High resolution time-lapse gravity field from GRACE for hydrological modelling

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Abstract

Calibration of large scale hydrological models have traditionally been performed using point observations, which are often sparsely distributed. The Gravity Recovery And Climate Experiment (GRACE) mission provides global remote sensing information about mass fluxes with unprecedented accuracy, which can be used for calibration of such models.

Mass concentration (mascon) parameters used at the Goddard Space Flight Center are spatial and temporal step functions of equivalent water height in predefined regions, estimated directly from the level-1B K-band Range-Rate (KBRR) data from GRACE. The mascon parameters are recovered through least squares inversion of a normal equation system, which is based on partial derivatives of the KBRR data residuals with respect to the mascon parameters. Spatial and temporal constraints are added for stability reasons, and the recovered mascon parameters represent mass redistributions on/near the surface of the Earth. A grid of $1.25^\circ \times 1.5^\circ$ and $1.5^\circ \times 1.5^\circ$ blocks\(^1\) (latitude $\times$ longitude) is used.

A simple water balance model of the Okavango River Basin covering parts of Angola, Namibia, and Botswana, is built using a modified Budyko type framework on each of seven sub-catchments, derived for the river basin from a digital elevation model. The hydrological model is initially calibrated to discharge and mass variations in a $1.25^\circ \times 1.5^\circ$ grid every ten days from five years of GRACE mascon only solutions, using a joint sequential calibration function.

Coupling of the mascon method with the hydrological model is done by chaining of partial derivatives, so that the normal equation system is solved for model parameters instead of mascon parameters. The mass variations from GRACE are relative, meaning that the origin is arbitrary, while the terrestrial water storage variations from model, are absolute. Thus, a bias exists between the model output and the GRACE derived mass variations, which must be accounted for by the use of bias parameters. One bias parameter is introduced for every mascon block, in order to account for the difference in level between the GRACE derived mass variations and the hydrological model, and spatial constraints on the bias parameters are used.

The coupling method is tested with different correlation distances on the bias constraint equations, and different scaling of the bias parameter constraints as well as the mascon parameter constraint equations. The results are evaluated by comparing the observed and simulated data with respect to the KBRR data, the discharge data, and the terrestrial water storage from the GRACE mascon only solutions used for

\(^1\)In the northern part of the study area blocks are smaller than in the southern part.
the initial calibration of the model. The discharge and terrestrial water storage data were also used for the initial joint model calibration.

In the coupled inversion, the adjustment of the hydrology parameter in the model is in general very small, since the model was already pre-calibrated. The terrestrial water storage output from the model, using the adjusted parameter value, shows a higher annual amplitude (14.79 cm) than the mascon only solution (12.09 cm), the 10-day spherical harmonic solutions from CNES/GRGS (8.85 cm), and the terrestrial water storage from GLDAS/Noah (11.39 cm), for the same area. The annual signal peaks around March to April. The timing of signal peaks for the model output is earlier than for the mascon only solution, but later than the GLDAS/Noah TWS and the CNES/GRGS SH solutions. The deviations are 10–20 days.

From this point of view, the tuning of hydrological models with KBRR data is certainly feasible, though highly time consuming and complicated at the moment. The method definitely has potential and should be tested with more model parameters and for larger models.
Dansk resumé

Storskala hydrologiske modeller er traditionelt set blevet kalibreret med punktobservationer, som ofte kun forefindes sparsomt. Gravity Recovery And Climate Experiment (GRACE) missionen leverer globale remote sensing informationer om massefluks med en hidtil uset nøjagtighed, som kan bruges til kalibrering af sådanne modeller.

Massekoncentrations (mascon) parametre, som bruges på Goddard Space Flight Center, er stepfunktioner der angiver ækvivalent vandhøjde i tid og rum, estimeret direkte fra level-1B K-Band Range-Rate (KBRR) data fra GRACE, over prædefinerede områder eller blokke. Mascon parametre bestemmes ved hjælp af mindste kvadraters inversion af et normalligningssystem, som er baseret på partielt afledte af KBRR data i henhold til mascon parametrene. Rummelige og tidslige bånd anvendes på parametrene, for at stabilisere løsningen, og de fundne mascon parametre repræsenterer masseomfordelinger på/nær Jordens overflade. Det anvendte grid består af 1,25°×1,5° og 1,5°×1,5° blokke 2 (breddegrad×længdegrad).

En simpel vandbalance model af Okavango flodbassinet, som dækker dele af Angola, Namibia og Botswana, er baseret på en modificeret Budykotype struktur (Zhang et al., 2008) på hvert af i alt syv små oplandsområder, som er beregnet for floden ud fra en topografisk model. Modellen er først blevet kalibreret til både vandføring og masse variationer i et 1,25°×1,5° grid hver 10. dag, ved brug af 5 års GRACE mascon løsninger, og en fælles kalibreringsfunktion.

Sammenkoblingen af mascon metoden med en hydrologisk model opnås ved at sammenkæde de partielt afledte, således at normalligningssystemet løses for model parametre i stedet for mascon parametre. Massevariationerne fra GRACE er relative, hvilket betyder at nulpunktet er arbitrært, hvorimod total vandmængde fra den hydrologiske model er absolut. Således eksisterer det en forskel i niveau mellem de to signaler, hvilket der må tages højde for ved hjælp af bias parametre. Én bias parameter introduceres for hver blok i modellen, for at tage hensyn til forskellen i mascon løsningen fra GRACE og resultatet fra den hydrologiske model. Bias parametrene pålægges rummelige bånd i inversionen på samme måde som mascon parametrene. Sammenkædningen testes ved brug af forskellige korrelationsaftstande på de bånd som bruges på bias parametrene, forskellig skalering af de ligninger som omhandler bånd på bias parametre og bånd på mascon parametre. Resultaterne evalueres udfra forskellen mellem simuleret og observeret data på tre forskellige typer data: KBRR data, flodens vandføring ved udmundingen og total vandmængde fra GRACE mascon løsningen, hvoraf vandføring og total vandmængde også blev  

2 Blokkene i den nordlige del af studieområdet er mindre end i den sydlige.
begge brugt ved den første kalibrering af modellen.

I den sammekoblede inversion er justeringen af den hydrologiske parameter i modellen generelt meget lille, eftersom modellen er prækalibreret. Den vandmængde som er resultatet af en modelkørsel med den justerede parameter, giver større amplitude af årstidssignalet (14,79 cm) end den mascon løsning som blev brug ved den første kalibrering (12,09 cm), 10-dages SH løsninger fra CNES/GRGS (8,85 cm) og total vandmængde fra GLDAS/Noah (11,39 cm), for det samme område. Årstidssignal er størst omkring marts-april måned. Tidspunktet for det største årstidssignal for modeloutputtet ligger tidligere end for mascon løsningen, men senere end for GLDAS/Noah og CNES/GRGS løsningerne. Afvigelserne er på 10–20 dage.

Samlet set er kalibrering af hydrologiske modeller ved brug af KBRR data bestemt muligt, selvom metoden i øjeblikket er meget tidskrævende og omstændelig. Metoden har potentiale, men bør testes med flere modelparametre og på større modeller.
Preface

This Ph.D. study is part of a large research project called HYDROGRAV, which is financed by Dansk Forsknings Råd and has been running in the years 2007 to 2010. The HYDROGRAV project aims at developing methodology for the routine assimilation of time-lapse gravity observations (both ground-based and space-borne) into hydrological models. The focus of this Ph.D. project is on the application of space-borne surveys from the Gravity Recovery and Climate Experiment (GRACE). The thesis includes one scientific paper, Krogh et al. (2010), which can be found in appendix C.

The partial derivatives of the GRACE range-rate data with respect to the mascon parameters, as well as the normal matrix operation program, SOLVE, which was used to invert the normal equation system, have kindly been supplied by NASA/Goddard Space Flight Center (GSFC), MD, USA. In addition, a number of small programs and UNIX shell scripts used to prepare files and run SOLVE were supplied. Parts of these were modified and extended by the author, to the point where a hydrological model can replace some of the mascon parameters. In this thesis, where programs developed or written by anyone other than the author are used, this is explicitly stated in the text.

During this Ph.D. program, I was given the opportunity to visit the Space Geodesy Group in the Planetary Geodynamics Laboratory at NASA/GSFC, which I very much enjoyed. It amounted to three visits, and was a great experience. A special thanks to the people at NASA/GSFC, and especially Dave Rowlands, for welcoming me and always being helpful.

Furthermore, I would like to thank the people around me who have all been a part of this process, my family, colleagues and advisors.
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<th>Description</th>
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<tr>
<td>95CI</td>
<td>95% Confidence Interval</td>
</tr>
<tr>
<td>CC</td>
<td>Correlation Coefficient</td>
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<tr>
<td>CHAMP</td>
<td>CHAllenging Mini-satellite Payload</td>
</tr>
<tr>
<td>CLSM</td>
<td>Catchment Land Surface Model</td>
</tr>
<tr>
<td>CMAP</td>
<td>CPC Merged Analysis of Precipitation</td>
</tr>
<tr>
<td>CNES/GRGS</td>
<td>Centre National d’Études Spatiales/ Groupe de Recherches de Géodésie Spatiale</td>
</tr>
<tr>
<td>CPC</td>
<td>Climate Prediction Center</td>
</tr>
<tr>
<td>CSR</td>
<td>Center for Space Research (University of Texas)</td>
</tr>
<tr>
<td>DEOS</td>
<td>Delft Institute for Earth Observation and Space Systems</td>
</tr>
<tr>
<td>DLR</td>
<td>Deutsches Zentrum für Luft- und Raumfahrt</td>
</tr>
<tr>
<td>d/o</td>
<td>(spherical harmonic) degree and order</td>
</tr>
<tr>
<td>ECMWF</td>
<td>European Centre for Medium-Range Weather Forecasts</td>
</tr>
<tr>
<td>ERA-Interim</td>
<td>ECMWF Re-Analysis-Interim</td>
</tr>
<tr>
<td>ET</td>
<td>Evapotranspiration</td>
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<tr>
<td>GFZ</td>
<td>Geoforschungszentrum Potsdam</td>
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<tr>
<td>GGM</td>
<td>GRACE Gravity Model</td>
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<tr>
<td>GLDAS</td>
<td>Global Land Data Assimilation System</td>
</tr>
<tr>
<td>GPS</td>
<td>Global Positioning System</td>
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<tr>
<td>GRACE</td>
<td>Gravity Recovery And Climate Experiment</td>
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<tr>
<td>GSFC</td>
<td>Goddard Space Flight Center</td>
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<tr>
<td>ITG</td>
<td>Institute of Theoretical Geodesy (University of Bonn)</td>
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<tr>
<td>JPL</td>
<td>Jet Propulsion Laboratory</td>
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<tr>
<td>KBRR</td>
<td>K-Band Range-Rate</td>
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<tr>
<td>LAGEOS</td>
<td>LAser GEOdynamics Satellite</td>
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<td>LB</td>
<td>Lower Bound</td>
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<tr>
<td>LEO</td>
<td>Low Earth Orbit</td>
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<td>LH-SST</td>
<td>Low-high SST</td>
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<td>LL-SST</td>
<td>Low-low SST</td>
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<td>LSM</td>
<td>Land Surface Model</td>
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<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration</td>
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<tr>
<td>NCDC</td>
<td>National Climatic Data Center</td>
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<tr>
<td>ORCHIDEE</td>
<td>Organising Carbon and Hydrology in Dynamic Ecosystems</td>
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<td>PET</td>
<td>Potential Evapotranspiration</td>
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<tr>
<td>PO.DAAC</td>
<td>Physical Oceanography Distributed Active Archive Center</td>
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<tr>
<td>RDC</td>
<td>(GRACE) Raw Data Center</td>
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<tr>
<td>SDS</td>
<td>(GRACE) Science Data System</td>
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<tr>
<td>SH</td>
<td>Spherical Harmonic</td>
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<td>SRTM</td>
<td>Shuttle Radar Topography Mission</td>
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<td>SST</td>
<td>Satellite-to-satellite tracking</td>
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<td>SWAT</td>
<td>Soil and Water Assessment Tool</td>
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<td>TRIP</td>
<td>Total Runoff Integrating Pathways</td>
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<tr>
<td>TRMM</td>
<td>Tropical Rainfall Measuring Mission</td>
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<tr>
<td>TWS</td>
<td>Terrestrial Water Storage</td>
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<tr>
<td>UB</td>
<td>Upper Bound</td>
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<tr>
<td>USAID</td>
<td>United States Agency for International Development</td>
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<td>UTCSR</td>
<td>Center for Space Research, University of Texas</td>
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<tr>
<td>WaterGAP</td>
<td>Water - Global Assessment and Prognosis</td>
</tr>
<tr>
<td>WBM</td>
<td>Water Balance Model</td>
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<tr>
<td>WGHM</td>
<td>WaterGAP Global Hydrological Model</td>
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Part I

Introduction
Chapter 1

Thesis background

This chapter will serve as an introduction to the work that has been done on calibration of large scale hydrological models with remote sensing data, as a part of this Ph.D. study. Firstly, the motivation and objectives will be outlined, then the scientific methods are presented shortly, and finally contents of the individual chapters will be outlined.

1.1 Motivation

Hydrological models are key scientific decision support tools in water resources management. Reliability of hydrological models is achieved and documented through calibration, i.e. the comparison of model results with field data. Traditionally, hydrological models have been calibrated with water level and discharge data. This data however, reflects hydrological conditions at the local scale, whereas in typical water resources management applications, much larger systems are considered. Moreover, the number of in-situ monitoring stations for many river basins has been decreasing during the past few decades, resulting in poor availability of reliable point observations of water level and discharge. Accurate hydrological models are also vital parts of modern climate prediction models. Seen in the light of the increasing frequency of extreme weather situations around the globe in recent years, the use of hydrological models is becoming still more important.

There is therefore an urgent need to improve the calibration of hydrological models through the use of innovative, large scale datasets. Satellite based remote sensing products provide a nearly global coverage, independently of country borders or local political situations. The Gravity Recovery and Climate Experiment (GRACE) provides space-borne gravity measurements with unprecedented accuracy and global coverage. Temporal variations of the Earth’s gravity field reflect, among other effects, temporal changes in terrestrial water storage (TWS) in the Earth system. Instrument accuracy has in the past been insufficient to measure the small changes in the gravitational acceleration, caused by changes in water storage, but with GRACE this obstacle has been overcome.
1.2 Objectives

The objectives of this thesis are threefold. First, a system of mascon blocks must be set up, covering Southern Africa and surrounding areas. A mascon only solution must be made, and different constraint approaches (regional vs. isotropic) must be tested. Secondly, a water balance model of the Okavango River should be build; and thirdly, the model must be coupled with the mascon inversion method, thus allowing to solve for model parameters instead of mascon parameters.

1.3 Scientific method

Processed GRACE gravity products are available from multiple processing centers as sets of spherical harmonic coefficients, with a spatial and temporal resolution of 400 km and 30 days, respectively. These fields are global in nature, and post-processing smoothing and averaging cause attenuation of the mass variation signal.

For this project, however, we apply the mass concentration (mascon) method, used at the National Aeronautics and Space Administration/Goddard Space Flight Center (NASA/GSFC), Maryland, USA. This method estimates mascon parameters, which are essentially cm of equivalent water storage, from precomputed differential range-rates based on the level-1B data from GRACE. The inversion is performed in a least squares sense, using a normal matrix operation program called SOLVE (Ullman, 1992a,b). The method can be applied on regional scales, and the nature of the method allows for conversion of some (or all) of the mascon parameters to hydrological parameters of any regional hydrological model, hereby solving for the hydrological parameters instead of the mascon parameters.

SOLVE is a part of GEODYN, which is an orbit-determination and geodetic parameter-estimation program developed by the Geodynamics Group at the Stinger Ghaffarian Technologies (SGT, Inc) for the Space Geodesy Laboratory at NASA/GSFC (http://terra.sgt-inc.com/geodyn/; http://terra.sgt-inc.com/solve/doc/).

A hydro-geophysical inversion approach is developed, consisting of fitting hydrological parameters of a regional river basin model, as well as mascon parameters of the surrounding areas. The outcome is a calibrated hydrological model as well as estimates of terrestrial water storage in the modeled area (from the model output tuned by the GRACE data) and surrounding areas (from the mascon parameters).

