



Evaluation of GRACE data for water resource management in Iberia: a case study of groundwater storage monitoring in the Algarve region

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ABSTRACT

Study region: Iberia, Algarve basin, South Portugal.

Study focus: This study evaluates the performance of several GRACE products in Iberia using the closure of the water budget. Then, it focusses on the Algarve region and explores the potential of GRACE as a tool of quantitative groundwater monitoring capable of bridging gaps in the existing ground-based network. Monthly data from GRACE, ancillary datasets from E-OBS, GLEAM, GRUN and ERA5, and groundwater level measurements from 12 karst-porous aquifers in the Algarve basin (5000 km²) are analyzed from 2004 to 2014.

New Hydrological Insights for the Region: When considering the closure of the water budget at the Iberian scale, GRACE Mascon solutions perform remarkably well and better than the products based on spherical harmonics. When considering only the Algarve region, the results are similar to the ones obtained for Iberia, but the GRACE solution that performs the best is the average of the CSR and JPL Mascon products. In spite of the Algarve's extremely small area when compared to the GRACE footprint, the satellite is capable of capturing the regionally averaged seasonal and de-seasonalized variations in observed groundwater storage (correlation between GRACE-derived and regionally averaged ground-based measurements is 0.82). For the first time ever at the regional Algarve scale, bounds are placed on the aquifer's storage properties which vary from 3.65×10^{-3} to 4.92×10^{-2} .

1. Introduction

The Algarve is a semi-arid region in the southwestern part of the Iberia Peninsula, where water demand for irrigation purposes is heavily dependent on groundwater. Evidence of a drying trend in this region is compelling (Guerreiro et al., 2017a) calling for the need of better aquifer monitoring. However, the quality and continuity of the existing ground-based monitoring network is at risk due to budget restriction in recent years. The motivation behind this study is to improve monitoring through the use of remote sensing datasets which can mitigate problems in the spatial and temporal coverage of groundwater levels in this region. Bearing in mind the doubts regarding the validity of using coarse resolution satellite data at such a local scale, the work begins by analyzing the

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performance of the various products at the scale of Iberia (Fig. 1).

Current knowledge of the global water cycle is increasingly dependent on the integration of conventional observations and remote datasets from satellite missions (Rodell et al., 2015). The first experiment providing satellite-based monitoring of groundwater changes at regional to global scales was the Gravity Recovery and Climate Experiment (GRACE), a joint mission between NASA and the German Aerospace center, primarily designed to provide measurements of the Earth’s gravity field (Tapley et al., 2004). Measurements of gravity carried out between 2002 and 2017 were based on the distance between two polar, sun-synchronous satellites separated 200 km apart, equipped with microwave K-band sensors, accelerometers and Global Positioning System receivers. The measurements,

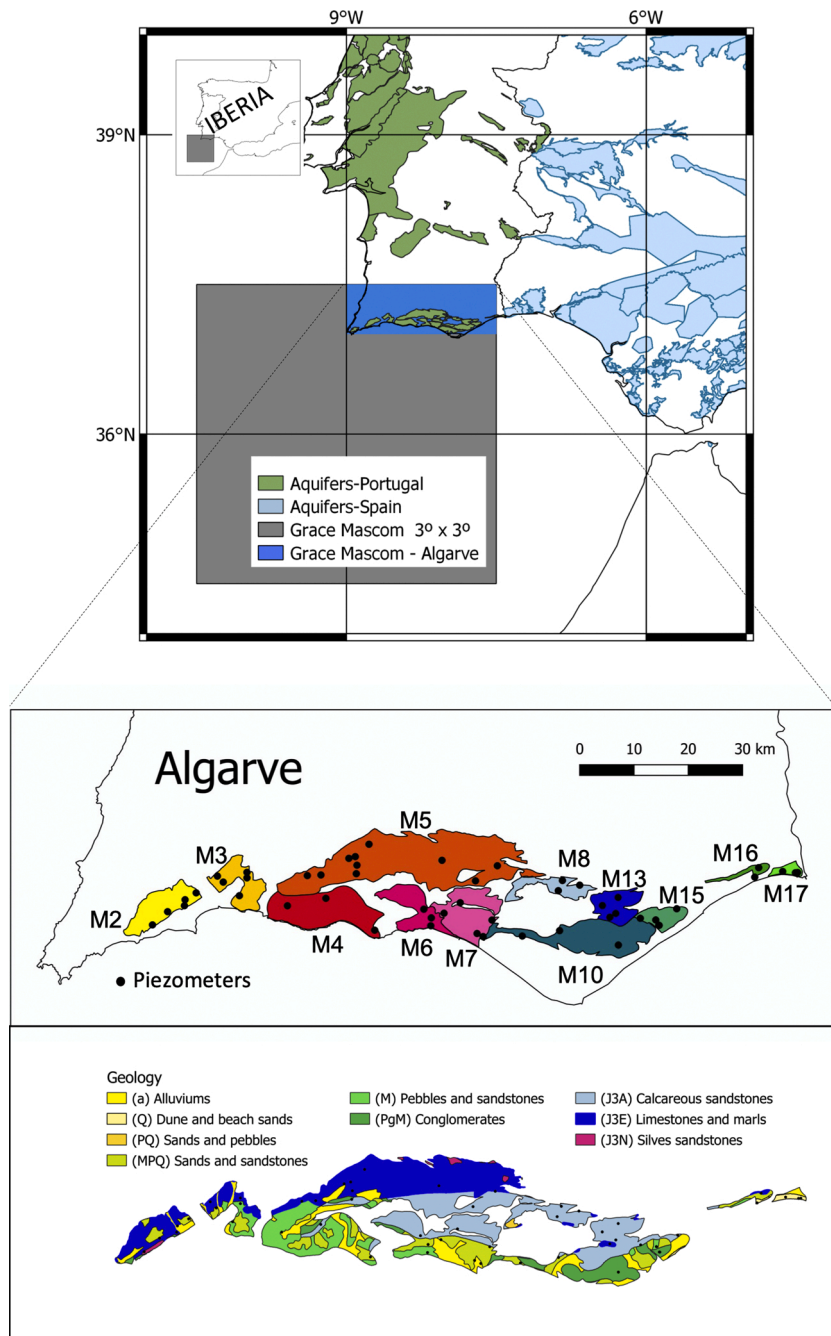


Fig. 1. Location of the study area. Map of southwest Iberia showing the groundwater bodies in Portugal and Spain, the 3° x 3° cell grid of the GRACE Mascon JPL product and its extent over land coinciding with the Algarve region. The zoomed region shows the studied aquifers systems (M2 to M17) in the Algarve and the location of the in-situ monitoring wells (black dots). The bottom map shows the surface geology of the studied aquifers.

added by other data as well as models, provided a global coverage of gravity changes reflecting mass changes in the Earth. Over land, these changes in mass are mainly due to changes in Total Terrestrial Water Storage (Δ TWS), an integrated measure of water storage that includes snow, surface water, soil moisture and groundwater. Over the past two decades GRACE-derived data has been shown to match in-situ measurements of groundwater levels in many large basins (Frappart and Ramillien, 2018; Rodell et al., 2004; Strassberg et al., 2007; Yeh et al., 2006), used to quantify the interannual variability of Δ TWS at some of the largest aquifers in the world (Cao et al., 2019; Huang et al., 2019; Humphrey et al., 2016), to estimate aquifer storage parameters (Bhanja et al., 2018; Sun et al., 2010) and to evaluate groundwater storage anomalies related to natural and anthropogenic forcing (Asoka et al., 2017; Rodell et al., 2018; Solander et al., 2017).

The processing chain of GRACE data involves a large number of corrections and uncertainties that introduce errors and impose restrictions on its use (Swenson and Wahr, 2006). One of the most important errors is the signal leakage between neighboring grid cells caused by the truncation of spherical harmonics and Gaussian filtering (Landerer and Swenson, 2012). For hydrological investigations it is commonly referred that the catchment size should not be less than the spatial resolution of the GRACE products $\approx 200,000 \text{ km}^2$ for Mascon and $\approx 300,000 \text{ km}^2$ for RL05 solutions (Vishwakarma et al., 2018). However, several studies showed that catchments smaller than this could be well observed by GRACE despite the resolution limitations (Becker et al., 2010; Ouma et al., 2015; Wang et al., 2011). For example, Biancamaria et al. (2019) showed good agreement between Δ TWS and hydrological models in the Garonne river basin in South West France ($50,000 \text{ km}^2$ drainage area), Liesch and Ohmer (2016) showed it was possible to estimate groundwater depletion from GRACE data in Jordan (over basins ranging from 1500 to $18,000 \text{ km}^2$), Hachborn et al. (2017) determined that GRACE is sufficiently sensitive to obtain a meaningful groundwater storage signal in southern Ontario ($45,000 \text{ km}^2$ area) and Rahimzadegan and Entezari (2019) showed that GRACE-derived estimation of groundwater-level changes can be used at local-scale in Iran with an acceptable accuracy (areas ranging from $5,000$ – $20,000 \text{ km}^2$). A major factor contributing to these recent successful applications is the progress in the processing algorithms of GRACE data, namely the development of global equal area Mascon products with reduced leakage errors across land/ocean boundaries and better signal to noise ratios, which makes them more suitable for regional applications (Wiese et al., 2016). However, these regional applications of GRACE data have to be evaluated against ground station measurements and this is the main objective of the present study.

