Geophysical Journal International

Geophys. J. Int. (2020) **221,** 1226–1231 doi: 10.1093/gji/ggaa073
Advance Access publication 2020 February 7
GJI Gravity, Geodesy and Tides

Impact of uncertainties of GOCE gravity model on crustal thickness estimates

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Accepted 2020 January 13. Received 2020 January 31; in original form 2019 December 13

SUMMARY

In the last few years many studies have applied data of satellite gravity sensors for solid Earth applications. The use of different methodologies has been shown to result in large variations in crustal thickness even when using the same data as source. It is, however, difficult to estimate what is a significant difference between such models. Up to now the impact of the inherent uncertainty of Gravity Field and steady-state Ocean Circulation Explorer (GOCE) data on solid Earth applications has never been quantified. With this study we will provide uncertainty boundaries for crustal modelling based on the GOCE TIM5 covariance matrix. Different noise realizations have been calculated using a Monte Carlo-like simulation and added to the TIM5 model coefficients. The resulting differences in crustal thickness amount to maximum ±0.2 km, which is less than 1 per cent of the total thickness, and much smaller than many other uncertainties involved in the inversion process.

Key words: Composition and structure of the continental crust; Gravity anomalies and Earth structure; Satellite gravity; Statistical methods.

1 INTRODUCTION

In recent years we have seen a sharp increase in publications using Gravity Field and steady-state Ocean Circulation Explorer (GOCE), or other satellite gravity data, for studying Earth structure. These studies used gravity models that are based on GOCE only data, satellite gravity only data, or combinations of satellite gravity data and terrestrial data (in which GOCE and other satellite gravity data are incorporated). The combined models have generally a high resolution (down to 10 km or even less) but inhomogeneous data coverage due to local regions with high resolution ground based data. GOCE and satellite only models have a much coarser resolution (around 80 km at best) but homogeneous coverage thereby showing strong spatial integrity of the data. Götze & Pail (2018) provide a recent review of various global gravity models and their use for geophysical modelling and interpretation. For some of these models also realistic error estimates in terms of a full covariance matrix is available, such as for the time-wise (TIM) GOCE-only model series (Pail *et al.* 2011), the GOCO satellite-only model series (Pail *et al.* 2010), or the combined gravity model XGM2016 (Pail *et al.* 2018). These error estimates result from the attempt to stochastically model all errors of the respective input data as realistically as possible. The advantage of full covariance matrices is that they enable to properly reflect spatially varying errors due to different data quality or observation geometries.

Most geophysical studies have focused on the crust or the whole lithosphere since the gravity signal is most sensitive for spatial variations in this depth domain (van der Meijde *et al.* 2013b). The most common Earth discontinuity to study is the Moho discontinuity, the boundary between the crust and the uppermost mantle. A wide range of methods have been used to retrieve information on the depth of this discontinuity, each with their own estimate of the uncertainty on the depth. The uncertainty estimates are very diverse and no common approach is used in calculating these. Most approaches are purely mathematical (e.g. Tenzer *et al.* 2012; Bagherbandi *et al.* 2013; Uieda & Barbosa 2017, and others), and only a few are based on actual validation using estimates from other sources and/or expert knowledge (e.g. Reguzzoni *et al.* 2013; van der Meijde *et al.* 2015; Afonso *et al.* 2019 and others). Another factors is related to differences between the gravimetric and seismic Moho, where isostasy based modelling approaches do not hold (Bagherbandi *et al.* 2013). Uncertainty estimates for derivation of the depth of the Moho discontinuity vary therefore widely, ranging from around 1 km, or less, for mathematical estimates, up to 6 km, or more, in case of validation with other Earth science based observations.