1.4 Thesis contents

The thesis is divided into three parts, where part I is the introduction. In part II the scientific methods will be outlined, and data sets presented; and in part III results will be presented, analyzed, and discussed, and conclusions will be listed.
1.4.1 Part I: Introduction

This chapter has outlined the motivation (1.1), objectives (1.2), and introduced the scientific methods (1.3) used in this Ph.D. project. In the remainder of part I, chapter 2 will introduce the basic concepts of gravity and gravity field representations (2.1), mass concentration parameters or mascons (2.2), and outline how gravity can be used for large scale hydrological applications (2.3). Furthermore, a review of previous works where GRACE data has been used in a new and innovative way will be given (2.4), and the study area (2.5), as well as the model (2.6) will be introduced.

The Gravity Recovery And Climate Experiment mission is described in chapter 3. Initially the mission objectives and follow-on plans are outlined (3.1), the method of satellite-to-satellite tracking is introduced (3.2), and the most important scientific instruments of the satellites are presented (3.3). The GRACE data levels (3.4) as well as static (3.5) and dynamic (3.6) gravity solutions from the GRACE mission are presented. Finally, problems with the GRACE data in relation to the mascon method are addressed (3.7).

1.4.2 Part II: Scientific Methods

Chapter 4 focuses on the Budyko-type water balance model that was built to represent the Okavango River basin. The original framework developed by Budyko (1958, 1975) and further expanded by Fu (1981), Koster and Suarez (1999) and Zhang et al. (2008) will be presented (4.1). The setup used in the model applied in this thesis is described (4.2), as well as the eight calibration parameters (4.3) and the spatial setup of the river basin model (4.4). Finally, the input data, which consist of precipitation and potential evapotranspiration computed from daily maximum and minimum temperatures, is described (4.5).

Chapter 5 outlines the method of sequential calibration of the Budyko-type water balance model. The calibration data (5.1) consist of discharge and terrestrial water storage. A joint objective function is used (5.2), balancing the influence of the two types of data by use of a weighting factor. The process of calibration (5.3) and the analysis of the calibration results (5.4) is outlined. Finally, the one-at-a-time sensitivity analysis method is outlined (5.5).

The theory of the mass concentration method is outlined in chapters 6 to 8, where chapter 6 is an introduction, chapter 7 is the description of the mascon method as it is used at the GSFC, and chapter 8 outlines the coupling of the mascon method with the hydrological model.

In chapter 6, the gravity potential at satellite altitude (6.1), the differential Stokes coefficients (6.2), and the mascon parameters are explained (6.3). The forward gravity model used for the forward computation of range-rates is described (6.4), the state vector parameters, which are parameters used to describe the position and velocity of a spacecraft, are explained (6.5), and the computation of partial derivatives though variational equations is outlined (6.6). Finally, issues regarding leakage of signal in mascon solutions are discussed (6.7) and the setup of mascon blocks used
over Southern Africa is presented (6.8).

Chapter 7 explains the setup of the normal equation system used in the least squares inversion (7.1). Next, spatial and temporal constraints (7.2), as well as the weighting of constraint equations relative to data equations, are outlined (7.3). Regional constraints, where an area is divided into separately constrained regions (7.4), and issues about limited temporal constraints on marginal periods of the time series are addressed (7.5). Lastly, the method of estimating the solution fit to the GRACE K-Band Range-Rate data is outlined (7.6).

In chapter 8, the expansion of the normal equation system needed for coupling is outlined (8.2), and the integration of the hydrological model is explained (8.1). Bias parameters are introduced to account for the difference in level between GRACE and the hydrological model (8.3), and the update of the a priori mascon parameter values, that are caused by the coupling with the hydrological model, is outlined (8.4).

1.4.3 Part III: Results, Analysis & Conclusions

Chapter 9 will go through the process of the calibration (9.1), and the testing of different weighting of the two data types, storage and discharge (9.2). Finally, the results of the sensitivity analysis will be presented and discussed (9.3).

In chapter 10, the inversion approach for the 5-year equivalent water storage product, from GRACE mascon only solutions, is outlined (10.1). A comparison with TWS from GLDAS/Noah and monthly UTCSR solutions for the same period is performed, with respect to time variable storage in the Okavango River Basin (10.2) and seasonal variations over Southern Africa in general (10.3).

Chapter 11 outlines testing of the coupled method (11.2), and the resulting mass variations are compared to GLDAS/Noah and UTCSR TWS for Southern Africa (11.3) and for the model area (11.4). Additionally, the change in storage caused by the parameter perturbation used to compute the partial derivatives in the coupling method, is described (11.1), and the model performance evaluated with respect to discharge and storage, for a period not used for calibration (11.5).

Chapter 12 provides a summary of the work published in Krogh et al. (2010), which is also a part of the Ph.D. project.

Final summing up, discussions and conclusions are given in chapter 13.
Combining gravity and hydrology

This chapter will introduce the reader to the concepts of gravity and its relation to hydrology. Furthermore, the Okavango River, which is the chosen study area, will be presented.

2.1 Gravity and gravity field representations

Newton’s law of gravitation states, that every particle attracts every other particle by a force $\vec{F}$ pointing along the line intersecting both points. The magnitude of the force is proportional to the product of the two masses ($m_1$ and $m_2$) and inversely proportional to the square of the distance between the particles ($r$) (Young and Freedman, 2000, eq. 12-1):

$$ F = \frac{G \cdot m_1 \cdot m_2}{r^2} \quad (2.1) $$

where $G = 6.67428 \cdot 10^{-11}$ m$^3$kg$^{-1}$s$^{-2}$ is the universal gravitational constant. Hence, for any two particles, a change in either mass ($m_1$ or $m_2$) or in distance ($r$), will result in a change in the magnitude of the gravitational attraction $F$. Applying this to an Earth-satellite system, a redistribution of the masses on or near the surface of the Earth $m_1$, will result in a change in the gravitational field affecting the satellite $m_2$. Over short periods of time, the most significant re-distribution of mass on the Earth’s surface is due to water storage changes (e.g. Tapley et al., 2004b; Wahr et al., 2004). No other substance moves as rapidly, except for the sudden shifting of land masses during earthquakes (e.g. Pollitz, 2006; Han et al., 2006, 2008). Whether studying hydrology, climatology, or oceanography, analyzing temporal variations in the gravity field is a powerful tool to estimate mass movements.

Global gravity fields are often expressed as spherical harmonic functions, consisting of a sine ($S$) and a cosine ($C$) coefficient, to describe the deviation from a perfect sphere. The geopotential $V$, defined as the potential exterior to the Earth including all solid and fluid components, can be expressed as an infinite series of spherical harmonics (Seeber, 2003, eq. 3.109):

$$ V(r, \theta, \lambda) = \frac{GM_E}{r} \left[ 1 + \sum_{l=1}^{\infty} \sum_{m=1}^{l} \left( \frac{R}{r} \right)^n (C_{lm} \cos m\lambda + S_{lm} \sin m\lambda) P_{lm} \cos \theta \right] \quad (2.2) $$
where $r$, $\theta$, and $\lambda$ are the spherical geocentric radius, latitude and longitude coordinates of the point where the geopotential is evaluated. $M_E$ is the Earth’s mass, $R$ is the Earth’s mean equatorial radius, $l$ and $m$ are the spherical harmonic degree and order (d/o), respectively, $P_{lm}$ are the associated Legendre functions, and $C_{lm}$ and $S_{lm}$ are the Stokes coefficients, also called spherical harmonic coefficients. The first term of the series ($GM_E / r$) describes the potential of a homogeneous sphere, while the following terms all represent what is called the disturbing potential, or the deviation from a perfect sphere (Seeber, 2003). In practice, equation (2.2) is truncated at a maximum degree $l_{max}$, and the shortest resolvable wavelength $\lambda$ at the Earth’s surface is then given by (Seeber, 2003, eq. 10.1):

$$\lambda = \frac{360}{l_{max}} \begin{array}{c} \text{[}\degree\text{]} \end{array} . \quad (2.3)$$

It is clear that with increasing $l_{max}$, an increasingly detailed representation of the gravity field can be achieved.

### 2.2 Mass concentrations

Mass concentration parameters (mascons) are another way of representing the gravity field. Mascons have been used since the late 1960’ies for lunar and other planetary mass recoveries from satellite tracking data. According to Lemoine et al. (2007a), the term mascon was first used by Muller and Sjogren (1968) for describing mass concentrations on the moon, detected by Lunar Orbiters. The mascon method is very applicable for recovering variations in the Earth’s gravity field at a temporal resolution as low as 10 days, which makes the method ideal for applications on GRACE data. In addition, the extend of a GRACE mascon solution does not have to be global, because the residual created in the GRACE data by a small mass anomaly, is centered on top of the anomaly. For all mascon solutions, spatial and temporal constraints are applied for stability reasons, since the amount of data recorded in 10 (or even 30) days is not enough to recover a gravity field without problems (e.g. Lemoine et al., 2007a, pers.com. D. Rowlands).

Mascon-derived mass variations, or any mass variation product, present a new calibration opportunity for the terrestrial water storage component of hydrological models, and can thus help close the water budget.

### 2.3 Gravity for large scale hydrological applications

Since the Gravity Recovery and Climate Experiment (GRACE) satellites were launched in March 2002, a unique dataset of the Earth’s static and dynamic gravity field has become available. For hydrological applications, the variations in the gravity field caused by terrestrial water storage are of great interest, and can be recovered by

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1 Five Lunar Orbiter missions were launched during 1966 and 1967, with the purpose of mapping the Moon’s surface (http://nssdc.gsfc.nasa.gov/planetary/lunar/lunarorb.html).
removal of tidal effects, and atmospheric and oceanic mass transports. Residual signals after removal of the background gravity models are dominated by hydrology, present day ice mass changes, and glacial isostatic adjustments in some areas.

Regional to large scale hydrological models have traditionally been calibrated with point observations of discharge and water level or head observations, which can be scarce and often of poor quality. Temporal mass variations recovered from GRACE, with accuracies corresponding to a few millimeters of water in regions the size of 400 km, present new opportunities for calibrating large scale hydrological models.

Large scale hydrological models (global to continental) are by Güntner (2008) divided into two types, land surface models (LSM) and water balance models (WBM). LSMs are typically based on energy and water fluxes and fully coupled heat and mass balance equations; and they are meant to represent the land surface in climate models. The water balance is usually not considered, and groundwater and surface water bodies are typically not modeled.

WBMs on the other hand, balance the input (precipitation \( P \)) and output (evapotranspiration \( ET \) and runoff \( R \)) of the model area with the change in storage \( \Delta S \):

\[
\Delta S = P - ET - R .
\] (2.4)

WBMs usually consider the entire water cycle, including soil water, groundwater and surface water, and are mainly developed to simulate stream flow at the catchment outlet.

Güntner (2008) points out that one major problem for all large scale hydrological models, is that they suffer from considerable uncertainties in model structure, process description, and forcing data, which leads to significant differences between model outputs. Typical calibration data used is discharge, since this has traditionally been the only available observable, before variations in total terrestrial water storage from GRACE became available. Calibration of LSMs with in-situ data is difficult since discharge is usually not simulated, and therefore many LSMs are not calibrated at all (Güntner, 2008).

From this perspective, the GRACE mission provides a unique data set to be used for large scale model improvement, as the estimated variations in terrestrial water storage can be used as a calibration dataset on global scales.

### 2.4 Review of previous works

The coupling of large scale hydrological models with remote sensing gravity data is still a relatively new discipline, and little research on model calibration with gravitational data has been published so far. More common is the comparison of model performance to available GRACE mass redistribution estimates, with or without tuning of the model. In this short review of published research on this area, I have chosen
to focus on studies that use GRACE data products in an innovative way, meaning anything other than merely comparing to a readily available GRACE gravity product. This includes data assimilation (Zaitchik et al., 2008; Kurtenbach et al., 2009), model calibration (Ngo-Duc et al., 2007; Werth et al., 2009), comparison and model tuning with range-rate observations instead of the available gravity products (Han et al., 2009), and application of regional mascon constraints (Boy et al., 2011).

Ngo-Duc et al. (2007) developed a water transfer scheme within the Organising Carbon and Hydrology in Dynamic Ecosystems (ORCHIDEE) LSM, which significantly improved the performance of the model compared to a GRACE land water product computed by Ramillien et al. (2005). The scheme includes the storage of water after it leaves the soil column, and before it reaches the ocean - essentially the amount of water stored in rivers and streams, and in short or longer time subsurface reservoirs. The GRACE land water solution used, is a spherical harmonic solution, based on a generalized least squares inversion of iterative nature. Big improvements were found over tropical basins, where the water stored in aquifers is estimated to account for about half of the seasonal variations, while high latitude areas had a smaller correlation between GRACE land water and model output than the tropical areas. It is concluded that this could be caused by simplification of snow parametrization or atmospheric forcing uncertainty.

Zaitchik et al. (2008) used an average of spherical harmonic solutions from the Geo-forschungszentrum (GFZ), the Jet Propulsion Laboratory (JPL), and Center for Space Research (CSR) for the period January 2003 to May 2006, for data assimilation of the Catchment Land Surface Model (CLSM) on the Mississippi river at sub-river basin scale. The CLSM is based on the topographic statistics of catchments, and forced with meteorological weather observations from the GLDAS forcing database of Rodell et al. (2004). For the assimilation, an iterative Ensemble Kalman Smoother (EnKS) scheme was used, with a fixed smoother window of one month (equal to the temporal resolution of the SH solution from GRACE). Comparisons are made with an open-loop simulation without data assimilation. The TWS simulations for the assimilation, are by design in-between the open-loop simulation and the TWS derived from GRACE data. Results showed significantly improved estimates of the amplitude and phase of the seasonal cycle of simulated groundwater compared to the open-loop simulation, when validated against groundwater measurements. Furthermore, the assimilation improved the phase of the annual cycle in estimated runoff, with no significant difference in mean annual runoff; again compared to the open-loop simulation. Finally, compared to the open-loop simulation, simulated TWS variability at watersheds of sub-observational scales, produced greater correlation coefficients to gaged river flow in seven of eight watersheds; with significantly higher correlation coefficients in five of eight watersheds.

Werth et al. (2009) used TWS changes together with discharge data, to calibrate the WaterGAP Global Hydrological Model (WGHM), for the time period 2003-2006. TWS changes were obtained from monthly GRACE time series of spherical harmonic global gravity fields expanded to degree and order 120 from the GFZ (GRACE Level-2 products, version GFZ-RL04). The focus was on the rivers Amazon, Mississippi and Congo, and they found that the multi-objective calibration improved the simulation results for all three river basins, compared to the WGHM standard version, in
the sense that the root mean squared errors were reduced by 40% to 80% with respect to discharge and 4% to 50% with respect to TWS changes. Largest improvement was achieved for the Amazon Basin and the smallest improvement for the Congo. They concluded that more accurate input data and a better calibration setting should be applied in order to improve the model further.

Han et al. (2009) used range-rate residuals from GRACE level-1B data, to estimate flow velocities in a combination of soil moisture from the Global Land Data Assimilation System/Noah (GLDAS/Noah) LSM, and river routing scheme from a Total Runoff Integrating Pathways (TRIP) model, over the Amazon Basin. They showed that the soil moisture water storage from GLDAS/Noah accounts for only 50% of the perturbation in inter-satellite range-rate observed from overflight of the Amazon Basin. The remaining perturbation could be simulated by application of the TRIP model on the GLDAS/Noah total runoff, with an overall effective flow velocity of 30 cm/s. Seasonal variations in the optimal flow velocity indicate, that lower flow velocities (as low as 10 cm/s) simulate the perturbations well in the peak water season (March-May), while higher velocities (up to 50 cm/s) are required for the rest of the year.

Kurtenbach et al. (2009) assimilated daily range-rate (level-1B) data with the WaterGAP Global Hydrological Model (WGHM), to produce daily snapshots of the gravity field to d/o 40. The method is based on modeled temporal variations, introduced in the level-1B data processing using a Kalman filter approach, to account for the reduced number of observations in one-day solutions compared to multiple-day solutions. An empirical auto-covariance function derived from the model is used in the estimation process, which causes the results to be unbiased towards the applied model, as only the stochastic correlation pattern is used. Improvements are seen in low signal areas like oceans and deserts, compared to weekly (d/o 30) and monthly (d/o 120) GFZ-RL04 solutions. The overall agreement between daily, weekly and monthly time series is good, and the daily solutions appear less noisy than the weekly solutions.