The Algarve is characterized by a warm Mediterranean climate, with a dry summer nearly 5 month long and low average annual rainfall. Groundwater in the region is vital to sustain agriculture and has been used as a backup system against temporary water shortages from immemorial time. In 2001 the emplacement of a public district water supply system based on dams enabled the shift from groundwater to surface water irrigation. However, operational problems and recent dramatic droughts (2004–2006, 2016–2017) pointed to the necessity of a mixed-source supply system using both surface and groundwater (Hugman et al., 2017; Stigter et al., 2006). Today, groundwater constitutes 88 % of the water used in agriculture, which in turn accounts for 60 % of the total water demand in the region. In the context of climate change the Algarve faces a major water resource management challenge. This is one of the regions in Europe where climate projections for 2041–2070 forecast the highest indexes of drought frequency and drought severity, under all emissions scenarios (Guerreiro et al., 2017b; Spinoni et al., 2018). In order to mitigate future water crisis there is an urgent need to maintain and improve the monitoring of groundwater resources in the area.

To our knowledge, this is the first study exploring the potential of GRACE to monitor groundwater storage changes in this part of the world (Iberia and Portugal in particular). The paper is structured in three parts: (1) The first is an assessment of different GRACE products using a water budget analysis based on precipitation, evapotranspiration and runoff obtained from public databases and re-analysis datasets. The aim is to determine which GRACE solution provides the best closure of the water budget, first in Iberia and then in the Algarve; (2) The second examines the match between GRACE-derived groundwater storage and in-situ groundwater level measurements obtained from a set of 51 piezometers, distributed across 12 aquifers in the Algarve. We apply a robust optimization method for estimating aquifer storage parameters, similar to the proposed by Sun et al. (2010), to obtain estimates of the storativity or specific yield distribution in the region. The optimization problem is formulated to explicitly account for uncertainty in remotely sensed and in-situ data by incorporating bounds on data variations; (3) Finally, groundwater time series are decomposed into trends, seasonal and residual components. This decomposition is of interest from the point of view of water resource management, since knowledge of water storage fluctuations is essential to establish relationships between water scarcity, climate forcing and human intervention.

2. Data

2.1. Study area

Mountain ranges in the Iberian Peninsula predominantly running from west to East have influenced the river network and the spatial configuration of the major river basins (Fig. 1). The topography and large weather circulation patterns generate a strong gradient in precipitation which decreases from north to south. As a result, river basins in the northern sector of the Peninsula have abundant yields while rivers in the southern sector have only modest mean annual streamflows. The Guadiana river, which defines the border between Portugal and Spain in southwestern Iberia, is the only major river at the edge of the Algarve and presents an annual streamflow of less than $4000 \text{ hm}^3/\text{year}$. The remaining rivers and streams in the Algarve have torrential character and there are no natural lakes. The areal extent of surface water held by dams is less than 1.4 % of the of the total area occupied by aquifers (SNIRH, 2020) and thus, surface water represents a very small fraction of the total available freshwater resources in the region.

In terms of geology the Algarve basin ($\sim 130 \times 40 \text{ km}$) is an E–W oriented sedimentary depocenter. It overlays a Paleozoic basement mainly composed of schists and greywackes cross-cut by Hercynian NNW–SSE to NW–SE and ENE–WSW faults which exerted a

significant tectonic control during sediment deposition (Ribeiro et al., 1979). The basin is composed of more than 3000 m of essentially marine sediments accumulated during Mesozoic and Cenozoic times (Manuppella, 1992). According to the geometry and permeability of the deposited lithologies, 17 aquifer systems were defined with predominantly karstic and porous detrital hydro-stratigraphic units (Almeida et al., 2000). This study focusses on 12 of these aquifers selected for their piezometric coverage (Fig. 1 and Table 1).

The Mesozoic sequence is essentially comprised of limestones, dolomites and marls of Jurassic age, that outcrop in the northernmost part of the study area, locally known as Barrocal (Fig. 1). This region is characterized by gentle hills and rocky soils, covered by Mediterranean vegetation and traditional crops such as olive, almond, fig and carob trees. The Jurassic and lower Cretaceous carbonate lithologies promoted the development of highly permeable karst formations that support some of the most important aquifers in the Algarve, such as the Querença-Silves (M5). The karstic depressions, covered by silts and clays, are nowadays mainly occupied by citrus orchards and vineyards, thanks to the widespread use of groundwater irrigation. Nevertheless, the irrigated area represents only around 4% of the total hydrographic basin being estimated that 24 % of the irrigation water returns to the groundwater reservoirs (APA, 2016). To the south, the Barrocal gives way to the coastal Algarve, a flattened region whose altitude does not generally exceed a few hundred meters. This region is largely covered by Cenozoic rocks, namely sandstones and bioclastic limestones from the Miocene, as well as Plio-Quaternary sands and gravels which are widespread distributed along the coast (Fig. 1).

A detailed description of all aquifers in continental Portugal is provided by Almeida et al. (2000). Most aquifers in the Algarve region are multi-layer mixed karst-porous systems, with the exceptions of M2, M5, M8, M13, classified as karst, and M17 classified as porous (Table 1). The Jurassic dolomites and limestones, as well as the Miocene carbonates, constitute the main water bearing formations in the majority of them. Like karst aquifers in general they show highly heterogeneous hydraulic properties. This is mainly due to spatial variations in the density and connectivity of the fracture network but is also controlled by variations in aquifer thickness, depth and lateral extent. Sands and gravels of Plio-Quaternary age often support shallow unconfined aquifer sections that are directly recharged by precipitation.

The climate in the Algarve region is temperate with hot and dry summers (Mediterranean of type Csa in the classification of Köppen-Geiger). The monthly average temperature ranges between 12 and 24 °C and the total annual rainfall is about 500 mm/year (1981–2010 climate normal) (IPMA, 2020). On average, about 42 % of the annual precipitation falls during the 3-month winter season (Miranda et al., 2002). Due to the orography, the precipitation decreases substantially from north to south, with coastal areas receiving on average less 70 % of precipitation than the hilly northern areas. The very low recharge rates in the Paleozoic metamorphic rocks to the north of the study area (10 % or less of the precipitation) force the generation of flash floods during precipitation episodes that is transformed in allogenic recharge when the limits of the more permeable lithologies of the Algarve sedimentary basin are intercepted to the south.

2.2. In-situ groundwater levels

The Portuguese National System for Water Resources maintains a nationwide groundwater level monitoring network and provides monthly time-series of measurements through its site (SNIRH, 2020). In the Algarve the observation network comprises 139 piezometers distributed among 17 aquifer systems, but not all piezometers have been operating continuously and some present evidence of sensor calibration problems or other lack of appropriate quality control. Therefore, a selection of 51 piezometer locations distributed over 12 aquifers (Fig. 1) was performed based primarily on the completeness and consistency of the time-series and secondly on a distributed geographic location sampling as many aquifers as possible. Preprocessing steps such as searching for outliers and interpolation for estimating missing values were carried out for all piezometric records before analysis. Initial screening detected some records containing inconsistent seasonal patterns that reveal the influence of human activity. These records were kept on purpose to check their departures from regional averages. The groundwater level data has a monthly frequency and spans the period from January 2004 to December 2014.

Table 1
Studied aquifers in the Algarve.

| Code | Name | Type | Area (km ²) | N. of wells |
|------|----------------------------------|--------------------------------|-------------------------|-------------|
| M2 | Almadena - Odeaxere | Semi-confined karst | 63.489 | 5 |
| M3 | Mexilhoeira Grande - Portimao | Semi-confined karst and porous | 51.707 | 5 |
| M4 | Ferragudo - Albufeira | Semi-confined karst and porous | 117.099 | 3 |
| M5 | Querença - Silves | Semi-confined karst | 317.839 | 11 |
| M6 | Albufeira - Ribeira de Quarteira | Semi-confined carbonate | 54.546 | 3 |
| M7 | Quarteira | Semi-confined karst and porous | 81.185 | 5 |
| M8 | S. Bras de Alportel | Semi-confined karst | 34.425 | 3 |
| M10 | S. Joao da Venda - Quelfes | Semi-confined carbonate | 113.305 | 3 |
| M13 | Peral - Moncarapacho | Semi-confined karst | 44.066 | 4 |
| M15 | Luz - Tavira | Semi-confined karst and porous | 27.720 | 5 |
| M16 | S. Bartolomeu | Semi-confined karst and porous | 10.595 | 2 |
| M17 | Monte Gordo | Unconfined porous | 9.616 | 3 |

2.3. GRACE water storage anomalies

Several solutions for GRACE total water storage monthly anomalies (deviations from the mean) denoted as Δ TWS, are available from different processing centers (University of Texas Center for Space Research (CSR) German Research Center for Geosciences (GFZ), Jet Propulsion Laboratory (JPL), among others). All released versions have processing chains involving corrections for gravity variations caused by atmospheric effects, ocean tides and glacial isostatic adjustment. In this study we use five solutions falling into two main categories of GRACE datasets: (1) the GRCTellus Land RL05 release of GRACE data from JPL, CSR and GFZ (available at <https://grace.jpl.nasa.gov/data/get-data/monthly-mass-grids-land>), and (2) the Mascon (mass concentration blocks) solutions from CSR (RL06) (available at <http://www2.csr.utexas.edu/grace>) and from JPL (RL06) (available at https://grace.jpl.nasa.gov/data/get-data/jpl_global_mascons).

The RL05 solutions from GFZ, CSR and JPL are released in grid form, available at $1^\circ \times 1^\circ$ resolution. They are derived from monthly Spherical Harmonic (SH) coefficients post-processed for truncation, de-stripping and spatial smoothing through the application of 300 km radius Gaussian filters (Landerer and Swenson, 2012; Swenson and Wahr, 2006). For land hydrological applications the monthly mass grids need to be multiplied by grids of scaling coefficients, which are gain factors based on numerical land hydrology models. The processing centers supply grids with the scaling coefficient and grids with estimates of total Δ TWS error resulting from a combination of measurement and signal leakage errors (Landerer and Swenson, 2012).

