A Technical Note on Least Squares Mascon Fitting to GRACE Satellite Data to Estimate Total Water Storage Changes in The Middle East

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Abstract:

Nowadays the twin satellite gravimetry missions, GRACE (Gravity Recovery and Climate Experiment) and GRACE -Follow On, provide a unique and alternative tool for monitoring and measuring Total Water Storage (TWS) changes at different spatial and temporal scales, from regional, continental to global, and from intra-seasonal to long-term scales. TWS is a key parameter for hydrological studies such as monitoring of groundwater storage changes. This chapter focus on a detailed description of a technique named least squares mascon fitting which has been used for monitoring of TWS changes for specific regions of the Middle East such as Iran, Iraq, Syria, eastern Turkey, northern Saudi Arabia, southern Saudi Arabia, and the area immediately west of the Caspian Sea using GRACE data. This chapter is also dealing with results of our current research in Iran's water main basins. It shows that GRACE and GRACE FO data can be used to estimate TWS changes at a basin scale. The mascon analysis has less leakage error and can be used for hydrological applications without applying any gain factors or any post-processing in compare with other solutions such as the spherical harmonic solutions.

Keywords: GRACE- GRACE Follow On- Total Water Storage- Mascon analysis

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1. Introduction:

The concept "mascon" stands for "mass concentration" and is a user-defined region of the Earth's surface. It originates from (Muller and Sjogren, 1968), who have used mascons to model the gravity field of the moon. There are three classes of GRACE mascon solutions that are used to study time-variable gravity. The first class of mascon solution is one in which an analytic expression for the mass concentration function is provided, and explicit partial derivatives relating the inter-satellite range-rate measurements to the analytic mascon formulation are used to directly estimate mass variations. An example of this first type of mascon solution is found in (Ivins et al., 2011), where spherical cap mascons are estimated directly from range accelerations to interpret the regional ice mass loss and Glacial Isostasy Adjustment (GIA) processes. The second class of mascon solution comes from the group at NASA Goddard Space Flight Center ((Luthcke et al., 2006), (Rowlands et al., 2010), (Sabaka et al., 2010), and (Luthcke et al., 2013)). This type of mascon solution shares commonality with the first type of mascon solution in the sense that the mascon basis functions are directly related to the inter-satellite range-rate measurements through explicit partial derivatives, which are used in the gravity estimation. The difference is that each mascon basis function is represented by a finite truncated spherical harmonic expansion, rather than an analytical expression, such that the functional representation of each mascon has signal power outside of the mascon boundary. Finally, the third class of so-called "mascon" solution or "Least Squares Mascon Fitting (LSMF)" are when users fit mass elements to spherical harmonic coefficients (Stokes coefficients from GRACE level 2 solutions) to reduce satellite measurement error, leakage error, and correlated error (striping error). These are not true mascon solutions in the sense that there is no direct relation between the formulation of the mass elements and the inter-satellite range-rate measurements (i.e., there are no explicit partial derivatives relating the observations to the state). Examples of this type of mascon solution include (Tiwari et al., 2009), (Jacobe et al., 2012), (Scharma et al., 2014), (Velicogna et al., 2014), and (Joodaki et al., 2014). In this chapter, we explain the third class of mascon solution in details and how it can be used to estimate TWS changes in a regional and a basin scale.

2. GRACE Data

The GRACE satellite mission was launched in March 2002 by NASA and the German Aerospace Center (DLR) (Tapley et al., 2004). It ended in October 2017, but the GRACE project has been continued by lunching GRACE Follow-On mission in May 2018. The GRACE project consists of two satellites, flying at an altitude of 450-500 km in identical near-polar orbits (89.5º inclination), with a separation distance of about 250 km. Continuous microwave measurements of the range between the two satellites, combined with data from on-board accelerometers and Global Positioning System (GPS) receivers, are used by the GRACE Project to determine global, monthly solutions for the Earth's gravity field at scales of a few hundred kilometers and greater. Those fields are derived as monthly sets of spherical harmonic ("Stokes") coefficients, and are made publicly available by the GRACE Project. These coefficients can be used to estimate month-to-month changes in mass stored on or near the Earth's surface, integrated over regions of a few hundred km or larger in scale (e.g., (Wahr et al., 1998)). The ability to observe an entire regional mass change without the need of spatial interpolation is a major strength of GRACE. But the lower bound on its resolution means that GRACE cannot determine precisely where the mass change within the region is coming from. In addition, GRACE can only deliver variations in water storage, not the total water storage itself.