Most recently, Boy et al. (2011) applied regional rather than global constraints (regional constraints will be explained in section 7.4) on high resolution (2° equal angle grid, every 10 days) mascons on the African continent, yielding higher spatial resolution than previous solutions. Two solutions are compared to the global solution of Sabaka et al. (2010), one with forward modeled hydrology from GLDAS/Noah, and one with no forward modeled hydrology. Validation is done by comparison with estimates of mass variations of 19 major lakes and reservoirs, derived from radar altimetry. They show that the forward modeled hydrology in general produces a better fit to the lake data, and that forcing with Tropical Rainfall Measuring Mission (TRMM) precipitation produces a better fit than CPC Merged Analysis of Precipitation (CMAP) forcing.

Cazenave and Chen (2010) provide an overview of the use of GRACE data in various geophysical fields, such as hydrology, ice sheet mass balances, oceanography and solid Earth studies like earthquakes and post glacial rebound. Günther (2008) focuses on the application of GRACE data to hydrological models in his review of the uses of GRACE data.
Chapter 2. Combining gravity and hydrology

2.5 Study area: The Okavango River

The target area for this study is the Okavango River system in Southern Africa (see figure 2.1). This area has very little in-situ data in the form of discharge, head, and weather observations, and is in this way ideal for the application of remote sensing gravity to hydrological model calibration.

The Okavango River originates in the southern highlands of Angola in south-western Africa. It essentially consists of two main tributaries, the Cubango to the west and the Cuito to the east, which join waters at the Angolan-Namibian boarder, and flows towards the south-east where the water is released into a huge wetland, called the Okavango Delta, in northern Botswana. The term delta however, is somewhat misleading since the wetland is closer to a combination of an alluvial fan and a braided river system, with river channels and small islands on top of a large sediment deposit (Milzow, 2008). The upstream part of the river system has a subtropical, humid climate with annual precipitation rates as high as 1300 mm/year, while the south-eastern part of the Okavango Delta, situated on the rim of the Kalahari Desert, has a semi-arid climate with only 450 mm of rain a year (see figure 2.2 and 2.3). The basin
is endorheic\(^2\), and when the water reaches the Okavango Delta, small parts are infiltrated while the majority of the water evaporates. During very wet years, the water may reach lake Ngami south of the Okavango Delta, and sometimes even travel as far as to the Makgardikgardi Salt Pans further towards the south-east.

Where the river enters Botswana, and before it spreads out in the Okavango Delta, a discharge station called Mohembo is placed. The annual variations in discharge at this place, are out of phase with the precipitation (figure 2.2), the peak is in April while the low flow period is in October and November. The area of the catchment upstream of Mohembo is approximately 170,000 km\(^2\), and this area is the only runoff generating area of the river basin (Milzow et al., 2011). The two rivers, Cuito and Cubango, originate from geologically different areas. The eastern part of the upstream catchment is dominated by thick deposits of Kalahari sands with hight hydraulic conductivity, whereas the sediments in the western part are primarily volcanic and metamorphic rocks with low hydraulic conductivity overlain only by a thin layer of sand. The variability in discharge from the two rivers, is very much affected by the difference in geology, resulting in greater variability from the Cubango (western river) due to high runoff compared to the Cuito (eastern river) where base flow is dominant (Hughes et al., 2006; Milzow et al., 2009).

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\(^2\)endorheic basin: a closed drainage basin that retains water and allows no outflow to other bodies of water such as rivers or oceans.
Figure 2.3: Mean annual precipitation in Africa for the period September 2003 to August 2008 in millimeters (mm). The model area is outlined in green, while the Okavango River network is shown in blue. Precipitation data was downloaded from http://data-portal.ecmwf.int/data/d/interim_daily in a 1.5°-grid every 12 hours.

2.6 Regional model of the Okavango River Basin

The model used in this study is a Budyko type model, following the framework of Zhang et al. (2008). It is a simple water balance model, consisting of a soil storage reservoir and a groundwater reservoir. The only two input data sets required are precipitation and potential evapotranspiration. For the purpose of simulating mass distributions within the river basin, a series of Budyko-type models each assigned to a sub-catchment area are used, making the river basin model semi-distributed. The sub-catchment mask used is the same as the one used by Milzow et al. (2011). It is derived from a digital elevation model based on Shuttle Radar Topography Mission (SRTM) data, and will be presented in chapter 4 (figure 4.7).

A one-at-a-time sensitivity analysis was performed for the model, evaluating the output of terrestrial water storage in areas corresponding to the mascon blocks used in the coupling approach.
Chapter 3

The Gravity Recovery and Climate Experiment (GRACE)

A short introduction to the Gravity Recovery And Climate Experiment (GRACE) mission and data is given in this chapter.

3.1 Mission objectives and follow-on

The twin GRACE satellites were launched in March 2002 as a joint US/NASA-German/DLR (Deutsches Zentrum für Luft- und Raumfahrt) project. The design lifetime was 5 years, and the mission objectives were to accurately map the global gravity field every 30 days, at a spatial resolution of 400 km (Tapley et al., 2004a). Furthermore, a minimum science requirement was to deliver a new model of the Earth’s static geoid with an error of less than 1 cm at a spatial resolution of 300 km, within the first year (Davis et al., 1999).

Well beyond the first 5 years of operation, the GRACE mission has recently been extended to the year 2012. The outstanding performance that GRACE has shown to monitor mass movements on and near the Earth’s surface, has led the US National Research Council Decadal Survey to recommend a GRACE-Follow-On mission for launch around 2017–2020 (Cazenave and Chen, 2010). Meanwhile, a GRACE-Gap-Filler mission is considered for launch around 2014–2015 (Cazenave and Chen, 2010; Tapley et al., 2010).

3.2 Satellite-to-satellite tracking

The Earth’s gravity field has for a long time been studied through satellite orbit perturbations, observed with GPS satellites and ground-to-satellite lasers. When one satellite in a low Earth orbit (LEO), is being tracked by satellites in higher orbits (like the GPS satellites), the mission is called a high-low satellite-to-satellite tracking mission (HL-SST). GRACE however, is a so-called low-low satellite-to-satellite tracking (LL-SST) mission, where two identical LEO satellites co-orbit, with an inter-satellite distance of a few hundred kilometers. LL-SST is a relatively new development in the
Chapter 3. The Gravity Recovery and Climate Experiment (GRACE)

Figure 3.1: Different satellite-to-satellite tracking missions. A) High-low satellite-to-satellite tracking in the CHAMP\(^1\) mission. B) Low-low satellite-to-satellite tracking in the GRACE mission.

\(^1\) CHAllenging Mini-satellite Payload. Launched in July 2000, and reentered the Earth’s atmosphere in September 2010. Developed to generate simultaneously highly precise gravity and magnetic field measurements over a 5-year period (http://science.nasa.gov/missions/champ/).

estimation of gravity fields, and GRACE is in fact the first mission of its kind. For gravity recovery, SH methods usually include GPS data, making the gravity solution a combined LL and HL product. For the mascon method, GPS data is not used.

In general, SST methods rely on the relationship between the parameters of the terrestrial gravity field (typically \(C_{lm}\) and \(S_{lm}\) coefficients of equation 2.2) and the observables from the satellite tracking (Seeber, 2003), which in the case of the GRACE mission is the relative velocity of the two satellites.

Because the GRACE satellites travel in the exact same orbit, only displaced by a few hundred kilometers, relatively local anomalies can be observed compared to SST missions where only one LEO satellite is used. When the GRACE satellites pass over a mass anomaly on or near the surface of the Earth, the leading satellite senses the anomaly first as it causes a small perturbation in the orbit. Shortly after, the trailing satellite experiences the exact same perturbation caused by the same anomaly, only slightly displaced in time. Hence, the residual created by the anomaly in the GRACE K-Band Range-Rate (KBRR) data (the change in inter satellite distance) is centered exactly on top the anomaly (Lemoine et al., 2007a; Rowlands et al., 2010).

The orbital height has a great effect on the resolution of the gravity field that can be recovered from the tracking data. The lower the orbit, the better the resolution, but also the more drag on the satellites and the shorter life time. The GRACE satellites were launched at an initial hight of approximately 500 km as a compromise of reduced drag and reduced resolution of gravity anomalies.

3.3 Instrumentation

The key element of the GRACE mission is measurement of the inter-satellite distance, as variations in the distance are caused by non-uniformities in the Earth’s gravitational field. To accurately measure the distance, a K-Band Ranging System is placed on each satellite, facing towards the other satellite. It transmits a signal of known frequency and wavelength to determine the inter-satellite distance. The
transmitted signal is then reflected on the other satellite, and the difference in phase between the transmitted and the reflected signal is measured, in order to determine the distance.

Orbit perturbations are not only caused by the Earth’s gravitational pull, but also by more direct factors like atmospheric drag and thrusting events. These factors are a source of error in estimating the gravity field from measurements of the inter-satellite distance. To measure the non-gravitational accelerations of the spacecrafts, an accelerometer is placed on both satellites. Additional ancillary instruments include GPS receivers for precise time-tagging and positioning, and attitude sensors which provide high precision inertial orientation of the satellites (Tapley et al., 2004a).

3.4 GRACE data levels

The initial data processing of the GRACE science data, is being handled by the three processing centers within the GRACE Science Data System (SDS): the NASA Jet Propulsion Laboratory (JPL), the Center for Space Research at the University of Texas, Austin (UTCSR), and the Geoforschungszentrum in Potsdam, Germany (GFZ). The SDS is designed to perform all tasks for gravity field processing to the production of monthly and mean gravity fields (Bettadpur, 2007b). The data products are being categorized according to the processing level that has been applied.

3.4.1 Level-0 data

The level-0 data is the raw GRACE data product, continuously passed to the GRACE Raw Data Center (RDC) at DLR in Neustrelitz. This data is divided into a scientific instrument stream and a spacecraft housekeeping stream, and placed in a rolling archive. From here, the SDS centers transfer the data to their own permanent archives (Bettadpur, 2007b). The interesting data for gravity field estimations are the inter satellite range-rate measurements ($\mu m/s$), but also accelerometer data and attitude and positioning data are important.

3.4.2 Level-1A data products

The level-1A processing step includes time-tagging to the satellite receiver clock and time-tag ambiguity corrections are performed. Furthermore the data is reformatted, and quality and editing control flags are added. This processing step is non-destructive, and the processing can be reversed to obtain the original level-0 data if desired, except for bad data packets. Ancillary data products needed for further processing are also included in the level-1A data (Bettadpur, 2007b).

3.4.3 Level-1B data products

The level-1B data is correctly time tagged and the sample rate is reduced. As for the level-1A data, level-1B data includes ancillary data needed for further processing.
The level-1B processing is possibly irreversible (Bettadpur, 2007b). For the mascon method, which will be described in detail in chapters 6 and 7, the level-1B data is used to fit mascon parameters through a least squares inversion.

### 3.4.4 Level-2 data products

The level-2 data product includes all gravity field and related products, derived from the previous processing level products. Ancillary data is also included (Bettadpur, 2007b).

### 3.5 Static gravity models

Common for a lot of static gravity field models, is that two versions are made; one where only satellite data is used (from GRACE and sometimes in combination with other missions, like LAGEOS\(^1\) and CHAMP), indicated by an S in the end of the name; and one where terrestrial information is used to constrain the model, indicated by a C in the end of the name.

Among the first gravity models (based on GRACE data) released was the GRACE Gravity Model v.01 (GGM01) from CSR, which was computed using data from 111 selected days between April and November 2002, and has an estimated accuracy of 2 cm up to d/o 70 (300 km), and 6 cm to d/o 90 (CSR, 2010b). A later CSR model (GGM02) was computed from 363 days of data from April 2002 through December 2003. The estimated RMS of geoid errors are \(\sim 0.7\) cm to d/o 70, with a maximum RMS error of \(\sim 0.9\) cm (CSR, 2010a). A GGM03 model also exists, computed from four years of data from January 2003 to December 2006. The constrained version (GGM03C) is complete to d/o 360 and is improved by a factor of 2 compared to GGM02 (Tapley et al., 2007).

GFZ also released a model about a year after launch (EIGEN-GRACE01S) based on only 39 days of data from August and November of 2002, complete to d/o 120 (some coefficients to 140) (GFZ, 2010). A later update (EIGEN-GL04C) was based on GRACE, LAGEOS and surface gravimetry and altimetry observations, complete to d/o 360. This version is used for the monthly level-2 product from GFZ (see table 3.2). The latest model from GFZ (EIGEN-5C) however, uses a total of 54 months of data from GRACE, combined with 14 years of LAGEOS data, and surface gravity observations, complete to d/o 360.

CNES/GRGS recently released a new mean field model, which was computed from 4.5 years of GRACE and LAGEOS data (EIGEN-GRGS.RL02.MEAN-FIELD). It is complete to d/o 160, and contains drift, annual and semi-annual terms and an offset for the 2004 Sumatra earthquake.

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\(^1\)LASer GEOdynamics Satellite. LAGEOS-1 launched in 1976, LAGEOS-2 in 1992, both in a height of app. 5900 km, and both still operational. (http://ilrs.gsfc.nasa.gov/satellite_missions/list_of_satellites/lag1_general.html)
Gravity field model | Group | \( l_{\text{max}} \)
--- | --- | ---
EIGEN-5C | GFZ | 360
http://op.gfz-potsdam.de/grace/results/

EIGEN-GL04C | GFZ | 360
Fürste et al. (2008); http://op.gfz-potsdam.de/grace/results/

GGM02S / GGM02C | CSR | 160/200
Tapley et al. (2005); http://www.csr.utexas.edu/grace/gravity/

GGM03S / GGM03C | CSR | -/360
Tapley et al. (2007); ftp://podaac.jpl.nasa.gov/pub/grace/doc/ReleaseNotes_csr_RL04.txt

EIGEN-GRGS.RL02.MEAN-FIELD | CNES/GRGS | 160
Includes time variable terms up to d/o 50.
Bruinsma et al. (2010);
http://grgs.obs-mip.fr/index.php/fre/Donnees-scientifiques/Champ-de-gravite/grace/static

ITG-Grace2010s | ITG | 180
http://www.igg.uni-bonn.de/apmg/index.php?id=itg-grace2010;
ftp://skylab.itg.uni-bonn.de/ITG-Grace2010/static/

Table 3.1: Recent static gravity models, derived from GRACE in combination with other satellite data and ground gravity observations. \( l_{\text{max}} \) is the maximum degree \( l \) to which the model is given.

Finally the Institute of Theoretical Geodesy (ITG) at the University of Bonn recently released a static field model (ITG-GRACE2010s), based on 7 years of GRACE-only data and complete to d/o 180.

It should be noted that a great number of different static gravity solutions derived from the GRACE data have been released, each better than the previous; and the ones mentioned here are only an extract.

In the mass concentration method, a background gravity model is needed to simulate differential range-rate observations with respect to the mass concentration parameters. At the NASA/GSFC the GGM02C gravity model is used as background field.

### 3.6 Dynamic gravity solutions

Dynamic gravity solutions all fall under the category of level-2 data products, defined in section 3.4. All processing centers in SDS provide monthly spherical harmonic (SH) solutions and the data products can be downloaded from the NASA Physical Oceanography Distributed Active Archive Center (PO.DAAC) website (see table 3.2) (Cazenave and Chen, 2010). Besides the internal SDS-groups, other research groups provide 10-day to monthly gravity solutions. Groups providing SH solutions include the Centre National d’Études Spatiales/Group de Recherche Geodesie Spatiale (CNES/GRGS), the Institute of Theoretical Geodesy at the University of Bonn (ITG), and the Delft Institute for Earth Observation and Space Systems (DEOS).
Table 3.2: Available GRACE gravity products from SDS centers, and external research groups. \( l_{\text{max}} \) is the maximum degree \( l \) to which the model is given.

1. The mean field GIF22a is a combination product of the 22-month time-series of UTCSR Release-02 products. Mean field to degree 120 was adjusted from GRACE data, while GGM02C (Tapley et al., 2005) coefficients are used from degree 121 to 200, and EGM96 (Lemoine et al., 1998) from degree 201 to 360 (Bettadpur, 2007c).

2. A 2° equal area grid.

From the NASA Goddard Space Flight Center (NASA/GSFC) a 4°×4° equal angle gridded mascon solution is available (e.g. Lemoine et al., 2007a), and recently a new mascon product with an improved spatial resolution of 2°×2° at the equator (equal area\(^2\)) has been developed (see e.g. Luthcke et al., 2008; Sabaka et al., 2010). Details and references for the solutions are presented in table 3.2.

For the work presented in Krogh et al. (2010), the CNES/GRGS SH solution and

\(^2\)The area of the blocks in the 2°×2° solution, is kept constant so that closer to the poles, the blocks span more than 2° in longitude.
the NASA/GSFC $4^\circ \times 4^\circ$ mascon solution, were compared to the recovered regional mascon solution, because of the same 10-day temporal resolution.

