270	7,65	1,09	4,52	6,56
602/43	-	144320	14550	6,12	1,75	3,86	4,37
602/76	-	149200	19450	8,53	0,88	3,89	9,05
602/178	-	145350	19250	7,23	2,51	5,45	4,72
602/187	-	150350	19100	5,33	1,13	3,11	4,20
602/242	-	146980	17100	6,98	1,86	4,67	5,12
602/311	-	144000	17130	7,31	1,48	4,53	5,83
603/38	-	152350	19020	5,00	0,25	2,56	4,75
602/78	LF5	151334	18172	3,95	-0,28	1,93	4,23
602/4	LF1	150016	18015	5,76	3,92	5,03	1,84
602/5	LF2	150033	18024	5,89	3,76	5,19	2,13
602/6	LF6	149812	18324	5,27	4,10	5,04	1,17
602/8	LF8	149806	18323	5,27	4,11	4,58	1,16
602/9	FD3	144016	14667	4,27	3,30	3,90	0,97
602/10	LF11	143898	14670	4,57	3,72	4,24	0,85

The location of the observation points constituting the historical piezometric network is presented on **Figure 10**. Historical head variations occurring at these points were analysed for the entire existent data records (from 1978 to 2007) nevertheless, only a fraction of this information (1989 to 2007 period) is presented on **Figure 11** since this information reflects the most recent variations on the aquifer’s piezometric surface , allowing for that reason an easier data interpretation.

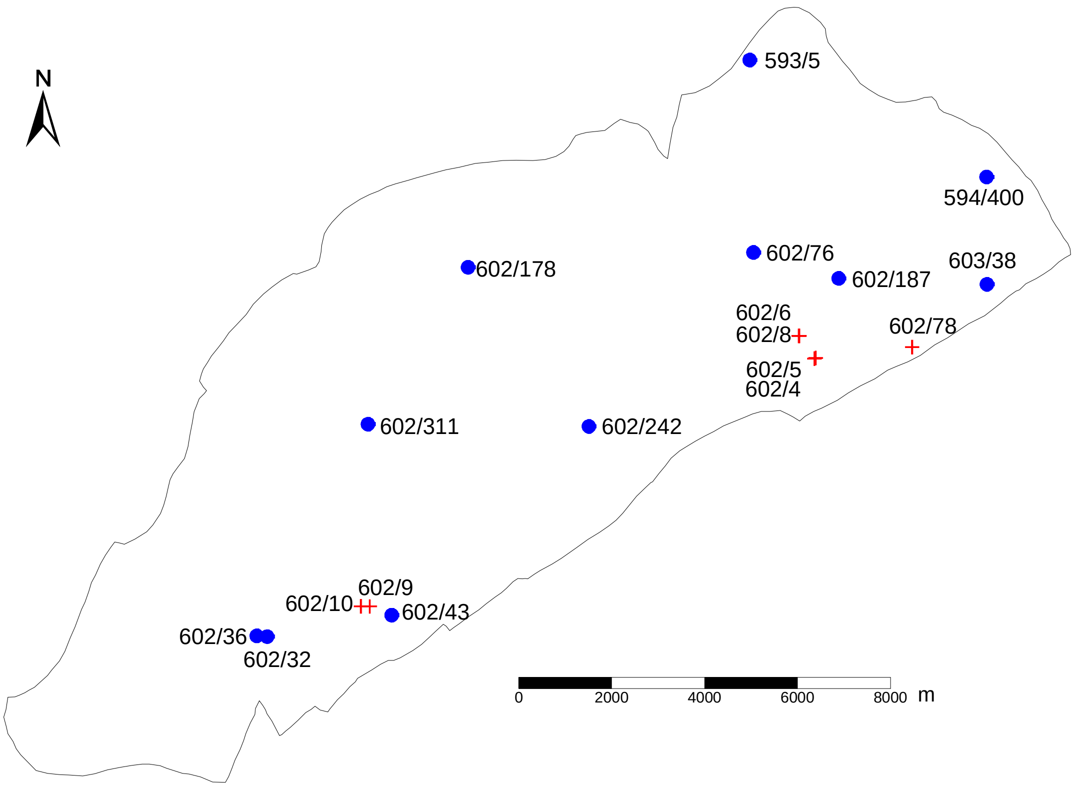

Figure 10 – Location of the historical data observation points. Observation points with data provided by INAG are represented by blue dots. Red crosses represent observation points with data made available by the Lagos Municipality.

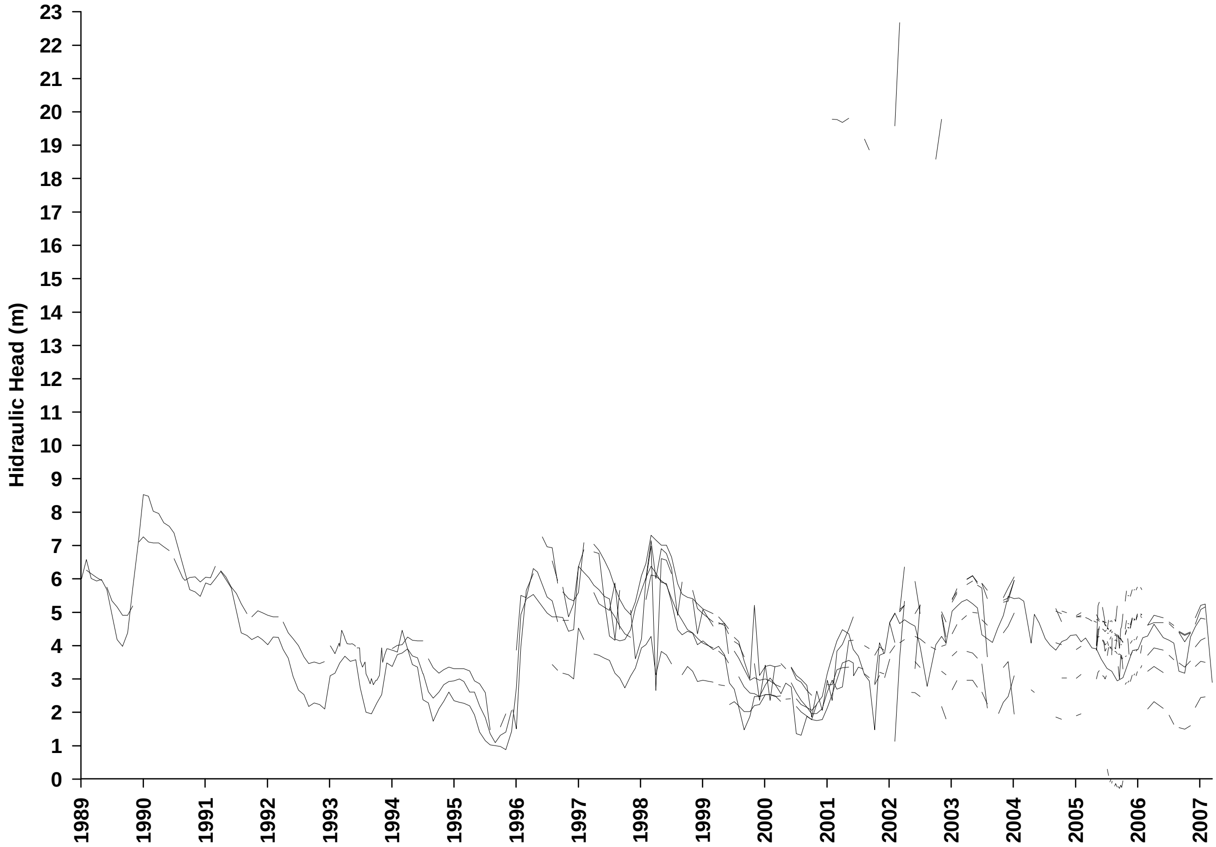

Figure 11 – Piezometric levels, from 1989 to 2007, obtained at 19 observation points located at AO.

The analysis on historical data hasn’t revealed significant variations at the water level. This indicates that the aquifer system has a high regulating power. It is relevant to point out that there is one observation point (CCDR ref. 602/78) where piezometric levels have remained below zero head values (i.e. below the average sea level) for a 3 month period (from July to October) in 2005. This stretch of time matches one of the most intensive periods of the 2004/2005 drought period which affected the entire Algarve region.

The observation point “602/78” (CCDR ref.) reveals the highest head values occurring at AO, and it located at the NE edge of the aquifer. It was therefore presumed that this area should be a recharge area with particularly low transmissivity values.

Subsequently, regional spatial head distribution patterns were analysed through the use of piezometric contours, with the objective of getting a better perspective of which are the dominant groundwater flow directions. Several piezometric contour maps were elaborated, using historical minimum, mean, median and maximum head values, and mean values for certain time periods (e.g. wet semesters/dry semesters, drought periods). On **Figure 12** an illustration of one of these contour maps, elaborated with basis on median historical values for the whole historical period 19 is presented, because of it’s relevance on the interpretation of the available data.

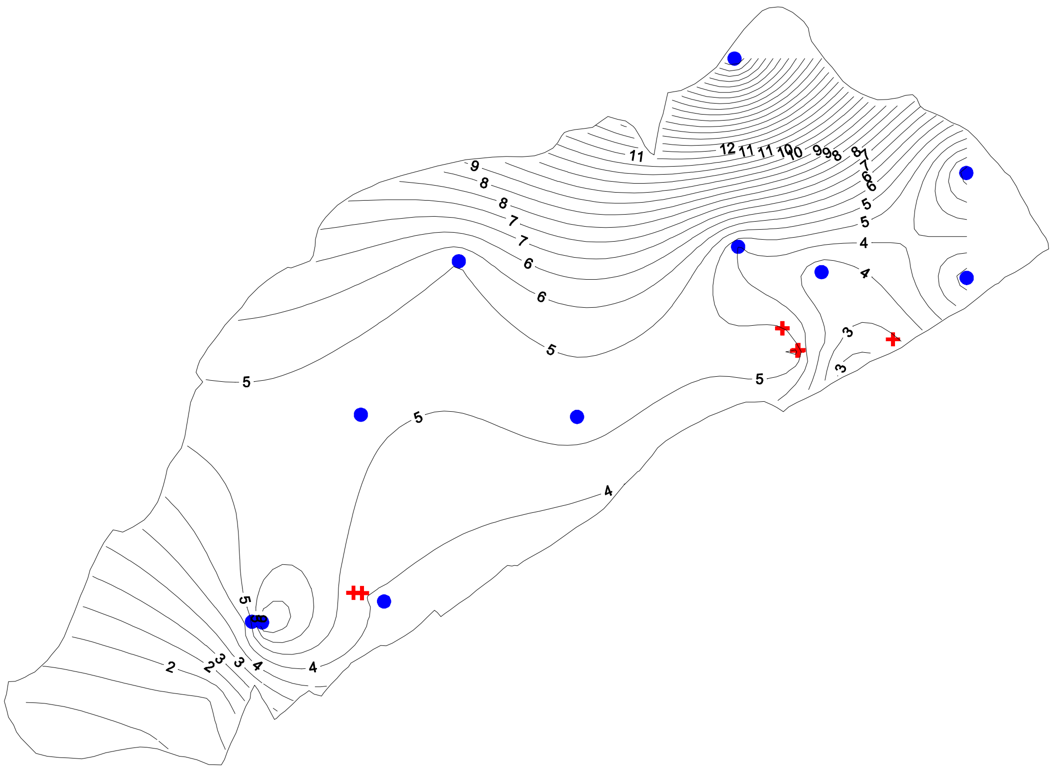

Figure 12 – Contours of the historical heads. Observation points with data provided by INAG are represented by blue dots. Red crosses represent observation points with data made available by the Lagos Municipality.

An analysis of the piezometric contour shows that the hydraulic gradient is higher on the NE part of the aquifer and lower at the two natural discharge areas, identified on **Section 2.4.2.**, which are situated at the SW limit of AO ("Boca do Rio") and at the "Ribeira de Bensafrim" (creek) estuary, SSE of AO. Regional flow should occur predominantly from NE to SW, with a slight local divergence SSE at the right section of AO. Surprisingly, a gradient occurring N to S can be identified on the middle section of AO, which according to the conceptual model shouldn't happen. At this point, the available data was considered insufficient for a coherent interpretation of the spatial head distribution.

Since extra field data was needed, additional field collection efforts were made. These efforts are presented on the next section.

2.5.2. Contribution of collected data for the improvement of the potenciometric analysis

Due to the lack of coverage on important aquifer sectors, an additional automatic piezometric network was designed and implemented at AO as part of the undergoing activities of the "POCTI/AMB/57432/2004" investigation project. Piezometric data was collected through the use of data loggers installed in 10 boreholes, distributed along aquifer sectors with less coverage (**Figure 13**); these data loggers acquired data within 2 hours time steps, from March 2007 to July 2007.