2.1. Low Degree Stokes Coefficients (n=0,1,2)

Because of the degree-0 Stokes coefficient is proportional to the total mass of the Earth and atmosphere, it is assumed constant, and it is not used in the computations of the time series of TWS changes. The geocenter motion is showed by the changes in degree-1 Stokes coefficients which cannot be derived from GRACE data. The absence of the geocenter motion might introduce an error in the TWS changes estimates ((Chambers et al., 2004); (Chen et al., 2005)). Degree-1 Stokes coefficients can be computed as described by (Swenson et al., 2008). The lowest-degree zonal harmonics, C_{20} Stoke coefficient is related to the Earth's oblateness. Because of the relative short separation length between the two GRACE Spacecrafts, the C_{20} coefficient cannot be well determined by GRACE. The C_{20} values provided in the level-2 data also show anomalous variability (e.g., (Chen et al., 2005)). Therefore, the monthly Satellite Laser Ranging (SLR) values for C_{20} coefficients derived from five SLR satellites (LAGEOS-1 and 2, Starlette, Stella and Ajisai) (Cheng et al., 2013) are used to replace the estimates from GRACE. This method is a well-established technique for determining independent degree-2 coefficients. The degree-1 coefficients, and SLR C_{20} coefficients and their associated standard deviations are continuously provided in the GRACE project Technical Notes (ftp://podaac.jpl.nasa.gov/pub/grace/doc).

2.2. Ocean's Gravity Contributions on Lakes and Water Reservoirs

The GRACE Project uses a global ocean model to remove the ocean's gravity contributions from the raw GRACE data before solving for the Stokes coefficients. But in that model, signals from large lakes and water reservoirs are not included, so there are nonnegligible signals in those areas which should be removed. The signal for each lake/water reservoir can be removed by computing the Stokes coefficients caused by a uniform 1 m rise of lake/water reservoir, and then scaling those coefficients using monthly altimeter estimates (Birkett et al., 2009) (http://www.pecad.fas.usda.gov/cropexplorer/global_reservoir/) of the lake/water reservoir surface height (see (Swenson and Wahr, 2007)).

3. Least Squares Mascon Fitting (LSMF) solution

Mascon is a user-defined area of Earth's surface and more than one mascon is necessary for this solution. In this solution, mascon amplitudes are fitted to the GRACE Stokes coefficients to obtain estimates of the monthly mass variability of each mascon. For each mascon, the set of Stokes coefficients are found such that they would be resulted by a unit mass distributed uniformly over that mascon. Let the degree n and order m Stokes coefficients for mascon *i* be (C^{i}_{nm}, S^{i}_{nm}). Let the actual, but unknown, mass of mascon *i* be M_i. The M_is for all mascons are estimated by fitting them simultaneously to the GRACE monthly Stokes coefficients.
Let (ΔC_{nm}, ΔS_{nm}) be the GRACE Stokes coefficients at time *t*, after removing the mean of all monthly solutions. The mean must be removed because otherwise contributions from the Earth's interior, which dominate the mean signal, would be misinterpreted as surface mass signals. As a result, GRACE can be used to determine change of total water storage, but not total water storage. Before fitting, the GRACE Stokes coefficients and the Stokes coefficients for each mascon are multiplied by $W_n\,(2n+1)/(1+k_n)$, where W_n are the coefficients of the Gaussian smoothing function, and the k_n are load Love numbers to transform these geoid coefficients into smoothed spherical harmonic coefficients of mass (Wahr et al., 1998). A Gaussian smoothing function is applied to the Stokes coefficients to reduce the noise in the monthly M_i time series. These modified Stokes coefficients are denoted with asterisks (i.e. $\Delta C^{*}_{nm}(t)$, $C^{*,i}_{nm}$, etc.) and the $\{M_i(t)\}$ are found such that they minimize the standard least squares merit function:

$$E=\sum_{n,m}\left[\left(\Delta C^{*}_{nm}(t)-\sum_{i} C^{*,i}_{nm}M_i(t)\right)^2+\left(\Delta S^{*}_{nm}(t)-\sum_{i} S^{*,i}_{nm}M_i(t)\right)^2\right] \qquad (1)$$

For each monthly time step, *t*, the $\{M_i(t)\}$ that minimize (1) solve

$$Y_j(t)=\sum_i B_{ji}\,M_i(t) \tag{2}$$

where

$$Y_j(t)=\sum_{nm}(\Delta C^*_{nm}(t)C^{*,j}_{nm}+\Delta S^*_{nm}(t)S^{*,j}_{nm}) \tag{3}$$

$$B_{ji}=\sum_{nm} C^{*,j}_{nm}\,C^{*,i}_{nm}+S^{*,j}_{nm}S^{*,i}_{nm} \tag{4}$$

The solution to (2) is

$$M_i(t)=\sum_j B^{-1}_{ij}Y_j(t) \tag{5}$$

Ideally, the solution for $M_i(t)$ would recover the true spatial average of mascon *i*'s mass: It means a spatial average that samples every point inside the mascon with a sensitivity of 1, and every point outside with a sensitivity of 0. Unfortunately, because of the finite number of harmonic degrees in the GRACE solution (for example, n_{max}=60 for CSR solutions), this is not the case. It is possible to determine the sensitivity kernel of each mascon solution, which not only provides insight into possible biases in those solutions but also can help when deciding how to choose mascon sizes, shapes, and locations.