### 3.7 Data problems in relations to the mascon method

The twin GRACE satellites make one observation every 5 seconds, amounting to approximately 17000 observations a day on a global scale. The target region for this study, Southern Africa and coastal ocean areas, is about 7% of that, which yields around 1200 daily observations. In reality the number is between 700 and 1200 a day, depending on the satellites’ ground track relative to the study area. For successful processing of a day’s worth of data a number of data files are needed, including range-rates, accelerometer data, attitude data, and GPS data. If any of these files are missing or corrupted, the day is skipped, which can result in some 10-day epochs being represented by only a few days of observations. Naturally, the less data used for estimation of 10-day mascon parameters, the less well determined the mascon parameters will be. This is reflected in the standard deviation returned by SOLVE from the inversion of the normal equation system.

The repeat time of the ground track (the time it takes before the satellites repeat the same ground track) for any satellite depends on the orbital height. For gravity field studies, a long repeat time is generally preferred to avoid large gaps between tracks, but at certain heights the repeat time can be very short (a few days). Figure 3.2A shows the repeat time as a function of orbital height for the GRACE satellites, while figure 3.2B shows the height of satellite GRACE-A from 2004 to 2010. In figure 3.2A, the upper number is the number of revolutions completed during the repeat period, which is given on the $x$-axis. Wagner et al. (2006) predicted that GRACE would reach the critical height of 450 km as early as 2008, resulting in a repeat period of only 3 days, by assuming a 17 m/day decrease in orbital height from January 2005. As can be seen on figure 3.2A and 3.2B, GRACE has not yet (Feb. 2011) passed 450 km. The slower than expected decrease in height was due to an unusually deep solar minimum during the past 5 years, causing less drag on the satellites than what would have been expected from an average minimum.

In general, long repeat times yield the best spatial sampling, and hence the best result when it comes to gravity fields. For the GRACE mission, the sampling problem manifests itself as striping at some degrees and orders, and cannot be avoided even when repeat periods are long. In spherical harmonic solutions, Gaussian smoothing is typically used to smooth the striping, but at the same time a part of the physical signal is removed, resulting in a dampening of the signal amplitudes. For the mascon approach the sampling problem is handled by constraining the mascon parameters in time and space. Furthermore, the block approach used in the mascon method, makes the distribution of ground tracks less important as long as enough sampling points are included in each block (pers.com. D. Rowlands).
Chapter 3. The Gravity Recovery and Climate Experiment (GRACE)

Figure 3.2: A) GRACE repeat periods (x-axis) as a function of orbital height (y-axis). Numbers above dots show the number of revolutions completed during the repeat period. The approximate date is shown for the points where the GRACE satellites have already passed. Modified from Klokočník et al. (2008). Timing information from Wagner et al. (2006) (<1/1/2004) and GRACE newsletters (>1/1/2004) (ftp://podaac.jpl.nasa.gov/pub/grace/doc/newsletters/). B) Orbital height of satellite GRACE-A in km since January 2004. Circles mark when the GRACE satellites pass through one of the repeat periods shown in window A. The numbers are: no. of revolutions / repeat period (days). The height is computed as the semi-major axis of the orbit minus the mean Earth radius (6378 km), and are retrieved from the GRACE newsletters (ftp://podaac.jpl.nasa.gov/pub/grace/doc/newsletters/).
Part II

Scientific Methods
Chapter 4

Model of the Okavango River

This chapter outlines the water balance model setup based on a framework presented originally by Budyko (1958, 1975), and the modifications applied for the model of the Okavango River, used in this study. Lastly, the parameters are discussed and the input data sets presented.

4.1 Budyko framework

The method of Budyko (1958, 1975), described as the Budyko framework in Zhang et al. (2008) is based on the water balance equation (Zhang et al., 2008):

\[
\frac{dS(t)}{dt} = P(t) - ET(t) - Q(t) \tag{4.1}
\]

where \(dS(t)/dt\) is the change in storage during time step \(t\), \(P(t)\) is the precipitation or incoming water, \(ET(t)\) is the evapotranspiration, and \(Q(t)\) is the runoff. If equation (4.1) is integrated over a sufficiently long period of time (several years or decades), the water balance becomes a steady-state equation. The net change in storage over this period of time will be zero (\(\Delta S = 0\)) so that the incoming water over time, is balanced by the outgoing water:

\[
P = ET + Q. \tag{4.2}
\]

For the estimation of mean evapotranspiration (\(\overline{ET}\)) Budyko (1958, 1975) reasoned that \(\overline{ET}\) would be smaller than both the available water (mean precipitation \(\overline{P}\)) and the available energy for evaporation (\(\overline{R}/\lambda\), where \(R\) is the net radiation and \(\lambda\) the latent vaporization of water\(^1\)) (Budyko (1958, 1975) in Koster and Suarez (1999)):

\[
\overline{ET} \leq \min(\overline{P}, \frac{\overline{R}}{\lambda}). \tag{4.3}
\]

He further assumed that precipitation and energy were the two most dominant factors on the evaporation. He called \(\overline{R}/\overline{P}\lambda\) for the index of dryness denoted by \(\phi\), and developed a relation between \(\overline{ET}\) and the index of dryness \(\phi\) (Budyko (1958, 1975) in

\(^1\)\lambda\) values at different temperatures are listed in table 4.2
Figure 4.1: \( \alpha \) as a function of \( w \) as it was defined by Zhang et al. (2008) for calibration purposes. The range of \( w \) is \([1, \infty]\), whereas the range of \( \alpha \) is \([0, 1]\).

Koster and Suarez (1999):

\[
\phi = \frac{R}{P \lambda} \quad (4.4)
\]

\[
\frac{ET}{P} = \left[ \phi \left( \frac{\tanh \frac{1}{\phi}}{1 - \cosh \phi + \sinh \phi} \right) \right]^{0.5} . \quad (4.5)
\]

One obvious problem with this method, was the lack of ability to take other factors than the dryness \( \phi \) into account. Fu (1981) developed a Budyko-like method for estimating mean annual evapotranspiration \( ET \), from mean annual precipitation \( P \) and potential evapotranspiration \( E_o \), and introduced a partitioning factor \( w \) (Zhang et al., 2008):

\[
\frac{ET}{P} = 1 + \frac{E_o}{P} - \left[ 1 + \left( \frac{E_o}{P} \right) \right]^{1/w} , \quad (4.6)
\]

where \( w \) has the range \([1, \infty]\). Fu’s equation (4.6) makes it possible to define different relationships between \( ET/P \) and \( E_o/P \) for different regions, by adjusting \( w \). Fu (1981) uses \( E_o/P \) as the index of dryness instead of \( R/P \lambda \), but the two are essentially similar as the radiation \( R \) is the main driver of the potential evapotranspiration \( E_o \).

Koster and Suarez (1999) successfully applied the Budyko relationship between \( ET \) and the index of dryness \( \phi \) (equation 4.5) on inter-annual scales, under the assumption that inter-annual changes in storage are much smaller than the fluxes. For shorter time step modeling (sub-annual or shorter), the equilibrium situation is not applicable, and storage changes must be considered. Zhang et al. (2008) applied the Fu-equation (4.7) at both daily and monthly time steps, no longer under the assumption of steady state, but by including storage changes in their model. For the purpose of model calibration Zhang et al. (2008) defined \( \alpha = 1 - 1/w \), where the range of \( \alpha \) is \([0, 1]\) (see figure 4.1):

\[
\frac{ET}{P} = 1 + \frac{E_o}{P} - \left[ 1 + \left( \frac{E_o}{P} \right)^{1/(1-\alpha)} \right]^{1-\alpha} . \quad (4.7)
\]
Figure 4.2: Ratio of mean annual evapotranspiration to precipitation $ET/P$ as a function of the index of dryness $\phi = E_o/P$ for different $\alpha$ values according to Fu’s equation (equation 4.7). Also shown is the Budyko relationship of $E/P$ as a function of the index of dryness $\phi = R/P\lambda$ (gray dotted line, equation 4.7).

Temporal averages are not used in equation (4.7), since steady state is not an assumption. Figure 4.2 shows the evaporation fraction $ET/P$ as a function of the index of dryness, at different $\alpha$ values (equation 4.7), as well as Budyko’s original curve of $ET/P$ (equation 4.5, gray dotted line). High $\alpha$ values correspond to high evapotranspiration efficiency, hence the closer $\alpha$ is to 1, the closer the $ET$ will be to either the demand limit ($E_o$) or the supply limit ($P$); whereas a low $\alpha$ will yield a low $ET$.

Zhang et al. (2008) also presents a top-down approach, starting out with the simplest possible model, only increasing complexity if deficiencies in the model performance are found. They used the Budyko-like curve of Fu (1981) for estimation of the fraction of incoming water that is withheld by the catchment (not becoming direct runoff), the fraction of retained water, after direct runoff, that is available for evapotranspiration (the rest will go to soil storage), and the fraction of water available after direct runoff that will actually be taken up by evapotranspiration.

For this study, problems in fitting the model to both gravity and discharge data, lead to expansion of the model by implementation of two additional water loss components, phreatic ET and flow loss. Furthermore, high direct runoff rates related to a few big rainfall events, pointed out a problem in modeling the release of runoff. To solve this, the discharge is routed through a linear reservoir, which smooths the runoff. This reservoir is not a reservoir physically located in a specific location, but represents various non-resolved smoothing processes and delays in the hydrological system.

---

2 phreatic water: ground water below the water table.
### 4.2 Model setup

The original Budyko framework has two storage compartments, the soil water and the groundwater. The incoming water in the form of precipitation, is partitioned into direct runoff, which goes to the river and disappears from the model, and retained water, which stays in the soil water reservoir. From here the water can either evaporotranspire and disappear, it can go to recharge of the groundwater, or it can remain in the soil storage compartment. Once the water reaches the groundwater compartment, the only way out is as base flow to the river (see figure 4.3).

Besides these processes, it was found useful to implement two additional loss processes, phreatic ET and flow loss. The phreatic ET is meant to simulate two processes: the process of groundwater moving upwards to the unsaturated zone in the soil where it is allowed to evaporotranspire, and the plant uptake of water directly from the saturated zone. To understand the need for the flow loss, it must be noted at this time that the model of the Okavango river, was set up to consist of seven Budyko-type sub-models. This will be explained further in section 4.4. The flow loss was introduced because the runoff travels around 700 km from the most upstream sub-models before it reaches the outlet at Mohembo. During this routing, the river looses water, some directly to ET and some initially to infiltration into the bank, and later to evaporotranspiration from the river bank. For simplicity, we assume instant evaporotranspiration from the bank, and remove ET from the river and the bank in the same time step it is produced.

The model is set up as a sequence of hydrological events, or a number of computations made from the input data, that are carried out every time step. These steps are outlined below. Further details on the model framework can be found in Zhang et al. (2008).

Of the incoming water (precipitation) in a time step $P(t)$, some will be retained by the catchment, and the rest will go directly to runoff. The partitioning of $P$ is done using Fu’s equation (equation 4.7), with $P(t)$ as the supply limit, and the maximum

![Figure 4.3: Budyko model framework and output signals. Modifications from the original framework are marked in blue. $P$: precipitation, $ET$: evapotranspiration, $ET_p$: phreatic evapotranspiration, $R$: recharge, $Q_d$: direct runoff, $Q_g$: groundwater base flow, $FL$: flow loss, $Q$: discharge at catchment outlet. $FL$ is computed from the sum of $Q_d$ and $Q_g$.](image-url)
amount of water that the catchment can retain in a given time step, as the demand limit $X_o(t)$:

$$\frac{X(t)}{P(t)} = 1 + \frac{X_o(t)}{P(t)} - \left[ 1 + \left( \frac{X_o(t)}{P(t)} \right)^{1/(1-\alpha_1)} \right]^{1-\alpha_1}. \quad (4.8)$$

$\alpha_1$ is the partitioning factor for the precipitation into retention and direct runoff, and the demand limit $X_o(t)$ is computed as the sum of unfilled space for storage in the soil $S_{max} - S(t-1)$, and the potential evapotranspiration $E_o$:

$$X_o(t) = (S_{max} - S(t-1)) + E_o(t). \quad (4.9)$$

Whatever water is not being retained, becomes direct runoff $Q_d(t)$ and hence contributes to the total runoff in the same time step it is being produced:

$$Q_d(t) = P(t) - X(t). \quad (4.10)$$

After initial runoff, the available water in the catchment is the sum of the retained water $X(t)$ and the water stored in the soil from the previous time step $S(t-1)$:

$$W(t) = X(t) + S(t-1). \quad (4.11)$$

The groundwater recharge $R(t)$ is then computed as the amount of available water $W(t)$, minus what is called the evapotranspiration opportunity $Y(t)$:

$$R(t) = W(t) - Y(t). \quad (4.12)$$

The evapotranspiration opportunity is also computed using the Fu-equation with the potential evapotranspiration $E_o(t)$ plus the max storage in the soil $S_{max}$ as the demand limit, and available water $W(t)$ as the supply limit:

$$\frac{Y(t)}{W(t)} = 1 + \frac{E_o(t) + S_{max}}{W(t)} - \left[ 1 + \left( \frac{E_o(t) + S_{max}}{W(t)} \right)^{1/(1-\alpha_2)} \right]^{1-\alpha_2}. \quad (4.13)$$

Next, the actual evapotranspiration $ET(t)$ is computed, also using Fu’s equation (equation 4.7), with the potential evapotranspiration $E_o(t)$ as the demand limit and again with the available water $W(t)$ as the supply limit:

$$\frac{ET(t)}{W(t)} = 1 + \frac{E_o(t)}{W(t)} - \left[ 1 + \left( \frac{E_o(t)}{W(t)} \right)^{1/(1-\alpha_2)} \right]^{1-\alpha_2}. \quad (4.14)$$

The partitioning factor $\alpha_2$ must be the same in equations (4.13) and (4.14), because the recharge to the groundwater is related to the evapotranspiration efficiency, in the sense that high evapotranspiration efficiency (high $\alpha_2$) gives a low recharge. Now, the soil water storage $S(t)$ is the leftover water after evapotranspiration, given by
the evapotranspiration opportunity $Y(t)$ minus the actual evapotranspiration $ET(t)$:

$$S(t) = Y(t) - ET(t). \quad (4.15)$$

The base flow from the groundwater reservoir is computed as a fraction of the groundwater storage from the previous time step, controlled by a parameter $d$:

$$Q_g(t) = d \cdot G(t - 1). \quad (4.16)$$

At this point the phreatic ET is computed. To stay in Budyko framework, Fu’s equation (4.7) was used. The demand limit is set to be remaining potential evapotranspiration after initial ET is subtracted ($E_o - ET$), and the supply limit is set as the amount of water in the groundwater reservoir, above a certain threshold ($G - G_{\text{min}}$ if $G > G_{\text{min}}$):

$$\frac{ET_p(t)}{G(t) - G_{\text{min}}} = 1 + \frac{E_o(t) - ET(t)}{G(t) - G_{\text{min}}} - \left[1 + \left(\frac{E_o(t) - ET(t)}{G(t) - G_{\text{min}}}\right)^{1/\alpha}\right]^{1/\alpha}. \quad (4.17)$$

The groundwater storage is then given by the sum of the remaining groundwater from the previous time step, and the recharge for the present time step, minus the phreatic ET:

$$G(t) = (1 - d) \cdot G(t - 1) + R(t) - ET_p(t). \quad (4.18)$$

Now all that is left to do, is to compute the flow loss. We assume a certain percentage of the runoff being lost pr. km, but only in the most downstream sub-catchments. The cumulated loss can be computed from the initial runoff $Q_d + Q_g$, the river length $l$, and the percentage lost pr. km $f_{\text{loss}}$:

$$FL(t) = (Q_d(t) + Q_g(t)) \cdot (1 - (1 - f_{\text{loss}})^l). \quad (4.19)$$

Figure 4.4 shows the reduction of the flow as a function of the river length, at different $f_{\text{loss}}$ values. For the Okavango River, the flow loss is only an important factor in the downstream sub-models, so to avoid having to set different $f_{\text{loss}}$ values for the individual sub-models, the loss is implemented on a maximum river length of 500 km for all sub-models, regardless of the distance from river origin to the outflow. Finally, the total discharge is then the sum of the direct runoff and the base flow for the given day, minus the flow loss:

$$Q_{\text{tot}}(t) = Q_d(t) + Q_g(t) - FL(t). \quad (4.20)$$

Equations (4.8) to (4.20) outline the computations that must be done for every time step in the modeling period.
4.2.1 Linear reservoir

For application on a river basin scale, the Budyko model is applied at a sub catchment level, so that the entire river basin model consists of a number of Budyko models. The runoff at the outlet of the river basin is then the sum of the runoffs from all the sub catchments (Budyko sub-models). However, summing the runoff might result in a spiky discharge because this assumes, that all runoff reaches the outlet in the same day it is produced in the sub-models. In reality, this is not the case, and not even great rainfall events produce a sudden rise and fall in discharge of large river systems. Furthermore, the direct runoff \( Q_d(t) \) is likely to produce spikes in the discharge at the outlet of each of the sub-models, because it is released at the same time step it enters the model as precipitation, whereas the water that goes through the groundwater reservoir is released gradually over a period of time. For the Okavango River Basin, the average travel time through the river from the furthest part of the catchment is only about 11 days (pers.com. C. Milzow), which is not particularly long when looking at annual signals. Hence, the delay once the water reaches the river is only of minor importance for a small river system like the Okavango. Other delay factors, which the linear reservoir will help simulate, are all the processes happening between the patch of land surface where the water falls and the river, since the model is not distributed on a fine scale. Smoothing the produced discharge from each sub model, will reduce potential spikes created by large rainfall events, and account for other delay factors that may or may not actually happen during the travel time in the river. For this purpose all discharge (\( Q_{tot} \)) is routed through a linear reservoir and hereby released gradually:

\[
Q_{out}(t) = Q_{out}(t-1) \cdot \exp\left(-\frac{\Delta t}{K}\right) + Q_{in}(t) \cdot \left(1 - \exp\left(-\frac{\Delta t}{K}\right)\right)
\]

where \( Q_{out} \) is the amount released from the reservoir, \( \Delta t \) is the time step, \( K \) is the reservoir constant, and \( Q_{in} \) is the inflow to the reservoir (from equation 4.20).
Table 4.1: Model parameters with upper and lower bounds used for calibration (chapter 5).