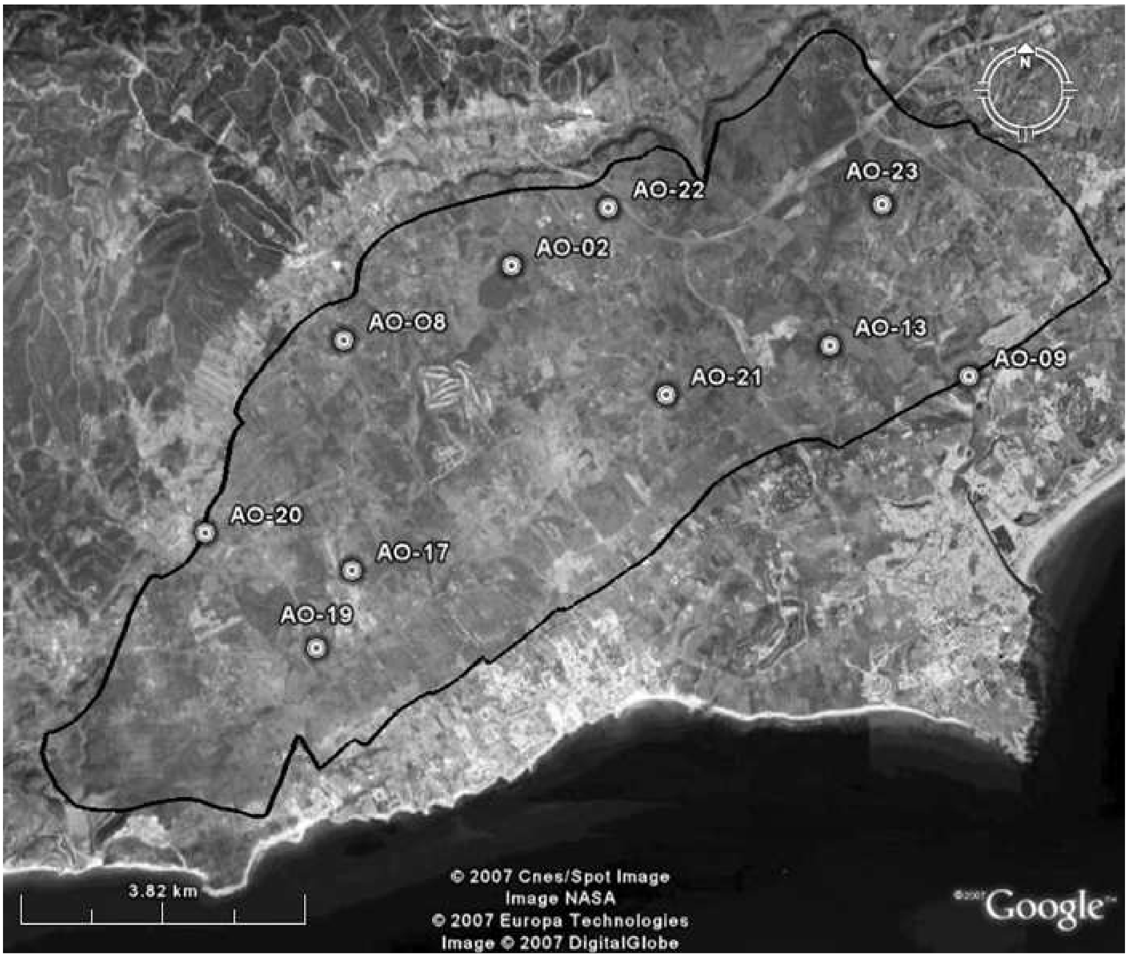

Figure 12 – Established network of automatic observation points. Image Source: Google Earth.

Manual data was also acquired within this process, for assessment of data quality, namely error measuring (**Figure 14**).

Figure 14 – Field collection of manual (left) and automatic data (right).

The observation points’ fieldwork reference, CCDR (“Comissão de Cooordenação e Desenvolvimento Regional”) reference, borehole reference, coordinates (Portuguese Military Coordinates, Lisbon Datum) and statistical data are presented on **Table 4**.

Table 4 – Observation points composing the Historical data network.

Fieldwork Ref.	CCDR Ref.	Borehole Ref.	X Coordinate	Y Coordinate	Max.	Min.	Mean	Range
AO-02	602/178	-	145350	19250	7,23	2,51	5,45	4,72
AO-08	-	-	143286	18416	5,14	4,10	4,77	1,04
AO-09	602/79	LF4	151565	17965	0,85	0,45	0,65	0,40
AO-13	602/6	LF6	149812	18324	5,27	4,10	5,04	1,17
AO-17	602/112	JK8	143376	15328	8,54	4,36	5,7	4,18
AO-19	-	-	142900	14298	5,09	4,52	4,82	0,57
AO-20	-	-	141418	15851	5,16	4,24	5,03	0,92
AO-21	-	-	147622	17601	3,95	3,44	3,66	0,51
AO-22	-	-	146846	20185	4,55	4,11	4,23	0,44
AO-23	-	-	150524	20210	5,33	3,34	3,88	1,99

After setting up these additional observation points, wider aquifer coverage was accomplished, enabling a better interpretation of the spatial head distribution, because at this point the available information consisted of historical data made available by official institutions from March 1978 to February 2007 and data collected automatically, through fieldwork, from March 2007 to July 2007. The resulting observation point coverage can be observed on **Figure 15**.

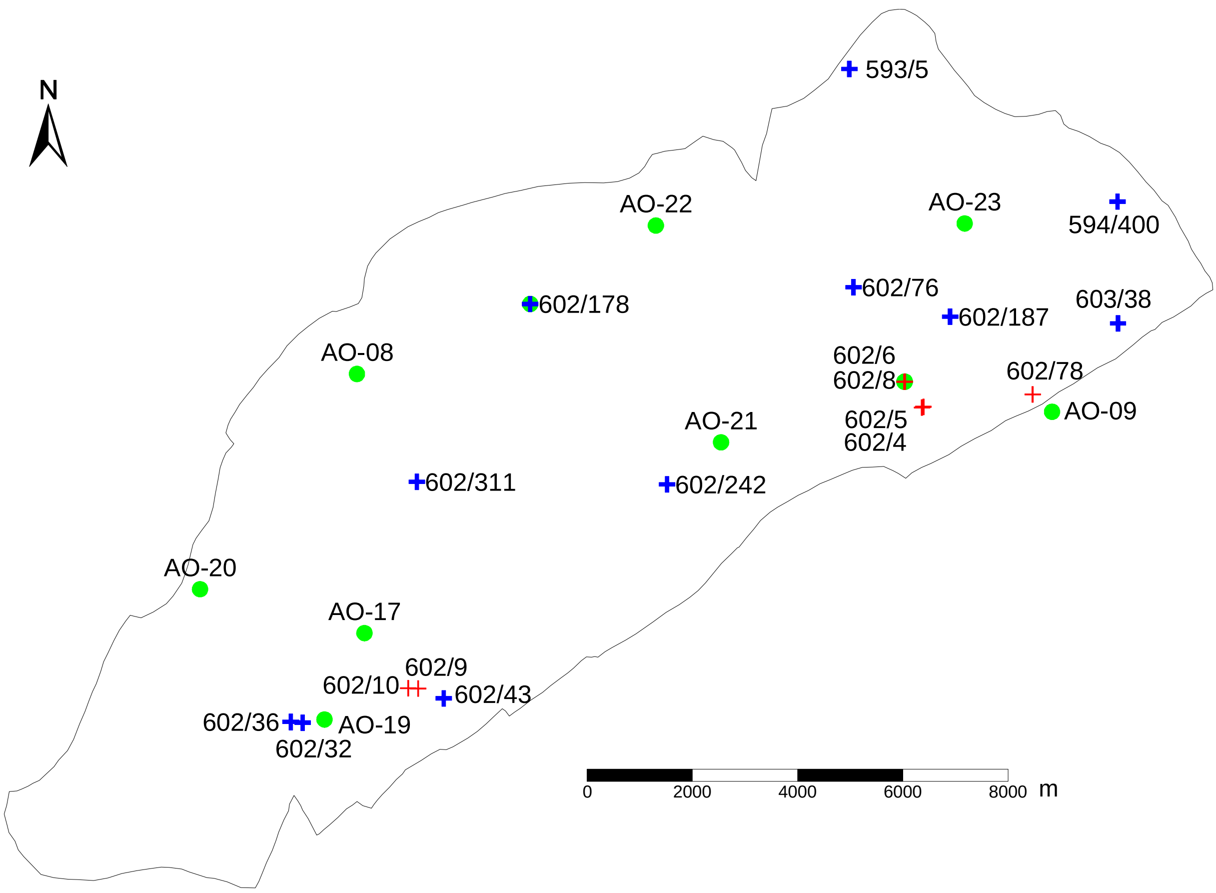

Figure 15 – Location of the data observation points. The data provided by INAG is indicated by the blue crosses. The red crosses represent the data made available by the Lagos Municipality. New automatically collected data is represented by the green dots.

The recently acquired piezometric data (**Figure 16)** was analysed in addition to existing data with the purpose of improving the information concerning flow directions and hydraulic head data variations. Only manually collected piezometric data was obtained at borehole Ref. AO-17 due to the occurrence of a technical impediment.

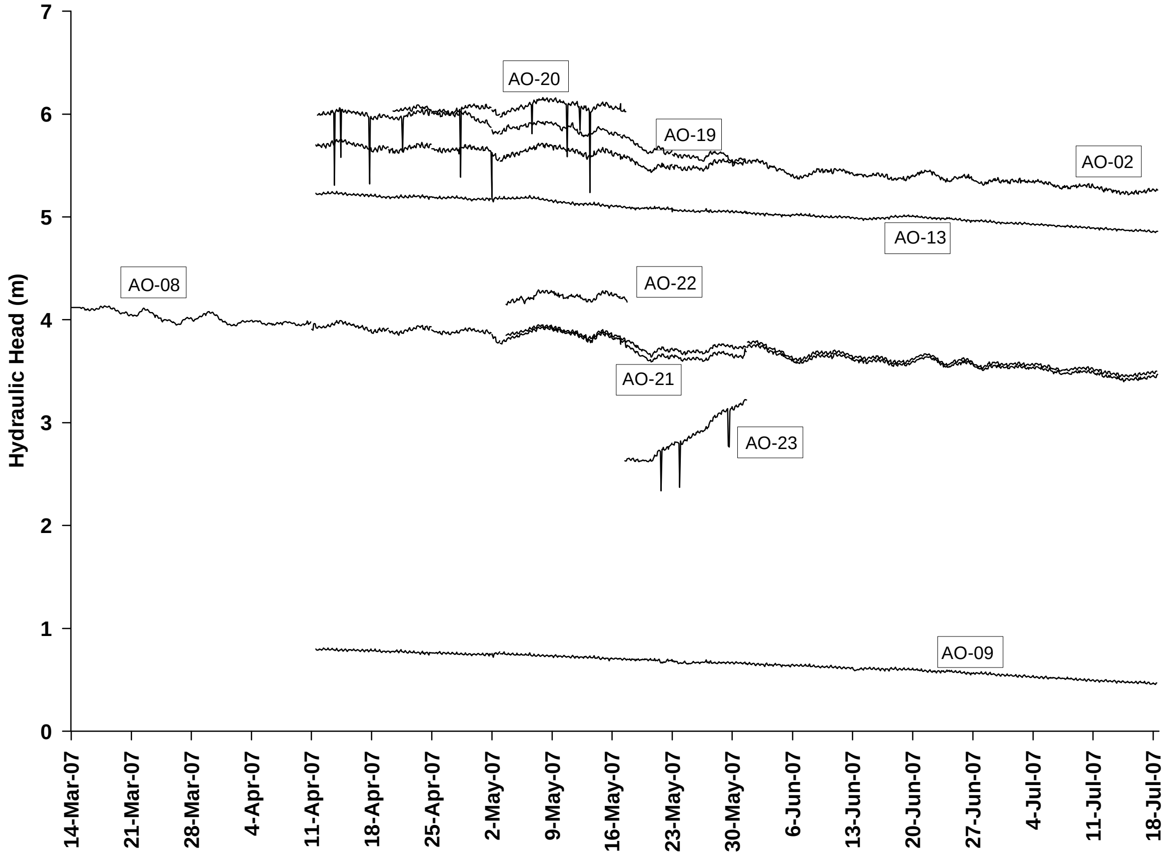

Figure 16 – Piezometric levels, from March 2007 to July 2007, obtained at 9 of the 10 observation points located at AO.

This quality improvement helped the elaboration of piezometric contours (**Figure 17**) showing higher coherence with the proposed conceptual regional model. The contours showed that regional fluid flows predominantly from NE (recharge area) to SW (discharge area of “Boca do Rio”). A N (recharge area) to S (discharge area at the estuary of the “Ribeira de Bensafrim” creek) flow can also be identified on the right section of AO.

