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Method Article

A groundwater security model based on hydraulic turnover times and flow compartments



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ABSTRACT

Starting with a log-linear relationship between groundwater discharge per unit drainage area (Q/A_b), hydraulic turnover time (t) and aquifer mobile storage (z), this study builds a groundwater security method at catchment scale. The method embeds previously published approaches to calculate Q/A_b , t and z , and relies solely on stream flow discharges and watershed areas. The ability to build a method on a couple of variables is remarkable. The method recasts the calculated variables as aquifer security indicators (S_Q , S_t and S_z), relating S_Q with yield capacity, S_t with self-depuration capacity and S_z with resilience. Groundwater security is the weighted product of S_Q , S_t and S_z . The method is validated with stream flow discharges and drainage areas concerning 294 hydrometric stations and their watersheds, located in continental Portugal. The results revealed a majority of moderately to highly secure watersheds, especially as regards S_t (> 62%), while 7–10% were classified as very highly secured in general (S_Q – S_t – S_z). The least secured basins are located in the more arid regions of continental Portugal (Northeast and south regions), as expected. The method can be easily transposed to any other region worldwide, with the necessary adaptations to regional climate, geological and topographic settings.

- Compile stream flow discharge data and organize them as natural logarithms and logarithmic variations as function of time, to estimate Q , t and z ;

- Recast the Q , t and z values as S_Q , S_t and S_z ratings, respectively, using the appropriate reclassification scales, and estimate watershed security levels, namely average security or customized (weighted) securities that highlight the contributions of Q/A_b (watershed yield), t (aquifer's self-depuration capacity) or z (aquifer's resilience);

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- Use the results to draw illustrative diagrams and spatial distribution maps.

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ARTICLE INFO

Method name: A groundwater security model based on hydraulic turnover times and flow compartments

Keywords: Hydraulic turnover time, Groundwater discharge, Watershed mobile storage, Aquifer self-depuration capacity, Aquifer yield capacity, Aquifer resilience, Sustainable water supply

Article history: Available online 20 June 2022

Specifications table

Subject Area;	Environmental Science
More specific subject area;	Groundwater hydrology
Method name;	A groundwater security model based on hydraulic turnover times and flow compartments
Name and reference of original method;	Pacheco, F.A.L., 2015. Regional groundwater flow in hard rocks. <i>Science of the Total Environment</i> 506–507, 182–195.
Resource availability;	Besides the Supplementary Materials provided with this submission, the authors are committed to provide additional data at the request of an interested scientist

Method details

The method introduced in this study to assess groundwater security conceives the underground portion of river basins as compartments with different volumes and storage capacity, and relates groundwater discharge rates from the compartments with hydraulic turnover times. Within this general framework, the larger and more porous river basins that yield massive groundwater volumes every year and can sustain them for a long time in the absence of replenishment, are viewed as the most secure. This is because they can persistently respond to large water demands and are capable to neutralize potential contamination from the surface considering the long-lasting underground pathways that allow contaminant attenuation through filtration, adsorption or chemical and biological decay. On the opposite side are the small low-porosity watersheds that yield just small volumes of groundwater annually and can sustain them for just short periods. In this case, the reason to be the least secure is that these watersheds can barely respond to large water demands and are readily affected by infiltration of contaminated surface waters given the short turnovers that hamper self-depuration. In between these two end-member compartments, there will be an assortment of other catchments with intermediate dimensions and hydraulic properties, gradients and turnover times, and hence with intermediate groundwater security.

The method is composed of three modules. The first module was coined “groundwater compartment” module and established a general log-linear regression between groundwater discharge rate and hydraulic turnover time that allowed the definition of groundwater compartments as function of watershed volume and effective porosity (*i.e.*, the catchment mobile storage). This relationship is the method’s core, because it gathered the above-mentioned elements of groundwater security in a single equation. Modules 2 and 3 were developed because implementation of module 1 requires prior estimation of those elements. Thus, the second module, termed “turnover time”, estimated the hydraulic turnover time of a watershed from a previously published method of Pacheco [1], and improved that method to additionally assess the groundwater discharge rate. It also used the log-linear relationship of module 1 to estimate the mobile storage (*z*) from the calculated groundwater discharge rate (*Q*) and hydraulic turnover time (*t*). Finally, the third module recast *Q*, *t* and *z* as security indicators (*S*) of aquifer yield, groundwater quality and aquifer resilience, respectively, and determined an average security for the basin as product of S_Q , S_t and S_z . This is why the module was called “security” module. The average security indicator can be customized to highlight the role of yield, quality or resilience, through power weighting of S_Q , S_t or S_z , respectively. The three modules are described in detail in the next subsections.