![Table 4.1](https://example.com/table41.png)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Mathematical</th>
<th>Practical</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Min. value</td>
<td>Max. value</td>
</tr>
<tr>
<td>$\alpha_1$</td>
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<td>1</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_3$</td>
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</tr>
<tr>
<td>$d$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
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<td>0.01$^1$</td>
</tr>
<tr>
<td>$K$</td>
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<td>Inf</td>
</tr>
<tr>
<td>$S_{max}$</td>
<td>0</td>
<td>Inf</td>
</tr>
<tr>
<td>$G_{min}$</td>
<td>0</td>
<td>Inf</td>
</tr>
</tbody>
</table>

$^1$At $f_{loss} = 0.01$, 99% of the water in the river will be lost during routing over a 500 km stretch (equation 4.19), so this is essentially the upper limit for $f_{loss}$.

units must be consistent, and in this case m$^3$/s was used for $Q$, and seconds (s) for $\Delta t$ and $K$ (but one time step is still 1 day). The effect of the linear reservoir on a sine curve input at different $K$ values is shown in figure 4.5. The code for implementation of the linear reservoir was written by P. Bauer-Gottwein.

![Figure 4.5](https://example.com/figure45.png)

Figure 4.5: Effect of using a linear reservoir (equation 4.21) at different $K$ values.

### 4.3 Parameters

The Budyko framework as described by Zhang et al. (2008) uses four parameters: $\alpha_1$, $\alpha_2$, $d$, and $S_{max}$. Besides these four parameters, the phreatic ET adds another two parameters: $\alpha_3$ and $G_{min}$; the flow loss adds yet another: $f_{loss}$; and the linear reservoir adds one final parameter: $K$. The parameters and their upper and lower bounds, are listed in table 4.1.

The three $\alpha$’s are partitioning parameters that can mathematically assume values
between 0 and 1. $\alpha_1$ controls the relation between retention and runoff (equation 4.8), in the sense that a low $\alpha_1$ will produce high initial runoff, and vice versa. In the Okavango area, the majority of the precipitation infiltrates or evaporates, and high direct runoffs are unrealistic. The lower limit for $\alpha_1$ can be set to 0.7 to avoid high direct runoffs.

$\alpha_2$ controls the relation between recharge, evapotranspiration and soil storage (equations 4.14 and 4.13), whereas $\alpha_3$ controls the phreatic ET (equation 4.17). For both $\alpha_2$ and $\alpha_3$, high values will yield a high ET and vice versa.

d is another partitioning factor that controls the relation between base flow and groundwater storage (equations 4.16 and 4.18), and can assume any value between 0 and 1. The value of $d$ determines how big a fraction of the stored groundwater, that is released as base flow in the current time step. The time it will take to empty the groundwater reservoir if recharge ceases, can be approximated by $1/d$ for $d$ close to 1, where the majority of the water is released in the following time step. When $d$ is smaller, the retention time is larger than $1/d$. Figure 4.6 shows the normalized storage $G$ and base flow $Q_g$ at different $d$ values as a function of time. If $d$ is smaller than $10^{-3}$, the approximated reservoir time is 1000 days (~3 years), which is probably about the upper limit for how long water stays in the groundwater reservoir in the Okavango area, so this could be a lower limit for $d$.

$f_{loss}$ controls the flow loss from the stream over the most downstream part of the river. At $f_{loss} = 0.01$ all water is lost over a 500 km stretch (see figure 4.4), so $f_{loss}$ should in general be small. A realistic upper limit could be $4.463 \cdot 10^{-4}$, which is equal to a total loss of 20%.

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**Figure 4.6:** Normalized groundwater storage $G$ (window A) and base flow $Q_g$ (window B) as a function of $d$ and time.
Chapter 4. Model of the Okavango River

The reservoir constant $K$ controls the release of water that goes to discharge or in other words, the smoothness of the discharge as well as the delay of the peak in discharge (see figure 4.5). When $K = 1$ day, the reservoir is effectively not a reservoir, since the water is leaving shortly after it enters, whereas a reservoir with $K = 1000$ days would take more than 1000 days to empty if inflow ceased. In principle the upper limit of $K$ is infinite, and should be well determined if discharge data is used for calibration. Nevertheless, an upper limit could be set at 500 days.

$S_{max}$ is the threshold parameter that controls how much water the soil profile can hold. This is used for computing the maximum retention $X_o$ (equation 4.9), and the evapotranspiration opportunity $Y(t)$ (equation 4.13). In this sense, a certain correlation with $\alpha_1$ and $\alpha_2$ is expected. In principle $S_{max}$ can have any positive value, but very high $S_{max}$ values are unrealistic, and an upper limit should be set to 500 mm.

$G_{min}$ is another threshold value. It defines a lower limit for how much water should be in the groundwater reservoir, for phreatic ET to take place. Like $S_{max}$ it has no mathematical upper limit, but since it was introduced to allow for phreatic ET, it should not be too high. Upper limit could be set to 200 mm.

4.4 Spatial setup

The spatial setup of the model, was based on seven sub-models corresponding to the seven sub-catchments outlined in figure 2.1. The catchments are directly adopted from the Soil and Water Assessment Tool (SWAT Gassman et al., 2007) model developed by Milzow et al. (2011), and the watershed delineation was done using a delineation tool in ArcSWAT. The derived $0.125\degree \times 0.125\degree$ mask is shown in figure 4.7.

The idea of modeling multiple sub-catchments instead of just one, is to obtain a certain spatial distribution. Furthermore, the input data that are used (temperature and precipitation), can be taken directly from the SWAT model of Milzow et al. (2011), easing the model construction.

4.5 Input data

The framework requires two input data sets, precipitation and potential evapotranspiration. The potential evapotranspiration is computed from the maximum and minimum daily temperatures, using the Hargreaves equation in the form given in Neitsch et al. (2005). The input data format and files are adapted from the SWAT model used in Milzow et al. (2011). Both data products are originally given in spatial grids, and then re-sampled to reflect one average time series pr. sub-catchment, using the mask shown in figure 4.7. Both data sets can be downloaded from the ECMWF website: http://data.ecmwf.int/data/.

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3 ArcSWAT is a graphical user interface to SWAT in ArcGIS
4.5.1 Precipitation

Milzow et al. (2011) shows that gridded precipitation products vary greatly over the Okavango River, from comparison of total annual precipitation from the Tropical Rainfall Measuring Mission (TRMM), the ERA-Interim reanalysis of the European Centre for Medium-Range Weather Forecasts (ECMWF), and the Famine Early Warning Systems Network (FEWS-Net). For this model, the FEWS-Net (Herman et al., 1997) and the ERA-Interim (Berrisfort et al., 2009) products were tested, and the ERA-Interim reanalysis was found to provide the best fit. The ERA-Interim product is produced from modeling of global circulation patterns, assimilated with a great number of observations, and is available from 1989 and onwards. The precipitation rate comes in a spatial resolution of 1.5° and temporal resolution of six hours. The data was extracted and processed to reflect the precipitation in mm/day at one precipitation station pr. sub-catchment by Milzow et al. (2011).

4.5.2 Potential evapotranspiration

The potential evapotranspiration is computed from the daily minimum and maximum temperatures from the ERA-Interim product from ECMWF (Berrisfort et al., 2009). This temperature product gives temperatures in 2 m elevation every three hours at a spatial resolution of 1.5°. Since temperature is not given continuously, but only eight times a day, peak values might not be represented. Milzow et al. (2011) compared the ECMWF data with hourly weather station records from in-situ sta-
Table 4.2: Latent heat of vaporization for water. From Brutsaert (2005, table 2.4).

<table>
<thead>
<tr>
<th>Temperature [°C]</th>
<th>Λ [MJ/kg]</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20</td>
<td>2.549</td>
</tr>
<tr>
<td>-10</td>
<td>2.525</td>
</tr>
<tr>
<td>0</td>
<td>2.501</td>
</tr>
<tr>
<td>10</td>
<td>2.477</td>
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<td>20</td>
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<td>30</td>
<td>2.430</td>
</tr>
<tr>
<td>40</td>
<td>2.406</td>
</tr>
</tbody>
</table>

In the Okavango River Basin from the National Climatic Data Center (NCDC). They found that the in-situ maximum and minimum temperatures were on average 0.1°C higher and -2.7°C lower than the ECMWF data, and a correction was applied to the maximum and minimum ECMWF temperatures by Milzow et al. (2011).

For the computations of the potential ET, the Hargreaves equation as it is described in Neitsch et al. (2005) is used:

$$\lambda E_o = 0.0023 \cdot H_0 \cdot (T_{max} - T_{min})^{0.5} \cdot (T_{avg} + 17.8)$$ (4.22)

where $E_o$ is the potential evapotranspiration (mm/day), $\lambda$ is the latent heat of vaporization for water (MJ/kg), $H_0$ is the extraterrestrial radiation (MJ/m²/day), $T_{max}$ and $T_{min}$ is the maximum and minimum air temperature for the given day (°C), and $T_{avg}$ is the mean air temperature for the given day (°C). The latent heat of vaporization for the relevant temperature range is shown in Table 4.2.

The extraterrestrial radiation $H_0$ is a function of the location on the Earth, and the position of the Earth in its orbit around the Sun (time of year):

$$H_0 = 37.59 \cdot e_0 \cdot [\omega \cdot T_{SR} \cdot \sin \delta \cdot \sin \phi + \cos \delta \cdot \cos \phi \cdot \sin(\omega \cdot T_{SR})]$$ (4.23)

where $e_0$ is the eccentricity correction factor for the Earth’s orbit, $\omega$ is the angular velocity of the Earth’s rotation (0.2618 rad/hr), $T_{SR}$ is the hour of sunrise, $\delta$ is the solar declination (rad), and $\phi$ is the geographic latitude (rad). The eccentricity correction factor $e_0$ is the square of the ratio of the mean Earth-Sun distance $r_0$ to the Earth-Sun distance at a given day $r$, which is a function of the day of the year $d_n$, as is the solar declination:

$$e_0 = \left( \frac{r_0}{r} \right)^2 = 1 + 0.033 \cdot \cos \left( \frac{2\pi d_n}{365} \right)$$ (4.24)

$$\delta = \sin^{-1} \left\{ 0.4 \cdot \sin \left[ \frac{2\pi}{365} \cdot (d_n - 82) \right] \right\}.$$ (4.25)

When using equations (4.24) and (4.25), leap years should not be taken into account, and February should always have 28 days. The hour of sunrise $T_{SR}$ depends on the geographical latitude $\phi$ (rad), the solar declination $\delta$ (rad), and the angular velocity of the Earth’s rotation ($\omega = 2\pi/24 = 0.2618$ rad/hr):

$$T_{SR} = \frac{\cos^{-1} \left( \frac{-\tan \delta \cdot \tan \phi}{\omega} \right)}{\omega}.$$ (4.26)

Equations (4.22) to (4.26) together with Table 4.2 provides the information needed to compute the potential evapotranspiration $E_o$ at a certain latitude ($\delta$), from daily maximum and minimum temperatures only.
Chapter 5

Sequential calibration & sensitivity analysis

This chapter describes the joint sequential calibration of the Budyko model to discharge and storage from isotropically constrained GRACE mascon solutions. The method for computing the mascon solutions is described in chapter 7, and the calibration results analyzed in chapter 9.

5.1 Calibration data

For the joint calibration two data sets were used; discharge from Mohembo gaging station in Botswana, and storage changes in the form of equivalent water layer thickness (mascons) derived from GRACE level-1B tracking data.

5.1.1 Discharge

One monitoring station on the Okavango River with more or less continuous readings for the period of interest exists in the area (Mohembo, see figure 2.1). Readings of discharge are given on a daily basis from 1974 to present, with minor parts missing. The data was kindly provided by the Department of Water Affairs of the government of Namibia and the Department of Water Affairs of the government of Botswana. For the purpose of the joint calibration, the period September 2003 to August 2008 was used.

5.1.2 Water storage from GRACE mascons

For the storage data, an isotropically constrained mascon solution (chapter 7) was used. The blocks have a size of $1.25^\circ \times 1.5^\circ$, and a total of 18 blocks are entirely or partly covered by one or more Budyko sub-models. The original data product used for water layer thickness recovery (partial derivatives of K-Band Range-Rates with respect to differential Stokes Coefficients), was provided by NASA/GSFC. As for the discharge data, the period September 2003 to August 2008 was used.
5.2 Objective function

The joint objective function is a combination of two sub-functions, one for discharge \( \Phi_q \) and one for storage \( \Phi_s \) respectively:

\[
\Phi = w \cdot \Phi_s + (1 - w) \cdot \Phi_q .
\]  

(5.1)

A weighting factor \( w \) is used to set the weight of the storage data relative to the discharge data. The two objective sub-functions are given by:

\[
\Phi_s = \frac{1}{n_s \cdot \sigma_s^2} \sum_{j=1}^{n_s} u_j \cdot (s_{obs,j} - s_{sim,j})^2
\]  

(5.2)

\[
\Phi_q = \frac{1}{n_q \cdot \sigma_q^2} \sum_{k=1}^{n_q} (q_{obs,k} - q_{sim,k})^2
\]  

(5.3)

where \( s_{sim} \) and \( q_{sim} \) are the simulated storage \( s \) and discharge \( q \) respectively, \( s_{obs} \) and \( q_{obs} \) are the observed data, \( n \) is the number of observations, and \( \sigma \) is the uncertainty on the data. The \( u \) in equation (5.2) is the weight on the individual storage residuals \( s_{obs} - s_{sim} \). This weighting of individual data points of the same data type, is introduced because the model and data resolution is different. The water storage from GRACE comes in blocks of 1.25\(^\circ\)×1.5\(^\circ\), whereas the model has irregular shaped sub-catchments as model "blocks" (see figure 4.7). This means that some mascon blocks will be completely covered by the model, while others will not; and most blocks will be represented in more than one sub-model. A mask of 0.125\(^\circ\)×0.125\(^\circ\) cells (see section 4.4), meaning that each mascon block has 120 cells, was designed to compute the weighted average of the involved blocks for each sub-model. The weight \( u_j \) is given by the number of cells in mascon \( j \) that is covered by the model, divided by 120.

The uncertainty on the data was set to \( \sigma_s = 0.75 \text{ cm} \) for the GRACE data, which was estimated to be the uncertainty of 4\(^\circ\)×4\(^\circ\) degree mascons by Lemoine et al. (2007a), and \( \sigma_q = 20 \text{ m}^3/\text{s} \) for the discharge data.