Most of the studies give a single value for the uncertainty, independent of the location of the estimate and the data models used (thereby ignoring the spatially variably quality of the combined gravity models). A few actually provide a spatial estimate of the variability of the Moho models. Reguzzoni *et al.* (2013) give a full spatially variable estimate of uncertainties, van der Meijde *et al.* (2013a) and Tugume *et al.* (2013) provide point-wise estimates based on comparison with seismological observations and derive average estimates for different tectonic domains. All these estimates are based on comparisons, sampling techniques like Monte Carlo simulations of variable input parameters, or statistical approaches (like multiple simulations with small distortions, or combinations thereof). Uncertainties in the modelling of the Moho depth as an effect of corrections or input data are only occasionally evaluated (e.g. terrain effects by Abrehdary *et al.* 2016; Szwillus *et al.* 2016). It might be very tricky to make a full uncertainty estimate of the depth of the Moho discontinuity due to the variable input models, different inversion techniques, and the inherent non-uniqueness of the inversion of gravity data. van der Meijde *et al.* (2015) studied a wide range of Moho models based on gravity-only, combined seismological and gravity, and seismological models only. They showed that variations are large between models, and differences can be as large as 20 km. Similarly, Grad *et al.* (2009) found differences up to 20 km between seismic based models for Europe. However, improving the understanding of error propagation is essential to at least understand the contribution by each component of the data and modelling.

One component that has not been evaluated is the propagation of satellite gravity sensor uncertainties to the Earth science models. It is therefore, till date, unknown how large this contribution is, and if it is significant in relation to the average Earth science or modelling uncertainty. This study will calculate the GOCE sensor intrinsic error contribution and its propagation through modelling into the final Moho model as previously calculated by van der Meijde *et al.* (2013a).

2 DATA AND METHODS

2.1 Satellite gravity data

The GOCE satellite has mapped our planet's gravity field in unprecedented detail. GOCE was the first spaceborne gravity gradiometer and carried six proof masses capable of observing detailed local changes in gravitational acceleration in three spatial dimensions with extremely high precision. It contributed unique gradient data to global gravity models, in particular at wavelengths down to 80 km.

The crustal thickness map used in this study is based on the inversion of the global gravity model GOCE TIM5 (Brockmann *et al.* 2014) that contains gravity gradient data from the GOCE mission (Drinkwater *et al.* 2003). Recently, a new model GOCE TIM6 was released, which is, similar to GOCE TIM5, based on the data of the complete GOCE mission, but with improved input gravity gradients. This improvement was mainly achieved by a modified gradiometer calibration strategy (Siemes *et al.* 2019). The resulting improvement compared to TIM5 is in the order of 20 per cent, but would not significantly change the results and conclusions of this study. We have used for this study the GOCE TIM5 release, because it corresponds to the model used by van der Meijde *et al.* (2013a), EIGEN-6C (Förste *et al.* 2011), when they calculated their gravity derived Moho for South America. We use that specific paper, and their results and error estimates for other modelling components, as a benchmark.

2.2 Noise realizations of gravity model

Model output of the GOCE TIM5 release is a set of spherical harmonic (SH) coefficients parametrizing the global gravity field up to SH degree 280, and the corresponding uncertainty estimates in terms of the full covariance matrix. For the present study, we use the model up to degree and order 200. Since realistic stochastic models for the main input observation types, that is gravity gradients and precise orbits, were included in the model generation, the resulting covariance matrix reflects the true error behaviour very realistically, which could be shown by external validation (Brockmann *et al.* 2014) applying validation methods as described in Gruber *et al.* (2011).

Based on the TIM5 covariance matrix $\Sigma(\hat{x})$, different noise realizations have been calculated using a Monte Carlo simulation and added to the TIM5 model coefficients $\hat{x}$, which contain the SH coefficient estimates in a pre-defined sorting. In a first step, a Cholesky decomposition was applied to the covariance matrix $\Sigma(\hat{x})$:

$$\Sigma(\hat{x}) = L\,L^T. \tag{1}$$

In a second step, the resulting lower triangular matrix L is applied to a uncorrelated random vector u with zero mean and unit variance, $u \in N(0,\ 1)$, resulting in a vector $d\tilde{x} = L\,u$ with the covariance properties of $\Sigma(\hat{x})$. This procedure was repeated with 10 random vectors u, resulting in 10 representative noise realizations of the GOCE TIM5 model. They were then added to the model coefficients $\hat{x}$ to result in 10 different 'noisy' GOCE TIM5 models: $\tilde{x} = \hat{x} + d\tilde{x}$.