Let $\Delta\sigma\ (\vartheta,\lambda,\ t)$ be the surface mass at co-latitude ϑ, longitude λ, and time t. Because the inverted mascon masses, M_i, are linearly related to the GRACE coefficients (through (5)), and those coefficients are linearly related to $\Delta\sigma(\vartheta,\lambda,\ t)$ (through Newton's Law of Gravity), there must be a linear relation between each M_i and $\Delta\sigma(\vartheta,\lambda,\ t)$. The most general linear relation has the form

$$M_i(t)=\int \Delta\sigma(\vartheta,\lambda,\ t)A_i(\vartheta,\lambda)a^2\sin\vartheta d\vartheta\ d\lambda \tag{6}$$

where $A_i(\vartheta,\lambda)$ is the sensitivity kernel for mascon i, and would ideally equal 1 for points inside the mascon and 0 outside, and *a* is the mean radius of the Earth. In order to explain about $A_i(\vartheta,\lambda)$, note that equations (2)–(4) imply a linear relation between M_i and the GRACE Stokes coefficients:

$$M_i(t)=\sum_{nm}\left[A^{C,i}_{nm}\Delta C_{nm}(t)+A^{S,i}_{nm}\Delta S_{nm}(t)\right] \tag{7}$$

where the factors $A_{nm}^{C,i}$, $A_{nm}^{S,i}$ can be determined as described below. The relation between the Stokes coefficients and $\Delta\sigma$ (ϑ,λ, t), implied by Newton's Law of Gravity, is (Wahr et al., 1998)

$$\begin{pmatrix}\Delta C_{nm}(t)\\ \Delta S_{nm}(t)\end{pmatrix}=\frac{3(k_n+1)}{4\pi\rho_{ave}a^3(2n+1)}\int \Delta\sigma(\vartheta,\lambda,t)P_{nm}(\cos\vartheta)\begin{pmatrix}\cos(m\lambda)\\ \sin(m\lambda)\end{pmatrix}a^2\sin\vartheta d\vartheta d\lambda \qquad (8)$$

where the $P_{nm}(\cos\vartheta)$ are Associated Legendre functions, and ρ_{ave} is the Earth's mean density. Putting (8) into (7) gives

$$M_i(t)=\int \Delta\sigma(\vartheta,\lambda,t)\,a^2\sin\vartheta d\vartheta d\varphi\sum_{nm}\frac{3(k_n+1)}{4\pi\rho_{ave}a^3(2n+1)}P_{nm}(\cos\vartheta)(A_{nm}^{c,i}(t)\cos(m\lambda)+A_{nm}^{s,i}\sin(m\lambda)) \qquad (9)$$

Comparing (9) with (6), the sensitivity kernel is:

$$A_i(\vartheta,\lambda)=\sum_{nm}P_{nm}(\cos\vartheta)\left(A_{nm}^{C,i}\cos(m\lambda)+A_{nm}^{S,i}\sin(m\lambda)\right)\frac{3(k_n+1)}{4\pi\rho_{ave}a^3(2n+1)} \qquad (10)$$

Consequently, the sensitivity kernel can be determined from knowledge of $A_{nm}^{C,i}$ and $A_{nm}^{S,i}$. We can determine these terms numerically, as follows.

Define a synthetic set of Stokes coefficients, where $\Delta C_{n'm'}(t) = 1$ for a single (n', m'), and all other Stokes coefficients are 0. Apply the fitting procedure described in (3)– (5) to this simple set of Stokes coefficients. From (7) we know the result for $M_i(t)$ equals $A_{n'm'}^{c,i}$. Repeating this for each (n', m'), and then for the $\Delta S_{n'm'}$'s as well, yields every $A_{n'm'}^{c,i}$, and $A_{n'm'}^{s,i}$, one at a time, which can then be put into (10) to obtain the sensitivity kernel. These steps can be repeated for every mascon i. It can be shown that the mascon sensitivity kernels have the following useful property. Let *i* and j represent any two mascons used in a simultaneous mascon fit, and let $A_i(\vartheta,\varphi)$ be the sensitivity kernel for mascon *i*. Then

$$\frac{1}{S_j}\int_{S_j} A_i(\vartheta,\varphi)\sin\vartheta d\vartheta d\varphi=\delta_{i,j} \qquad (11)$$

where S_j is the surface area of mascon j: it means that the area-averaged sensitivity kernel of a mascon is 1 over itself and 0 over any other mascon used in the simultaneous inversion. This implies that if a mass anomaly is distributed uniformly across a mascon, the solution for that mascon will deliver the true mascon average, and that this mass anomaly will not contaminate the solution for any other mascon.