5.3 Calibration process

The Budyko model was calibrated using an internal least squares adjustment function \texttt{lsqnonlin}\(^1\) in Matlab. The \texttt{lsqnonlin} function is a curve fitting function for non-linear problems of the form:

\[
\min_x \| F(x) \| = \min_x \left( \sum_{i=1}^{n_F} F_i(x)^2 \right)
\]  

(5.4)

where the suggested minimization function \( F(x) \) is the difference between the simulated and observed data \( F(x) = f_{sim}(x) - f_{obs} \), and \( x \) is a vector of input parameters, in this case \( x = [\alpha_1, \alpha_2, \alpha_3, d, floss, K, S_{max}, G_{min}] \). In other words, there is a value

\(^1\)http://www.mathworks.com/help/toolbox/optim/ug/lsqnonlin.html
\( F_i(x) \) for every data point \( i \) that is used for calibration, and the calibration process aims at minimizing \( F_i(x) \) as well as \( \sum F(x)^2 \). Since a joint calibration is performed, by minimizing the objective value \( \Phi \) of the joint objective function (equation 5.1), \( F(x) \) is created so that:

\[
\sum F(x)^2 = \Phi. \tag{5.5}
\]

The number of elements in \( F(x) \) is the sum of the number of storage and discharge data points \( n_F = n_s + n_q \). From equations (5.1), (5.2), (5.3), and (5.5) the following can be obtain:

\[
F_1(x)^2 + F_2(x)^2 + \ldots + F_{n_F}(x)^2
= \frac{w}{n_s \cdot \sigma_s^2} \cdot \sum_{j=1}^{n_s} \left( s_{\text{sim},j} - s_{\text{obs},j} \right)^2 + \frac{1-w}{n_q \cdot \sigma_q^2} \cdot \sum_{k=1}^{n_q} \left( q_{\text{sim},k} - q_{\text{obs},k} \right)^2. \tag{5.6}
\]

Writing out the individual elements of equation (5.6) yields:

\[
F_1(x)^2 = \frac{w}{n_s \cdot \sigma_s^2} \cdot \left( s_{\text{sim},1} - s_{\text{obs},1} \right)^2 \quad \Leftrightarrow \quad F_1(x) = \sqrt{\frac{w}{n_s \cdot \sigma_s^2}} \cdot \left( s_{\text{sim},1} - s_{\text{obs},1} \right)
\]

\[
F_2(x)^2 = \frac{w}{n_s \cdot \sigma_s^2} \cdot \left( s_{\text{sim},2} - s_{\text{obs},2} \right)^2 \quad \Leftrightarrow \quad F_2(x) = \sqrt{\frac{w}{n_s \cdot \sigma_s^2}} \cdot \left( s_{\text{sim},2} - s_{\text{obs},2} \right)
\]

\[
\vdots \]

\[
F_{n_s}(x)^2 = \frac{w}{n_s \cdot \sigma_s^2} \cdot \left( s_{\text{sim},n_s} - s_{\text{obs},n_s} \right)^2 \quad \Leftrightarrow \quad F_{n_s}(x) = \sqrt{\frac{w}{n_s \cdot \sigma_s^2}} \cdot \left( s_{\text{sim},n_s} - s_{\text{obs},n_s} \right)
\]

\[
F_{n_s+1}(x)^2 = \frac{1-w}{n_q \cdot \sigma_q^2} \cdot \left( q_{\text{sim},1} - q_{\text{obs},1} \right)^2 \quad \Leftrightarrow \quad F_{n_s+1}(x) = \sqrt{\frac{1-w}{n_q \cdot \sigma_q^2}} \cdot \left( q_{\text{sim},1} - q_{\text{obs},1} \right)
\]

\[
F_{n_s+2}(x)^2 = \frac{1-w}{n_q \cdot \sigma_q^2} \cdot \left( q_{\text{sim},2} - q_{\text{obs},2} \right)^2 \quad \Leftrightarrow \quad F_{n_s+2}(x) = \sqrt{\frac{1-w}{n_q \cdot \sigma_q^2}} \cdot \left( q_{\text{sim},2} - q_{\text{obs},2} \right)
\]

\[
\vdots \]

\[
F_{n_s+n_q}(x)^2 = \frac{1-w}{n_q \cdot \sigma_q^2} \cdot \left( q_{\text{sim},n_q} - q_{\text{obs},n_q} \right)^2 \quad \Leftrightarrow \quad F_{n_s+n_q}(x) = \sqrt{\frac{1-w}{n_q \cdot \sigma_q^2}} \cdot \left( q_{\text{sim},n_q} - q_{\text{obs},n_q} \right)
\]

It is now clear that the minimization function \( F(x) \) consists of two parts, one for storage and one for discharge:

\[
F(x) = \begin{cases} 
\sqrt{\frac{w}{n_s \cdot \sigma_s^2}} \cdot \sum_{j=1}^{n_s} \left( s_{\text{sim},j} - s_{\text{obs},j} \right), & \text{if } 1 \leq i \leq n_s \\
\sqrt{\frac{1-w}{n_q \cdot \sigma_q^2}} \cdot \sum_{k=1}^{n_q} \left( q_{\text{sim},k} - q_{\text{obs},k} \right), & \text{if } n_s + 1 \leq i \leq n_s + n_q
\end{cases}. \tag{5.7}
\]
5.4 Calibration analysis

During the calibration process, some parameters were excluded from the calibration, and kept fixed at an estimated realistic value. This was done for example if two parameters showed a correlation coefficient close to 1, or if the calibration would adjust the parameter to infinite or unrealistic values. For the purpose of identifying these parameters, the following analysis tools were used.

5.4.1 Confidence intervals

Confidence intervals (95%) for the parameters that represent the best fit, were computed using the \texttt{nlparci} function in Matlab

\begin{equation}
\text{ci} = \text{nlparci}(x, \text{res}, 'jacobian', J),
\end{equation}

given the optimal parameters set \(x\), the residuals of all data points (sim-obs) \(\text{res}\), and the Jacobian matrix \(J\). All three are returns from \texttt{lsqnonlin}.

5.4.2 Correlation coefficients

In some cases model parameters are correlated, so that a certain change in the output might be achieved by updating either of two parameter. When two parameters are strongly correlated, they cannot be estimated simultaneously. The correlation coefficient \(CC_{ij}\) for a pair of parameters \(i\) and \(j\), can be computed from the covariance of the two parameters \(C_{ij}\) and their standard deviations \(\sigma_i\) and \(\sigma_j\):

\begin{equation}
R_{ij} = \frac{C_{ij}}{\sigma_i \cdot \sigma_j} = \frac{C_{ij}}{\sqrt{\text{var}_i} \cdot \sqrt{\text{var}_j}} = \frac{C_{ij}}{\sqrt{C_{ii}} \cdot \sqrt{C_{jj}}}. \tag{5.9}
\end{equation}

The standard deviation on parameter \(i\) is given by the square root of the variance \(\text{var}_i\), which is obtained from the diagonal of the covariance matrix \(C_{ii}\). The covariance matrix \(C\), is computed from the Jacobian matrix \(J\), which is returned by the \texttt{lsqnonlin} function (Galassi et al., 2001, Section: Nonlinear Least-Squares Fitting):

\begin{equation}
C = (J^T \cdot J)^{-1}. \tag{5.10}
\end{equation}

Correlation coefficients larger than \(\pm 0.95\) are considered high, and simultaneous estimation of both parameters with reasonable confidence intervals, is not possible.

5.4.3 Weighting of data types

So, how does one identify the optimal weight \(\omega\) for the joint calibration of two types of data? Because a local search algorithm was used, initially a few calibration runs were performed from different starting points with a weight of 0.5 on the storage

\(^2\text{http://www.mathworks.com/help/toolbox/stats/nlparci.html} \)
data ($w = 0.5$). The `lsqnonlin` minimization function was then used to find the smallest minimum, near the smallest of the minimums already identified. The adjusted parameter values were evaluated, based on how realistic the model output were in the sense of the amount of groundwater, soil storage, evapotranspiration and so forth. Hereafter a number of calibration runs were carried out with different weights $w$, all starting off relatively close to the selected optimal parameter set. The parameter values, confidence intervals and correlation coefficients were evaluated, and an optimal weighting of the two data types was chosen. The results of this analysis will be described in section 9.2.

5.5 Sensitivity analysis

The sensitivity approach used is a one-at-a-time sensitivity analysis, performed at the location in the parameter space where the model was already adjusted to. Regarding the coupling with the mascon method, it is assumed that the sensitivity does not change much for small adjustments in the parameter values, since the model is already calibrated with respect to both storage and discharge, and thus the parameters fairly well adjusted to fit these data sets. First, a reference model run is made. Then, for each parameter in the analysis, perturbation of the parameter value is done followed by a model run, which is then compared to the reference model run. The sensitivity $S = \Delta M / \Delta P$ is computed as the difference in output between two model runs (the reference run $M_{\text{ref}}$ and the perturbed run $M_{\text{perturb}}$), with respect to the difference in the parameter $P$:

$$S = \frac{\Delta M}{\Delta P} = \frac{M_{\text{perturb}} - M_{\text{ref}}}{P_{\text{perturb}} - P_{\text{ref}}}.$$  

Since the model area is very small, and the size of the sub-catchments is way below the GRACE resolution, there is no point in trying to estimate parameters on a sub-catchment scale. Therefore parameters are estimated on a river basin scale. For the model used in this study, all parameters have the same value in all sub-catchments. However, in interest of preserving the opportunity to use different starting values at each sub-catchment, a scaling factor $s_i$ on all parameters of the same type $p_{ij}$ is estimated instead of the parameter value itself:

$$\Delta p_{ij} = (p_{ij})_{\text{perturb}} - (p_{ij})_{\text{ref}} = (p_{ij})_{\text{ref}} \cdot (1 + s_i) - (p_{ij})_{\text{ref}} = (p_{ij})_{\text{ref}} \cdot s_i.$$  

In equation (5.12) $\Delta p_{ij}$ is the perturbation of the hydrology parameter, $i$ is the parameter type (for example $\alpha_1$), $j = 1, ..., n$ is the sub-catchment, and $n$ is the number of sub-catchments, whereas $s_i$ (scaling factor) is the parameter that is solved for in the least squares inversion. This approach can naturally only be used if the model parameter has a non-zero reference value. Since the scaling parameter is the one being estimated in the least squares inversion, the sensitivity (5.11) is computed with respect to the scaling parameter $s_i$, so that

$$\Delta P_i = \Delta s_i = (s_i)_{\text{perturb}} - (s_i)_{\text{ref}} = s_i - 0 = s_i.$$  

41
A different sensitivity ($S_{t,b}$) will be computed for each block ($b$) at every epoch ($t$), and the quadratic mean sensitivity ($S_{rms}$) of a parameter is computed, to get an estimate of the total sensitivity for the parameter:

$$S_{rms} = \sqrt{\frac{\sum_t \sum_b S_{t,b}^2}{n_t \cdot n_b}}$$

where $t = 1, ..., n_t$, $b = 1, ..., n_b$,  

(5.14)

$n_b$ is the number of blocks, and $n_t$ the number of epochs.
Chapter 6

The mascon method I: Introduction

The gravity recovery method applied in this study is the mascon method, which is also used at the NASA Goddard Space Flight Center. The word mascon is short for mass concentration, and a mascon parameter represents a deviation from the a priori mean field and forward models, either as a mass surplus or a mass deficit in a small area (Rowlands et al., 2010). The deviation is considered as a uniform mass layer (in cm of water) over a predefined region, during a specified time interval. This way, mascon parameters become temporal and spatial step functions, over predefined epochs and spatial blocks.

This chapter will introduce the method of mascon parameters, while chapter 7 outlines the normal equation systems used to solve for them, and the constraints needed to compensate for insufficient amounts of data at small time scales. Chapter 8 outlines the coupling with the hydrological model and the transformation of mascon parameters to hydrology (model) parameter. Appendix A provides a short list of expressions used in this and the following two chapters, and can be used as look-up.

6.1 Gravity fields

The following definitions and normalizations are taken from Rowlands et al. (2010) and Bettadpur (2007a), but originate from earlier works like Heiskanen and Moritz (1967) and Torge (2001). The gravitational potential (or geopotential) at satellite altitude is given by:

\[
U(r, \theta, \lambda) \approx \frac{GM_E}{R} \left[ \sum_{l=1}^{l_{\text{max}}} \sum_{m=0}^{l} \left( \frac{R}{r} \right)^{l+1} \mathcal{P}_{lm}(\sin \theta)(\bar{C}_{lm} \cos m\lambda + \bar{S}_{lm} \sin m\lambda) \right] 
\] (6.1)

where \(r, \theta, \) and \(\lambda\) are the spherical geocentric radius, latitude and longitude coordinates of the point where the geopotential is evaluated; \(GM_E\) is the product of the universal gravitational constant \(G\) and the Earth’s mass \(M_E; R\) is the Earth’s mean semi-major axis; \(l\) and \(m\) are the spherical harmonic degree and order; \(\mathcal{P}_{lm} = N_{lm} \cdot P_{lm}\) (Bettadpur, 2007a) are the fully normalized associated Legendre functions, \(N_{lm}\) is the normalization factor; and \(\bar{C}_{lm}\) and \(\bar{S}_{lm}\) are the fully normalized Stokes coefficients,
which can be computed from the normalized Legendre functions. The Legendre function normalization is a so-called $4\pi$-normalization, meaning that the integral of the square of each spherical harmonic over a unit sphere $S$ is equal to $4\pi$:

$$\int_S \left[ P_{lm}^j (\sin \theta) \left\{ \frac{\cos m\lambda}{\sin m\lambda} \right\} \right]^2 dS = 4\pi \quad (6.2)$$

resulting a normalization of the stokes coefficients:

$$\left\{ \overline{C}_{lm}, \overline{S}_{lm} \right\} = \frac{1}{(2l+1)M_E} \times \int \int \int_{\text{Global}} \left( \frac{r_M}{R} \right)^l P_{lm}^j (\sin \theta_M) \left\{ \frac{\cos m\lambda_M}{\sin m\lambda_M} \right\} dM \quad (6.3)$$

where $(r_M, \theta_M, \lambda_M)$ are the coordinates of the mass element $M$ in the integrand.

### 6.2 Differential Stokes coefficients

The aforementioned deviation from the a priori mean field and forward models, can also be regarded a differential mass. In order to calculate the gravity potential at satellite altitude of a differential mass at the surface of the earth, we make use of the fact that a change in the gravitational potential caused by this differential mass can be expressed as a set of differential potential coefficients (or differential Stokes coefficients), which can be added to the mean field to get a full gravity field expansion (derived from Chao et al. (1987) in Rowlands et al. (2010)):

$$\left\{ \Delta \overline{C}_{lm}(t), \Delta \overline{S}_{lm}(t) \right\} = \sigma_j(t) \cdot \left[ \frac{(1 + k'_l R^2)}{(2l-1)M} \right] \int \overline{P}_{lm}^j (\sin \theta) \left\{ \frac{\cos m\lambda}{\sin m\lambda} \right\} d\Omega. \quad (6.4)$$

The evaluation of the integrals is restricted to a predefined region, $j$. In equation (6.4) $k'_l$ is the loading Love number of degree $l$, $\sigma_j(t)$ is the differential surface mass at epoch $t$ for region $j$, $d\Omega$ is the solid angle surface area of the region where $\sigma_j(t)$ is applied: $d\Omega = \cos \theta d\theta d\lambda$. The differential surface mass $\sigma_j$ is the differential mass of the unit area (differential surface mass) in kg pr. m$^2$. The loading Love number is included to account for the elastic yielding by the Earth under the differential surface mass $\sigma_j$.

### 6.3 Mascon parameters

It is clear from equation (6.4), that the relationship between the differential surface mass $\sigma_j(t)$ and the differential Stokes coefficients ($\Delta \overline{C}_{lm}$ and $\Delta \overline{S}_{lm}$) is linear. The differential surface mass $\sigma_j(t)$ is given in kg · m$^{-2}$, but might as well be expressed in water layer thickness $h_j(t)$, since 1 cm of water over 1 m$^2$ has a weight of 10 kg: $\sigma_j(t) = h_j(t) \cdot 10 \text{[kg cm}^{-1} \cdot \text{m}^{-2}] \text{ (Rowlands et al., 2010)}$. Using this conversion in equation (6.4), the thickness of the water layer $h_j(t)$ becomes a scale factor on a pre-computed set of differential Stokes coefficients, each representing a 1 cm thick layer of water (Rowlands et al., 2010):
\[
\begin{align*}
\begin{cases}
\Delta C_{jlm}(t) \\
\Delta S_{jlm}(t)
\end{cases} & = h_j(t) \cdot \left[ \frac{10 \cdot (1 + k_j^l) R^2}{(2l - 1) M} \right] \int \mathcal{P}_{lm}(\sin \theta) \left\{ \begin{array}{c}
\cos m \lambda \\
\sin m \lambda
\end{array} \right\} d\Omega.
\end{align*}
\]

where \( h_j(t) \) is also called a mascon parameter. Mascon parameters are recovered from satellite tracking data, by chaining of partial derivatives. The computation of partial derivatives of tracking data with respect to Stokes coefficients is done by the use of variational equations, which will be outlined in section 6.6; whereas the partial derivatives of the Stokes coefficients with respect to the mascon parameters can be computed from equation (6.5).