Groundwater compartment module

The flow of groundwater (Q , L^3T^{-1}) through the section of an aquifer is proportional to flow velocity (v , LT^{-1}) and effective section area ($A_e = A \times n_e$, L^2 , where n_e is the aquifer's effective porosity):

$$Q = vA_e \tag{1}$$

On the other hand, velocity is a cinematic relationship between a path length (L , L) and the time required to travel along the path (t , T):

$$v = \frac{L}{t} \tag{2}$$

The replacement of Eqs. (2) in (1) gives:

$$Q = \frac{LA_e}{t} = \frac{V_e}{t} \tag{3}$$

where V_e (L^3) represents the effective aquifer's volume also known as mobile aquifer storage. If Q is the discharge of groundwater from a river basin that was assessed at time t , then V_e is the mobile catchment storage. If both terms of Eq. (3) are now divided by the basin's area (A_b , L^2), the result is:

$$\frac{Q}{A_b} = \frac{V_e}{A_b t} = \frac{z}{t} \tag{4}$$

where $z = V_e/A_b$ (L) is the mobile catchment storage per unit basin area. If logarithms are finally taken from the left- and right-hand sides of Eq. (4), the result is:

$$\log\left(\frac{Q}{A_b}\right) = \log(z) - \log(t) \tag{5}$$

A projection of $\log(\frac{Q}{A_b})$ (LT^{-1}) as function of $\log(t)$ (T) describes a straight-line $y = a + bx$, with $b = -1$ and $a = \log(z)$. Thus, it is possible to use this outcome to draw a general $\log(\frac{Q}{A_b})$ versus $\log(t)$ diagram composed of straight lines with slope -1 ($b = -1$) and intercept- y values pre-defined at certain values of $a = \log(z)$. The line corresponding to $z=0$ would represent a totally impermeable catchment ($n_e = 0$) or the boundary between the surface and groundwater compartments ($V = 0$). Other lines can be given specific meanings. For example, a line drawn for $z \leq 1$ m can be used to limit below the soil plus saprolite (altered rock layer) compartment whereas if drawn for $1 < z \leq 10$ m can be used to limit the shallow groundwater compartment. The deep groundwater compartment can be bounded below by the $10 < z \leq 100$ m lines and finally the very deep groundwater compartment by the $z > 100$ m line. These boundaries are not universal but are acceptable for Portuguese watersheds considering results from various studies [2–5]. Other geologic, topographic and climate settings may change these limits, but users can adapt the boundaries to their own settings. The diagram can be further divided by vertical lines representing pre-defined hydraulic turnover times. Thus, within the z compartments, there will be regions of fast (e.g., $t < 1$ year) to slow (e.g., $t > 100$ year) flow, representing watersheds of similar storage capacity but with different hydraulic conductivity and/or gradient. Taken altogether, the limits imposed to z and t , coupled with the range of Q/A_b values, define sectors in the diagram that can be interpreted from the standpoint of groundwater security. In general, the larger the Q/A_b , z and t the best for security. Larger values of Q/A_b ensure improved capacity to attain water demand for activities while larger values of z warrant resilience against hydrologic drought. Moreover, larger values of t safeguard longer contact between dissolved pollutants and aquifer materials that allow more efficient contaminant attenuation through filtration, adsorption or decay processes. Thus, starting from a simple log-linear regression (Eq. (5)), the proposed method is capable to assess water security from quality as well as quantity viewpoints.

Having defined the groundwater flow compartments, as function of Q/A_b , z and t , the diagram can be populated with $\log(\frac{Q}{A_b})$ and $\log(t)$ values relative to actual watersheds. The plot of a real watershed over the compartments allows to envisage which type the watershed represents. However, before doing that, a method is required to estimate the groundwater discharge and the hydraulic turnover

time at catchment scale. The present study resorted to a model developed by Pacheco and published in 2015 [1] that estimates t as function of stream flow discharge, which will now be improved to estimate groundwater discharge as well. A detailed description of the method is presented in the next subsection.

Hydraulic turnover time module

Similarly to Eq. (4), the hydraulic turnover time of a watershed has been equated to [6]:

$$t = \frac{Vn_e}{Q} \quad (6)$$

where t (T) is the time, Vn_e (L^3) is the mobile catchment storage, with V (L^3) equated to the watershed volume and n_e (dimensionless) to its concomitant effective porosity, and Q (L^3/T^{-1}) is the average groundwater discharge. A direct use of Eq. (6) to estimate the hydraulic turnover time implies the prior assessment of its components, but Pacheco [1] reduced the required data to Q when the equation is combined with a formula for n_e deduced from a recession flow method, namely the Brutsaert method [7–9].