2.3 Model calculations

The TIM5 models with different noise realizations $\tilde{x}$ were all processed in a similar way to retrieve crustal thickness. The modeling approach applied is an implementation (Gómez-Ortiz & Agarwal 2005) of the Parker–Oldenburg iterative inversion method (Parker 1973; Oldenburg 1974), similar to the application on South America by van der Meijde *et al.* (2013a). The inversion results in a simple two-layer model with Moho topography as the interface, and is based on the assumption that the entire gravity signal is caused by Moho topography. Surface topography and subsurface inhomogeneities are not considered in the model and have been corrected for, *a priori*. The effect of surface topography has been removed by a Bouguer correction. A correction has been also applied for sediment basins. The sediment correction is based on sediment thickness information retrieved from a global sediment thickness map on a 1° x 1° degree scale (Laske & Masters 1997). The density contrast was assumed constant at 200 kg m^{-3}. This is based on the average density value of the central layer in the digital soil map (Laske & Masters 1997) which is around 200 kg m^{-3} less than the 2670 kg m^{-3} used for rocks in the Bouguer correction.

A low-pass filter is included in the inversion procedure to ensure convergence of series due to unstable behaviour at higher frequencies (Gómez-Ortiz & Agarwal 2005). The upper boundary was set to a wavelength of approximately 200 km. This low-pass filter justifies the use of satellite-only models of limited spatial resolution. In Götze & Pail (2018) it is discussed that omission errors, that is higher-frequency signals which are not parametrized by global satellite-only gravity models, can have significant amplitudes especially in topographic rough areas. In our case we used GOCO TIM5 up to SH degree and order 200, so that the omission error is composed of gravity signals with spatial wavelengths lower than