4. Results

4.1. Time series estimates in the Middle East

By using LSMF solution, as described in section 3, to 114 months, from February 2003 to December 2012, of GRACE Release 05 Stokes coefficients, from the Center for Space Research (CSR) at the University of Texas (data available at http://podaac.jpl.nasa.gov), we construct time series of GRACE TWS changes for specific regions of the Middle East, chosen largely to coincide with political boundaries. The entire region is subdivided into seven mascons: Iran, Iraq, Syria, eastern Turkey (east of 35° longitude), northern and southern Saudi Arabia (north and south of 25° latitude), and the region immediately west of the Caspian Sea (Figure 1).

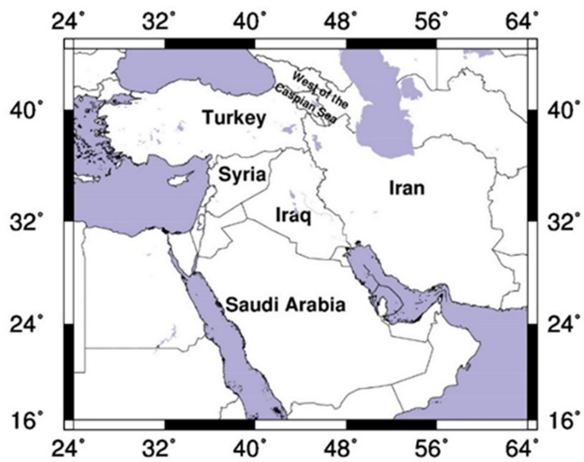


Figure 1. The mascons which have been used to estimate time series of TWS changes in the Middle East

As mentioned in section 2., the GRACE data is modified with replacing the low degree coefficients and removing the signal from the Caspian Sea and from two large lakes in the region: Lake Tharthar in Iraq and Lake Urmieh in Iran. The Stokes coefficients are contaminated with short-wavelength noises that have striping pattern (Kusche et al., 2009). In this case study, de-striping of the coefficients is done by using a 100 km Gaussian smoothing function. The use of a smaller Gaussian radius instead of a decorrelation filter results in noisier monthly time series but improves the characteristics of sensitivity kernels (Eq. 10). Figure 2, for example, shows the sensitivity kernel for the Iran mascon, when fitting all seven mascons to the Stokes coefficients. The kernel's value is small outside Iran and is close to unity inside Iran, but it does depart somewhat from those ideal values.

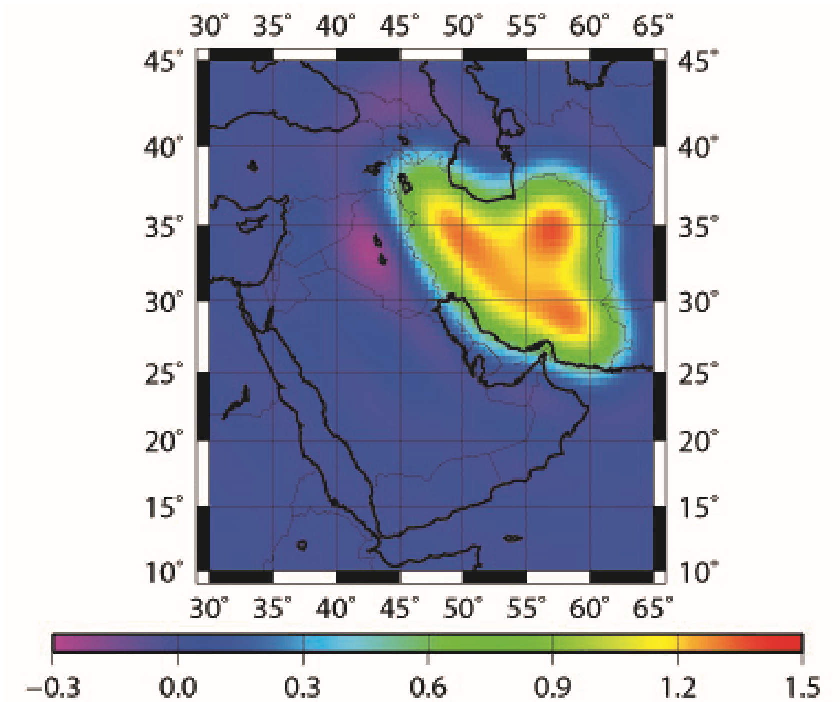


Figure 2. The sensitivity kernel for Iran

Figure 3 compares the GRACE estimate of total water storage variability for Iran, with a land surface model such as version 4.5 of the Community Land Model (CLM4.5) (Oleson et al., 2013). To extract a seasonally varying time series from the GRACE TWS and the total CLM4.5 water storage output, 12-month and 6-month periodic terms are fitted to both data sets across a 13-month sliding window. The black and red curves show result that have been smoothed to reduce sub-seasonal noise; the blue and green curves show the long-period (i.e. interannual and secular) components of the black and red curves. Note that the GRACE and model results agree well at seasonal periods, and they both show a sharp decrease in water storage that started with the onset of the drought, in 2007. The model results seem to have leveled off, and even recovered some, by 2009. The GRACE results, however, show a continuing water loss. Since CLM4.5 does not include an anthropogenic component, we interpret the increasing difference between GRACE and CLM4.5 as evidence of post-2007 anthropogenic groundwater loss.