The Brutsaert method used the so-called Boussinesq equation established in 1903 to describe the drainage from an ideal unconfined rectangular aquifer bounded below by a horizontal impermeable layer and flowing laterally into a water channel. The solution for that equation has the general form of a power function:

$$\frac{dQ}{dt} = aQ^b \quad (7)$$

where Q (L^3/T^{-1}) represents the groundwater discharge and t (T) is the time, while a and b represent hydraulic coefficients. The a coefficient relates with the groundwater reservoir's characteristics and b with the stream flow regime, namely the short-time or high-flow ($b = 3$) and the long-time or low-flow ($b = 1$) regimes. In the work published in 1998, Brutsaert and Lopez [9] derived the following solution for the short-time regime:

$$a = \frac{1.13}{Kn_e z^3 l^2}, b = 3 \quad (8a)$$

where K (LT^{-1}) is the hydraulic conductivity, n_e (dimensionless) the effective porosity, z (L) the aquifer thickness and l (L) the length of upstream channels intercepting groundwater flow. The long-time regime is adequately described by the so-called linear solution of Boussinesq published in 1903:

$$a = \frac{0.35\pi^2 K z l^2}{n_e A_b^2}, b = 1 \quad (8b)$$

where A_b (L^2) is the upland drainage area. In his work of 2015, Pacheco noted that when Eqs. (8a) and (8b) are combined and z is equated to V/A_b , the effective porosity becomes written as:

$$n_e = \frac{1.98}{V\sqrt{a_1 a_3}} \quad (9)$$

where a_i represents the value of a when $b = i$ (1 or 3). Besides, He further noted that by combining Eq. (9) with Eq. (1), the estimation of hydraulic turnover time simplifies to:

$$t = \frac{1.98}{Q\sqrt{a_1 a_3}} \quad (10)$$

meaning a formulation solely dependent on average groundwater discharge (Q) and flow regimes (a_1 and a_3). According to the Brutsaert method, the values of a_1 and a_3 can be read in a scatter plot $\ln(DQ_t/Dt)$ versus $\ln(Q_t)$, where Q_t is the stream flow discharge measured in a hydrometric station located at the outlet of a catchment. In that plot, the lower envelope to the scatter points is represented by two straight lines, one with a slope $b = 1$, and the other with a slope $b = 3$, and the y-values where these lines intercept $\ln(Q_t) = 0$ are the parameters a_1 and a_3 .

Table 1

Security classes of Q/A_b , t and z . They were adapted to the pilot application that spans a large number of Portuguese watersheds.

Security class	Q/A_b range (m/year)	t range (year)	z range (m)
1	< 0.01	< 10	< 1
2	0.01–0.1	10–100	1–10
3	0.1–0.5	100–500	10–50
4	0.5–1	500–1000	50–100
5	> 1	> 1000	> 100

In the present study, the average groundwater discharge (Q) is also determined from the scatter plot $\ln(DQ_t/Dt)$ versus $\ln(Q_t)$. In that diagram, the lines of slope 1 and 3 intersect each other at Q_{max} , which represents the maximum groundwater discharge in the low-flow regime because the intersection point separates the low-flow regime (only groundwater discharge) from the high-flow regime (groundwater + surface water discharge). In the present study, Q_{max} is used as proxy to the maximum possible groundwater discharge. To estimate Q_{max} , the user draws a vertical line through the intersection point of slope 1 and 3 lines and reads $\ln(Q_{max})$ at the independent variable axis (X-axis). On the other hand, the scatter point plotted most to the left in the low-flow regime region represents the lowest possible groundwater discharge in the available stream flow record (Q_{min}). In this case, drawing a vertical line through this point allows the reader to estimate $\ln(Q_{min})$ at the intersection of this line with the independent variable axis. Finally, the (geometric) average groundwater discharge will be given by:

$$Q = \exp\left(\frac{\ln(Q_{min}) + \ln(Q_{max})}{2}\right) \tag{11}$$

After the determination of Q and t , z can be estimated using Eq. (5).

Security module

As mentioned above, variables Q/A_b , t and z can be recast as indicators of groundwater security. Variable Q/A_b describes security from a quantity (yield) standpoint, as larger yields ensure a better response to water demand and especially peaks of demand. Variable t describes security from a quality viewpoint because of its relationship with pollution attenuation. And finally, variable z looks at security from the side of aquifer resilience, because a larger mobile storage allows a better adaption of water supply systems to variations of aquifer replenishment through infiltration of precipitation, namely to long periods of meteorologic and hydrologic drought.

The security module recasts Q/A_b , t and z as security indicators (S_Q , S_t and S_z , respectively) through reclassification. Considering the log-linear relationship between the three variables (Eq. (5)), reclassification will be also log-linear. The security indicators increase as function of increasing values of their parent variables, because yield, quality and resilience security increase as Q/A_b , t and z increase. The security classes cannot be defined universally because they are likely dependent on regional settings such as climate, geology or topography. For the present study, adapted to the pilot application in continental Portugal, the security classes were defined as depicted in Table 1.