The Mascon solutions are an improved version of GRACE products with reduced leakage errors at ocean-continent boundaries, which are more appropriate to regional studies, especially in coastal regions. The CSR Mascon is based on spherical harmonic coefficients and is available at native $1^\circ \times 1^\circ$ resolution although it is released at 0.25° (Save et al., 2018, 2016). Relative to previous CSR solutions the RL06 Mascon uses a newly defined grid which better split tiles along the coastline to minimize the leakage between land and ocean signals. Since this product does not use empirical de-stripping or filtering, there is no need to apply any additional scaling factors to this solution.

The JPL Mascon (RL06) uses an alternative form of gravity field basis functions with a-priori constraints in space and time to minimize the effect of measurement errors (Watkins et al., 2015; Wiese et al., 2016). Despite provided with a spatial sampling of 0.5° in both latitude and longitude, the JPL Mascon grid has a native resolution of $3^\circ \times 3^\circ$ in size (Fig. 1 shows the extent of the JPL Mascon grid cell used to study the Algarve region). We apply a set of optional gain factors for continental hydrology applications, derived from the CLM hydrology model, which are designed to study mass change signals at sub-mascon resolution. These land-grid scaling factors, as well as the scaled uncertainty estimates associated to each Mascon, are also provided within the same data directory as the Mascon data. As grid cells along coastlines (such as the one in Fig. 1) contain mixed land and ocean signals we use the CRI-filtered version of the mascon solution. This version of the data employs a Coastline Resolution Improvement (CRI) filter in a post-processing step to separate the land and ocean portions of mass within each land/ocean mascon. The joint effect of the CRI filter and gain factors has been shown to reduce leakage errors when determining the mass balance of large hydrological basins of up to 30 %, with local improvements ranging from 38 % to 81 % (Wiese et al., 2016)

For visualization purposes Fig. 2 displays an example of a snapshot at one particular month (January 2016) of the five GRACE

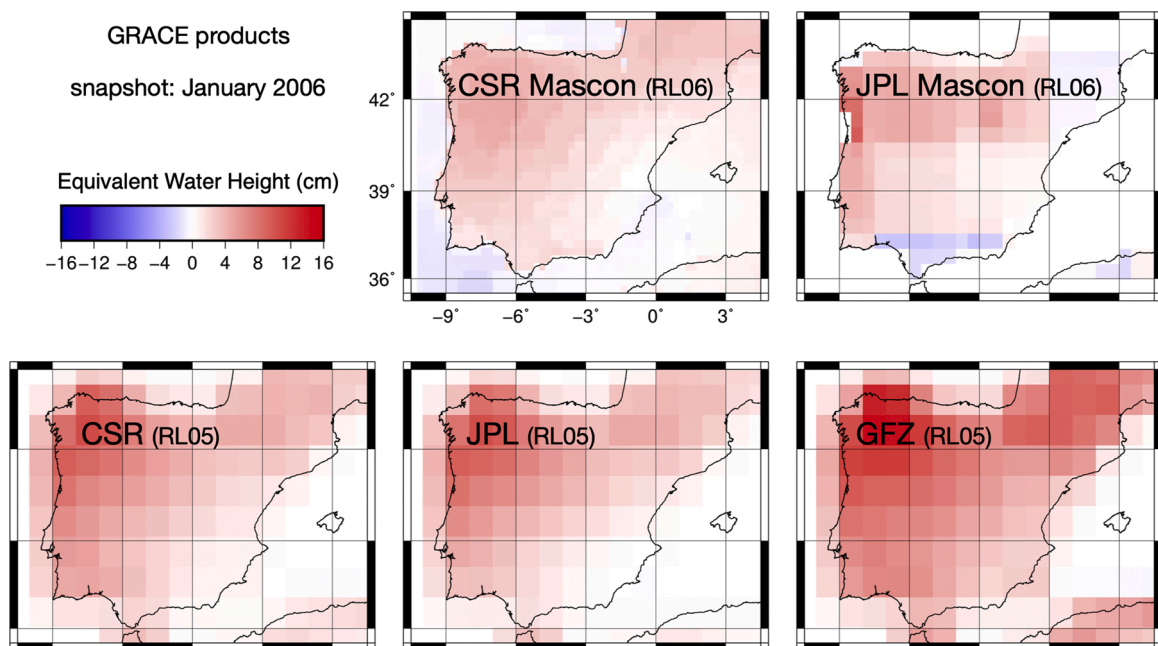


Fig. 2. Example of a snapshot (January 2006) of the five different GRACE products over Iberia showing differences in spatial resolution and range of equivalent water height (or thickness).

solutions in Iberia as provided by the processing centers (after application of the scaling factors). The solutions represent total water storage anomalies expressed in units of equivalent water height (in cm). The image highlights differences in the pixel resolution and the much better discrimination of land and ocean regions in the Mascon products (at the top) in comparison with the solutions based on truncated spherical harmonics (at the bottom).

Since water budgets are based on land variables (described in the next section) we use a wet-dry mask grid computed using the shoreline database of the Generic Mapping Tools (Wessel et al., 2019) to isolate the land part of the GRACE products over Iberia. Spatial averages, also known as zonal means, over the masked grids produce the GRACE-Iberia time-series displayed in Fig. 3. Time-series corresponding to spatial averages over the Algarve region are obtained in the same way but are limited to the region between $7^{\circ} - 8^{\circ}$ W of longitude and $37^{\circ} - 38^{\circ}$ N of latitude (GRACE-Algarve). All time-series represent anomalies in total water storage relative to the 2004–2014 time-mean baseline.

2.4. Ancillary data

Public available estimates of precipitation, evapotranspiration, runoff and soil moisture are used for two purposes: (1) provide alternative independent estimates of the total water balance used for GRACE validation over Iberia and the Algarve, and (2) provide estimates of the different components of the water cycle, needed for the disaggregation of Δ TWS in the Algarve. A flowchart showing the main datasets and processing steps is shown in Fig. 4.

The balance between precipitation, evapotranspiration and runoff constitutes the simplest estimate of the water budget or net flux of water between the atmosphere and the Earth's surface. Monthly precipitation data with a spatial resolution of 0.1° is extracted from the E-OBS gridded dataset (v20.0e) which is based on ground-station observations. This dataset is currently maintained and provided by the European Climate Assessment & Dataset project (<https://www.ecad.eu>). Monthly grids of evapotranspiration and volumetric soil moisture are obtained from the third version of the Global Land Evaporation Amsterdam Model (GLEAM v3) at 0.25° spatial resolution (<https://www.gleam.eu>). GLEAM is a set of algorithms dedicated to the estimation of terrestrial evaporation and root-zone soil moisture from satellite data (Martens et al., 2017). It uses the Priestley and Taylor equation to calculate potential evaporation based on observations of surface net radiation and near-surface air temperature, as well as combination of satellite, ground-station and reanalysis input data. Other estimates of soil moisture, such as the provided by the earth2Observed project (<https://www.earth2Observe.eu/>) were also tested but gave essentially the same results as the GLEAM estimates. Runoff data was extracted from GRUN, an observation-based gridded global reconstruction of monthly runoff timeseries (Ghiggi et al., 2019). The dataset corresponds to the ensemble mean of 50 reconstructions obtained from a machine learning model with different subsets of data and is provided at 0.5° spatial resolution from 1902 to 2014.

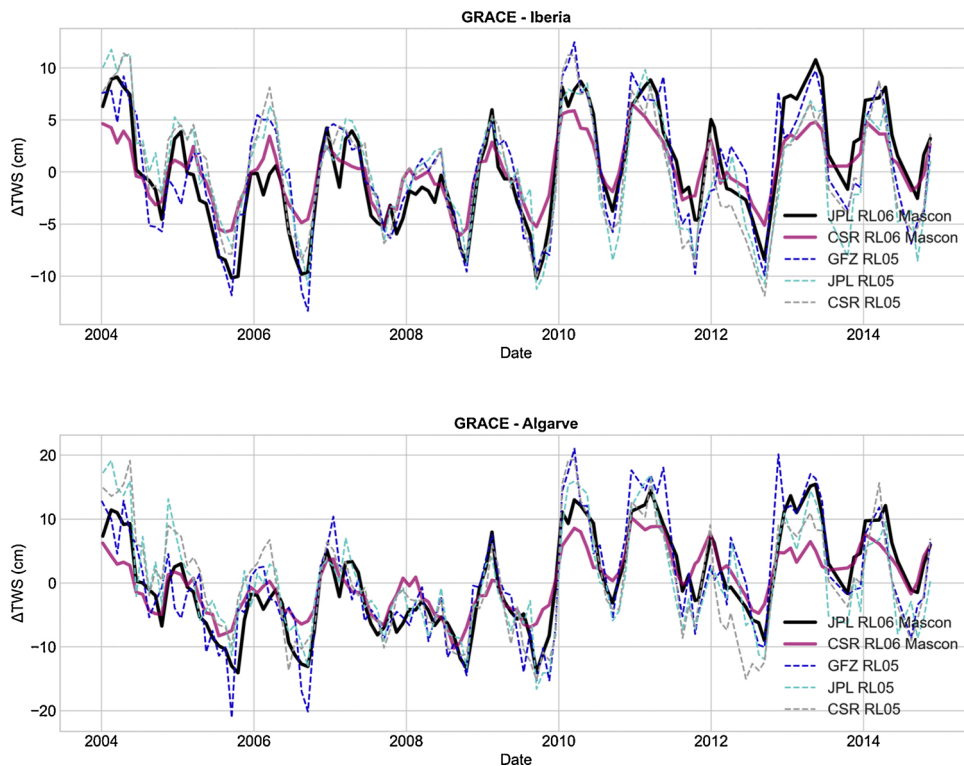


Fig. 3. Total water storage anomalies (Δ TWS) time-series computed from the five GRACE products over Iberia and over the Algarve region. The anomalies correspond to spatial averages of equivalent water thickness relative to the 2004–2014 time-mean baseline.