The GRACE results for the other mascons such as Iraq, eastern Turkey, northern and southern Saudi Arabia all agree well with the CLM4.5 results at seasonal periods and their long-period components show a similar abrupt decrease in 2007 (Figure 4). In eastern Turkey the GRACE results subsequently recover, though not as rapidly as the CLM4.5 results.

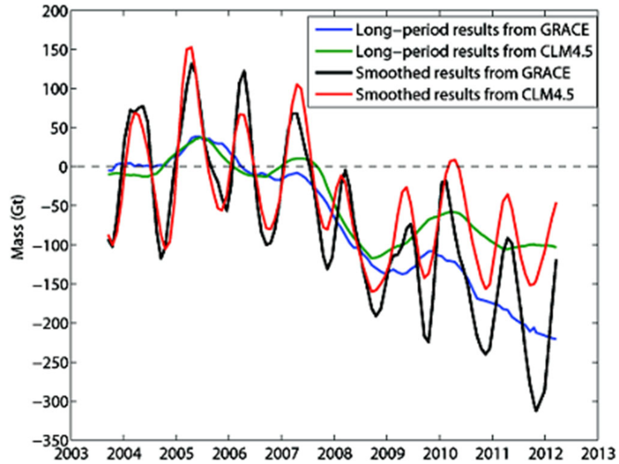


Figure 3. Changes in TWS, in gton, for Iran.

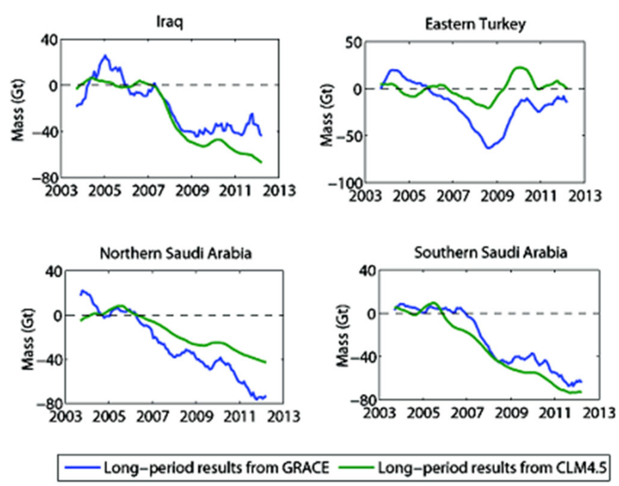


Figure 4. Changes in TWS, in gton, for Iraq, Eastern Turkey, Northern and Southern Saudi Arabia

4.2. Time series estimates in Iran's water main basins

Figure 5 shows six main water basins in Iran including: Caspian Sea basin (175051 km^2), Urmieh lake basin (52000 km^2), Persian Gulf and Oman sea basin (424029 km^2), Central Plateau basin (825000 km^2), Eastern Boundary basin (106000 km^2), and Gharaghom basin (44295 km^2). We estimate time series of GRACE TWS for each basin by using LSMF solution. We assume each basin as a mascon and fit mass amplitudes for each of these mascons, simultaneously, to the GRACE monthly data as described in section 3. We thereby obtain monthly times series of mass variability for each of those basins during 2002-2017. Modifying the GRACE Stokes coefficients and the other necessary modifications such as removing the lake signal and smoothing radius are done as described in section 4.1.

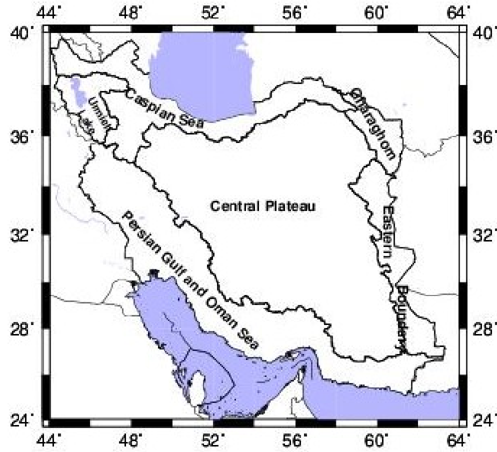


Figure 5. Iran's main water basins

Because GRACE data have finite resolution, it is impossible to obtain a perfect unweighted average of mass variability within a basin, no matter what technique is used for the GRACE analysis or what basin is considered. Results from a mascon fitting method are no exception. For example, a GRACE estimate for the mass change in the central plateau basin will include contamination from mass variations outside it and will not weight every point inside it equally. Effects of mass variations outside the central plateau basin can be reduced by using a sensitivity kernel (Eq. 10) for the central plateau basin, when fitting all six mascons to the Stokes coefficients (Figure 6).