The average security of a river basin is defined by a weighted product of partial securities (S_Q , S_t and S_z), i.e.:

$$S = S_Q^{wq} \times S_t^{wt} \times S_z^{wz} \tag{12}$$

where wq , wt and wz are the weights (importance) attributed to the S_Q , S_t and S_z indicators, respectively. By default, the weights are all equated to 1 (all indicators are equally important), but they can be customized to raise the importance of a specific indicator. In that case, the weight of an indicator can be set to values between 1 and 3, providing that the other weights are set to values between 0 and 1, and that the sum of weights is always 3, i.e.

$$wq + wt + wz = 3, \text{ for all combinations of } wq, wt \text{ and } wz \tag{13}$$

Table 2

Levels of groundwater security and corresponding ranges of S as determined by Eq. (12).

Level of security	S range
Very low	1
Low	1–2
Moderate	2–12
High	12–36
Very high	36–80
Exceptional	80–125

Setting the sum of weights fixed to a constant value keeps the range of S values relatively uniform and hence allows a direct comparison among weighted and unweighted security diagrams or maps. If the weight of an indicator is set to 3 (and the other weights to 0), then the resulting diagram or map will represent groundwater security from a single standpoint (yield, quality or resilience).

The calculated S values (Eq. (12)), if weights are all 1, range from 1 to 125. The final step of security module is to set up a qualitative scale that levels groundwater security between very low and exceptional, hinged on five classes of S . The criterion used to define the class boundaries was: (1) class 1 is defined when all indicators are 1 (i.e., $S_q = 1$ and $S_t = 1$ and $S_z = 1$); (2) the class is set to $i + 1$ if the calculated S is larger than a reference case where two indicators are equal to i and one indicator is equal to $i + 1$. Based on this criterion, the levels and ranges of groundwater security are depicted in Table 2.

Data and software requirements

The groundwater security method is minimalist as regards data requirements. It fully operates with a dataset of daily stream flow discharges measured at the outlet of target watersheds, complemented with watershed boundaries and areas. In general, the records of stream flow discharge can be downloaded from the websites of public water resource management institutions, and saved as spreadsheets. Sometimes, these institutions also provide shapefiles / geodatabases with the delineation and geometric characterization of watersheds located upstream the sites where the stream flow discharges were measured. If not available, the stream flow discharges can be measured on site with appropriate hydrometric stations, and the watershed boundaries interpreted from Digital Elevation models using conventional terrain modeling tools embedded in GIS software.

The three modules comprising the groundwater security method can all be implemented in Microsoft Excel software using solely the stream flow discharge measurements and watershed areas (e.g., Fig. 1a,b below). The results (e.g., security indicators) can then be used in more sophisticated statistical computer packages for appealing representations. Here, the STATISTICA software of Statsoft (<https://www.statistica.com/en/>) was used to draw contour plots (e.g., Fig. 2a–d) and histograms (Fig. 3a–d), whereas the ArcGIS Pro-of ESRI (<https://www.esri-portal.pt/pt-pt/arcgis/produtos/arcgis-pro/overview>) was used to draw spatial distribution maps (Fig. 4a–d).

Strong points and gaps

Strong point 1: novelty. The method has the capacity of unraveling three important viewpoints of groundwater security using a single equation (Eq. (5)), namely aquifer yield capacity, aquifer self-depuration capacity and aquifer mobile storage (resilience to prolonged drought periods), which is remarkable. Strong point 2: minimal data requirements. The method relies on a couple of readily available variables: daily stream flow discharge and watershed area. Gap: parameter estimation dependent on user experience. The subjectivity of determining a_1 , a_3 , Q_{\min} and Q_{\max} from Fig. 1a is a source of uncertainty.