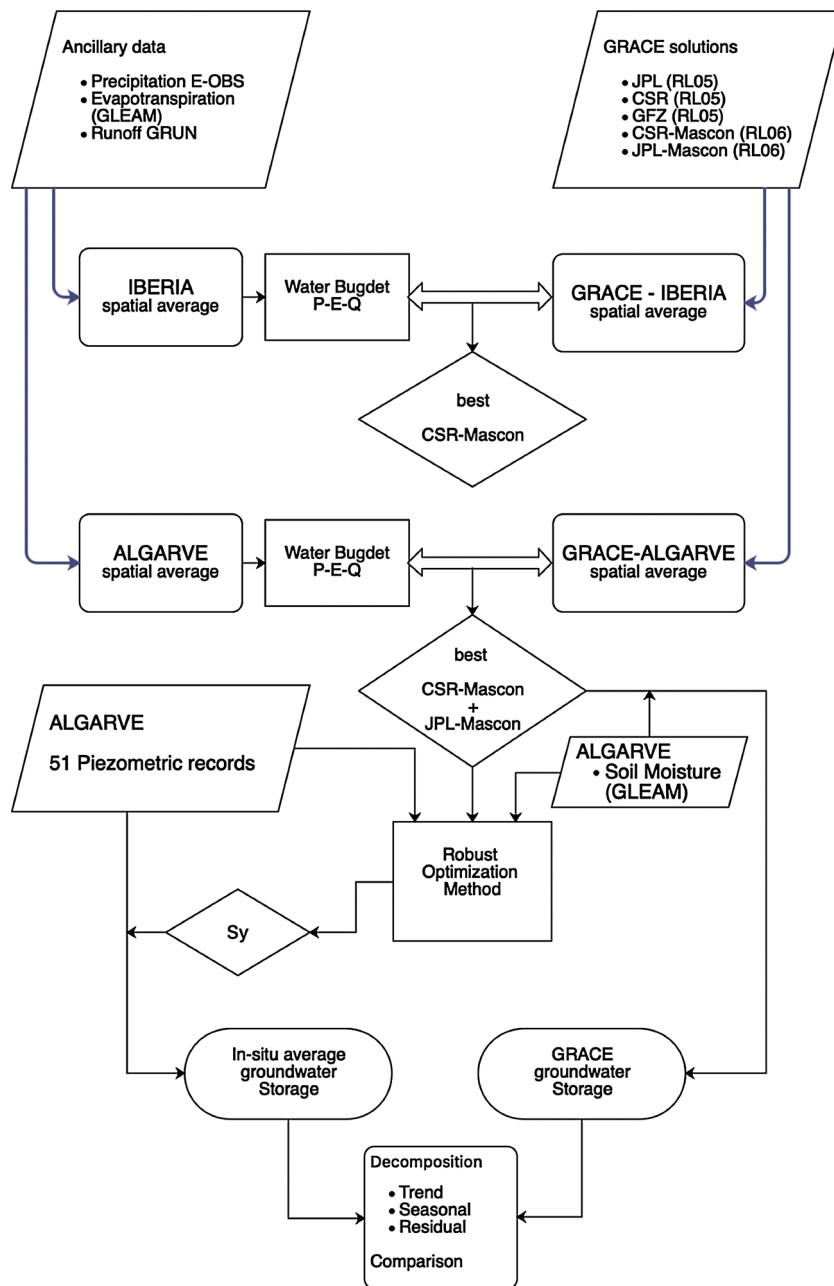


Fig. 4. Flowchart showing the datasets and main steps of the processing sequence.

Aiming at checking the hydrological consistency between different products the basin-scale water budget is also computed using the ERA-5 reanalysis data, available from the Copernicus Climate Change service (C3S) Climate data store (<https://cds.climate.copernicus.eu>). The variables extracted from the ERA-5 land global grids are the precipitation, evaporation and runoff, with monthly frequency and spatial resolution of 0.1°.

3. Methodology

3.1. Assessment of GRACE products: closure of the water budget

Time variations in total water storage ($\partial TWS/\partial t$) are computed from the monthly scaled GRACE time-series using a central difference formula,

$$\partial TWS/\partial t \approx (\Delta TWS_{t+1} - \Delta TWS_{t-1})/2 \quad (1)$$

where t represents a given month. At a regional scale, these variations are related to discharge runoff (Q), precipitation (P) and evapotranspiration (E) via the water budget equation,

$$\partial TWS/\partial t + Q = P - E \quad (2)$$

3.2. Validation of GRACE-derived groundwater storage variations in the Algarve

Groundwater storage changes derived from GRACE are typically computed by subtracting the other components of the water budget from ΔTWS (Rodell and Famiglietti, 1999). In semi-arid environments with negligible surface water components and no snow, the changes in total water storage measured by GRACE can simply be partitioned into changes in groundwater storage (ΔGWS) and changes in soil moisture (ΔSM), so that the water budget equation becomes,

$$\Delta GWS = \Delta TWS - \Delta SM \quad (3)$$

In order to compare ΔGWS derived from GRACE with in-situ observations, it is necessary to convert groundwater levels measurements into groundwater storage changes. A common way of making this conversion is to use the equation (Bhanja et al., 2018; Hachborn et al., 2017; Nanteza et al., 2016; Sun et al., 2010; Swenson et al., 2006),

$$\Delta GWS_{OBS} = S \Delta h \quad (4)$$

Where S is the storativity (dimensionless) and Δh are the changes in hydraulic head observed in-situ. This equation derives from the relation $V_w = SA\Delta h$ between the volume of water V_w drained from an aquifer with overlying surface area A and the average decline in head Δh (Eq. 3.35 from (Fetter, 2001)). In a confined aquifer the storativity is the product of the specific storage S_s and the aquifer thickness b (one-dimensional approximation),

$$S = S_s b \quad (5)$$

$$S_s = \rho_w g (\alpha + n\beta) \quad (6)$$

Where ρ_w is the water density, g is the acceleration of gravity, α is the compressibility of the mineral aquifer skeleton, n is the porosity and β is the compressibility of the water. In a confined aquifer when the head falls, the water released comes from the entire thickness of the aquifer and is accounted for by the compressibility of the mineral skeleton and the compressibility of the pore water. The value of the storativity of confined aquifers ranges from 5×10^{-3} to 5×10^{-5} (Freeze and Cherry, 1979). In an unconfined aquifer the storativity is (Fetter, 2001),

$$S = S_y + S_s b \quad (7)$$

Where in addition to the water expelled or stored in connection to the specific storage and saturated thickness, we have also to consider the specific yield S_y . The specific yield represents the volume of water that a rock will yield by gravity drainage. It is defined as the ratio of the volume of water that drains from the pore spaces owing to the attraction of gravity, to the total rock volume. The value of S_y is several orders of magnitude greater than $S_s b$ for an unconfined aquifer, and therefore in this case the storativity is usually taken to be equal to the specific yield. The usual range for S_y is 0.01–0.30 (Freeze and Cherry, 1979). In the present case study where the aquifer systems are mainly carbonate karst aquifers, sometimes covered and alternating with porous detritic hydrostratigraphic units, the flow domains present transitional characteristics varying between unconfined, confined and semi-confined systems. Therefore, we expect to have transitional storativity values varying between those of typical confined and unconfined aquifers.

It is not possible to simply solve Eq. 4 because S is unknown in the majority of the aquifers considered in this study. In addition, the relative contribution of soil moisture to the total water variations is uncertain and that uncertainty needs to be taken into account. To solve the problem this study uses a robust optimization method similar to the proposed by Sun et al. (2010) to infer aquifer storage parameters from a set of linear equations,

$$S_j \Delta h_j = \Delta TWS - k_j \Delta SM \quad (8)$$

Where j represents each individual in-situ observation, Δh_j is the change in hydraulic head relative to the 2004–2014 average at each piezometer, and k_j is a local weighting factor for soil moisture that can be considered proportional to the local soil layer thickness. The two unknowns in this equation S_j and k_j are determined at an individual piezometer basis using the Generalized Reduced Gradient (GRG) algorithm which is an extension of the reduced gradient method designed to accommodate inequality constraints. The lower and upper bounds on the storativity were set to 1×10^{-9} and 0.3, respectively. The weighting factor k_j is set as an unconstrained non-negative variable. First, the objective function (Eq. 8) is rewritten to match the form $f(S_j, k_j) = 0$. Then, the solver looks at the gradient or slope of the objective function as the input values (or decision variables) change and decides that it reached an optimum solution when the partial derivatives equal zero. We implement the GRG solver in Excel (solver add-in) using the multistart option which creates a randomly distributed population of initial values that are each evaluated using the traditional GRG algorithm. By starting multiple times from different initial conditions this option increases the chance of finding a solution that is a global rather than a local minimum. The method is applied repeatedly at each individual observation, that is, for each j . Finally, after finding the best S at each

location, the ability of GRACE to monitor groundwater storage is evaluated by comparing the in-situ ΔGWS_{obs} (from Eq. 4) with the GRACE-derived ΔGWS (from Eq. 3).