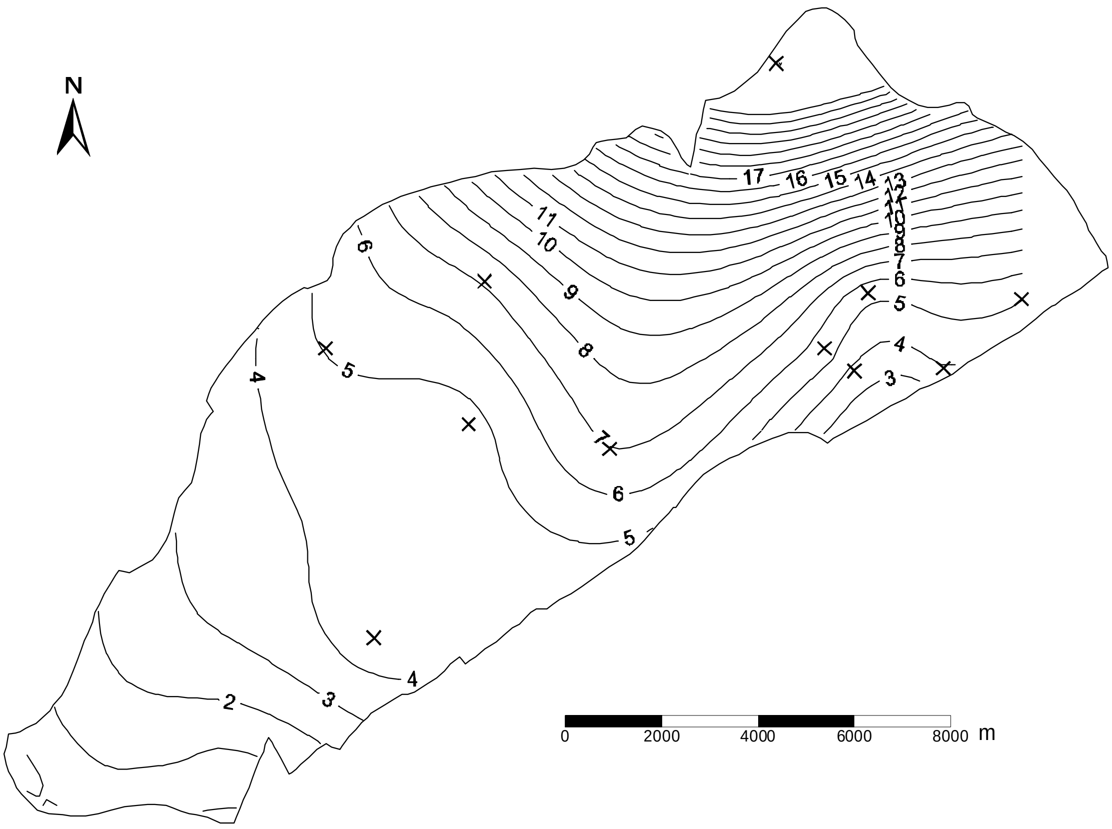

Figure 17 – Contours of the analysed heads. The selected points used for contouring are shown as “x” marks.

The elaboration of these contours contributed a great deal for the subsequent definition of constant transmissivity zones inside AO which allowed to distinguishing the hydraulic behaviour of different hidroestratigraphic units integrating the aquifer system. The subdivision of these zones took place on the basis of the character of the piezometric contours since there is little obvious variation in geology throughout the study area.

3. General framework of the modelling process

The physical principles supporting the simulation of the hydraulic behaviour of the aquifer system are thoroughly explained by Huyakorn & Pinder (1983). In this section, a brief description is presented, according to Monteiro (2001):

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)+Q=S_s\frac{\partial h}{\partial t} \tag{1}$$

where:

- K_{xx}, K_{yy} and K_{zz} are the values of hydraulic conductivity [LT^{-1}] along the x, y and z Cartesian axis that are assumed to be parallel to the directions of greater hydraulic conductivity, h is the hydraulic potential [L], Q is a volumetric flux per volume unit [$L^{3}T^{-1}L^{-3}$] that represents fluid gains and losses and S_s is the specific storage, necessary to simulate transient variations on the reserved volume of water [L^{-1}].

Hydraulic conductivity is defined by the expression:

$$K=\frac{\rho g k}{\mu} \tag{2}$$

where ρ is the water density [ML^{-3}]; g is the gravity's acceleration [LT^{-2}]; k is the intrinsic or geometric permeability [L^2] and μ is the dynamic viscosity [$ML^{-1}T^{-1}$];

The piezometric level, also denominated as hydraulic potential (h, [L]), corresponds to the energy each mass unit of the fluid, if kinetic energy is neglected, and it is expressed as the sum of the elevation potential, z [L] of the fluid and the pressure potential, p [$ML^{-1}T^{-2}$] at a given point:

$$h=\left(\frac{p}{\rho g}\right)+z \tag{3}$$

Specific storage [L^{-1}] is defined by the expression:

$$S_s=\rho g\left(\alpha+n\beta\right) \tag{4}$$

Where α is the compressibility of the porous media [LT^2M^{-1}], n is the effective porosity (non-dimensional) and β is the water compressibility [LT^2M^{-1}].

Equation (1) is frequently expressed on a simplified manner, using the divergence and gradient differential operators:

$$S_s \frac{\partial h}{\partial t} + div\left(-[K]\overrightarrow{grad}\, h\right) = Q \tag{5}$$

While describing the particular case of flow on permanent regime, the variables are time-independent. On this case, equation (5) is reduced to equation (6):

$$div\left(-[K]\overrightarrow{grad}\, h\right) = Q \tag{6}$$

The parameter's dimensional analysis shown before is only valid for 3D elements. An oversimplification is necessary for the simulation of flow on bi-dimensional and one-dimensional spaces. The discretization technique used to simulate the hydraulic running of the aquifer on the scope of the present study encompasses the use of linear bi-dimensional finite elements with three nodes. On this case, the conductive parameter used is transmissivity, T [L^2T^{-1}], which is obtained multiplying K by the aquifer's saturated thickness.

$$div\left(-[\mathrm{T}]\,\overrightarrow{grad}\, h\right) + Q = 0 \tag{7}$$

The total simulated budget will be equal to zero, because a medium permanent state of the aquifer is represented, i.e., recharge and discharge have the same value at the flow domain global scale.

For transitory simulations the capacitive three-dimensional parameter described before, S_s [L^{-1}], is replaced for the storage coefficient S [-] that is obtained multiplying S_s by the aquifer's saturated thickness.

4. Methodology of inverse calibration of the flow model

On this section the concepts associated to the inverse method and the calibration software PEST (Doherty 2002) will be described in detail.

The use of inverse models, such as the non-linear least-squares regression, enhances the analysis scope for groundwater flow models. Nowadays the most significant limitation to using this technique is due to the lack of information on the necessary requisites for its implementation, as well as on the benefits it brings.

The benefits obtained through the use of inverse models can be presented in the following manner (Poeter & Hill, 1997):

1. Faster determination of best fit parameter values.
2. Quantification of:
    i. Calibration quality;
    ii. Data limitations and needs;
    iii. Confidence limits on parameter estimates and predictions.
3. Identification of issues that are easily overlooked during non-automated calibration.

The use of inverse models eases the assessment on the reliability of prevision due to the fact that results involve not only estimated parameters, hydraulic potentials and flow, but also confidence intervals, applied to both. This amplifies the scope of analysis for results.

Sensibility analysis, standard deviations and correlations can be used as support for evaluating estimated values, as well as the model's calculated results, checking if the data supplied to the model is sufficient or if it is necessary to introduce new data to enhance its performance.

Fundamentally, the calibration process is the same using inverse modelling or manual approaches. In both cases parameter values and other model aspects are adjusted until the dependent variables (heads and flows) match field observations.

The fundamental difference between the two calibration approaches, which is generally referred as the main benefit of inverse modelling, consists on the ability to determine automatically parameter values that produce a better fit between observed and simulated hydraulic heads and flows.

If estimated parameter values corresponding to the best fit are outside the range of expected values, this is a fundamental indication about the validity of the conceptual model and the changes that might be needed.

The time consuming nature of intuitive parameter value adjustment limits the range of alternative constructed models that are considered and, given the lack of rigorous analysis of parameter correlations, variance/covariance, and residuals, there is no assurance that the estimated parameter values for any model are 'the best'. Consequently, conclusive model discrimination is nearly impossible (Poeter & Hill, 1996).

With inverse models used to determine parameter values that optimize the fit of the model results to the field observations for a given model configuration, the modeller is freed from tedious trial-and-error calibration involving changes in parameter values so more time can be spent addressing insightful questions about the hydrologic system (Poeter & Hill, 1996).

4.1. Parameter estimation through inverse modelling

Instead of supplying only model geometry, material properties, and boundary conditions, the modeller can also enter the data used for calibration, i.e., the parameter definition, field observations (for example, measurements of hydraulic heads and flows), independently determined values of the parameters (usually called "prior information"), and variances of the measured hydraulic heads, flows, and parameters.

After implementing the model with initial parameter estimates, an automatic calibration code:

1) determines the differences (residuals) between observed and simulated values of heads, flows, and parameters, at all locations and times in the model; 2) squares the residuals to eliminate negative values and emphasize the larger residuals; 3) weights the importance of

each squared residual by the amount of uncertainty the modeller specifies for each observation, as expressed by the inverse of observation error variances; 4) sums the weighted residuals to obtain an overall measure (an objective function) of how well the field observations match the model simulated values ("goodness of fit"); 5) calculates sensitivities (i.e., how much the simulated heads and/or flows would change given a change in the parameter values); and 6) uses the sensitivities and residuals to adjust the parameter values to minimize the objective function; 7) repeats steps 4 through 6.

4.2. Decreasing parameter correlation and consideration of nonlinearity

Correlation can be calculated between any pair of estimated parameters, using standard linear methods, and can range between -1.0 e +1.0. Absolute values near one indicate that coordinated linear changes in parameter values would cause the same heads and flows at observation points.

Decreasing parameter correlation from 1,0 to 0,98 is typically enough to individually estimate the parameter values.

Flow observations (e.g., groundwater discharge along a stream reach) generally decrease the correlation between parameters that is present in cases where only head observations are available.

Calculated parameter correlations depend on the parameter values because the inverse problem for ground-water flow is nonlinear with respect to most parameters of interest – that is, hydraulic heads and flows are not a linear function of the estimated parameters, so that sensitivities are different for different parameter values.

This nonlinearity is sometimes a confusing concept for ground-water hydrologists because they are used to thinking of the ground-water flow equation as linear when applied to confined layers, a characteristic which allows application of the principle of superposition. That is, however, linearity of the differential equation that relates hydraulic head to space and time given fixed parameters values, not linearity of hydraulic head with respect to parameters.

Independently measured values of the parameters (e.g., transmissivities from aquifer tests) can be used to decrease correlation, and this often is useful in complex problems. In such a case, the objective function includes not only the difference between observed and simulated heads and flows but also the difference between observed and estimated parameter values (Poeter & Hill, 1997).

4.3. The Correlation Coefficient

The correlation coefficient, R provides a measure of the simulation's "goodness of fit", as defined on Cooley & Naff (1990). Unlike the objective function, the correlation coefficient is independent on the number of observations involved in the parameter estimation process, and of the absolute levels of uncertainty associated with those observations. Hence, the use of this measure of goodness of fit allows the results of different parameter estimation exercises to be directly compared.

The correlation coefficient, R, is calculated as (Doherty, 2002):

$$R = \frac{(w_i c_i - m)(w_i c_{oi} - m_o)}{\left[(w_i c_i - m)(w_i c_i - m)(w_i c_{oi} - m_o)(w_i c_{oi} - m_o)\right]^{1/2}} \qquad (8)$$

where:-

c_i is the i'th observation value,

c_{0i} is the model-generated counterpart to the i'th observation value,

m is the mean value of weighted observations, and

m_o is the mean of weighted model-generated counterparts to observations.

Generally, R should be above 0,9 for the fit between model outputs and observations to be acceptable (Hill, 1998).

4.4. Observation errors, weighting, and the calculated error variance

Field observations include error, and model representations are never a perfect reflection of field conditions, thus the minimum sum-of-squared residuals value always is larger than zero in field applications.

To use nonlinear regression, the modeller needs to assign variances (or standard deviations or coefficients of variation that are used to calculate variances) to all observations. The variances can reflect estimated measurement error and, sometimes, model error.

For example, if the modeller estimates that there is a 95 % probability that the true head is within +/-0,5 m of the observed head and that a normal probability distribution applies, then a normal probability distribution table can be used to determine that +/-0,5m is 1,96 standard deviations. Consequently, $1.96\sigma = 0{,}5$m and the standard deviation, σ, is 0,26 m.

The variance is the square of the standard deviation (σ^2), or 0,066 m^2. Each squared residual is weighted by the inverse of the variance (weight = $1/\sigma^2$) before the sum-of-squared residuals value is calculated, so observations which the modeller regards as less prone to error (smaller variance) have more importance in determining the parameter values (Poeter & Hill, 1997).