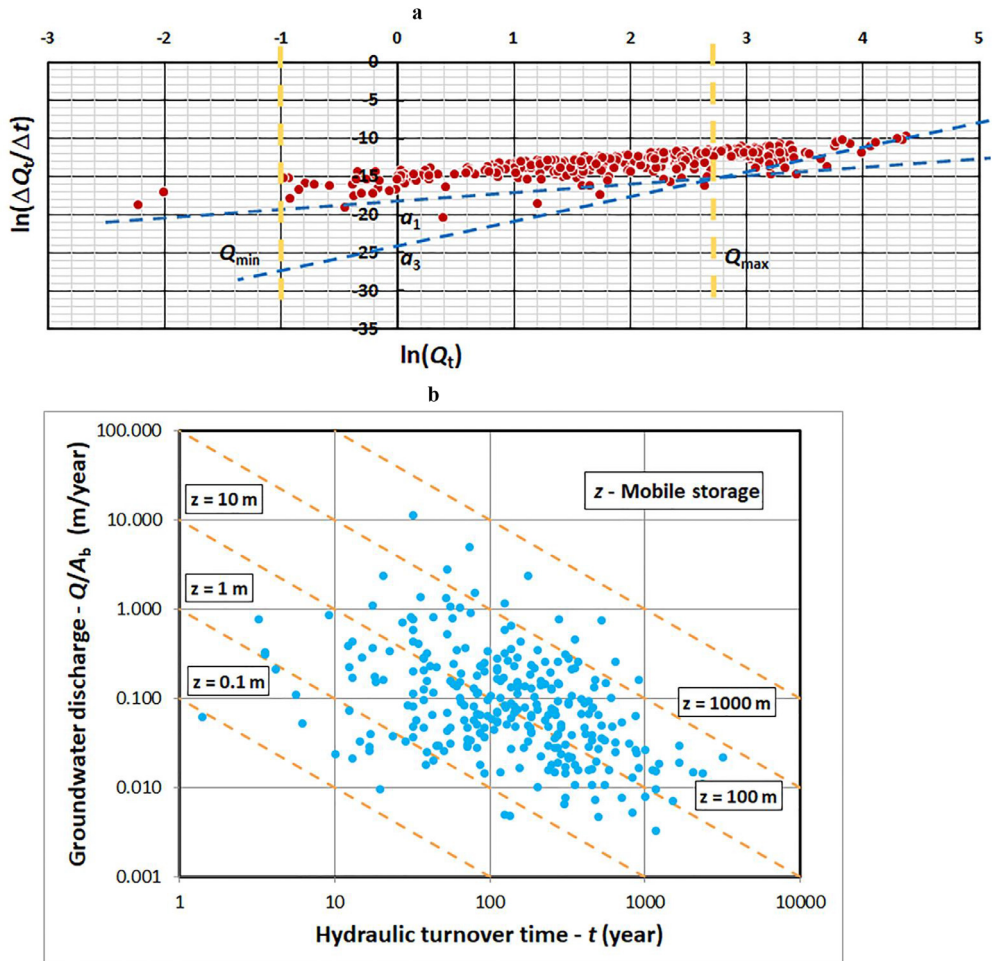


Fig. 1. a – Example of how to apply the Brutsaert method to stream flow discharge data. The example refers to station 03 J/02H. The raw data and full implementation of the method can be consulted in the Supplementary Materials (Spreadsheet 2). 1b – Distribution of 294 Portuguese watersheds (blue circles) as function of groundwater discharge (Q/A_b), hydraulic turnover time (t) and watershed mobile storage (z).

Method validation

Data preparation and method implementation

The method is exemplified with streamflow discharges and drainage areas relative to 294 watersheds located in continental Portugal, spanning an ample range (several orders of magnitude) of these values: $0.02 < \text{stream flow discharge (m}^3/\text{s)} < 517.13$; and $2.6 \times 10^6 < \text{drainage area (m}^2) < 9.7 \times 10^{10}$. The data were retrieved from the Portuguese System for Information on Water Resources, at the URL <http://snirh.apambiente.pt>. The Supplementary Materials (Spreadsheet 1) contain the list of basins and of hydrometric stations located at the basin outlets, namely information on basin's name and drainage area, as well as on station's code, name, geographic location (latitude, longitude, altitude) and average stream flow discharge. Spreadsheet 2 can be consulted to see how the Brutsaert method was applied to one of the hydrometric stations (03 J/02H), namely: (1) how the values of a_1 and