Using the spatial average of the error provided by the GRACE processing centers (measurement and leakage errors) we estimate a regional ΔTWS error of 2.15 cm in the Algarve region. The ΔSM error is estimated to be 2.66 cm, corresponding to the upper bound of the standard deviation of the spatial average of soil moisture. The error in GRACE-derived ΔGWS is computed by propagating ΔTWS and ΔSM errors following Rodell and Famiglietti (2002) and is on average 3.4 cm.

3.3. Groundwater storage in the Algarve: trends and seasonality

The Hodrick-Prescott (HP) filter is a data decomposition technique applied in time-series analysis to reveal long-term trends and isolate short-term fluctuations (Hodrick and Prescott, 1997). The method offers advantages over linear regression analysis when nonlinear trends are present and has been successfully applied in GRACE related studies over the past few years (Bhanja et al., 2018, 2016; Sun, 2013). In order to separate the trend component of a time-series the HP filter minimizes the objective function,

$$\sum_{t=1}^m (y_t - \bar{y}_t)^2 + \lambda \sum_{t=2}^{m-2} [(\bar{y}_{t+1} - \bar{y}_t) - (\bar{y}_t - \bar{y}_{t-1})]^2 \tag{9}$$

Where y_t is a time-series, \bar{y}_t is the trend term computed using time steps of t , $t + 1$ and $t - 1$ and λ is a smoothing parameter recommended to be equal to 129,600 for monthly frequency data (Ravn and Uhlig, 2002). Once the trend is determined, the cyclical (seasonal) components are computed as deviations from the trend ($y_t - \bar{y}_t$). The HP filter is applied to the average groundwater storage computed as the mean of the in-situ observations over the entire Algarve region according to,

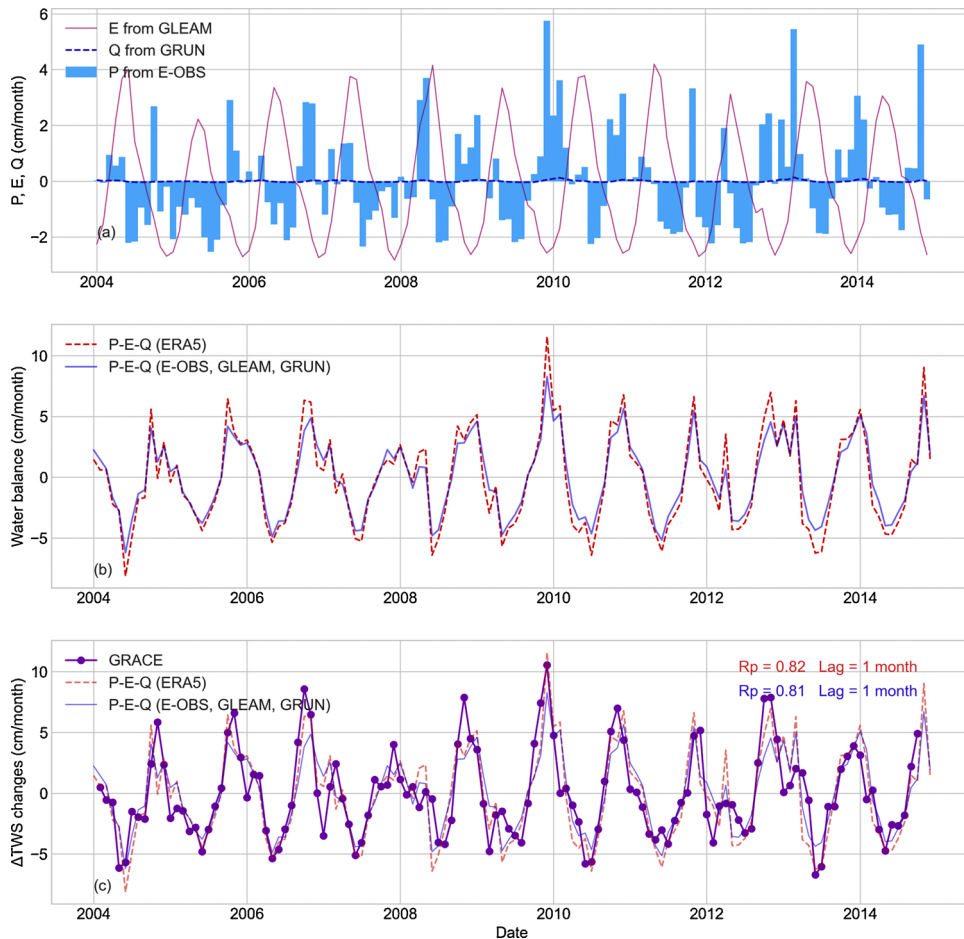


Fig. 5. All time-series correspond to spatial averages over continental Iberia (a) Components of the water budget: precipitation P, Evapotranspiration E and runoff Q. (b) Two estimates of the water budget: P-E-Q from E-OBS,GRUN, GLEAM and the same from ERA5. (c) Time changes in ΔTWS from GRACE (CSR-M) compared to the water budget.

$$\Delta\widehat{GWS}_1 = \sum_j^N W_j S_j \Delta h_j \text{ with } W_j = 1/N \tag{10}$$

where N is the total number of piezometers and $S_j \Delta h_j$ come from Eq. 8. This hypothesis acknowledges the heterogeneity inside each aquifer and gives equal weight W_j to every piezometer. Alternatively, we also computed the average groundwater storage considering the aggregated contributions from each aquifer (e.g. Hachborn et al., 2017; Sun et al., 2010),

$$\Delta\widehat{GWS}_2 = \sum_1^{12} W_i \bar{S}_i \Delta h_i \text{ with } W_i = A_i/A \tag{11}$$

Where \bar{S}_i is the median value of the storativity at each aquifer, Δh_i is the mean observed groundwater level anomaly and W_i is the aquifer's weight, considered proportional to the ratio between the aquifer's area A_i and the total area A of the 12 aquifers in the studied region.

Following the application of the HP filter, the annual cycle (monthly climatology) is removed from the seasonal component to obtain a de-seasonalized (residual) groundwater level time series. The association between the observed and GRACE-derived seasonal and de-seasonalized components is quantified using the Pearson's coefficient of correlation (Rp). The association between trends is found to be non-linear which prevents the use of Pearson's correlation coefficient.

4. Results

4.1. Closure of the water budget over Iberia and the Algarve

The performance of the different GRACE products is assessed using the water budget equation (Eq. 2) and the ancillary datasets. Fig. 5a shows some of these ancillary datasets averaged over Iberia, namely, P extracted from E-OBS, E from GLEAM and Q from GRUN,

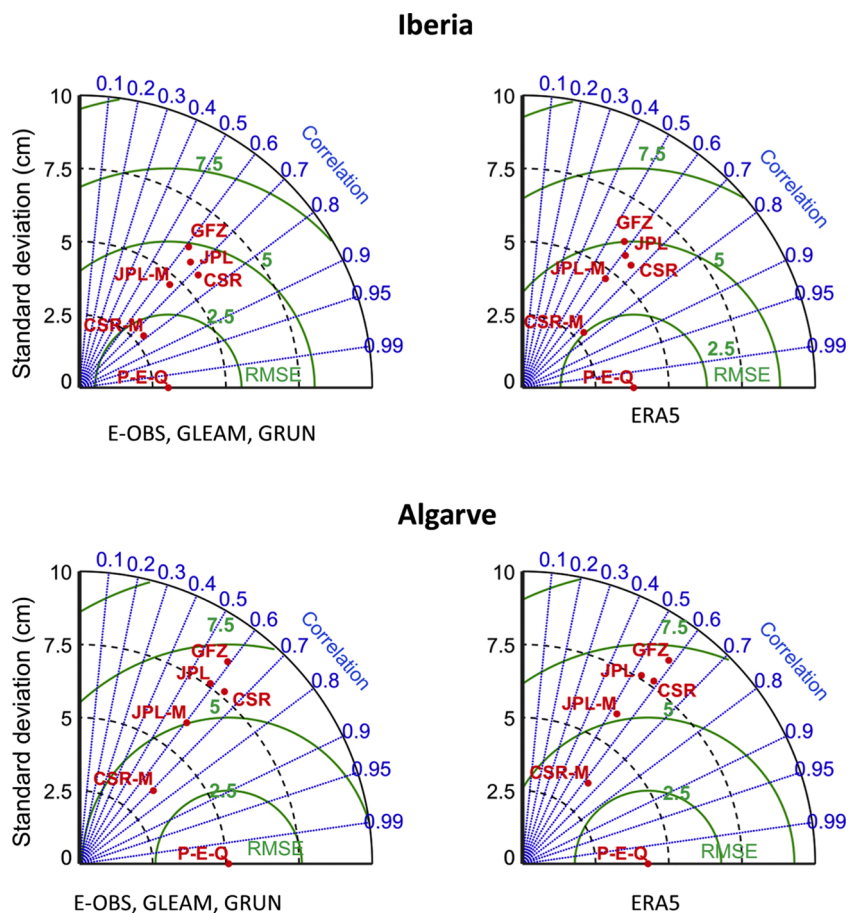


Fig. 6. Taylor diagrams showing the correlation coefficients, standard deviations and root mean square errors (RMSE) between ΔTWS from GRACE products and the two independent estimates of the water balance, for Iberia and for the Algarve region.

expressed as anomalies in cm/month relative to the 2004–2014 time-mean baseline. The analysis of their relative magnitude shows that precipitation and evapotranspiration are the main components of the Iberian water budget, contributing to 63.2 % and 32.3 % of the total water changes, respectively, while runoff accounts for only 4.5 % of the variance. The two independent estimates of P-E-Q (based on the above and on the re-analysis product ERA5) are consistent (Fig. 5b) and produce nearly identical fits to the time variations of the GRACE data (Fig. 5c). Time variations of the CSR-M GRACE Mascon solution (computed according to Eq. 1) show good agreement to the water budget, with a Pearson's coefficient of about 0.8 and a time lag of maximum correlation of 1 month (Fig. 5c). Similar time-evolution patterns and relationships among components of the water budget are obtained when considering the averages over just the Algarve region (time-series not shown). At this more local scale, precipitation and evapotranspiration contribute to 65 % and 35 % of the total water change and runoff contributes to less than 0.5 % of the total variance. Thus, in semi-arid regions without major rivers or lakes, such as the Algarve, surface waters are often considered negligible.