The objective function, Φ, corresponds to the sum of squared deviations between model outcomes and corresponding field data. The lower it is the better is the model calibrated (Vecchia & Cooley, 1987). **Figure 18** shows contours of the objective function in two-parameter space. In most instances, the region of "allowed parameter space" where the objective function is low enough for the model to be considered as calibrated is long and thin as is shown in the shaded region of this figure.

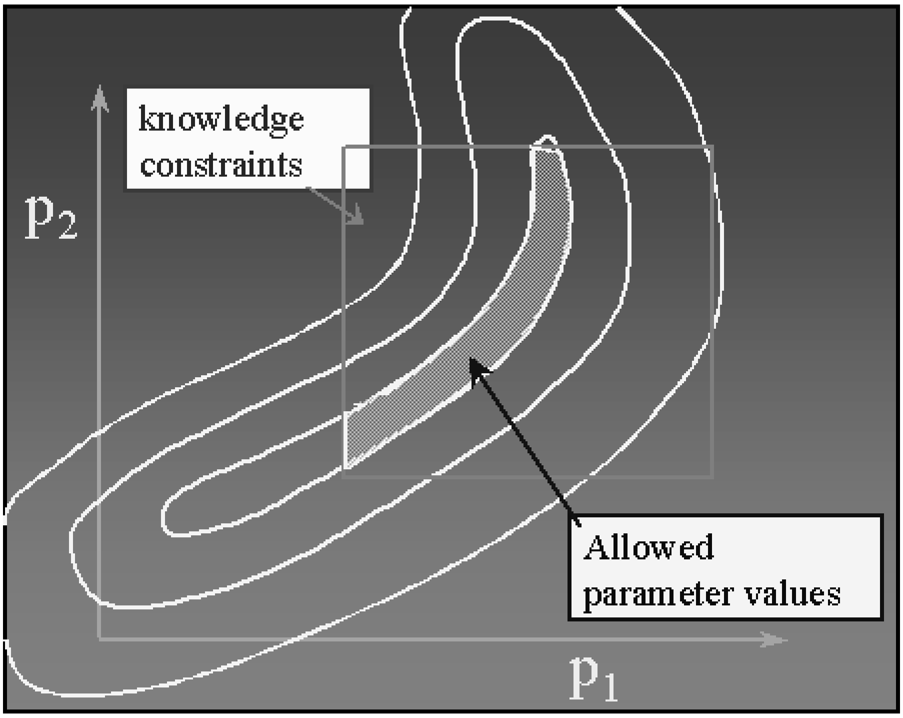

Figure 18 - Contours of the objective function in parameter space (white lines). "Allowed parameter space" is shown shaded. Knowledge and physical constraints are shown as a grey square. Source: Vecchia & Cooley (1987).

Any parameter set within this area can be considered to calibrate the model. Note that it is not only calibration conditions which enforce constraints on parameter values; in most cases knowledge and physical constraints result in the imposition of realistic bounds on parameter values as well. These bounds are also shown on **Figure 18** (Vecchia & Cooley, 1987).

4.5. The Gauss-Marquardt-Levenberg algorithm as realized in PEST

PEST (which is an acronym for Parameter ESTimation) is an automatic calibration code that has the potential to adjust the model's parameters until model-generated results fit a set of observations as closely as possible.

To calibrate a model, PEST needs to know observed values of the variables characterizing the aquifer system; in this case it is necessary to provide the calibration algorithm with the values of hydraulic heads measured at a set of points distributed along the flow domain, associated to the finite element network nodes.

Essentially, the PEST procedure consists on comparing the numeric flow model simulated head values with observed values for the same points, computing the difference between both.

The sum of squared deviations between model outcomes and corresponding field data is the objective function that the algorithm is set to minimize.

Based on piezometry information, available for the set of calibration points, the algorithm changes the value of transmissivity parameters, in an iterative fashion, for a range of previously defined zones, until these can achieve the best fit between simulated values of head and observed values, which corresponds to the minimum value of the objective function. (Doherty, 2002)

PEST uses the Gauss-Marquardt-Levenberg algorithm for nonlinear parameter estimation. For linear models, parameter estimation can be achieved in one step. However, for non-linear problems, parameter estimation can only be achieved by an iterative process. How this iterative estimation works is briefly reviewed here, following the formulation in Doherty (2002), and according to the interpretation of Kunstmann *et al.* (2006).

The relationship between parameters and model-generated output can be represented by a function M which maps the n-dimensional parameter space into the m-dimensional "observation" space. It is required that this function is continuously differentiable with respect to all model parameters for which estimates are sought. Supposing that for the set of parameters to be estimated in the hydrological model (comprising the parameter vector p_0) the corresponding set of model-calculated heads is h_0, i.e.

$$h_0 = M(p_0) \tag{9}$$

A parameter vector p that differs slightly from p_0 then produces a model output q that can be approximated to (Taylor's theorem):

$$q \approx q_0 + J \cdot (p - p_0) \tag{10}$$

Here, J indicates the Jacobian matrix of M, consisting of m rows (one for each observation of model output) and n columns. J_{ij} indicates the derivative of the i-th observation with respect to the j-th parameter.

Inverse hydrogeologic modelling means that a set of model parameters is estimated for which the model generated hydraulic heads is as close as possible to the observed hydraulic heads.

In the least square sense this means that a set of parameters has to be found for which the objective function χ^2, defined as

$$\chi^2 = (h_{obs} - h_0 - J\cdot (p - p_0))^t \cdot W \cdot (h_{obs} - h_0 - J\cdot (p - p_0)) \tag{11}$$

is a minimum (superscript "t" denotes the transposed matrix). Here, h_{obs} represents the observed head values and h_0 the modelled head values. W is a $m\times m$ diagonal matrix whose entries w_{ii} are the squares of the weights attached to the i-th observation**.** Introducing these observation weights allows a higher contribution to the objective function for observations that have a higher reliability. The weights do not necessarily have to sum up to unity. Often they are chosen inversely proportional to the standard deviation of the measurements (Doherty, 2002).

A new estimate for the parameter p can be obtained by

$$p = p_0 + u \tag{12}$$

with the upgrade vector

$$u = (J^t \cdot W \cdot J)^{-1} \cdot J^t \cdot W \cdot (h_{obs} - h_0) \tag{13}$$

where superscript "−1" denotes the inverse matrix. Since Eq. (10) is only approximately correct, so also is Eq. (13). Hence, the vector p (defined by Eq. 12) adding the parameter upgrade vector u to the current parameters values h_0 does not guarantee to yield the minimum of the objective function. The new set of parameters contained in p must then be used as a new starting point in determining a further parameter upgrade vector and so forth.
Marquardt (1963) and Levenberg (1944) *in* Kunstmann *et al.* (2006) changed Eq. (13) to

$$u = (J^t \cdot W \cdot J + \alpha I)^{-1} \cdot J^t \cdot W \cdot (h_{obs} - h_0) \tag{14}$$

where "I" denotes the $n\times n$ identity matrix and parameter "α" has been introduced (the Marquardt parameter). When α is zero, Eq. (14) is equivalent to Eq. (13). When α is high, the direction of u approaches that of the negative gradient vector g, defined as

$$g_i = \frac{\partial \chi^2}{\partial p_i} \tag{15}$$

which can be expressed as

$$g = -2J^t \cdot W \cdot (h - h_0) \tag{16}$$

The advantage of this strategy is a faster convergence to the minimum of the objective function χ^2, in particular when parameters are correlated. Details on the strategy of how PEST chooses the Marquardt parameter a can be found in (Doherty, 2002).

PEST uses a secant's approximation for approximating the Jacobian matrix J. This is achieved by perturbation of the parameters to be estimated (by 1 % e.g.). In fact, estimating n parameters requires n perturbed model runs and one unperturbed run, i.e. n+1 model calls for every iteration within PEST.

Based on the Jacobian matrix the sensitivity of each parameter with respect to all observations can be calculated by

$$s_i = (J^t.W.J)_{ii}^{1/2} / m \tag{17}$$

with m: number of observations and *i* indicating the number of the parameter.

Relative parameter sensitivity rs_i is then defined as the product of s_i and the parameter value p_i :

$$rs_i = s_i \cdot p_i \tag{18}$$

5. Description of the implemented regional flow model

On **Section 2**, a global characterization of the studied aquifer system was made, considering numerous aspects which are essential for the definition of AO's conceptual model. Nevertheless, these aspects are necessary, but not sufficient for building a groundwater flow model. It is vital and necessary to define how the transmissivity parameter is spatially distributed along the aquifer's area.

Moreover, it is well known that hydraulic parameters obtained from pumping tests in individual boreholes are not adequate to obtain realistic representations of aquifers. For that reason, the simulations further presented on **Section 8** of this thesis are based in a synthetic bi-dimensional numerical representation of the AO, where the conductive parameter transmissivity (*T*) was estimated by inverse modelling for zones where the behaviour of piezometers allows a reasonable fitting of field data using a single value of T with.

A number of previous model variants were elaborated in the last years to simulate AO's state variables in order to understand its hydraulic behaviour. These efforts led to the construction of the finite element model which was the basis for the model presently calibrated on this thesis.

On this section a number of steps, carried out during the process of building the direct model (in opposition to the model presented on **Section 8** which was calibrated by an inverse automatic method) will be presented.

5.1 Finite Element Mesh

The first step taken on the construction of the finite element model which was the basis for the model presently calibrated on this thesis, consisted on the definition of a non-structured finite element mesh (**Figure 19**), whilst the assignment of properties to elements was not taken into consideration (Vieira & Monteiro, 2003).

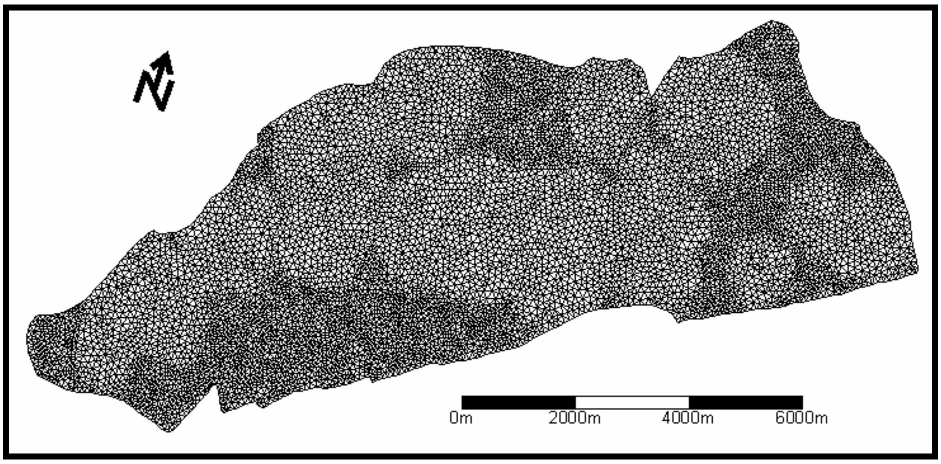

Figure 19 – Finite element mesh generated for the simulation of AO. Source: (Vieira & Monteiro, 2003).

The mesh was generated using the Delaunay TMesh method, which was developed at the Swiss Institute of Technology (Laboratory of Geology, Lausanne, Switzerland) and is composed of 7494 nodes and 14533 triangular finite elements. In order to generate the mesh, the aquifer's limits, proposed by Almeida *et al.* (2000), the system's geologic cartography (Manuppella, 1992), the hydrographical coverage and a database containing important water points (wells and piezometers, containing relevant information regarding head measurements or groundwater quality and springs) were taken into consideration.

5.2. Boundary Conditions

Hydraulic potentials were imposed where discharges are known to occur, according to the information referred on **Section 2.4.2.** (Monteiro *et al.*, 2003). The potentials were imposed on recharge areas, at the juxtaposition of the ribeira de Bensafrim and Vale do Barão creeks' watercourses, only where its altitude was known to be lower in relation to the historic piezometric values of the surrounding area. The display of the resulting imposed potentials can be observed on **Figure 20**.