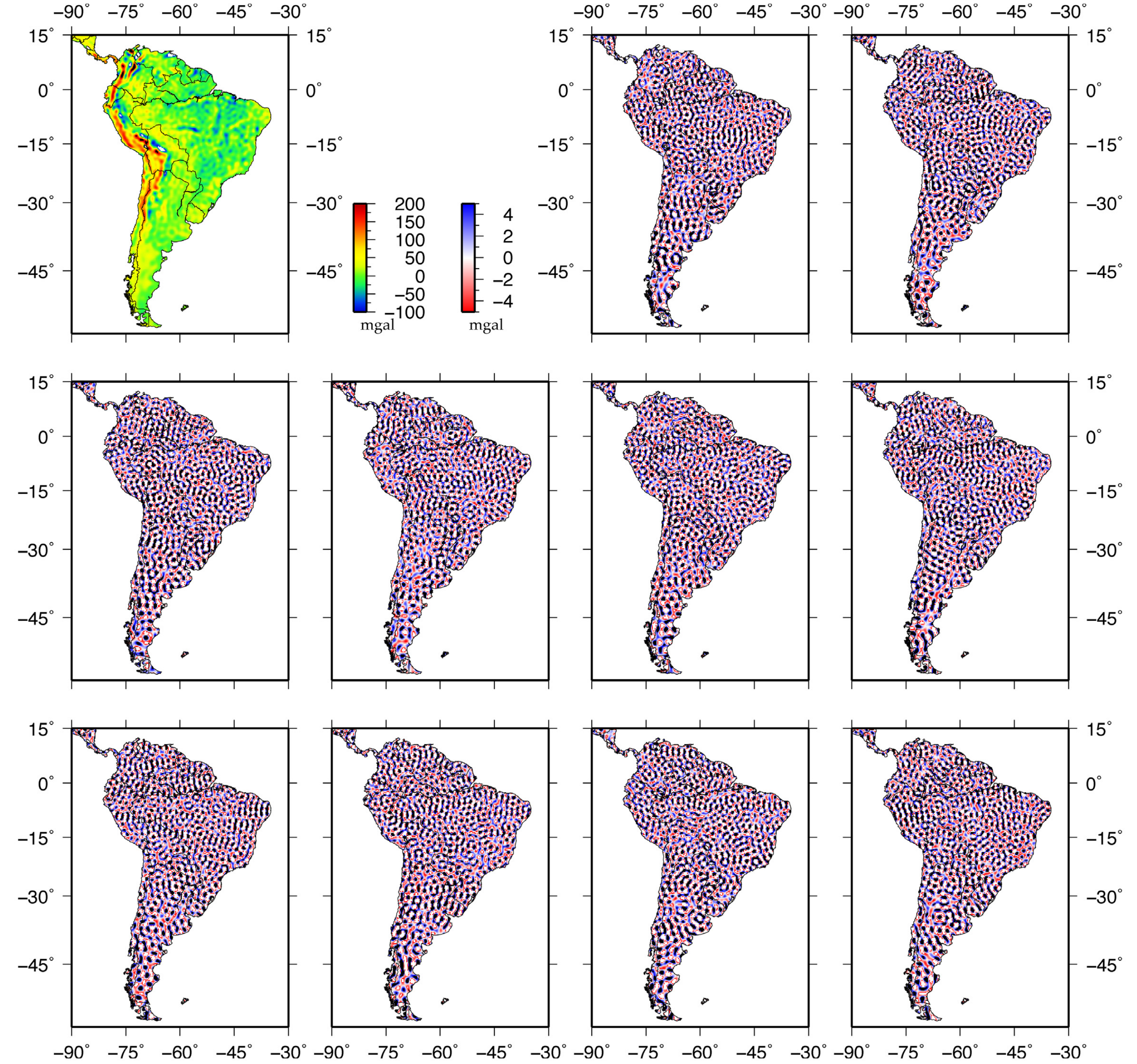

Figure 1. Error realizations.

100 km. However, they will be largely filtered out by the processing step of low-pass filtering with an upper boundary of about 200 km wavelength. In this analysis no other parameters have been varied. The required starting (initial) Moho depth and the density contrast between the lowermost crust and uppermost mantle have been the same as in van der Meijde *et al.* (2013a) in which also further details on the data processing can be found. For each realization of the uncertainty estimates, we have used the undisturbed inversion result by using the SH coefficient set $\hat{x}$, and subtracted the realization $\tilde{x}$ with the error coefficients added to it.

3 RESULTS AND DISCUSSION

The final gravity model, after corrections, is shown in the top-left panel of Fig. 1. The total range of values is around 300×10^{-5} m s^{-2} (or mGal) for the continent of South America (only the continent is shown to increase visibility of structure). The other 10 panels show 10 random error realizations based on the GOCE TIM5 covariance matrix. No apparent pattern is visible in the error realizations. The distribution of positive and negative errors, varying between -5 and 5 mGal, has no relation to structure, or seems otherwise influenced by the Earth, like topographic effects. There is no relation to high and low values of the gravity model and possible patterns visible in one realization are not visible in the other realizations. This is to be expected, because the error structure resulting from the GOCE mission is not signal-correlated, and shows as the only systematic feature a latitude-dependent pattern, which is related to the changing ground track density of the GOCE orbit due to meridian convergence, and a slight latitudinal variation of mean orbit altitude. This feature, however, is not directly visible in the error realizations of Fig. 1, because the standard deviation per latitude varies only between 0.8 and 0.95 mGal within the latitude range of South America, with the maximum at a latitude of about 20°S.