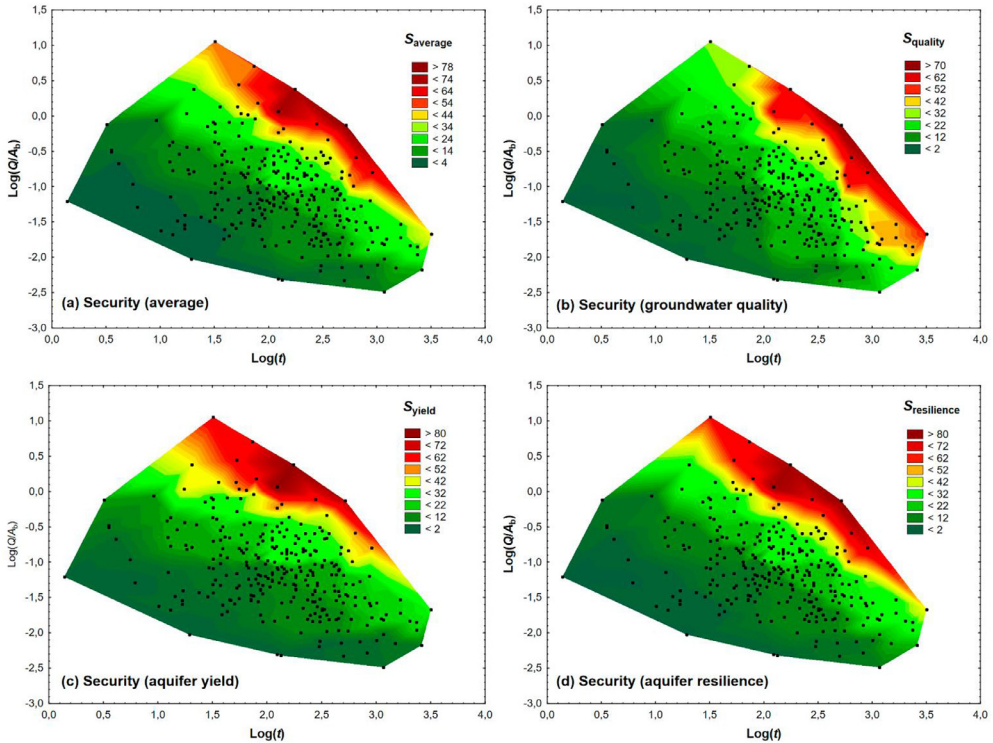


Fig. 2. Distribution of groundwater security (shaded areas) as function of groundwater discharge (Q/A_b), hydraulic turnover time (t) and catchment mobile storage (z): (a) $S_{average}$ – unweighted security; (b) $S_{quality}$ – groundwater security highlighting the role of hydraulic turnover time; (c) S_{yield} – groundwater security highlighting the role of Q/A_b ; (d) $S_{resilience}$ – groundwater security highlighting the role of z .

a_3 were estimated from the $\ln(DQ_t/Dt)$ versus $\ln(Q_t)$ diagram; (2) how the values of $\ln(Q_{max})$ and $\ln(Q_{min})$ were estimated from the same graph; and (3) how the previous values were coupled with the average Q value (Eq. (11)) to estimate t using Eq. (10). The stream flow discharges depicted in Spreadsheet 2 refer to daily records, which were summarized as monthly averages before being used with the Brutsaert method. The scatter diagram plotting $\ln(DQ_t/Dt)$ versus $\ln(Q_t)$ is also represented in Spreadsheet 2 and reproduced in Fig. 1a for illustrative purposes. The DQ_t/Dt quotient was estimated as $(Q_{i+1} - Q_i)/(t_{i+1} - t_i)$, where subscript i refers to a month. The graphic's abscissa was estimated as $\ln[(Q_{i+1} + Q_i)/2]$. The dashed lines were drawn with slope 1 and slope 3 just below the cloud of points. It is worth noting the haziness of drawing these lines, because it is frequent that some points scatter significantly below the main cloud. In those cases, the dashed lines can be drawn so 90% of the points are located above them [10,11]. A vertical orange line was passed through the intersection of slope 1 and slope 3 lines to obtain $\ln(Q_{max})$. Another vertical line was passed through the lowest continuous set of $\ln(Q_t)$ values to obtain $\ln(Q_{min})$. Two points at the left of this line were not considered in this assessment because they were assumed outliers. The intercept-y of the dashed lines in Fig. 1a are $\ln(a_1) = -20$ and $\ln(a_3) = -25$ which, for an average groundwater discharge of $Q = 2.34 \text{ m}^3/\text{s}$ (or $7.38 \times 10^7 \text{ m}^3/\text{year}$), implies a hydraulic turnover time of $t = 158.6$ years for station 03 J/02H (River Vez basin). By drawing plots similar to Fig. 1a, but relative to the other 293 hydrometric stations listed in the Supplementary Materials, hydraulic turnover times and average groundwater discharges were calculated for all studied basins. The results are listed in Spreadsheet 3 of Supplementary Materials and range from: $t = 1.39$ to 3185.79 years; $Q/A_b = 0.003$ to 11.32 m/year.