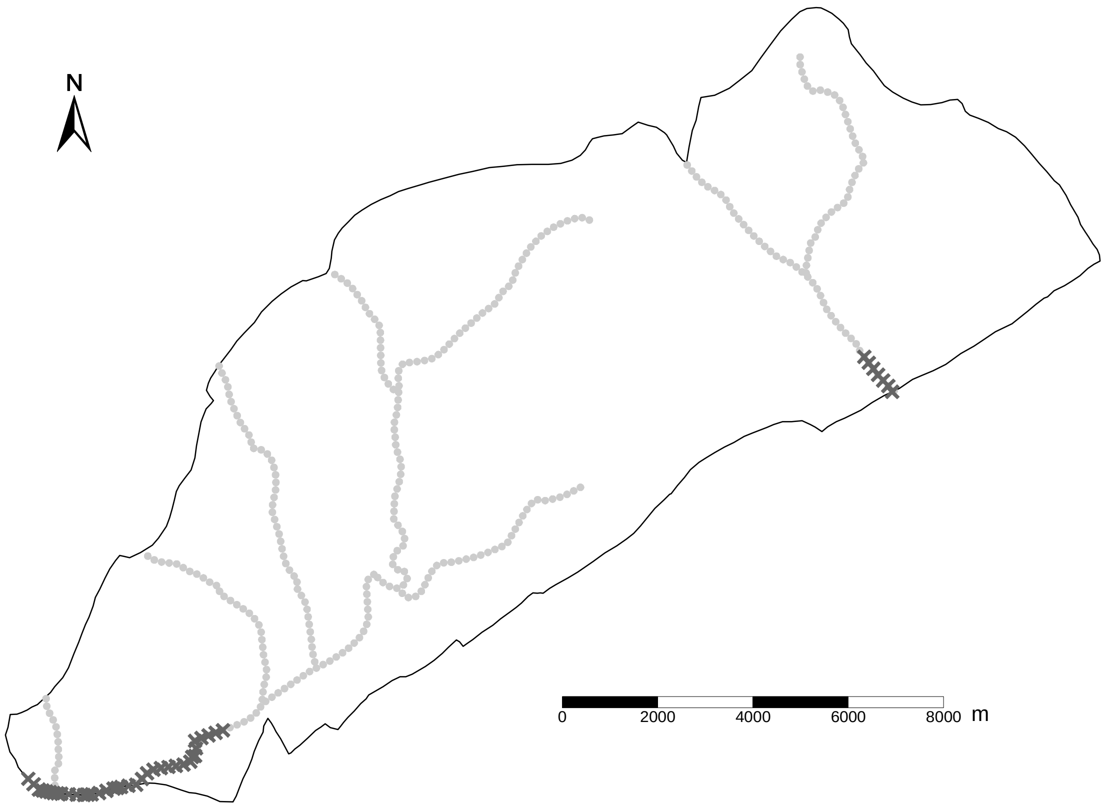

Figure 20 – Watercourses of creeks (light grey lines) and imposed potentials (dark grey crosses) at areas where there is known evidence of occurrence of discharge episodes.

5.3. Recharge

Recharge values were calculated according to a criteria defined by Vieira & Monteiro (2003), which is explained on **Section 2.4.1.**. The authors have considered both the spatially distributed values of precipitation calculated by Nicolau (2002), as described on **Section 2.3.**, and the fraction of precipitation assumed to occur for each of the rising lithologies on the aquifer area. The average infiltration rate resulting from the shown recharge distribution is 40,3%. The model's recharge distribution along the aquifer area can be seen on **Figure 21**.

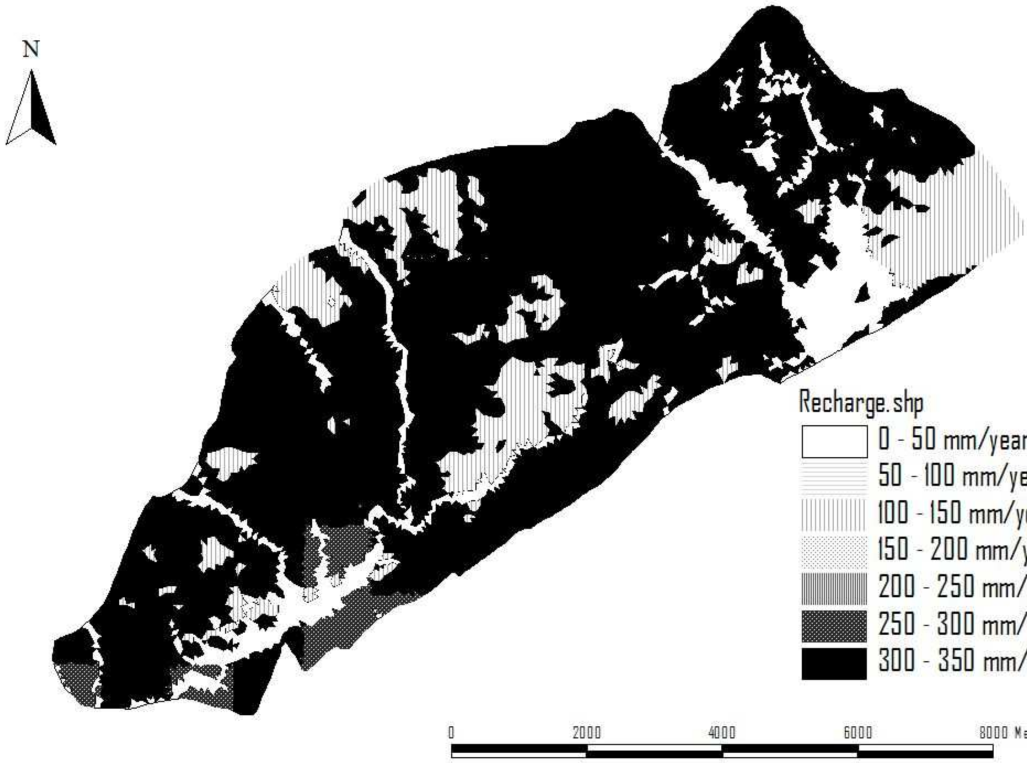

Figure 21 – Recharge attributed to each one of the elements of the FEN used on the simulation of underground flow on the AO.

6. Model variants based on homogeneous representations of the flow domain

Previous model versions of the AO finite element model, which was presented on the preceding section, considered transmissivity as being homogeneous along the aquifer area. The hydraulic behaviour AO was analysed with the support of a number of simulations carried out in the last years, using these “direct” models. The present section of the thesis will focus on a brief exposition of two of these simulations.

6.1. Simulation of the natural water balance

One of the model’s variants was conducted by Vieira & Monteiro (2003) and pretended to simulate the natural water balance of AO. On this simulation, a constant transmissivity value of 1000 m^2/day was used for the whole area of the aquifer (63,5 km^2). Recharge was ascribed according to the method described on **Section 2.4.2.** and the distribution of precipitation infiltraton rates along the aquifer area is the same as illustrated on **Figure 21**.

Potentials were imposed in the same way as described on **Section 5.3.**. The simulated piezometric surface is represented by the contours shown on **Figure 22**.

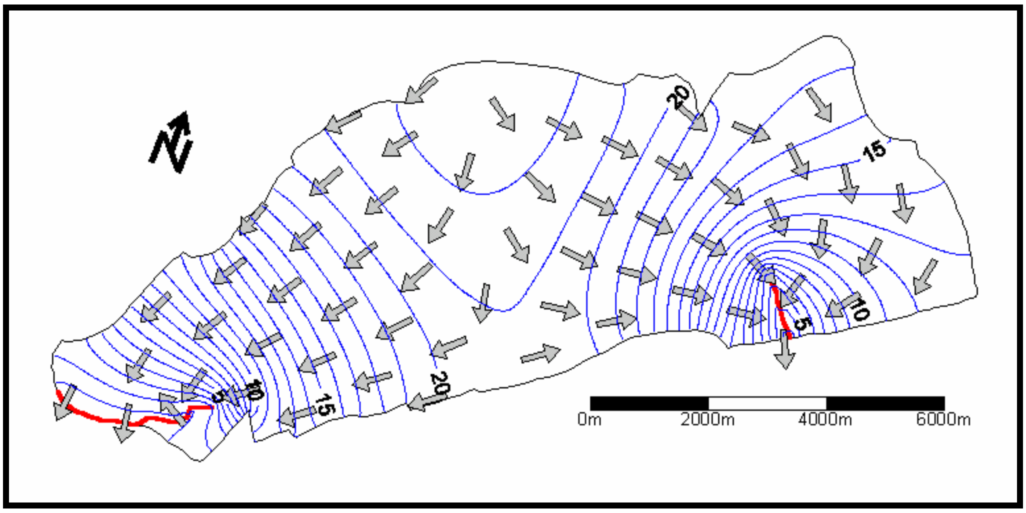

Figure 22 – Simulation head contour map (black thin lines). Imposed potentials (black thick lines) at areas where there is evidence of occurrence of discharge episodes. The flow pattern is represented by arrows. Source: Vieira & Monteiro (2003).

It can be observed that the aquifer's regional groundwater flow pattern reflects the influence of the imposed potentials on the two discharge areas**.** Flow converges from the N central section of AO to the "Boca do Rio" area (red line at the W sector of AO) and to the estuary of "Ribeira de Bensafrim" creek (red line at the E sector of AO). According to the simulation results of this model's version, the estimated average recharge for the AO is $16{,}6\times10^{6}$ m^{3}/year.

6.2. Simulation of the water balance considering a hypothetical water use

While pursuing the objective of analysing the impact of the hypothetic implementation of a golf course (in the vicinity of "Espiche"), Monteiro (2005) developed a subsequent version of the model presented on **Section 6.1.,** which considered, (beyond the simulation of with AO's natural hydraulic behaviour) a hypothetic water withdrawal for irrigation occurring from 6 hypothetical boreholes inside the limits of this aquifer system (**Figure 23**).

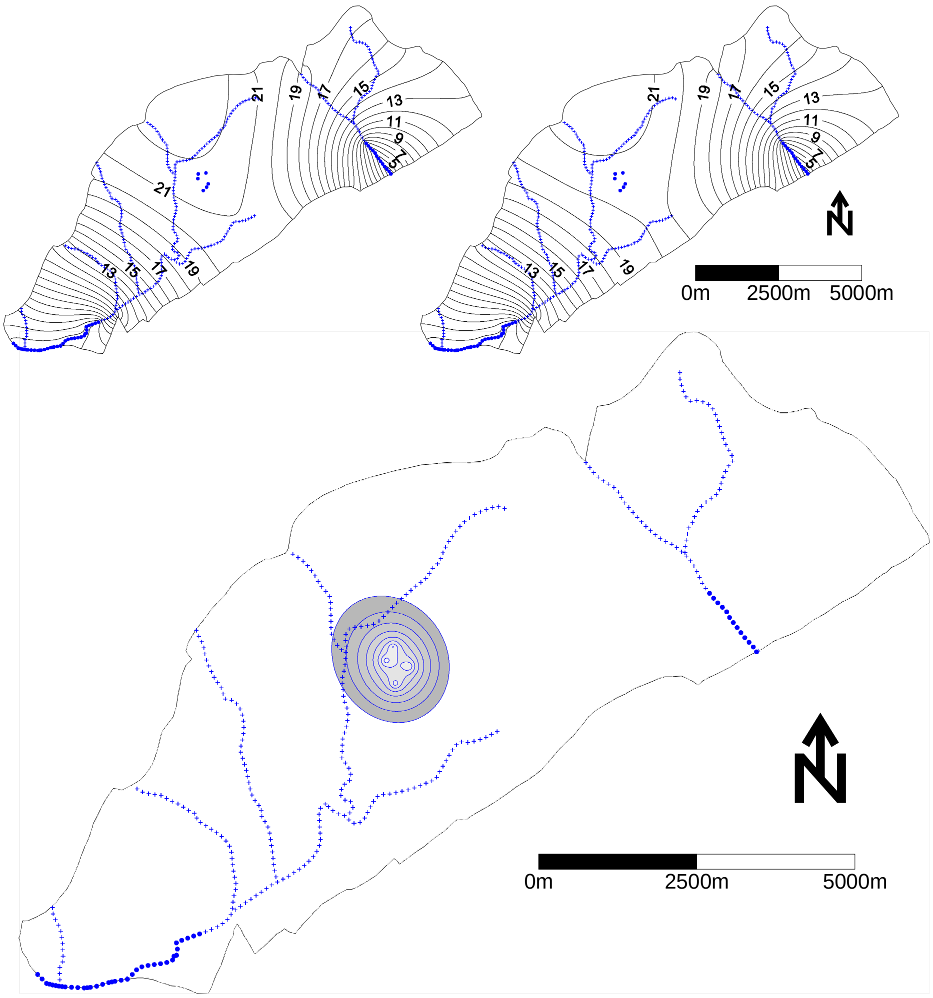

Figure 23 – Simulation of the hydraulic behaviour of AO on natural regime (above and left) and considering withdrawals occurring on 6 boreholes (above and right). Below, residuals between both simulation results, (with values equal to or greater than 1m), show a cone of depression on AO's regional piezometric pattern, caused by withdrawals. Source: Monteiro (2005).

Withdrawals occurring on these points totalled 5×10^5 m^3/year. Residuals between the simulation of the hydraulic behaviour of AO on natural regime and the simulation of the hydraulic behaviour of AO considering withdrawals occurring from 6 boreholes, show the existence of a cone of depression on the regional piezometric pattern (residuals with values equal to or greater than 1m), produced by the hypothetic withdrawals.

7. Limitations on the representation of AO as a homogeneous flow domain

Up to this thesis, all previous model versions of the AO finite element model considered transmissivity homogeneous throughout all of the aquifer area, i.e. they were direct models.

This assumption is very likely to be a limitation whilst a simulating of the hydraulic behaviour of regional karst aquifers is necessary, because these are highly heterogeneous in nature, since they are dominated by either secondary or tertiary porosity, or both.