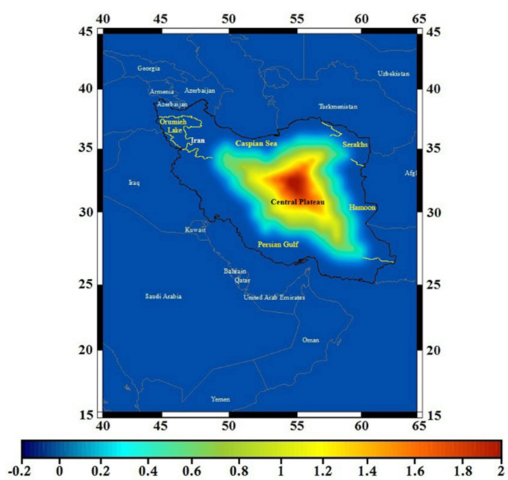
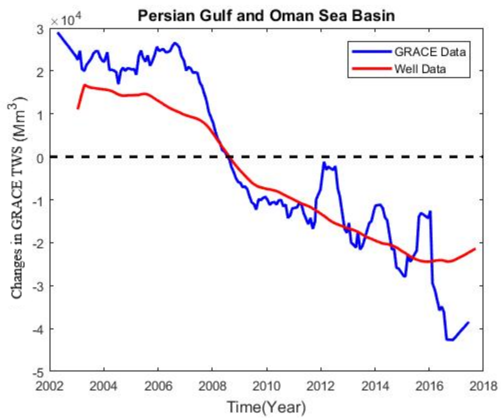


Figure 6. The sensitivity kernel for the central plateau

Figure 7 compares changes in the GRACE TWS for the six main water basins of Iran, with variation of groundwater level data from observation wells. There are 17,865 active observation wells in the whole of Iran. To obtain time series of groundwater level changes in the six main water basins, each main water basin is divided into several sub-basins, and each sub-basin is divided into several study areas. The Thiessen polygon method has been used to make a time series of the groundwater level changes across each study area. Then we scale up it for each study area by multiplying it by the ratio: ($\frac{\text{area of the study area}}{\text{area of the Thiessen polygon}}$).



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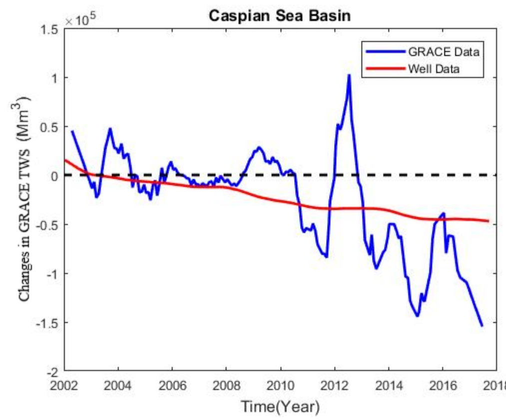

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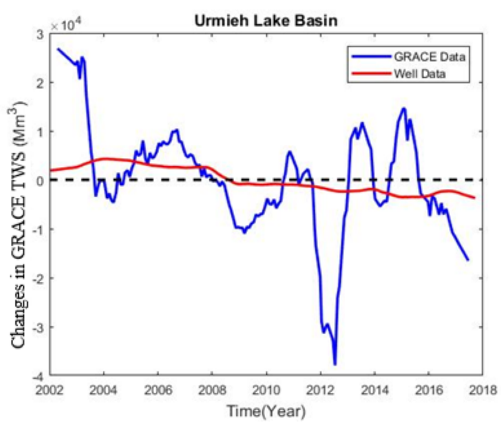

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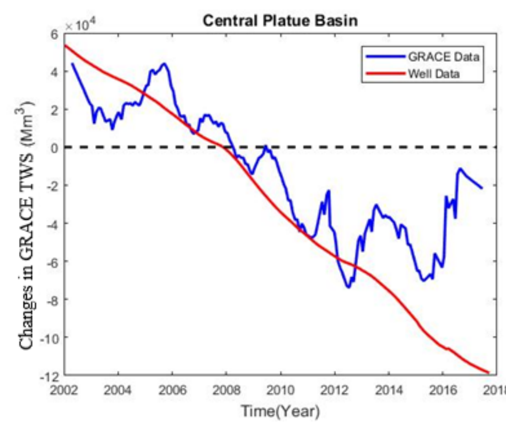