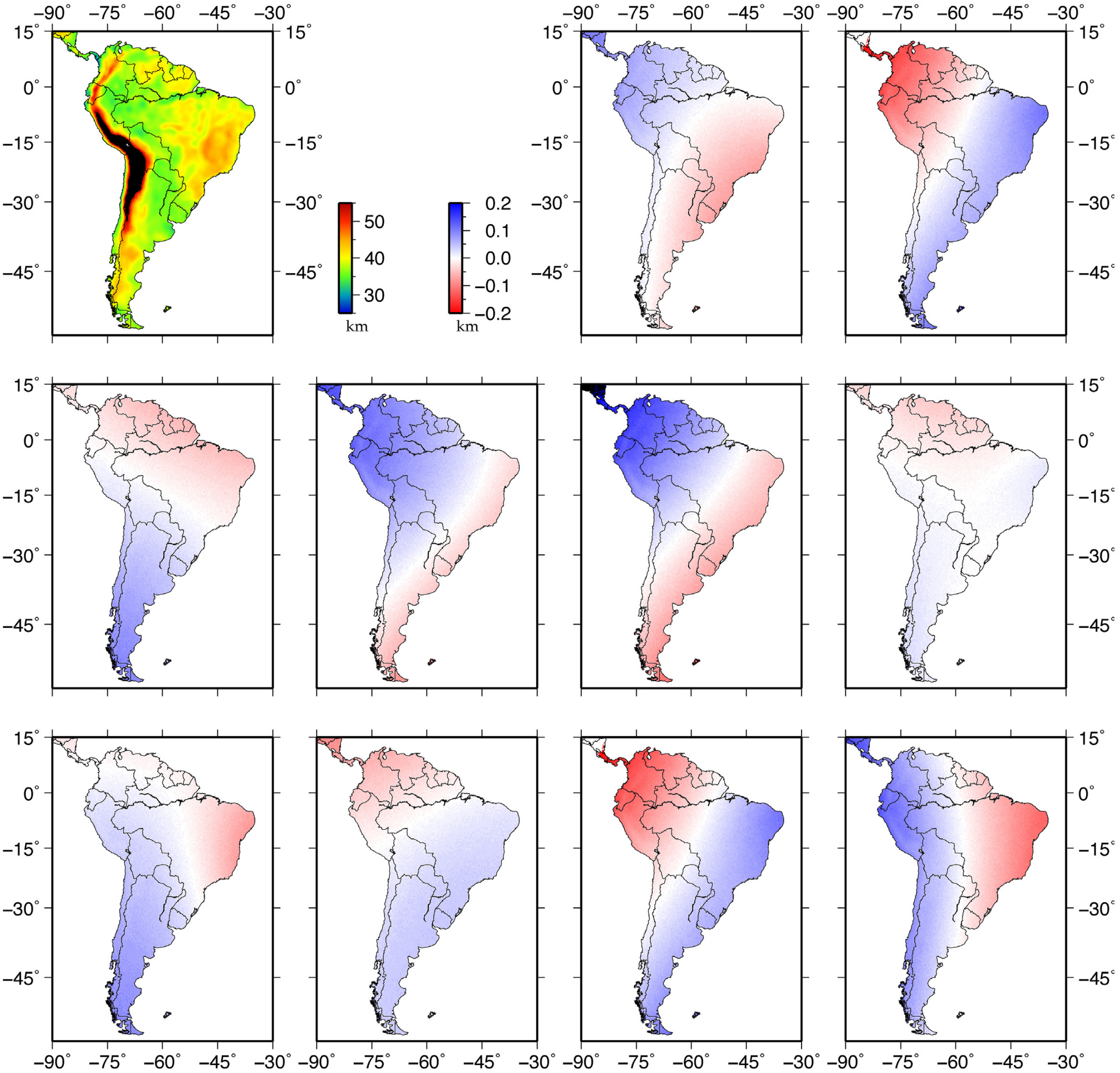

Figure 2. Propagated uncertainties.

The error is, at maximum, 5 per cent of the total (corrected) gravity field.

These error realizations $d\tilde{x}$ have been added to the gravity field $\hat{x}$ and then inverted for crustal thickness following the approach by van der Meijde *et al.* (2013a). The results in Fig. 2 show the final crustal thickness model in the top-left panel. The other 10 panels show the difference between the final model and the 10 models where the error estimates were added to the total gravity field before inversion. So, these 10 panels show the excess thickness due to the GOCE gravity field uncertainties. The total thickness variations amount to maximum 0.2 km, positive or negative. In most of the panels the difference is much smaller, often less than 0.1 km. There are no distinct patterns visible in any of the models related to Earth structure or topography. The model differences are, generally, very smooth and show a clear gradient over the continent. This gradient is not directly a result of the error realizations, but show the impact of these error variations in the fitting of the Fourier surface through the data (see Gómez-Ortiz & Agarwal 2005, for specific details on the method), and is therefore directly related to the modelling approach used. The overall propagation of the GOCE sensor uncertainties into the crustal thickness modelling is damped. The uncertainties contributed up to 5 per cent to the input gravity field. After inversion, however, the GOCE sensor related uncertainty is less than 1 per cent of the total crustal thickness. It is possible that for other modelling techniques the propagated error is larger or smaller or shows a different pattern. The long-wavelength shape of uncertainty is due to the fitting of a Fourier surface through the data. Alternative modelling approaches will most likely not show this same pattern but something that fits with the chosen modelling approach for these studies.