In order to assess the efficiency of the direct finite element model in characterizing the real spatial distribution of state variables, simulated head results at observation points (considering a homogeneous transmissivity value of $1{,}14\times10^{-02}$ m/s for all of the aquifer area) were compared with the real piezometric data already shown on **Section 2.5**. The distribution of recharge rates along the aquifer area is the same as illustrated on **Figure 21**.

It must be stressed that the simulation which delivered these results was fully performed during the course of the work which led to the subsequent AO finite element model calibration using an indirect method (further explained on **Section 8**).

The calculated head results obtained from the direct simulation are displayed on **Table 5**. For measured observation points which had a coordinate position in close proximity to an adjacent point, the mean head value was set on an equidistant position in space, between the pair.

Table 5 – Measured and calculated hydraulic heads obtained through the non–calibrated simulation. On paired observation points' references signalled with "*", an average measured head value was assumed.

Observ. points	Measured (m)	Calculated (m)	| Residuals | (m)
AO-16,15*	4,42	18,73	14,31
AO-08	5,14	24,15	19,01
AO-06	4,69	24,22	19,53
AO-02	7,23	25,21	17,98
602/242	6,98	23,47	16,49
AO-14,13*	5,27	13,34	8,07
AO-01	3,79	8,26	4,47
602/187	5,33	14,49	9,16
AO-10	3,95	10,24	6,29
593/5	22,73	21,17	1,56
603/38	5,00	15,35	10,35

The correlation between measured and simulated hydraulic head shown on **Figure 24** provides an illustration of the limited effectiveness in the results of the simulation, since most points are far away from the x=y curve.

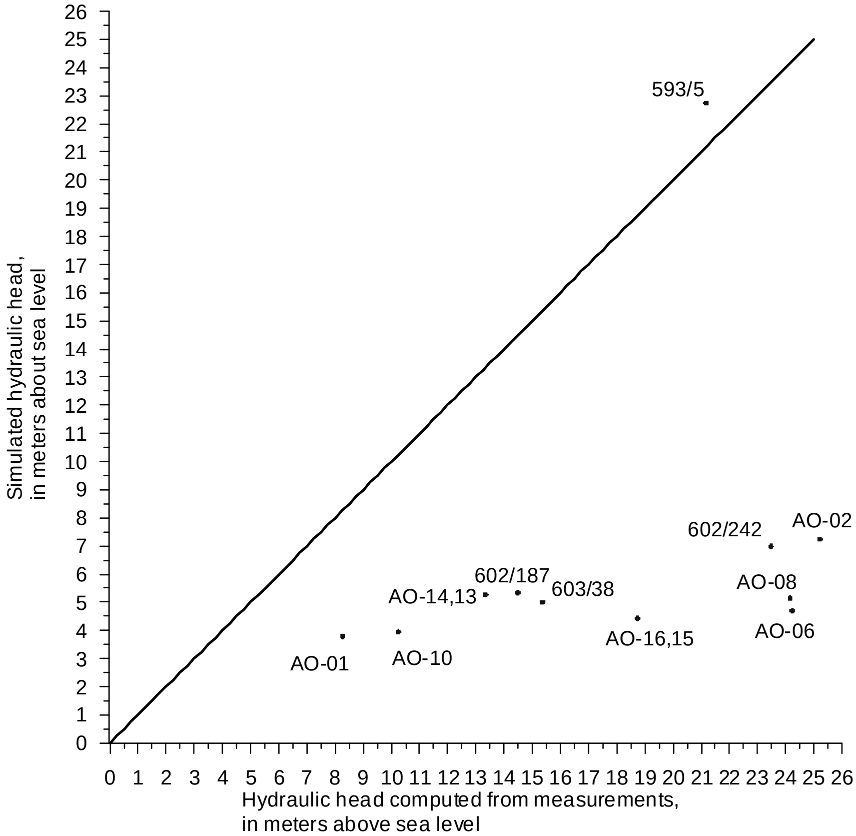

Figure 24 – Model calibration cross-plot of observed vs. calibrated head values.

The equipotential contours displayed on **Figure 25** show a poor fit between both values of measured and calculated hydraulic head. Both the configuration of the regional pattern and the order of magnitude of head values are not equivalent in almost all of the aquifer area. Little similarity between equipotential lines can only be observed near discharge areas where potentials where imposed.

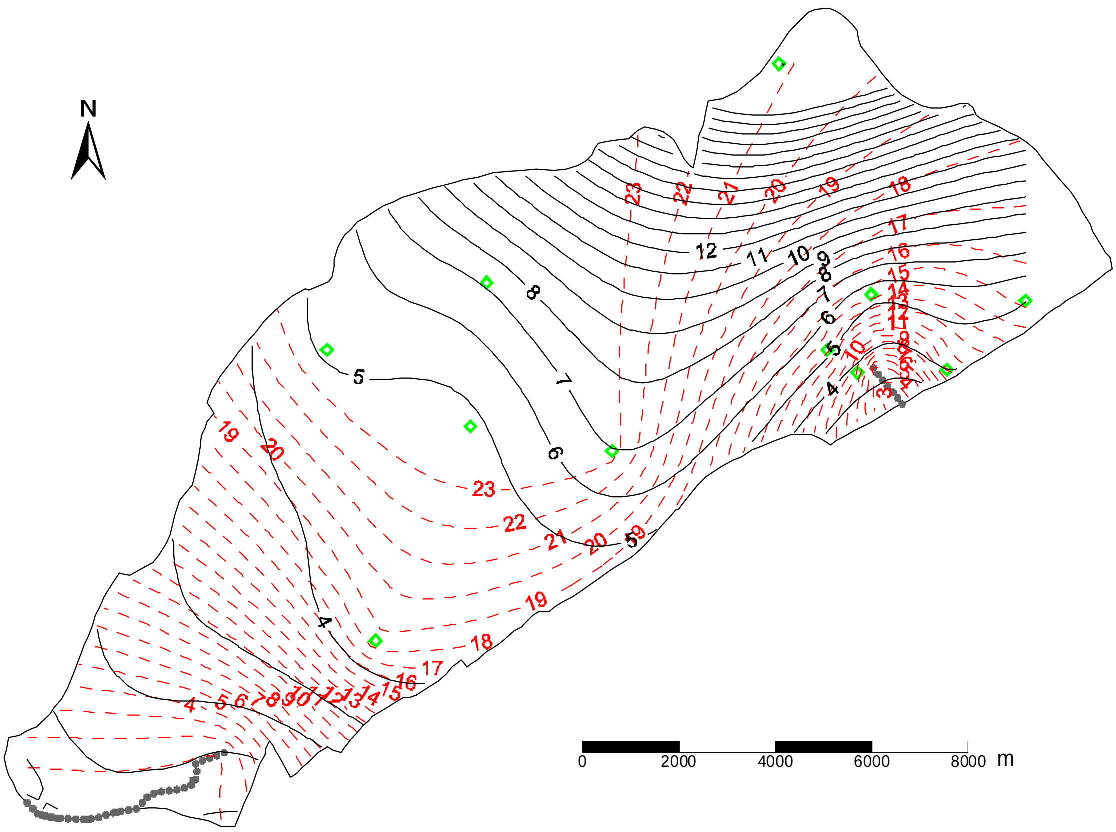

Figure 25 – Equipotential lines contoured from simulated (dashed red lines) and measured (black lines) hydraulic heads at observation points (green lozenges). Imposed potentials are shown in grey.

The poor fit obtained by the modelled results here illustrated shows how important it is to assign coherent transmissivity values to the modelled area. The subsequent section describes the method of characterization of the spatial distribution of transmissivity on the Almádena-Odeáxere aquifer system through automatic calibration. This method actually consists of an attempt to improve the simulation accuracy of the aquifer's hydraulic behaviour already achieved at this stage.

8. Inverse calibration of the model

8.1. Setting of constant transmissivity zones

In order to calibrate the model using measured heads, constant T zones were defined inside the aquifer area. These zones were set in such a way that they could allow to distinguishing the hydraulic behaviour of different hydrostratigraphic units integrating the aquifer system.

The subdivision of these zones took place mainly on the basis of the character of the piezometric contours since there is little obvious variation in geology throughout the study area. This particular assumption is supported by the calibration methodology carried out by Doherty (1998) which has already led to the construction of groundwater models capable of achieving an excellent fit between model-generated and field hydraulic results.

During the process of calibration, differently “zoned” variants were tested, with the purpose to obtain a set of parameters able to produce the best possible fit between measured and calculated hydraulic potentials. The variant which latter revealed the best calibration results is presented on **Figure 26**.

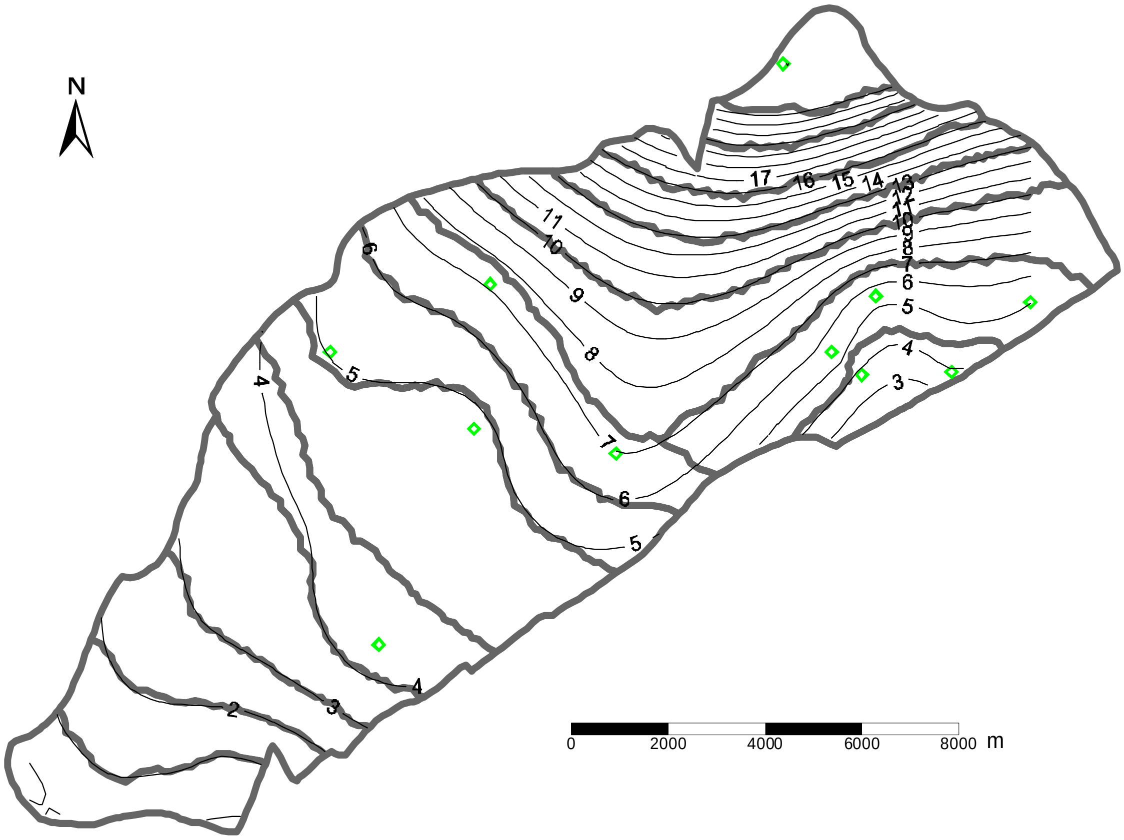

Figure 26 – Transmissivity zones' setting (thick grey lines) and piezometric contours on the basis of its configuration (black thin lines). Observation points used for the contour generation are shown as green rhombi.

After the definition of the constant T zones, additional "fictional" observation points (guide points) were added to some of these zones, in order to supply the conceptual model with the necessary information to calibrate the finite element model. Because these guide points were added, the contours of the resulting head distribution are slightly different from the original (contours on **Figure 27** when comparing to contours on **Figure 26**). Nevertheless, as far as the representation of the reality by the conceptual model is concerned, the change caused is unremarkable.