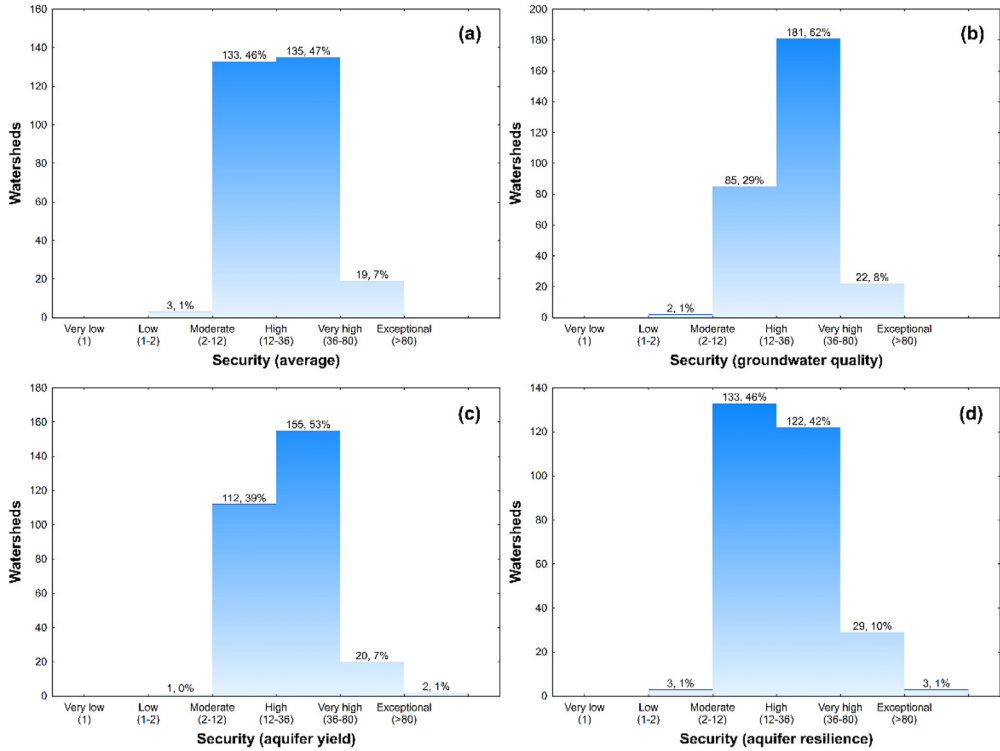


Fig. 3. Groundwater security histograms: (a) $S_{average}$; (b) $S_{quality}$; (c) S_{yield} ; (d) $S_{resilience}$. Additional information in the caption of Fig. 2.

It is worth recalling here that turnover times determined by Pacheco in 2015 [1] were based on average Q_t and not on average Q and hence are likely underestimated.

Having estimated the hydraulic turnover times for all river basins, the 294 Q/A_b versus t points were plotted in the groundwater security diagram (Fig. 1b). The studied basins span various groundwater compartments (various orders of z), which is not surprising given the range of drainage areas that span > 4 orders of magnitude ($2.6 \times 10^6 < \text{drainage area (m}^2) < 9.7 \times 10^{10}$).

A brief summary of results in the tested area

The groundwater security of watersheds is represented in Fig. 2a-d. The allocation of security ratings to the watersheds is in keeping with the classes of Table 1 (security indicators) and Table 2 (security levels as determined using Eq. (12)). The allocation of S_Q , S_t and S_z , as well as the calculation of S , are provided as Supplementary Materials (Spreadsheet 4). Fig. 2a describes unweighted security while Fig. 2b-d result from a customization of weights. In the case of Fig. 2b, $w_t = 1.5$ and $w_q = w_z = 0.75$, meaning that this figure highlights the contribution of hydraulic turnover time (protection of groundwater quality) to groundwater security. Fig. 2c and d were drawn with the purpose to highlight the roles of yield and resilience, respectively, and, in those cases, the weights were set up as follows: $w_q = 1.5$ and $w_t = w_z = 0.75$ (Fig. 2c); $w_z = 1.5$ and $w_q = w_t = 0.75$ (Fig. 2d). In all these figures, the vast majority of watersheds plot where security scores range from 2 to 36, meaning that they are moderately to highly secured. There are even a significant number of watersheds with very high security (points plotted over the red-shaded areas). The histograms of security, with identification of counts and percentages of count, are presented in Fig. 3a-d, as