Taylor diagrams summarize best the strength of the statistical association between time series using the Pearson correlation coefficient, the root-mean-square error (RMSE), and the standard deviation. They are useful to compare the skill of different models or datasets and have been computed to compare GRACE and P-E-Q estimates at both the regional scale of Iberia and the more local scale of the Algarve (Fig. 6). The GRACE solution that agrees best with the water budget (P-E-Q) will lie the closest to the observation point on the x-axis. All diagrams show that the RL05 solutions from GFZ, CSR and JPL are the poorer performing since they present the largest RMSE (Fig. 6). Although all products perform better at the Iberian scale, as expected, the Mascon products have actually good scores in the Algarve, not differing much from the scores obtained at the Iberian scale. These results gave us the necessary confidence to proceed with the evaluation of the GRACE products as a tool of quantitative groundwater monitoring in the Algarve (presented in the next sections).

In Iberia the best Mascon solution is the CSR-M since it shows the smallest RMSE, the better correlation with P-E-Q and the best standard deviation (Fig. 6). In the Algarve, the CSR-M and the JPL-M Mascon solutions are similar in terms of correlation coefficient but one of them (CSR Mascon) underestimates the variability in amplitude of the observations (standard deviation of about 5 cm) while the other (JPL Mascon) overestimates it. The best fit to the water budget closure in the Algarve region is thus provided by an average of the GRACE Mascon products (arithmetic mean of CSR-M and JPL-M). This result is independent of the ancillary datasets since the results for ERA5 are almost identical to the results for E-OBS, GLEAM and GRUN. Other studies have also shown that averaging GRACE products can be advantageous since it reduces random, uncorrelated errors resulting from individual solutions (Cao et al., 2019; Xiao et al., 2015).

4.2. Comparison between GRACE and in-situ groundwater data in the Algarve

This section is focused in the Algarve region where groundwater level data collected from 51 piezometers is compared to the GRACE Mascon average solution. Fig. 7a shows the relative magnitudes of ΔTWS and ΔSM converted into units of equivalent water height (cm). The weighting factors calculated through the robust optimization fitting constrain the soil moisture variability to be

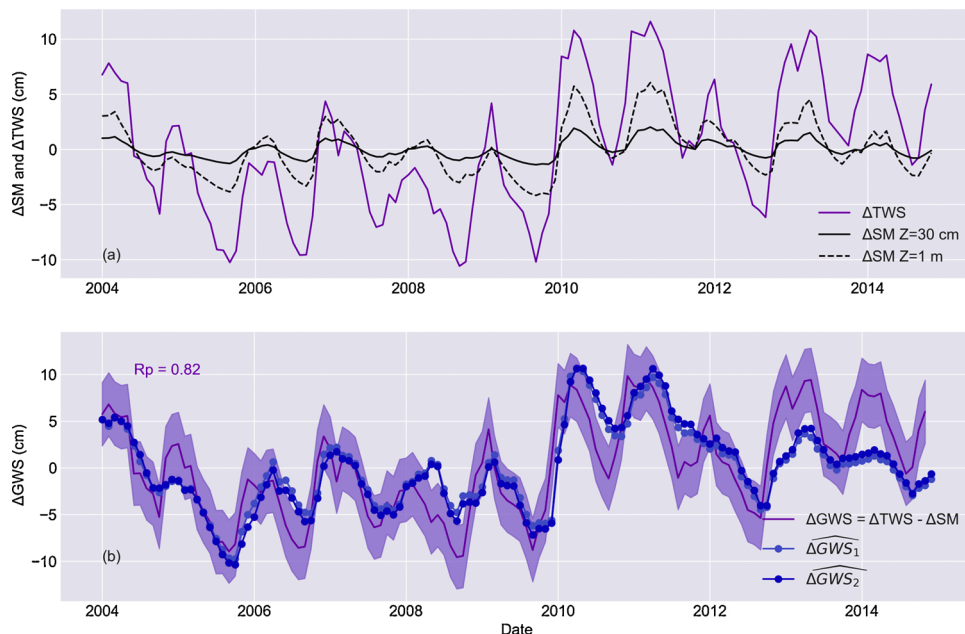


Fig. 7. All time-series correspond to spatial averages over the Algarve region. (a) GRACE Mascon ensemble ΔTWS and upper and lower bound of ΔSM . (b) Groundwater storage anomalies derived from GRACE (ΔGWS and error in light shading) and from ground measurements ($\Delta \widehat{GWS}_1$ and $\Delta \widehat{GWS}_2$).

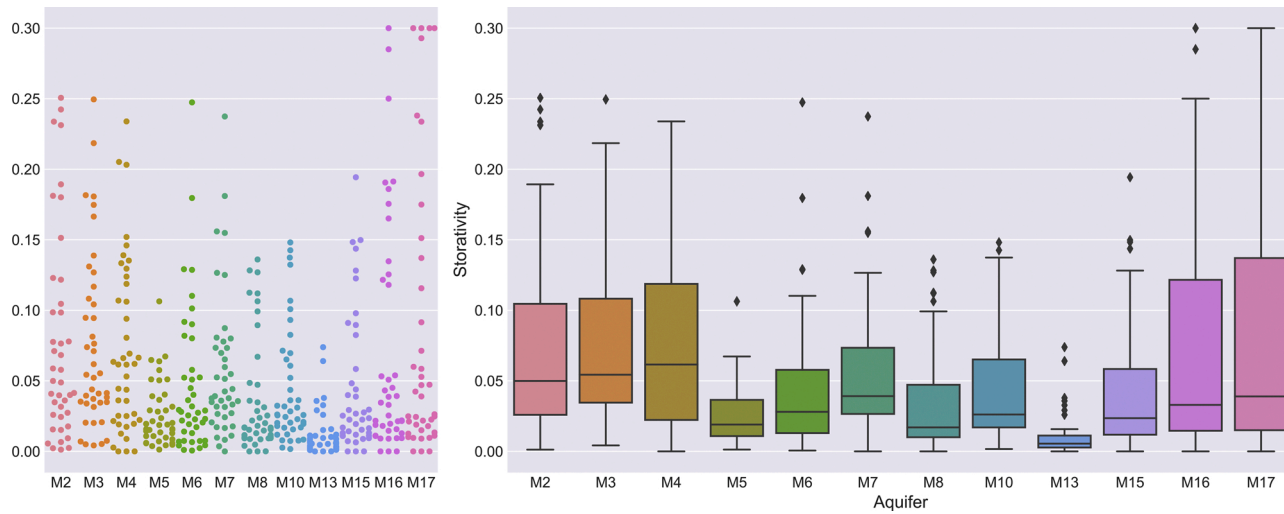


Fig. 8. Statistical distribution of the storativity estimates for aquifers M2 to M17. Boxes represent median, quartile and extreme values. Outliers are a function of the inter-quartile range. More data is presented in [Table 2](#) and Table SM1 (supplementary material).

limited to the upper 30 cm of the soil column at most locations (1 m is the upper bound attained at just few locations). Therefore, changes in soil moisture are estimated to contribute to only a small fraction (up to 16 % but only 2% on average) of the total water storage changes in the Algarve.

The comparison between the in-situ groundwater storage and the satellite-based estimate ($\Delta TWS - \Delta SM$) is displayed in Fig. 7b. The two forms of spatial averaging considered in this study (using Eq. 10 and using Eq. 11) produce almost identical time-series of regionally averaged in-situ groundwater storage, $\widehat{\Delta GWS}_1$ and $\widehat{\Delta GWS}_2$. The reason for this is that the number of piezometers per aquifer is roughly proportional to the aquifer's area. The GRACE-derived and in-situ data portray consistent variations and have a correlation coefficient of 0.82 (Fig. 7b). The main deviations between GRACE and the in-situ observations occur after 2012 and are attributed to gaps in the satellite time-series. Thus, in order to extend the satellite lifespan and save battery the GRACE satellite has been switched off periodically for 4–5 weeks every 5–6 months since 2011 (Landerer and Swenson, 2012). Excluding this exceptional period, GRACE can monitor the basin-integrated change of groundwater storage in the Algarve with good accuracy.

The storativity computed from the robust fitting method is displayed in Fig. 8 aggregated per aquifer. The median S ranges from 3.65×10^{-3} to 4.92×10^{-2} , showing large variability within the same aquifer. Inter-aquifer variability for S is high as also shown by coefficients of interquartile variation ranging from 63 % in M10 (S. Joao da Venda - Quelfes) to over 79 % in M17 (Montegordo), as well as by wide ranges, with S estimates in some aquifer systems attaining the maximum programmed ranges (i.e., 1×10^{-9} to 0.3) (Table 2). Such variability may be explained by the fact that aquifer systems are mostly constituted by overlaying unconfined and confined aquifers with varying (and in many cases still unknown) degrees of connectivity and independence. In consequence, the median Sy values show nonsignificant differences between aquifer systems (Kruskal-Wallis chi-squared (11) = 393.29, Dunn post-hoc test, $p > 0.05$ - see supplementary material). For the purpose of studying the relationship between GRACE signal and that of the aquifer systems, this variability should be considered as a property of the system, which nonetheless still allows good agreements between GRACE estimated values and field estimates, as shown in Table 2. Taken together the regionally averaged storativity for the Algarve aquifers is 2.4×10^{-2} .