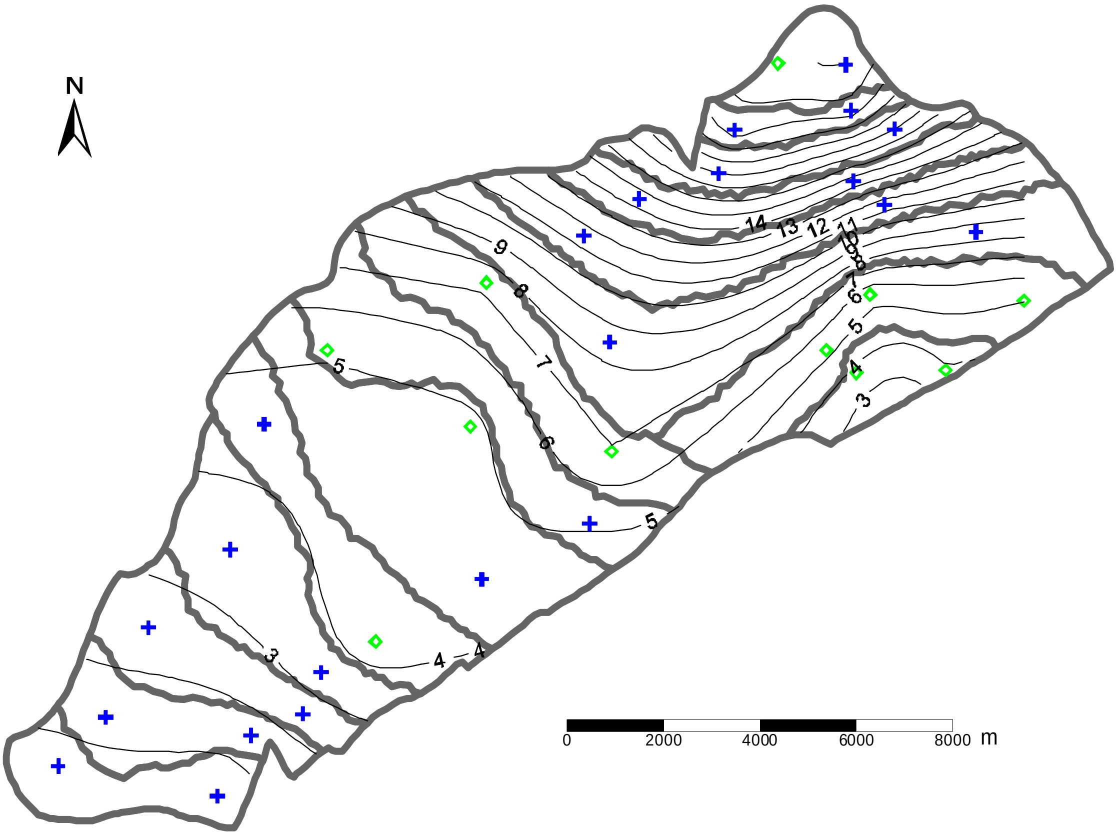

Figure 27 – Additional guide observation points (blue crosses) addressed to the defined zones of constant transmissivity (thick grey lines), original observation points (green rhombi) and new head contours (black thin lines).

8.2. Analysis of the simulation results

8.2.1. Goodness of Fit

The extent to which model outputs are in agreement with their field-measured counterparts is apparent from the value of the sum-of-squared weighted residuals (objective function), Φ, as explained on **Section 4.4.**. The calibration algorithm (which was used in parameter estimation mode) has automatically lowered the objective function as far as possible.

Another measure of goodness of fit is provided by the correlation coefficient, R, as defined in **Section 4.6.**. It is consensually accepted that R should be above 0.9 for the fit between model outputs and observations to be acceptable (Hill, 1998).

A comparison of the R and Φ values for different calibrated versions of the model, using distinct zone setting alternatives is shown on **Table 6**. The version referred as 5.1 on this table corresponds to the version which obtained the best results and for which the zoning shown on **Section 8.1.** was used. The following discussion and illustration of results will specifically address this version.

Table 6 – Comparison between 3 different calibrated versions of the model. Version 5.1 obtained the best results

Version Reference	5	5,1*	5,2
Objective function, Φ	5,928	4,56	5,12
Correlation Coefficient, R	0,9981	0,9967	0,9962

The correlation between measured and simulated hydraulic heads on the simulation version 5.1 reveals a significant increase on the effectiveness of the simulation. Hence, a successful automatic calibration was carried out (**Figure 28**).

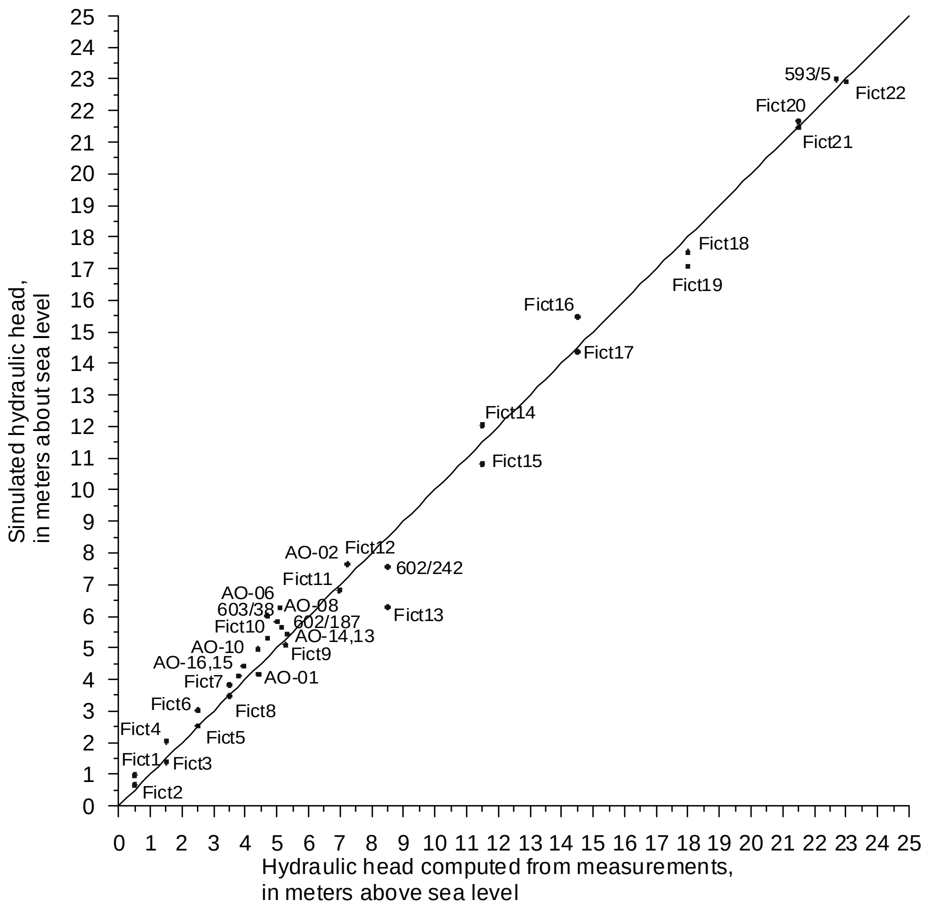

Figure 28 – Model calibration cross-plot of observed vs. calibrated head values (version 5.1).

The equipotential lines contoured from measured and calculated hydraulic head displayed for the simulated version 5.1 shows a fairly good fit between both sets of values. Both the configuration of the regional pattern and the order of magnitude of head values are equivalent in nearly all of the aquifer area (**Figure 29**).

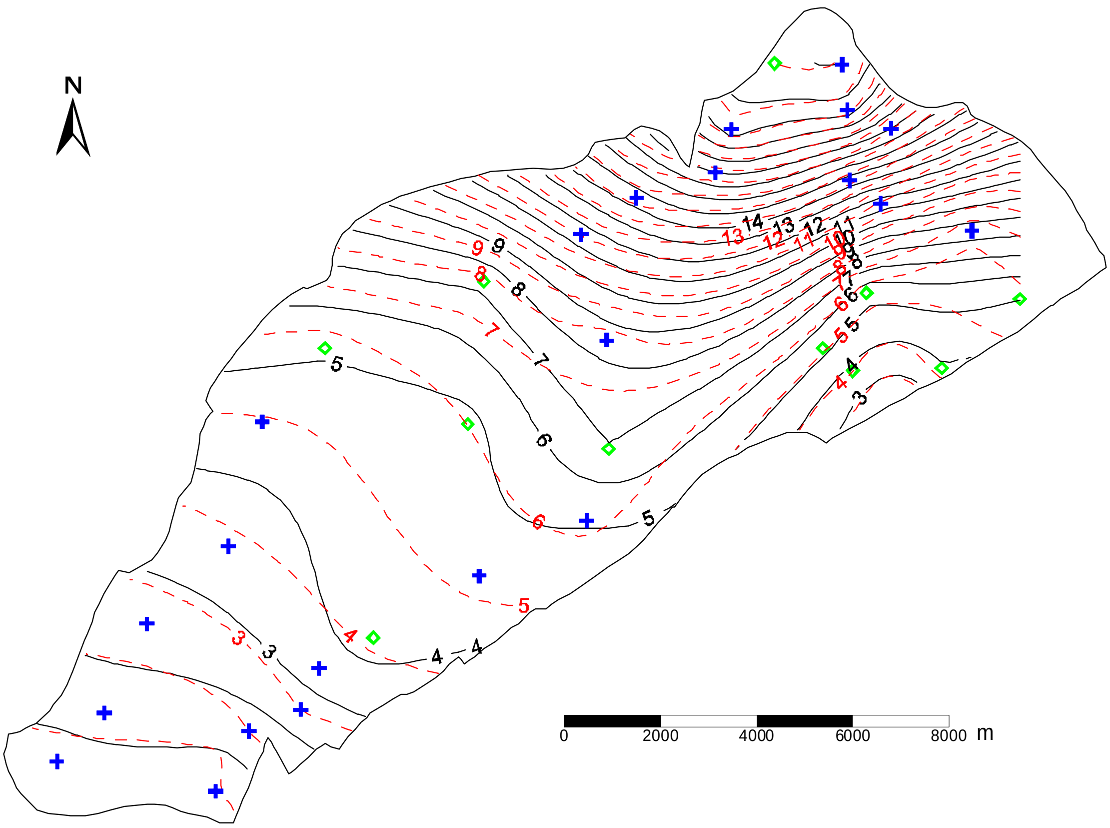

Figure 29 – Equipotential lines contoured from the calibrated model's simulated (dashed red lines) and measured (black lines) hydraulic heads at observation points (green lozenges). Additional guide observation points are represented by blue crosses.

8.2.2. Spatial distribution of transmissivity

The transmissivity values obtained for version 5.1 at each of the designed zones are shown on **Figure 30**. These values ranged from 86 m^2/day ($1{,}0 \times 10^{-03}$ m^2/s) to 8158 m^2/day ($9{,}4 \times 10^{-02}$ m^2/s) and show a fairly realistic distribution throughout the AO area, since the automatic setting of transmissivity has placed higher T values where flux would be expected to pass through faster pathways and lower T values where higher head gradients exist hence increasing consistency with the proposed conceptual model.

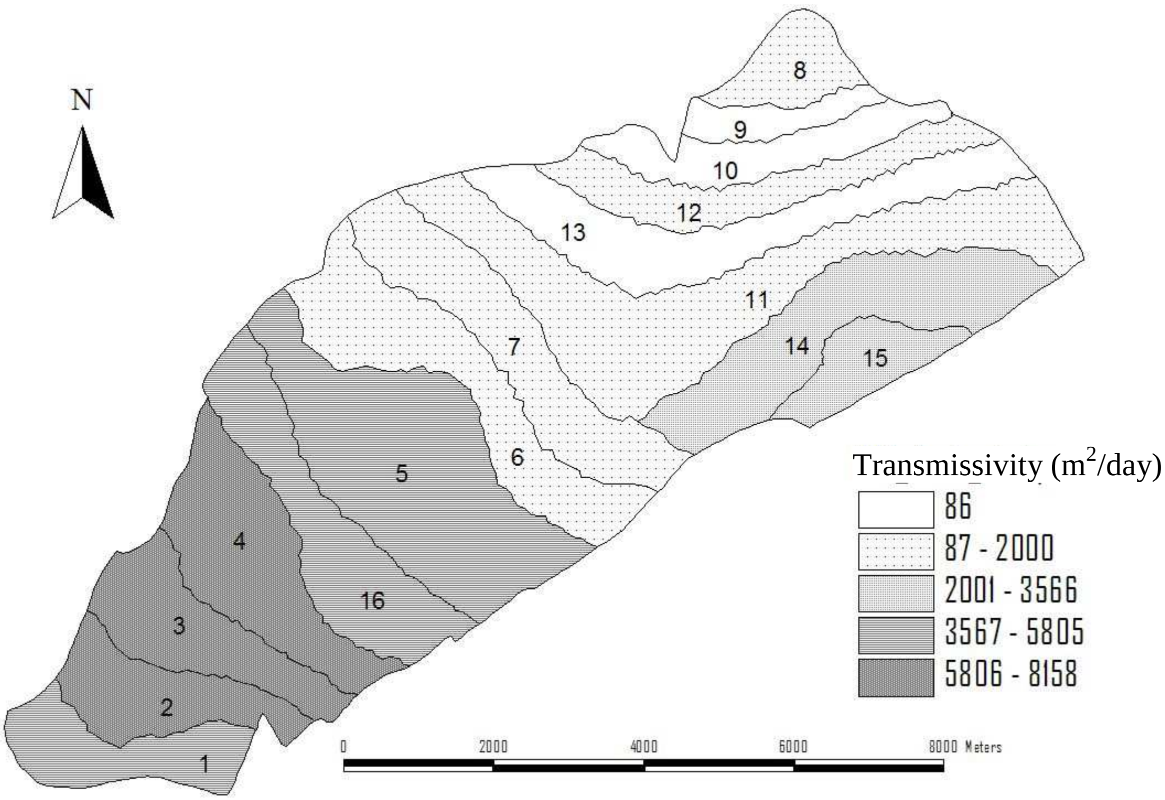

Figure 31 – Transmissivity zones set for the automatic calibration process (identified by numbers) and resulting distribution of regional transmissivity in m^2/day (greyscale pattern).