### 6.4 Forward gravity model

The mean gravity field used in the forward modeling of the differential range-rates, consists of a number of different components. Several different processing models have been used at GSFC. For the work presented is this Ph.D. project, two of these models have been applied; v.02 and v.06. For both models, the following components are included: The static field is simulated by the GGM02C (see table 3.1) constrained with terrestrial gravity information from Center for Space Research (CSR), University of Texas (Tapley et al., 2005), complete to d/o 150 for v.02, and d/o 200 for v.06. Atmospheric gravity contribution is based on operational surface pressure grids from ECMWF, complete to d/o 90 every 3 hours. The ocean tides are modeled with the Goddard/Grenoble Ocean Tide model 2004 v.7 (GOT4.7) every 3 hours to d/o 50, with some main constituents (O1, K1, S2, M2) to d/o 70 (Ray, 1999; Ray and Ponte, 2003).

Additionally for the v.06 processing, the majority of the terrestrial water storage (TWS) signal is forward modeled by using the Global Land Data Assimilation System (GLDAS)/Noah land surface model, with observation based forcing, in a 0.25\degree grid every 3 hours. Precipitation forcing from the Climate Prediction Center Merged Analysis of Precipitation (CMAP) is used (Rodell et al., 2004). Snow and canopy water was removed from the GLDAS TWS, and major mountain glacier areas were zeroed out using a 0.25\degree mask (Raup et al., 2000). An issue when including a hydrological signal in the mean gravity model, is the matter of ensuring a zero total mass change in the entire Earth system from epoch to epoch. This was handled by adding a uniform layer of water on all ocean blocks in every epoch, balancing the deficit or surplus created on the land masses due to the added hydrological model (Sabaka et al., 2010; Boy et al., 2011).

Sabaka et al. (2010) found that including GLDAS in the mean gravity model (v.06 processing), generally improved the performance of the mascon parameters, reducing daily RMS values of the KBRR residuals, as well as leakage from land areas with large seasonal variations. The improvement is probably due to the starting point for the inversion being closer to the true value, thus reducing the influence of non-linearity in the partial derivatives of the KBRR data with respect to the mascon parameters.
Chapter 6. The mascon method 1: Introduction

<table>
<thead>
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<th>Model</th>
<th>resolution</th>
<th>v.02</th>
<th>v.06</th>
</tr>
</thead>
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<tr>
<td>Static gravity field</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>GGM02C          (^{[1]})</td>
<td>d/o 150</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Static gravity field</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ECMWF operational surface pressure grids</td>
<td>d/o 90 @ 3h</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Induced oceanic time-variable gravity (non-barotropic response)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOG2D from ECMWF atm. pressure and winds           (^{[2]})</td>
<td>d/o 90 @ 6h</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Ocean Tide Modeling</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GOT4.7          (^{[3]})[4]</td>
<td>d/o 50 (O1, K1, S2, M2 d/o 70)</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Continental water storage in non-glacial areas</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GLDAS/Noah      (^{[5]})[6]</td>
<td>d/o 90 @ h3</td>
<td>x</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.1: Selected forward gravity models used at GSFC.


Forward modeling GLDAS, means that the total hydrology signal from a mascon solution must be computed by adding the GLDAS signal to the mascon parameters that are recovered from the least squares inversion. In the remaining part of this thesis, reference to a mascon solution is always a reference to the complete hydrology signal, whether it was directly solved for (with v.02 partials) or reconstructed by adding GLDAS to the recovered mascon parameters (v.06 partials).

The partial derivatives computed from the v.02 forward model were used for the work published in Krogh et al. (2010), while the v.06 partials were used for all other mascon solutions presented in this thesis.

6.5 State vector parameters

The trajectory of an orbiting body can be described by just six initial parameters. The six parameters (position \( p = (x, y, z) \) and velocity \( v = (\dot{x}, \dot{y}, \dot{z}) \)) are commonly called a set of state vector parameters or simply a state vector. The orbit computation requires updating of the parameters at each epoch. In the case of the GRACE mission, where two satellites in identical orbits are in play (see chapter 3), the number of state vector parameters is twelve (six pr. satellite). A classic Cartesian coordinate representation however, is not a must, and in some cases other coordinate representations can be more favorable. The mascon method used at NASA/GSFC uses the baseline between the two satellites as one state vector, and the state vector of the midpoint of the baseline as the other, instead of the two Cartesian state vectors for the individual satellites. The midpoint state vector, is the average of the two Cartesian state vectors, and the position coordinates are converted to spherical coordinates; declination of the midpoint (\( \delta \)), right ascension of the midpoint (\( \alpha \)), and distance between the midpoint and the Earth’s center of mass (\( \rho \)) (see figure 6.1A), whereas the velocity vector remains Cartesian (\( \dot{x}, \dot{y}, \dot{z} \)) (figure 6.1B). The baseline vector is the difference between the two original Cartesian state vectors (see figure 6.2), and is converted to spherical coordinates (\( \ell, \theta, \psi, \dot{\ell}, \dot{\theta}, \dot{\psi} \)) in a local coordinate system, centered at the midpoint of the baseline between the two satellites (Rowlands et al., 2002). The twelve state vector parameters are listed in table 6.2.
Table 6.2: The twelve state vector parameters used in the mascon approach for the two GRACE satellites. $P_1$ to $P_3$ are the position parameters for the baseline midpoint in a spherical coordinate system (see figure 6.1A), while $P_4$ to $P_6$ are the velocity (or rate-of-change) parameters for the baseline midpoint in Cartesian coordinates (see figure 6.1B). $P_7$ to $P_9$ are the spherical coordinates used to describe the baseline (difference) vector (see figure 6.2), while $P_{10}$ to $P_{12}$ are the rate-of-change in spherical coordinates for the baseline vector. $P_7$ to $P_{12}$ are in a local coordinate system centered at the baseline midpoint (see figure 6.2). From Rowlands et al. (2002).

<table>
<thead>
<tr>
<th>$P_i$</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_1$</td>
<td>$\rho$ distance of baseline midpoint from the Earth’s center of mass</td>
</tr>
<tr>
<td>$P_2$</td>
<td>$\delta$ declination of baseline midpoint</td>
</tr>
<tr>
<td>$P_3$</td>
<td>$\alpha$ right ascension of baseline midpoint</td>
</tr>
<tr>
<td>$P_4$</td>
<td>$\dot{x}$ inertial X component of baseline midpoint velocity</td>
</tr>
<tr>
<td>$P_5$</td>
<td>$\dot{y}$ inertial Y component of baseline midpoint velocity</td>
</tr>
<tr>
<td>$P_6$</td>
<td>$\dot{z}$ inertial Z component of baseline midpoint velocity</td>
</tr>
<tr>
<td>$P_7$</td>
<td>$l$ baseline vector length</td>
</tr>
<tr>
<td>$P_8$</td>
<td>$\theta$ baseline vector pitch</td>
</tr>
<tr>
<td>$P_9$</td>
<td>$\psi$ baseline vector yaw</td>
</tr>
<tr>
<td>$P_{10}$</td>
<td>$\dot{l}$ baseline rate-of-change vector magnitude</td>
</tr>
<tr>
<td>$P_{11}$</td>
<td>$\dot{\theta}$ baseline rate-of-change vector pitch</td>
</tr>
<tr>
<td>$P_{12}$</td>
<td>$\dot{\psi}$ baseline rate-of-change vector yaw</td>
</tr>
</tbody>
</table>

Figure 6.1: Midpoint state vector. COM = Center Of Mass. A) Position vector of the baseline midpoint in spherical coordinates ($\rho, \delta, \alpha$). Declination ($\delta$) is the angle between the XY-plane and the position vector. Right ascension ($\alpha$) is the angle between the X-axis and the projection of the position vector to the XY-plane. Inclination ($i$) is the angle between the orbit plane and the XY-plane. B) Velocity vector of baseline midpoint in Cartesian coordinates ($\dot{x}, \dot{y}, \dot{z}$).
Chapter 6. The mascon method I: Introduction

Figure 6.2: A) Baseline state vector in local coordinate system. The X'Y'-plane is perpendicular to the position vector of the baseline midpoint (ρ, δ, α), so that the Z'-axis points away from the Earth’s center of mass. The Y'-axis points towards North, and the X'-axis towards the East. Pitch (θ) is the angle between the X'Y'-plane and the baseline vector. Yaw (ψ) is the angle between the X'-axis and the projection of the baseline vector on X'Y'-plane. The magnitude (l) is the length of the baseline vector.

B) Projection of the baseline vector on to the X'Y'-plane of the local coordinate system, at different locations of the orbit.

Rowlands et al. (2002) concluded that it is not necessary to estimate all twelve parameters in local, short arc, gravity solutions, but that sufficient improvement of the residuals can be obtained by estimating only three state vector parameters along with the gravity parameters. They found that the RMS of the residuals improved from 200 µm s\(^{-1}\) to less than 0.1 µm s\(^{-1}\) for 15-minute arcs, by including the baseline rate-of-change vector pitch (P\(_{11}\) or ˙θ), the baseline rate-of-change vector magnitude (P\(_{10}\) or ˙l), and the baseline vector pitch (P\(_{8}\) or θ) in the solution.

Consequently, only three of the twelve state vector parameters are estimated simultaneously with the mascon parameters. The a priori values of the state vector parameters, are estimated from a forward GEODYN run on the mean gravity field described in section 6.4. For global mascon solutions, this is the final estimation of the initial state vector parameters, but for local solutions (like those used in this study), only a subset of the global data is used. Adjustments must be made to the state vector parameters, since a smaller dataset will give a better fit of the parameters compared to the initial a priori values. State vector parameters are commonly referred to as arc parameters, and this term will be used in the rest of this document.

6.6 Variational equations

The acceleration \(\ddot{x}\) of a spacecraft can be expressed as a function of the spacecraft position \(x\), velocity \(\dot{x}\), time \(t\) since the initial epoch \(t_0\), and a dynamical parameter set \(p\) (GTDS, 1989):

\[
\ddot{x}(t) = F(x(t), \dot{x}(t), t, p) \tag{6.6}
\]
where \( \mathbf{p} \) is a vector of parameters, containing the initial state vector parameters \( \mathbf{x}(t_0) \) and \( \dot{\mathbf{x}}(t_0) \), and constant model parameters pertaining to drag, gravitational harmonic coefficients etc., in union denoted \( \mathbf{p}^* \):

\[
\mathbf{p} = [\mathbf{x}(t_0), \dot{\mathbf{x}}(t_0), \mathbf{p}^*].
\] (6.7)

The parameters in \( \mathbf{p}^* \), include all parameters that will have an effect on the acceleration of the satellite, including gravity or Stokes coefficients. Differentiation of equation (6.6) with respect to the dynamical parameters of \( \mathbf{p} \) yields the following matrix equation (GTDS, 1989):

\[
\frac{\partial \ddot{\mathbf{x}}(t)}{\partial \mathbf{p}} = \frac{\partial \dot{\mathbf{x}}(t)}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} + \frac{\partial \dot{\mathbf{x}}(t)}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} + \left( \frac{\partial \ddot{\mathbf{x}}(t)}{\partial \mathbf{p}} \right)_{\text{explicit}} .
\] (6.8)

Equation (6.8) expresses the change in acceleration \( \ddot{\mathbf{x}} \) (left-hand-side) due to the change in location \( \mathbf{x} \) caused by the changed parameter in \( \mathbf{p} \) (first term on the right-hand-side), the change in velocity \( \dot{\mathbf{x}} \) due to change in \( \mathbf{p} \) (second term), and the direct effect of the changed coefficient on the acceleration \( \dot{\mathbf{x}} \) (third term denoted "explicit").

The force model \( F(.) \) from equation (6.6) is a set of equations describing the external forces acting on the spacecraft. In \( F(.) \) there is an explicit equation for every force, which in union explains the majority of the accelerations. The last part is caused by the initial state parameters \( \mathbf{x}(t_0) \) and \( \dot{\mathbf{x}}(t_0) \). The initial state parameters affect all components of the acceleration at the starting epoch, and therefore also at all other epochs, but there is no explicit equation or force associated with them. They are hence given implicit in all equations in the force model.

At the initial epoch, the location and velocity are not different from the initial state regardless of the parameter in the denominator of \( \partial \ddot{\mathbf{x}} / \partial \mathbf{p} \), except for the initial state parameters, and only the explicit or direct effect of the change in the parameter is causing a change in the acceleration \( \ddot{\mathbf{x}} \):

\[
\frac{\partial \ddot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} = \frac{\partial \dot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{x}(t_0)}{\partial \mathbf{p}} + \frac{\partial \dot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{x}(t_0)}{\partial \mathbf{p}} + \left( \frac{\partial \ddot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} \right)_{\text{explicit}}
\]

\[
= 0 \cdot \frac{\partial \dot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} + 0 \cdot \frac{\partial \dot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} + \left( \frac{\partial \ddot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} \right)_{\text{explicit}}
\]

\[
= \left( \frac{\partial \ddot{\mathbf{x}}(t_0)}{\partial \mathbf{p}} \right)_{\text{explicit}} .
\] (6.9)

When the parameter \( p_i \) in the denominator is an initial state parameter, the explicit term is always equal to zero, since no explicit equation exists.

Given that the acceleration \( \ddot{\mathbf{x}} \) is the second and the velocity \( \dot{\mathbf{x}} \) the first derivative of the position \( \mathbf{x} \) with respect to \( t \), equation (6.8) can be written as:
\[ \frac{\partial}{\partial \mathbf{p}} \left( \frac{d^2 \mathbf{x}(t)}{dt^2} \right) = \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} + \frac{\partial \dot{\mathbf{x}}(t)}{\partial \mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{p}} \left( \frac{d \mathbf{x}(t)}{dt} \right) + \left( \frac{\partial \ddot{\mathbf{x}}(t)}{\partial \mathbf{p}} \right)_{\text{explicit}} \]  

(6.10)

and by application of the assumption that the time \( t \) and the parameter set \( \mathbf{p} \) are independent, the differentiation with respect to \( t \) and \( \mathbf{p} \) can be interchanged to obtain (GTDS, 1989):

\[ \frac{d^2}{dt^2} \left( \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} \right) = \frac{\partial \dot{\mathbf{x}}(t)}{\partial \mathbf{p}} \cdot \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} + \frac{\partial \ddot{\mathbf{x}}(t)}{\partial \mathbf{p}} \cdot \frac{d}{dt} \left( \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} \right) + \left( \frac{\partial \dddot{\mathbf{x}}(t)}{\partial \mathbf{p}} \right)_{\text{explicit}}. \]  

(6.11)

From here, a system of linear differential equations called variational equations, is easily set up (GTDS, 1989):

\[ \ddot{\mathbf{Y}}(t) = \mathbf{A}(t) \cdot \mathbf{Y}(t) + \mathbf{B}(t) \cdot \dot{\mathbf{Y}}(t) + \mathbf{C}(t) \]  

(6.12)

where

\[ \mathbf{A}(t) = \left[ \frac{\partial \ddot{\mathbf{x}}(t)}{\partial \mathbf{x}} \right]_{3 \times 3}, \quad \mathbf{B}(t) = \left[ \frac{\partial \ddot{\mathbf{x}}(t)}{\partial \mathbf{x}} \right]_{3 \times 3}, \quad \mathbf{C}(t) = \left[ \left( \frac{\partial \ddot{\mathbf{x}}(t)}{\partial \mathbf{p}} \right)_{\text{explicit}} \right]_{3 \times n_p} \]  

(6.13)

\[ \mathbf{Y}(t) = \left[ \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} \right]_{3 \times n_p}, \quad \dot{\mathbf{Y}}(t) = \left[ \frac{d}{dt} \left( \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} \right) \right]_{3 \times n_p}, \quad \ddot{\mathbf{Y}}(t) = \left[ \frac{d^2}{dt^2} \left( \frac{\partial \mathbf{x}(t)}{\partial \mathbf{p}} \right) \right]_{3 \times n_p} \]  

(6.14)

and \( n_p \) are the number of elements in vector \( \mathbf{p} \).