4.3. Trends and seasonality of groundwater storage changes

Considering the results of the previous section, It can be argued that the good correlation found between satellite and in-situ groundwater storage anomalies is just due to the seasonal and annual cycles. In order to exclude this hypothesis, the total signals

Table 2
Statistics for the estimated S per aquifer system.

| Code | IQR | Min | P25 | Median | P75 | Max | cqv (%) | Range | Field S | Reference |
|------------------|----------|----------|----------|----------|----------|----------|---------|-------|--|--|
| M2 | 8.55E-02 | 3.68E-06 | 2.35E-02 | 4.61E-02 | 1.09E-01 | 3.00E-01 | 65 | 0.3 | | |
| M3 | 9.12E-02 | 9.82E-05 | 1.47E-02 | 4.43E-02 | 1.06E-01 | 3.00E-01 | 76 | 0.3 | | |
| M4 | 1.01E-01 | 1.49E-03 | 1.47E-02 | 4.92E-02 | 1.16E-01 | 3.00E-01 | 77 | 0.3 | | |
| M5 | 2.30E-02 | 3.56E-05 | 5.60E-03 | 1.32E-02 | 2.86E-02 | 3.00E-01 | 67 | 0.3 | Storativity: 5×10^{-3} and 2×10^{-2} ; specific yield: $1 \times 10^{-3} - 7.5 \times 10^{-2}$ | Almeida e Silva (1983), Silva (1988), Hugman et al. (2012) |
| M6 | 5.85E-02 | 6.02E-04 | 1.04E-02 | 3.02E-02 | 6.89E-02 | 3.00E-01 | 74 | 0.3 | Storativity: $10^{-3} - 10^{-4}$; specific yield: $2 \times 10^{-2} - 4 \times 10^{-2}$ | Monteiro et al. (2013) |
| M7 | 5.37E-02 | 3.62E-05 | 1.17E-02 | 3.51E-02 | 6.54E-02 | 3.00E-01 | 70 | 0.3 | Storativity: $10^{-3} - 10^{-4}$; specific yield: $2 \times 10^{-2} - 4 \times 10^{-3}$ | Monteiro et al (2013) |
| M8 | 3.08E-02 | 1.88E-04 | 6.25E-03 | 1.52E-02 | 3.71E-02 | 3.00E-01 | 71 | 0.3 | | |
| M10 | 4.26E-02 | 1.60E-03 | 1.24E-02 | 2.47E-02 | 5.50E-02 | 3.00E-01 | 63 | 0.3 | | |
| M13 | 7.23E-03 | 2.47E-05 | 1.92E-03 | 3.65E-03 | 9.15E-03 | 2.64E-01 | 65 | 0.3 | | |
| M15 | 4.11E-02 | 1.04E-05 | 9.90E-03 | 2.05E-02 | 5.10E-02 | 3.00E-01 | 67 | 0.3 | | |
| M16 | 1.06E-01 | 1.04E-05 | 1.66E-02 | 3.51E-02 | 1.23E-01 | 3.00E-01 | 76 | 0.3 | | |
| M17 | 1.33E-01 | 1.04E-05 | 1.79E-02 | 4.24E-02 | 1.51E-01 | 3.00E-01 | 79 | 0.3 | Storativity: 10^{-4} ; specific yield: 0.18 | Afonso (1983); Diamantino and Lobo Ferreira (2002) |
| Regional Average | 5.26E-02 | 3.68E-06 | 8.58E-03 | 2.38E-02 | 6.12E-02 | 3.00E-01 | 75 | 0.3 | | |

IQR: interquartile range; cqv: coefficient of quartile variation $(P75-P25)/(P75 + P25) \times 100$.

are decomposed into trends, seasonal and residual patterns and the correlations re-computed for each component. The results are only shown for the GRACE-derived and in-situ $\widehat{\Delta GWS}_1$ time-series (Fig. 9) since $\widehat{\Delta GWS}_2$ would lead to equivalent conclusions. Trends obtained with the HP filter are non-linear and slightly positive over the period of study (Fig. 9a). GRACE overestimates the positive tendency and is found not suitable to examine the trend of groundwater storage in the Algarve, especially after 2012. The seasonal components on the other hand show very good matches having a correlation coefficient of 0.85 (Fig. 9b). The anomalies are typically positive in winter/spring and negative in summer/autumn and range from -10 to +10 cm. Fig. 9c shows the de-seasonalized signals which expose periodicities larger than 12 months. These components are useful to detect exceptionally wet and dry periods lasting for more than one hydrological year. The major droughts that affected the Iberian Peninsula in 2004–2006 and 2011–2012 can be clearly identified, as well as the anomalously wet years of 2010 and 2011. The regional impact of these extreme events is evident in both the ground-based $\widehat{\Delta GWS}_1$ and GRACE estimates. In addition, the degree of association between the de-seasonalized GRACE and in-situ time series ($R_p = 0.82$ in Fig. 9c) demonstrates that the good match described in the previous section is not just due to the seasonal and annual variations. Overall, GRACE performs well in capturing the multi-year deficits and surplus of groundwater storage in the Algarve basin. The observed multi-year deficits and low-frequency cycles are related to low-frequency oscillations in the amount of precipitation, which in turn are associated to climate patterns such as the North Atlantic Oscillation and the East Atlantic pattern (Neves et al., 2019).

The results also show a time-lag of about 1–2 months between GRACE and the average of the in-situ measurements (Fig. 9b). However, the delays of the in-situ observations relative to the satellite data reflect the local hydrogeological properties at the piezometric locations, such as transmissivity and depth to the water table, and are not a regional uniform feature. Sites dominated by porous or fractured rocks and shallow water tables have a fast response to heavy rainfall events (for instance in winter 2010) and are more likely to be well synchronized with GRACE. In the study area the aquifers that most visibly belong to this category are M16 and M17 (supplementary data). In the opposite extreme the aquifers having the largest damping of high-frequencies and greater lags relative to GRACE are M5, M6 and M7.

Another advantage of comparing residual components (Fig. 9c) is the detection of possible anthropogenic activity. The negative

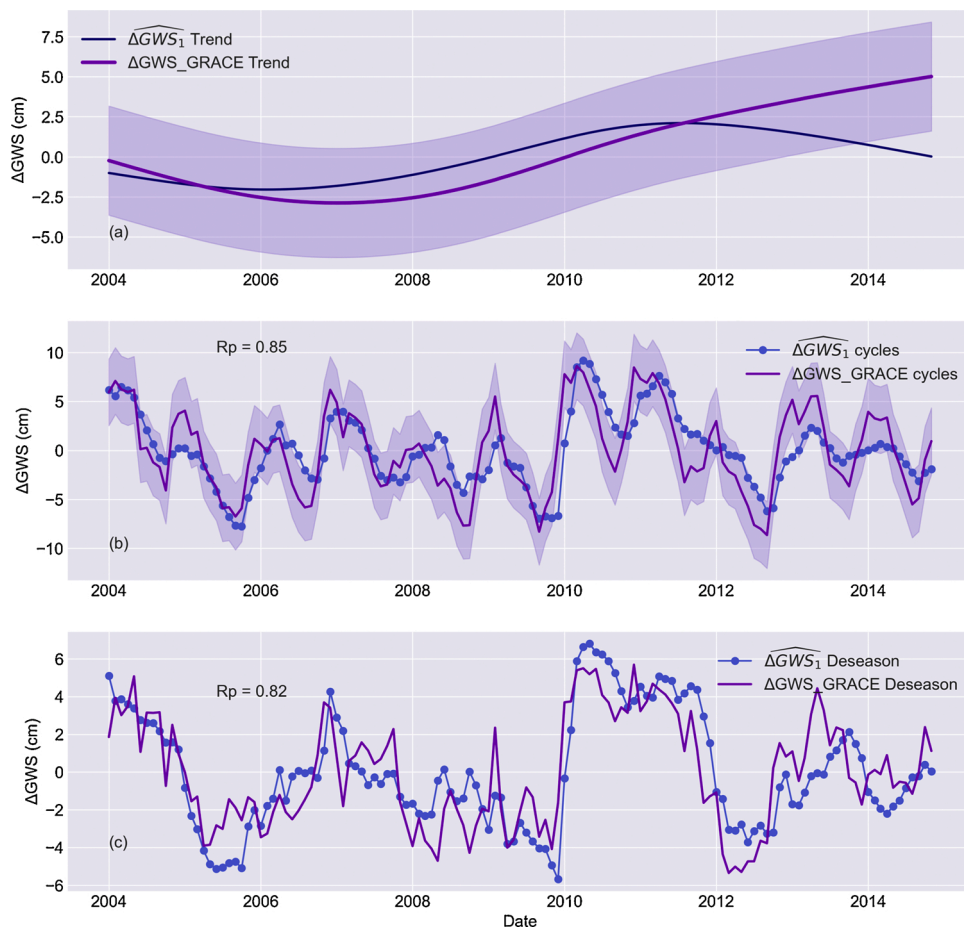


Fig. 9. Decomposition of ΔTWS and $\widehat{\Delta GWS}_1$ shown in Fig. 7b. (a) Trend, (b) Seasonal and (c) De-seasonalized components (annual cycle removed). GRACE error in light shading and R_p indicates the Pearson's correlation coefficient between time-series.

peak in groundwater storage observed during 2005 is probably related to drought-induced abstraction. In that period (2004–2006 drought) all existing dams in the Algarve were almost depleted and restrictions on water use were imposed for all economic sectors, with exceptional measures being taken to avoid the total disruption of the public water system. When the public water supply could not be ensured by surface waters, emergency boreholes were made and the old boreholes were reactivated (Nunes et al., 2006). Unfortunately, there is still no proper data on groundwater pumping as most boreholes are privately owned and keep no abstraction records. Climate-induced pumping contributing to fast resource depletion at an integrated basin scale can be easily detected using comparisons with GRACE. Applying the same methodology at an individual aquifer level may be useful to detect sharp local deviations from the regional average. For example, the most outstanding examples of negative deviations in summer 2005 occur in aquifers M13 and M15 (supplementary data). Note that for individual aquifers similar conclusions can be drawn if in-situ averages such as $\Delta\widehat{GWS}_1$ (rather than GRACE) are considered as the regional reference. They will be harder to compute and not as readily available as the satellite data though.