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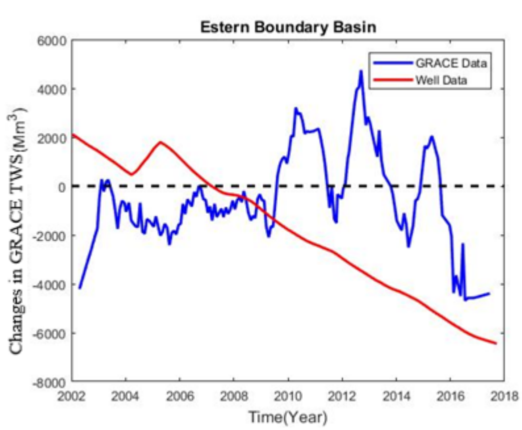

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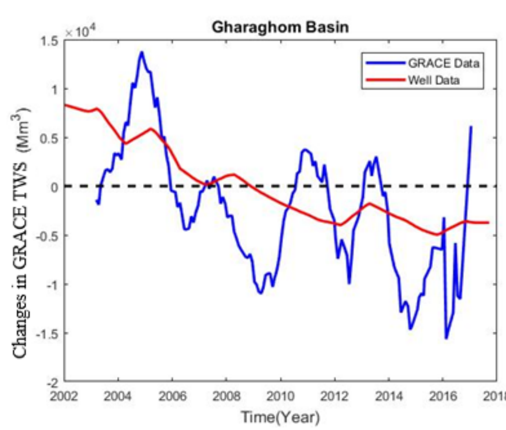


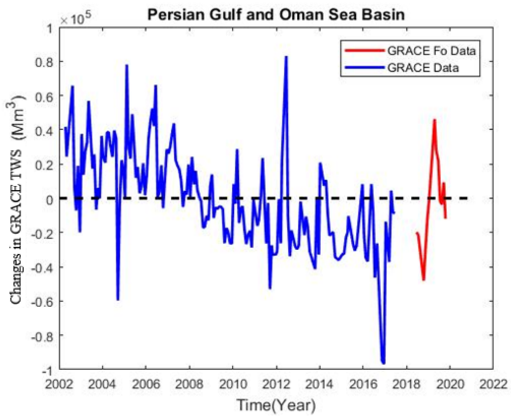
(f)

Figure 7. Changes in GRACE TWS, in Million cubic meter (Mm^3), compared with monthly values inferred from the well data, across (a) the Persian Gulf and Oman Sea basin, (b) the Caspian Sea basin, (c) Urmieh Lake, (d) Central Plateau, (e) Eastern Boundary, and (f) Gharaghom basin.

The total change in groundwater storage across each sub-basin is computed by adding together the scaled change in groundwater storage of all its study areas. The same procedure is carried out for each main water basin. Note that the GRACE and well results both show a sharp decrease in water storage that started with the onset of the drought, in 2007 and most of the GRACE long-term water loss is due to a decline in groundwater storage. Using a smaller Gaussian radius results in noisier monthly time series and some fluctuation in the GRACE long-term variability.

4.3. Time series estimates of TWS from GRACE and GRACE FO in Iran's main water basins

Figure 8 shows time series of water storage variability, in Million cubic meter (Mm^3), from GRACE and GRACE FO during 2002 to 2020 for six main water basins of Iran. As described in sections 4.2, mascons are chosen largely to coincide with boundaries of six main water basins of Iran (see Figure 5). By using LSMF solution, as described in section 3, to 163 months, from April 2002 to August 2017, of GRACE Release 06 Stokes coefficients, and to 15 months from May 2018 to October 2019, of GRACE FO Release 06 Stokes coefficients, both of the Center for Space Research (CSR) at the University of Texas (data available at https://podaac-tools.jpl.nasa.gov/drive/files/allData), we construct time series of GRACE/GRACE FO TWS changes for the six main water basins. In order to include the degree-1 geocenter terms, we follow the methodology of (Swenson et al., 2008). The degree-1 coefficients are recalculated consistently for each GRACE/GRACE-FO solution. We replace the GRACE/GRACE FO results for the lowest-degree zonal harmonic coefficient, C_{20}, with those obtained from Satellite Laser Ranging (Cheng et al., 2013). All harmonics are smoothed with a 100 km radius Gaussian smoothing function (Wahr et al., 1998). In all of the water basins, time series of water storage variability from GRACE/GRACE FO line up well across the data gap from mid-2017 to mid-2018. The GRACE/GRACE FO results consist mainly of short-period, seemingly random fluctuations, superimposed on long-period variability. The short period fluctuations represent the effects of GRACE/GRACE FO measurement errors and month-to-month errors in the modeled water storage quantities. The long-period variability, which stands out more clearly after smoothing the GRACE/GRACE FO results, represents changes in total water storage. The most obvious characteristic of that variability is a steady groundwater loss during this 18-year period.