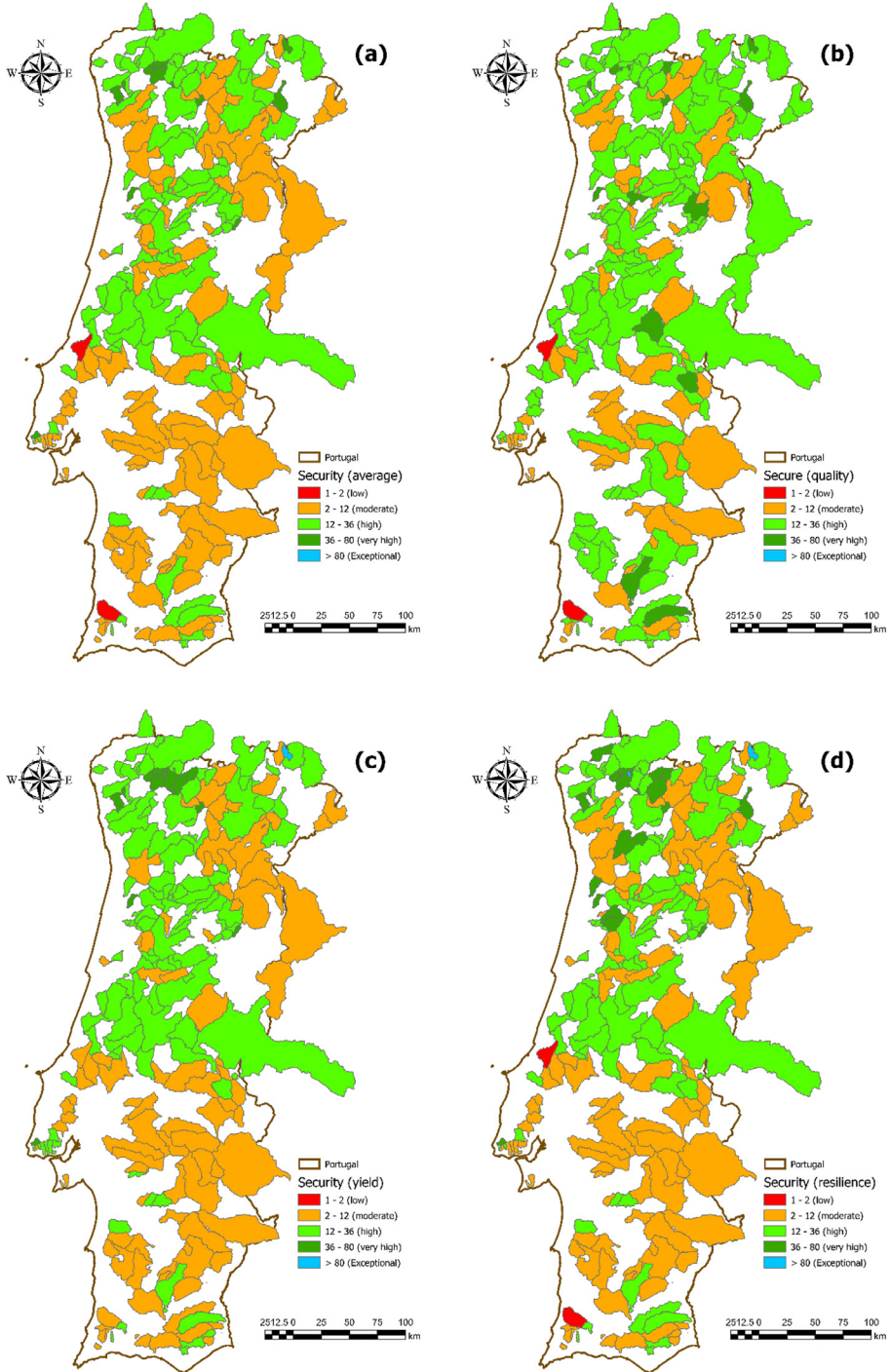


Fig. 4. Groundwater security of continental Portugal watersheds, as estimated with the proposed method: average(a) and highlighting groundwater quality protection (b), aquifer yield (c) and aquifer resilience (d).

complement to the diagrammatic representation of Fig. 2a–d. These figures point to 7–10% of very high security watersheds and > 60% watersheds highly secured for groundwater quality.

The spatial distribution of groundwater security is displayed in Fig. 4 for the average (a), quality (b), yield (c) and resilience (d) scenarios. It is evident the concentration of moderately secure basins in the more arid regions of continental Portugal (Northeast and South, where precipitation is low), and the general highly secure basins concerning quality.

Supplementary material and/or Additional information: The Supplementary Materials are composed of four spreadsheets: (1) list of watersheds used to validate the groundwater security method. The spreadsheet contains information on basin's name and drainage area; the code, name and location information about the hydrometric station located at the basin's outlet; (2) exemplification of how to apply the Brutsaert method to one hydrometric station (Fig. 1a); (3) summary of hydraulic turnover times and projection of Q/A_b versus t values on the groundwater security diagram (Fig. 1b); (4) Base data and calculation of security indicators (S_Q , S_T and S_Z) and security levels (S_{average} , S_{quality} , S_{yield} and $S_{\text{resilience}}$) used to produce Fig. 2 (diagrammatic representation of security levels as function of groundwater discharge, hydraulic turnover time and catchment mobile storage), Fig. 3 (histograms of security levels) and Fig. 4 (spatial distribution of security levels).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

For the authors integrated in the CITAB research center, this work was supported by National Funds of FCT – Fundação para a Ciência e Tecnologia, under the project UIDB/04033/2020. The author integrated in the CITAB research center is also integrated in the Inov4Agro – Institute for Innovation, Capacity Building and Sustainability of Agri-food Production. The Inov4Agro is an Associate Laboratory composed of two R&D units (CITAB & GreenUPorto). For the author integrated in the CQVR, the research was supported by National Funds of FCT – Fundação para a Ciência e Tecnologia, under the projects UIDB/00616/2020 and UIDP/00616/2020.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:[10.1016/j.mex.2022.101766](https://doi.org/10.1016/j.mex.2022.101766).

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