Table 3 shows the Pearson's correlation coefficients computed between GRACE and in-situ total, seasonal and residual components at individual aquifers, in the form of a heat map. It provides a direct overview of which aquifers are the ones where GRACE has the greatest potential for being used as a complementary tool of groundwater storage monitoring. Aquifer M4 stands out as the aquifer whose fluctuations are best captured by the satellite in the time span of this study.

5. Discussion and future perspectives

5.1. Errors and limitations due to GRACE resolution

The suitability of GRACE to represent large-scale freshwater variations has been demonstrated around the world (Rodell et al., 2018; Tapley et al., 2019). However, at regional scales the use of GRACE satellite data for monitoring aquifers is questionable, requiring a case-by-case validation (e.g. Becker et al., 2010; Biancamaria et al., 2019; Hachborn et al., 2017; Rahimzadegan and Entezari, 2019). GRACE data close to its spatial resolution limit (~200 km for Mascon products) is known to suffer from low signal to noise ratio and from leakage errors across neighboring regions. Ancillary data employed by processing centers to invert ΔTWS , such as outputs from glacial isostatic adjustment, atmosphere, ocean and land models, have their own source of uncertainties which also increase with increasing resolution. Another source of error when considering GRACE data are the gaps resulting from the periodic

Table 3

Match between GRACE and in-situ ΔGWS at individual aquifers (Pearson's correlation coefficient).

| | Original time-series | Seasonal components | De-seasonalized |
|------------|-------------------------|------------------------|-----------------|
| M2 | 0.62 | 0.75 | 0.78 |
| M3 | 0.67 | 0.83 | 0.75 |
| M4 | 0.87 | 0.85 | 0.76 |
| M5 | 0.78 | 0.75 | 0.81 |
| M6 | 0.75 | 0.76 | 0.75 |
| M7 | 0.8 | 0.75 | 0.73 |
| M8 | 0.74 | 0.72 | 0.59 |
| M10 | 0.78 | 0.81 | 0.77 |
| M13 | 0.54 | 0.66 | 0.51 |
| M15 | 0.66 | 0.72 | 0.66 |
| M16 | 0.51 | 0.78 | 0.76 |
| M17 | 0.58 | 0.83 | 0.8 |

satellite shutdowns to save battery life, especially after 2012 (Landerer and Swenson, 2012). At the scale of Iberia and also Algarve, some mismatch between time variations in Δ TWS and net-fluxes of precipitation, evaporation and runoff via the water budget equation, can also be due to errors not only in GRACE but also in the ancillary datasets themselves (ERA5, GRUN, E-OBS, GLEAM).

An application of GRACE to monitor groundwater storage changes at the scale of Iberia is out of the scope of this study. Acknowledging the large degree of uncertainty associated to GRACE at small scales, we tested the use of GRACE in the Algarve not as an alternative but as a complementary tool to the in-situ existing network. This study demonstrates the feasibility of using GRACE as a fast and relatively reliable form of estimating regionally integrated changes in groundwater storage in the Algarve. Despite its extremely small area when compared to the GRACE footprint, the correlation between in-situ and satellite data in the Algarve (with Pearson's correlation coefficient of 0.82) is comparable to values reported in the literature, for example, 0.58 in the High Plains aquifer (Strassberg et al., 2007), 0.6 in East Africa (Nanteza et al., 2016), 0.71 in Southwest China (Huang et al., 2019), ranging from 0.33 to 0.91 over the major river basins in India (Bhanja et al., 2016) and from 0.55 to 0.74 in Jordan (Liesch and Ohmer, 2016). Three factors may explain the good match obtained at this small scale: (1) the good performance of Mascon products regarding the separation of land and ocean signals at this particular location, (2) the fact that aquifers in the Algarve are isolated, far from other neighboring water masses and the only significant water reservoirs in the area, and (3) the fact that the extent of the Algarve region coincides with the extent of the GRACE JPL Mascon pixel over land (Fig. 1).

5.2. Future perspectives

When computing the net balance of groundwater storage in the Algarve region (integral of the in-situ observed groundwater anomalies) it is found that the net values are negative for the majority of the aquifers and that the average loss in the Algarve region is 4 cm of equivalent water thickness. This generalized depletion is not evident when analyzing only the trends. Thus, the net effect of the seasonal variations is what contributes the most to the groundwater storage decrease observed between 2004 and 2014. The time span of this study is too short to conclude whether this is a persistent feature, although climate model projections for this region leave no doubt about an existing drying tendency (Spinoni et al., 2018). Model projections for Iberia are also alarming showing an intensification of drought conditions for the main Iberian international basins with multi-year droughts reaching a drought severity index DSI-12 of up to 800 % (i.e. 8 years of mean annual rainfall missing) and an average of 80 % of basin areas experiencing extreme drought by the end of the century (Guerreiro et al., 2017b).

Given the disturbing observations of declining groundwater storage throughout the world, GRACE may add value to hydrological investigations in areas where there is a significant fraction of groundwater abstraction (Döll et al., 2014). Several studies in different parts of the globe present evidence of groundwater depletion based on GRACE satellite data, for instance in Southeast Australia (Leblanc et al., 2009), India (Rodell et al., 2009) and California Central Valley (Scanlon et al., 2012). Groundwater over-abstraction in periods of drought is one of the factors that most contributes to the long-term depletion of aquifers. With an increasing frequency and duration of meteorological droughts expected for Iberia and the Algarve in the coming years (Spinoni et al., 2018) it becomes urgent to find and adjust ways of identifying the onset of groundwater droughts. In 2011, NASA started distributing operational wetness/-drought indicators for shallow groundwater and soil moisture based on the assimilation of GRACE into a land-surface model (Houborg et al., 2012). More recently, other groundwater drought indices have been proposed based on GRACE anomalies, which can detect and monitor droughts resulting from either natural or anthropogenic variations (Li and Rodell, 2015; Thomas et al., 2017). GRACE-based indices have the advantage of providing basin-integrated estimates and of overcoming the lack of in-situ observations, in space or in time. However, these indices have to be validated locally because sometimes they are found to be not suitable (Van Loon et al., 2017). Although studies like this have not yet been conducted in Iberia, the present work provides an optimistic outlook for the use of such indices in the region. Monitoring the onset of groundwater drought using all available data sources is vital to achieve an adaptable planning of water management capable of mitigating the negative impacts of drought.

6. Conclusions

Data from ground-station observations (E-OBS, GRUN), land-surface models (GLEAM) and atmospheric reanalysis (ERA5) indicate that the main components of the water budget in Iberia (Algarve) are precipitation and evapotranspiration, contributing to approximately 63 % (65 %) and 32 % (35 %), respectively, of the total water storage changes. Among the 5 GRACE products tested in this study, the one that produces the best fit to the closure of the water budget in Iberia is the CSR Mascon, and in the Algarve is the average of the CSR and JPL Mascon solutions (release RL06). It is concluded that GRACE provides a consistent representation of the hydrological cycle and thus, can be used as an aid in monitoring climate-related water mass transports in both Iberia and the Algarve.

GRACE data in the Algarve has large uncertainties due the small size of the study area. The lack of field measurements of soil moisture and of aquifer storage properties adds extra uncertainties in the validation of the GRACE-derived groundwater changes. Nonetheless, the robust optimization method used in this study provides some bounding constraints on the above factors, and produces realistic results consistent with the existing field measurements. It is estimated that soil moisture contributes to only a small fraction (between 2% and 16 %) of the total water storage variations. The storativity parameters of the aquifers, in turn, are bounded to range between 3.65×10^{-3} and 4.92×10^{-2} with a median value of 2.4×10^{-2} . The inferred storage properties show great spatial variability, even within the same aquifer, in agreement to the great heterogeneity inherent to the multilayer and karst characteristics of most aquifers in the Algarve.

Groundwater is the main responsible for total water storage anomalies captured by GRACE in the Algarve. The association between satellite-derived and in-situ data is good (correlation coefficient of 0.82) even after removing the trend, seasonal and annual cyclic

components. We conclude that GRACE is effectively capable of capturing the regionally integrated groundwater storage changes in the Algarve with good accuracy, being also able to capture the multi-year deficits and surplus resulting from the natural fluctuations driven by climate. GRACE is therefore recommended as a complementary and diagnostic source of hydrologic data in Iberia and in particular the Algarve region.

CRedit authorship contribution statement

Maria C. Neves: Conceptualization, Methodology, Writing - original draft, Writing - review & editing. **Luis M. Nunes:** Methodology, Validation, Writing - review & editing. **José P. Monteiro:** Writing - review & editing.

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.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:<https://doi.org/10.1016/j.ejrh.2020.100734>.

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