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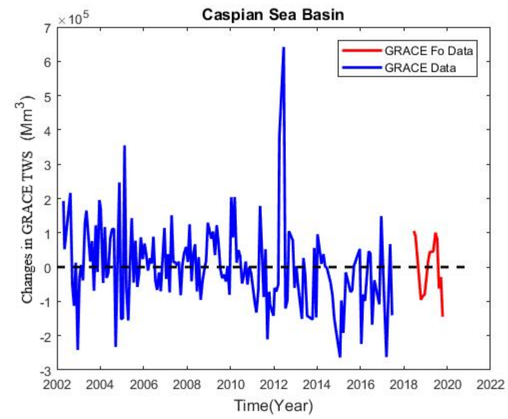

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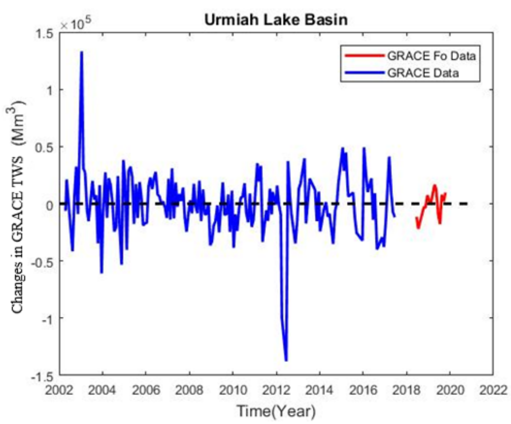

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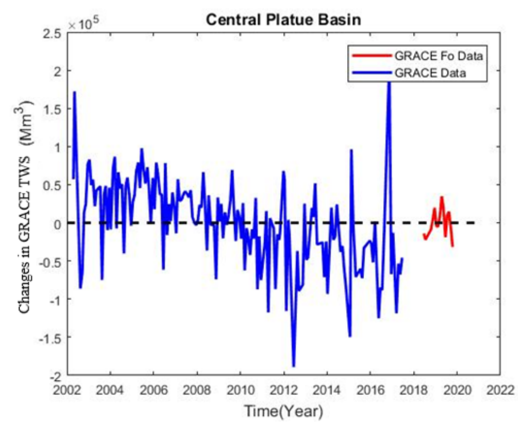

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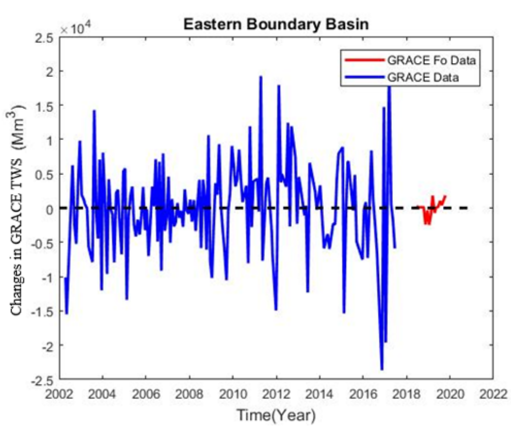

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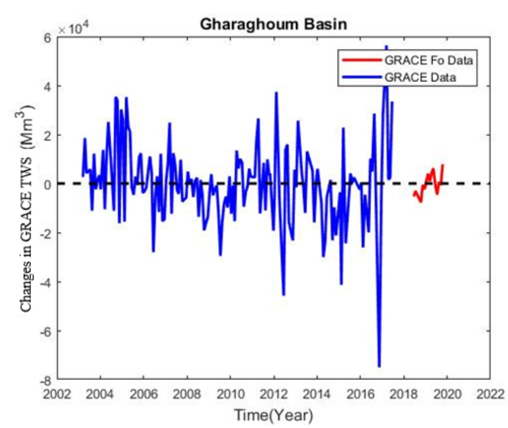

(f)

Figure 8. Changes in GRACE/GRACE FO TWS, in Million cubic meter (Mm^3), across (a) the Persian Gulf and Oman Sea basin, (b) the Caspian Sea basin, (c) Urmieh Lake, Central Plateau, (d) Eastern Boundary, and (e) Gharaghom basin.

5. Summary and Conclusions

Total Water Storage (TWS) is a basic element of the hydrological cycle and a key state variable for land surface-atmosphere interaction. However, measuring TWS in a comprehensive way for different storage compartments and beyond the point scale is a challenge. Gravity measurements are influenced by water storage due to the Newtonian attraction of masses. Observations of temporal gravity changes provide a direct and depth-integrated measure of water storage change. GRACE and GRACE Follow On (GRACE FO) missions are two valuable satellite missions for measuring of temporal gravity changes. A standard method to compute time series of TWS changes using temporal satellite gravity data, named spherical harmonics solution, has been described in (Wahr et al., 1998). In this chapter, we have demonstrated the Least Squares Mascon Fitting (LSMF) solution to GRACE and GRACE FO data to estimate time series of TWS changes in two spatial scales: at a regional scale in the Middle East and at a basin scale in the six main water basins of Iran. The results show that the LSMF technique is a useful method to estimate time series of TWS changes using the satellite gravity data in both basin and regional scales. The GRACE and GRACE FO data line up across the data gap at a basin scale.

6. References

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