Considering that $K = T / b$, and an aquifer thickness, b, of 1000 m, hydraulic conductivity, K (m/s) was calculated with basis on T (m^2/s) values characterising AO at regional scale (**Table 7**).

Table 7 – Regional results of transmissivity and conductivity for each defined zone at version 5.1.

Zones	T (m^2/day) $\times 10^{+02}$	T (m^2/s) $\times 10^{-02}$	K (m/s) $\times 10^{-05}$
1	57,77	6,69	6,69
2	81,58	9,44	9,44
3	72,40	8,38	8,38
4	73,63	8,52	8,52
5	51,04	5,91	5,91
6	14,19	1,64	1,64
7	20,00	2,31	2,31
8	13,53	1,57	1,57
9	0,86	0,10	0,10
10	0,86	0,10	0,10
11	16,84	1,95	1,95
12	17,91	2,07	2,07
13	0,86	0,10	0,10
14	27,26	3,16	3,16
15	35,66	4,13	4,13
16	58,05	6,72	6,72

Regional conductivity values ranged from $1{,}0\times10^{-6}$ m/s to $9{,}44\times10^{-5}$ m/s, with mean and median values reaching $3{,}92\times10^{-5}$ m/s and $2{,}73\times10^{-5}$ m/s respectively.

A comparison between regional hydraulic conductivity values calculated using the calibrated version of the model and hydraulic conductivity values calculated with basis on transmissivity values (assuming that $K = T / b$) obtained through pumping tests at 16 different boreholes (Reis, 1993), is shown on **Figure 32.** Conductivity values determined at well scale range from $1{,}94\times10^{-6}$ m/s to $1{,}02\times10^{-4}$ m/s, with mean and median values reaching $2{,}36\times10^{-5}$ m/s and $1{,}14\times10^{-5}$ m/s respectively.

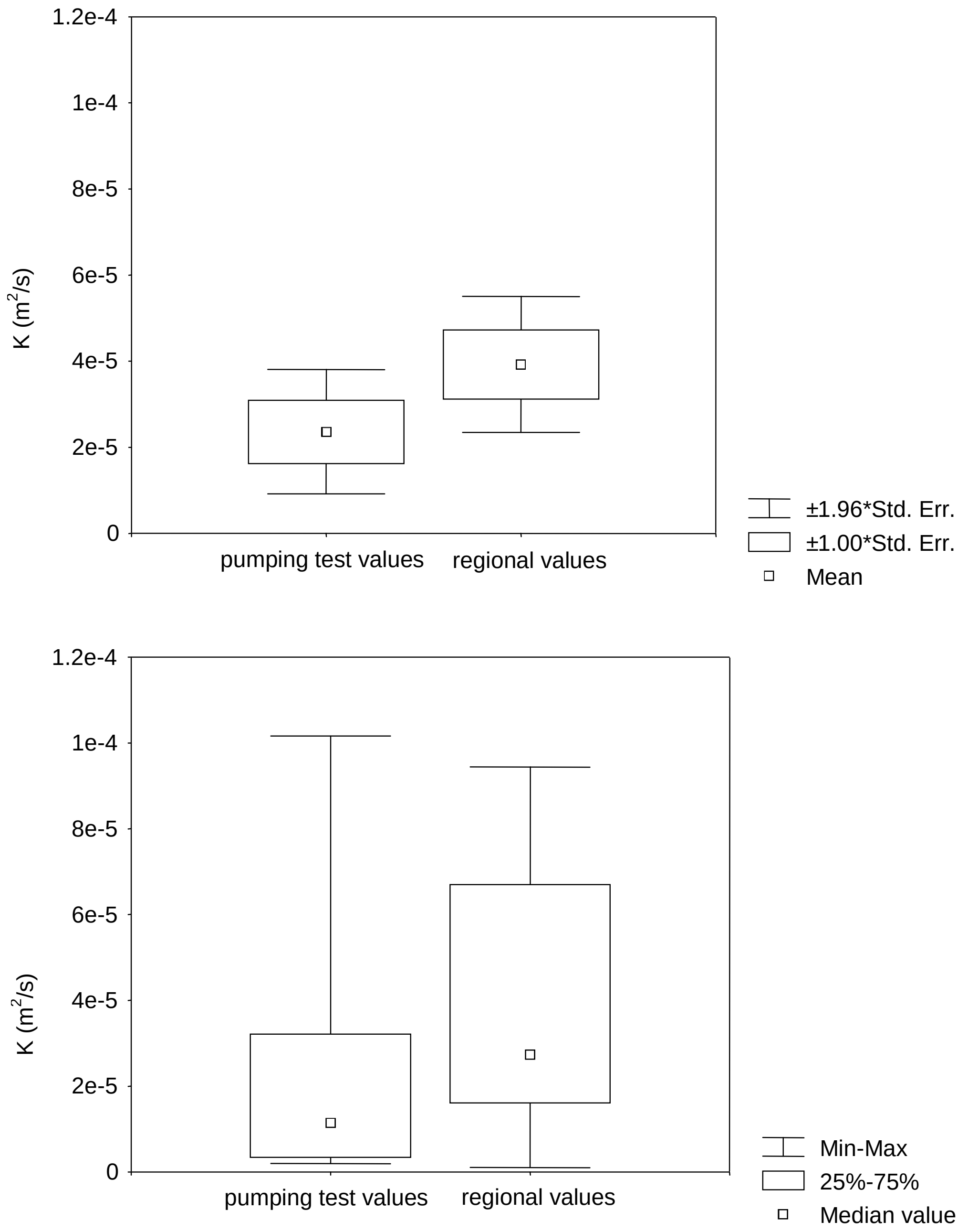

Figure 32 – Hydraulic conductivity (K) comparison between regional values and values determined from the interpretation of pumping tests (m/s). Mean and standard deviation errors are represented above. Range, median and 25 %-75 % quartiles are represented below.

Conductivity values calculated with basis on transmissivity values (assuming that $K = T / b$) obtained by Almeida *et al.* (2000) through the use of pumping tests range between $2{,}9\times10^{-7}$ m/s and $2{,}4\times10^{-5}$. Also in this case the calculated regional transmissivity values have revealed to be higher.

As discussed on **Section 1.2.**, hydraulic conductivity values determined at regional scale were, as expected, actually higher than values determined at well scale with pumping tests. These values reflect the change in hydraulic conductivity with scale. This scale effect is particularly marked in flow domains where diffuse and conduit flow is overlapped in a complex flow pattern. The variation of hydraulic conductivity values with scale, foreseen by Kiraly (1975), is closely related to the shape and dimension of different kinds of voids developed in that kind of rocks and is expressed in **Figure 33**.

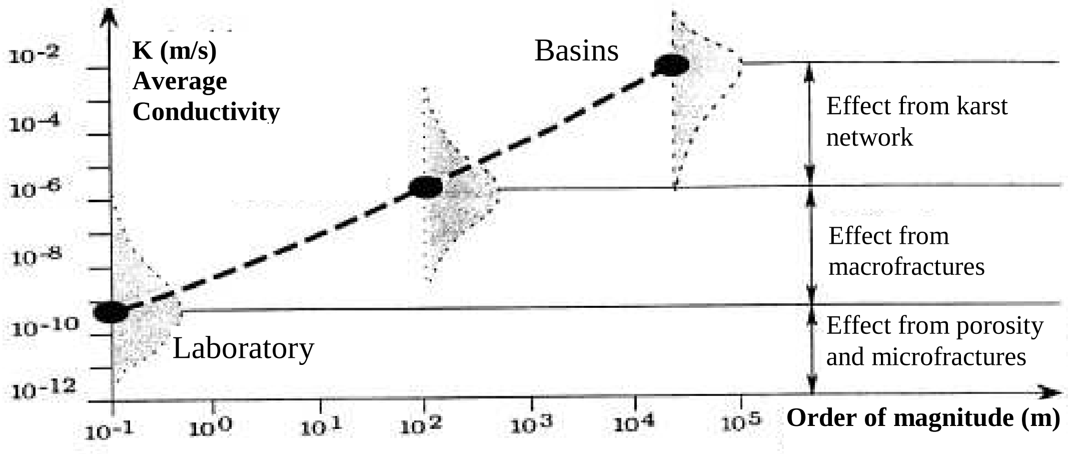

Figure 33 – Scale effect in karst aquifers hydraulic conductivity. Adapted from Kiraly (1975)

Depending on their spatial extent three scales can be defined: the rock matrix, the local and the regional scales.

At the lower extreme of the scale, porosity and hydraulic conductivity, depend on the existence of intercrystalline voids, moldic voids and microfractures, with dimensions ranging from sub-micrometers to millimetres. The volume of these voids tends to change according to the dominant active geologic processes. In some cases the porosity tends to be enhanced due to the dissolution of calcite and dolomite, the dominant minerals in carbonate rocks. In some other cases the hydraulic conductivity and porosity may be reduced due to calcite precipitation and cementation. This is identified as laboratory (or rock matrix) scale and is associated to the analysis of samples with few cm^3 in dimension.

At an intermediate scale (local or well scale) the parameters are related to structures with dimensions varying from few meters to few hundred meters. In many cases that scale is in the order of the aquifer thickness. At this scale the hydraulic parameters depend on the distribution and connectivity of the voids in rock matrix and on the existence of fractures.

At regional, or even at aquifer scale, a more or less developed network of dissolution channels exists. In well developed karst aquifers these structures can control the flow pattern in the entire flow domain. In other cases more or less independent branches of channels are observed in different sectors of an aquifer system. Another important difference between the fracture network at well scale and karstic channels at regional scale is the fact that the former are characterised by a configuration where one of the dimensions in space (aperture) is much smaller than the other two ones. In the case of karstic channels, this rule cannot be generalised as their shapes vary from among a large set of geometries (Monteiro, 2001).

9. Final remarks

Previously to the present work, the context of application of the AO flow model has been the assessment of coherence between the existent conceptual models, field data and the results obtained through the implementation of numeric finite element models.

After this initial stage, the absence of estimations on hydraulic parameter values able to distinguish the hydraulic behaviour of different hydroestatigraphic units was identified as an important factor to fulfil.

The parameter characterization made by Reis (1993) and Almeida *et al.* (2000) with basis on pumping tests, and the Logan method, only allowed to calculate transmissivity at borehole scale, where the tests were performed. Hence, up to the present work, the spatial distribution of transmissivity values at regional scale could not be characterized at the AO using these results.

The lack of regionally distributed hydraulic parameter values only allowed the possibility to use numeric models to simulate groundwater flow at regional scale using homogeneous parameter values, applied to the whole aquifer area. It has therefore been assumed that the determination of the spatial distribution of transmissivity should be the main challenge respecting the calibration of the model implemented during the course of the present work.

The main advantage of using an inverse calibration methodology to attain the thesis main objectives consisted on the automatic way in which the process took place. The speed and effectiveness of the used algorithm allowed several variants of the model to be tested. In opposition, if a trial-and-error approach was used, an enormous effort would have been necessary; in order to exhaustively interpret the generated results and to carry out the identification and change of the parameter values expected to be able to improve the models' performance. Moreover, these efforts would be made, without any assurance of a convergence to an optimal solution.

Diverse variants having distinct configurations of homogeneous zones of transmissivity were defined. The variant presented on **Section 8.1.** corresponds to the zone configuration that produced the best fit between measured hydraulic heads and heads simulated by the model. This variant shows a correlation coefficient, R, of 99.7% and a value of 4.56 m for the sum of squared deviations between model outcomes and corresponding field data. These results show a very reasonable fit between measured and simulated head values.

The model's calibration results provided the first estimate on the regional transmissivity values distribution, which range from 86 m^2/day to 8158 m^2/day, allowing step further on the reliability of future simulations of spatial distribution and temporal evolution of state variables (hydraulic head and natural outflows).

Further investigations, could involve the use of the calibrated model to develop transient variations of the AO model, which could consider the variation of recharge and withdrawals in time and allow determining e.g. the aquifer's storage.

Beyond the worth of the obtained results, it is expected that the present work may allow a broader diffusion of this calibration approach which at the present time is insufficiently known and applied outside the academic circles. Moreover, the present work also opens the possibility for the development a future model-based regional management of AO water reserves with obvious advantages to what respects to the rational use of groundwater in the Algarve region.

10. References

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