The GOCE sensor uncertainties are also much smaller than the modelling or Earth science related uncertainties. Uncertainties for the final crustal thickness model were estimated based on a regulated variation of the modelling input parameters. In order to investigate the uniqueness of our crustal thickness map, van der Meijde *et al.* (2013a) performed several inversions using a range of values for critical parameters, such as the starting Moho depth and the density contrast across the Moho interface. The density contrast over the Moho varies strongly globally and between studies, roughly between 280 and 480 kg m^{-3} (Dziewonski & Anderson 1981; Martinec 1994; Bassin *et al.* 2000; Sjöberg & Bagherbandi 2011; Tenzer *et al.* 2012). For assessing the modelling uncertainty the density contrast was varied with 50 kg m^{-3} and with 1 and 2 km steps for the initial starting value of the Moho depth. This resulted in a combined effect of, on average for the whole continent, of ±3 km variation. This uncertainty is much larger, at least 10-fold, compared to the GOCE sensor related uncertainties.

We have evaluated here the so-called commission error, errors that we know that are there and that are measurably added to the data. On the other hand we also have an omission error, that is the omitted high-frequency signals that are not observed by gravity missions due to limited spatial resolution. These are extremely hard to estimate since they can't be calculated directly because they are not in the data. For most of the models it is expected though that these high frequency signals have very little effect on the Moho since the Moho is, in general, a reasonably smooth discontinuity. There can be a larger omission error in areas that are geodynamically very active, like steep mountain ranges, (complex) subduction zones, and sharp continent–ocean boundaries where the Moho can vary sharply over a short spatial distance. Estimates for these variations, from a modelling perspective and based on earth science related parameter variations, are given in van der Meijde *et al.* (2013a), Tugume *et al.* (2013) and van der Meijde *et al.* (2015). These earth science and modelling errors can be relatively large, and are a combination of, for example limitations in modelling approach that do not allow for sharp variations, but also might have a contribution from omission errors. Omission errors can be reduced by applying combined instead of satellite-only gravity field models (Götze & Pail 2018). In our processing, we expect that the omission error of gravity signals beyond SH degree and order 200 is insignificant, because of the 200 km low pass filter applied during inversion (*cf.* Section 2.3).

4 CONCLUSIONS

We have evaluated the propagation of TIM5 covariance matrix $\Sigma(\hat{x})$, noise realizations into Earth science modelling. As an example we evaluated the uncertainty contribution in crustal thickness modelling in South America, following an earlier publication. We observed that the total absolute maximum sensor error can contribute up to 5 per cent of the gravity signal , but is in most cases 2 per cent or less. After modelling, we found that the GOCE sensor uncertainty contribution in crustal thickness is less than 1 per cent of the total crustal thickness. This is much smaller than Earth science related uncertainties in Moho depth modelling. The contribution is small for our example but might be higher for other modelling approaches. The pattern is mostly dominated by the modelling technique applied. There is no visible relation to subsurface structure and/or surface topography. We finally concluded that the uncertainty in the global gravity models are not the main error contributor of Moho depth uncertainties.

ACKNOWLEDGEMENTS

This work was partly funded by the Netherlands Organisation for Scientific Research (NWO), grant number ALW-GO-AO/11-30. The standard repository for global gravity models (coefficients) is the ICGEM portal (http://icgem.gfz-potsdam.de/). Additionally, the coefficients and covariance matrices of GOCE models are provided by the ESA Virtual Archive (http://eo-virtual-archive1.esa.int/GOCEGravityModels.html).

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