Satellite tracking data like the KBRR measurements can be expressed as a simple function of the spacecraft position at the measurement epoch. The partial derivative of the KBRR measurement with respect to the state vectors can easily be found and chained with \( \mathbf{Y} \) and \( \dot{\mathbf{Y}} \) from equation (6.14), to get the partial derivatives of the KBRR measurements with respect to the gravity coefficients \( \mathbf{C} \) and \( \mathbf{S} \), which are part of \( \mathbf{p}^* \):

\[ \frac{\partial \text{KBRR}}{\partial \{ \mathbf{C}, \mathbf{S} \}} = \frac{\partial \text{KBRR}}{\partial \{ \mathbf{x}, \dot{\mathbf{x}} \}} \cdot \frac{\partial \{ \mathbf{x}, \dot{\mathbf{x}} \}}{\partial \{ \mathbf{C}, \mathbf{S} \}}. \]  

(6.15)

The same is valid for the differential range-rates \( \Delta \text{KBRR} \) with respect to the differential Stokes coefficients \( \Delta \mathbf{C} \) and \( \Delta \mathbf{S} \).
6.7 Signal leakage

Signal leakage is in general a big problem with gravity solutions from GRACE. It is typically manifested around land areas with high signal amplitude, where the signal cannot be contained in the area where it originates, but leaks into surrounding areas. The leakage can typically be identified in nearby oceans, since forward modeled oceanic gravity ideally results in a zero mass variation over the oceans, but the problem exists everywhere because the sensed mass deviations are sensed by GRACE over a greater area. Rowlands et al. (2010) show that a layer of water, 20 cm thick, over a $4^\circ \times 4^\circ$ area at the equator, will be sensed by GRACE up to 800 km away (see figure 6.3), which might cause leakage of the signal from one area to another. Even though KBRR measurements from GRACE are of differential nature, the resolution of the variations in the gravity field that can be recovered is limited. For spherical harmonic gravity solutions, GPS data are often used in combination with KBRR data, which will worsen the leaking problem, since GPS observations in general perform worse than the KBRR data when it comes to isolating gravity responses (Sabaka et al., 2010). The mascon solutions however, do not use GPS data, thus making the problem of leakage smaller. Furthermore, the v.06 forward model used in this thesis (see section 6.4), has hydrology forward modeled in the form of GLDAS/Noah. The hydrological contribution to time variable gravity is by far the largest, when traditional disturbing signals have been removed. This starts off the normal equation system closer to the "truth" compared to the situation where hydrology is not forward modeled. Since only one iteration is performed, the a priori guess is important and the closer to the truth, the smaller the leakage problem will be (Sabaka et al., 2010).
6.8 Mascon setup in Southern Africa

The target area of this study is Southern Africa, particularly the four major river basins, Zambezi, Okavango, Limpopo, and Orange. Unfortunately, unforeseen complications during the method development, resulted in too little time to set up models for all four river basins. Instead only one model is used, a model of the Okavango River upstream of the gaging station at Mohembo (see figure 2.1).

The mascon system covers a total area of 36.75° in latitude and 34.5° in longitude. The area has been divided into 644 mascon blocks of 1.25° × 1.5° (latitude × longitude) north of 26°S, and 1.5° × 1.5° south of 26°S (figure 6.4). This region is big compared to the area of interest, which is the aforementioned river basins (Zambezi, Okavango, Limpopo, and Orange), but the relatively wide margin of 6°–7° is needed to avoid marginal effects from incomplete range rate forward modeling, due to masses deviating from the static field outside the region that is not being forward modeled. This is avoided by using a wide margin, because range-rates are only affected locally by differential masses (Rowlands et al., 2010).

Additionally, each block was assigned to a hydrological region, of which the area has 29. The blocks have been numbered continuously according to the sub-region and main region they belong to. Figure 6.4 shows river basin outlines in green, and the outline of the original mascon regions in gray. The model area is outlined in pink, whereas the affected mascon blocks (transformed blocks) are encircled in red. The blocks are numbered continuously, starting with blocks in the Zambezi Basin, followed by the Okavango, the Limpopo, and the Orange Basin. This order is however not necessary, and blocks can be numbered in any order.
Figure 6.4: Map of the mascon block setup in Southern Africa used in this study. The green lines outline the river basins, Zambezi, Okavango, Orange and Limpopo, derived from a digital elevation model based on data from the Shuttle Radar Topography Mission. The gray straight lines outline the separation of mascon blocks into river basin specific regions. The magenta part of the Okavango river basin outlines the model by C. Milzow that is used in this study, and the red straight lines encircles the mascon blocks used for the model-mascon coupling.
Chapter 7

The mascon method II:
Geophysical least squares inversion

This chapter is the second of three chapters about the mascon method. The setup of the normal equation system consisting of data and constraint equations is outlined. Furthermore, regional constraints as well as a weighting function for the constraints are introduced. Appendix A provides a short list of expressions used in this chapter, and can be used as look-up.

7.1 Normal equation system setup

The partial derivatives of the differential KBRR data $\Delta KBRR$ with respect to the mascon parameters $h_j$, are computed through the use of variational equations (section 6.6). The partial derivatives are arranged in a matrix $A$, so that

$$A_{ij} = \frac{\partial \Delta KBRR_i}{\partial h_j} = \frac{\partial \Delta KBRR_i}{\partial \{\Delta C_{lm}, \Delta S_{lm}\}_j} \cdot \frac{\partial \{\Delta C_{lm}, \Delta S_{lm}\}_j}{\partial h_j}. \quad (7.1)$$

As mentioned in the previous section, each partial derivative $\partial \{\Delta C_{lm}, \Delta S_{lm}\}_j/\partial h_j$ is independent of the a priori values of the parameters. However, this is not true for the $\partial \Delta KBRR_{comp,j}/\partial \{\Delta C_{lm}, \Delta S_{lm}\}_j$ partial derivatives, which change as a function of the a priori mass distribution. This means that it might be beneficial to perform a few iterations by recomputing the partial derivatives $A_{ij}$ and re-adjusting the mascon parameters. Orbit computations are however quite time consuming, and should be avoided if possible. Using an accurate background model can help reduce the effect of the non-linearity, because the partial derivatives can be assumed linear in the proximity of the point at where they were computed in the first place. This is the reason that hydrology from GLDAS/Noah is included in the v:06 forward gravity model, and is probably why it improves the mascon estimates compared to a forward model without hydrology (section 6.4).

When $A$ has been computed, the following equation system can be set up, relating the mascon parameters $h$ to the data residual $y$, which is the difference between the computed and the observed KBRR data (equation 7.3), through the partial derivatives from equation (7.1):
\[ A \cdot h = y \]  
(7.2)

\[ y_i = \Delta KBRR_i = KBRR_{obs,i} - KBRR_{comp,i} \cdot \]  
(7.3)

The mascon parameters \( h \), are the deviation from the mean field plus all know time varying contributions, including storage from GLDAS/Noah. The number of KBRR observations in one day for the study region is approximately 700-1200, whereas the number of mascon parameters is 644 every ten days. Hence, the number of equations in (7.2) is much larger than the number of parameters, so the system overdetermined and cannot be expected to be solved exactly for all parameters \( h_j \). Instead a least squares approach is used, minimizing the sum of squares of the errors between the left and the right hand side of the equation:

\[ \hat{h} = \min_h \| y - A \cdot h \| \]  
(7.4)

where \( \hat{h} \) is the best estimate of \( h \), and \( \| \cdot \| \) denotes the sum of squares of (\( \cdot \)). Provided that all columns of \( A \) are linearly independent, which is the case because the water height was perturbed in only one region at a time, the minimization is achieved by solving the following normal equations (Weisstein, 2010):

\[ A^T \cdot A \cdot h = A^T \cdot y \]  
(7.5)

The normal matrix \( A^T \cdot A \) has the dimensions \( (n_{par}, n_{par}) \), and is hence significantly smaller than \( A \) \( (n_{obs}, n_{par}) \), because \( n_{obs} \gg n_{par} \). If the system is non-linear, the partial derivatives in \( A \), will depend on the location in the parameter space, and thus not be constant. In that case, the procedure is to use an iterative approach by solving for \( h \), recomputing \( A \) at the new \( h \), and then solve for \( h \) again, until no further improvements are made. As mentioned in relation to equation (7.1), this particular problem is non-linear to some extent, but when starting with \( h \) being as close to zero as possible (by including all known time variable contributions), no significant improvement is made in the second iteration.

### 7.2 Spatial and temporal constraint equations

In equation (7.5) the mascon parameters \( h \) (which are a mass step function in time and space) are not constrained by any geo- or hydro-physics and, for the solution to be stable, mathematical constraints might be needed; especially if small regions and short time periods are used. This is done by adding a number of constraint equations to the system in equation (7.5). Each constraint equation ties a pair of mascon parameters \( h_i \) and \( h_j \) to each other, requiring that the difference between the two parameters \( h_j \) and \( h_i \) is equal to a constraint \( c \):

\[ h_j - h_i = c \]  
(7.6)
This equation will however rarely be fulfilled, but something close to equality will be obtained after the least squares inversion. The residual of the constraint equation \( z_{ij} \) is equal to the difference between the desired difference \((h_j - h_i)_{\text{optimal}}\) (which is equal to \(c\)) and the actual difference \((h_j - h_i)_{\text{actual}}\):

\[
z_{ij} = (h_j - h_i)_{\text{optimal}} - (h_j - h_i)_{\text{actual}}.
\] (7.7)

For the mascon parameters, the optimal difference is zero, because we want neighboring mascons to have values very close to each other, so equation (7.6) becomes \(h_j - h_i = 0\) and the residual will only depend on the actual values of the mascon parameters \(h_i\) and \(h_j\):

\[
z_{ij} = 0 - (h_j - h_i)_{\text{actual}} = (h_i - h_j)_{\text{actual}}.
\] (7.8)

Residual for all equations in the normal equation system, are computed both before and after the least squares adjustment. The adjustment ensures that

\[
\sum \text{resid}^2_{\text{after}} < \sum \text{resid}^2_{\text{before}}
\] (7.9)

even if the individual residuals might be larger, the sum of the squared residuals will be smaller. If both \(h_i\) and \(h_j\) start off at zero (which is the case for a system that only has mascon parameters), the residual for the constraint equations before will be zero, whereas the residuals after will probably not; but the residuals of the data equations will be smaller after the adjustment than before, so the total sum of the squared residuals will be smaller after the adjustment.

When adding the constraint equations to the normal equation system of equation (7.5), the system becomes:

\[
(A^T A + C^T C) \mathbf{h} = A^T \mathbf{y} + C^T \mathbf{z}
\] (7.10)

where \(C\) has the size \((n_{\text{cnst}}, n_{\text{par}})\) and holds the partial derivatives of the constraint equations (equation 7.6) with respect to the mascon parameters \(h\), and \(z\) contains the constraint residuals (equation 7.8) on each pair of mascons constrained in \(C\). The partial derivatives of the constraint equation (equation 7.6) with respect to each parameter \(h_i\) and \(h_j\) is:

\[
\frac{\partial(h_j - h_i)}{\partial h_i} = -1 \quad \text{and} \quad \frac{\partial(h_j - h_i)}{\partial h_j} = 1.
\] (7.11)

An example of a constraint matrix of five parameters, is shown in figure 7.1.
Chapter 7. The mascon method II: Geophysical least squares inversion

Figure 7.1: Example of a constraint matrix (or equation system) tying five parameters ($h_1$ to $h_5$), through ten constraint equations (cnst1 to cnst10). The number of constraint equations is always equal to $(m^2 - m)/2$ for $m$ parameters, provided that all parameters are tied to all other parameters. Blank spots symbolizes zeros and * denotes the actual values of the parameters (see equation 7.8).

7.3 Weights on constraint equations

In equation (7.10) all data and constraint equations are weighted equally, which is not ideal for acquiring variability in the mass distribution. Assuming that all mascons (in time and space) are tied together via constraints, the number of constraint equations is $(m^2 - m)/2$ for $m$ mascon parameters, and will thus dominate the system completely due to the vast amount of constraints compared to the amount of mascon parameters. Furthermore, mascon parameters located far from each other in time and space will naturally be further from each other in value than a neighboring pair of mascon parameters, consequently far-away-mascons should not be constrained as tightly as close-to-each-other mascons. Therefore higher weights are assigned to the data than to the constraint equations, and the weights on the constraint equations are distance dependent, following (Rowlands et al., 2010):

$$w_{ij} = S \cdot \exp \left( 2 - \frac{d_{ij}}{D} - \frac{t_{ij}}{T} \right). \quad (7.12)$$

In equation (7.12) $w_{ij}$ is the weighting on the constraint equation linking mascons $i$ and $j$, $d_{ij}$ is the spatial distance between mascon parameters $i$ and $j$, $t_{ij}$ is the distance in time between mascons $i$ and $j$, $D$ is the correlation distance, $T$ is the correlation time, and $S$ is a scaling factor used to adjust the weights on the constraint equations relative to the weight on the data equations. $S$ is chosen so that the diagonals of the normal matrix of the constraint equations ($C^TWC$) are never more than 10% of the diagonals of the normal matrix of the KBRR observation equations ($A^TVA$), which means that $S$ typically is less than $10^{-3}$ if the weight on the data is 1 (Lemoine et al., 2007a; Rowlands et al., 2010). Lower weights like $10^{-4}$ was found to produce too noisy solution by Lemoine et al. (2007a), who also states that the scaling factor $S$ might vary from region to region. The data equations are all applied equal weights. Equation (7.10) now becomes

$$\left( A^TVA + C^TWC \right) h = A^TVy + C^TWz, \quad (7.13)$$

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where $V$ is the weight on the data and $W$ is the weight on the constraints, both are diagonal matrices. The correlation constants $D$ and $T$ in equation (7.12) must be large enough to effectively constrain neighboring mascon parameters, but also small enough to allow spatial and temporal variation. Rowlands et al. (2005, 2010) found that $D$ equal to one block spacing, as well as $T$ equal to one time step (typically 10 days) works well. For monthly solutions no temporal constraints are needed. For the solutions presented in this thesis, a correlation distance $D$ of 130 km, a correlation time $T$ of 10 days, and scaling factors $S$ of $10^{-4}$ and $2 \cdot 10^{-4}$ was used.

Equation (7.13) can be reduced to:

$$D \cdot h = u$$  \hspace{1cm} (7.14)

where $D$, $h$, and $u$ have the sizes $(n_h \times n_h)$, $(n_h \times 1)$, and $(n_h \times 1)$ respectively, $n_h$ is the number of parameters in $h$,

$$D = A^TVA + C^TWC, \quad \text{and} \quad u = A^Tv + C^Wz.$$  \hspace{1cm} (7.15)

The complex system of multiple matrices in equation (7.13) is thus reduced to a simple equation system similar to equation (7.5), where $D$ would correspond to $A^T A$ and $u$ to $A^T y$. The normal equation system in (7.14) is inverted and solved for the mascon parameters $h$ using SOLVE (Ullman, 1992a), which is part of the GEODYN software. SOLVE is also used to write the constraint equations, given lists of parameters that are to be constrained to each other.
Chapter 7. The mascon method II: Geophysical least squares inversion

7.3 Regional constraints

The constraint approach described above, will smooth spatial and temporal high frequency oscillations in the recovered gravity variations more or less, depending the constraint constants ($D$ and $T$, equation 7.12), and the weight on the constraints ($S$, equation 7.12). For various reasons, it might be useful to separate geographical regions, such as land and ocean, or glaciers and land (Luthcke et al., 2006, 2008). This can be done by removing any constraint equation relating the two areas. In figure 7.3, regional constraint equations are shown for 4 blocks at 2 epochs = 8 mascon parameters, where blocks 1 and 2 are kept separate from blocks 3 and 4. Constraining all 8 parameters to each other, would require 28 constraint equations, whereas in this example, all equations relating block 1 or 2 to either block 3 or 4 (at both epochs), has been removed. Krogh et al. (2010) describes a study where the regional constraint approach is used on river catchments and sub-catchments (see figure 7.4), whereas the rest of the work in this dissertation was done with just two regions: land and ocean.

7.5 Producing long time series

One obvious problem with the outlined least squares inversion, is that long time series are impossible to solve for, due to increased computation time for large equation systems. In my experience, when solving for 25 months (75 epochs) instead of 13 months (39 epochs), the computation time is multiplied by approximately six. So naturally, it will be more convenient to solve for one year at a time, and then patch solutions together. This approach however, gives rise to another problem, regard-
ing the temporal constraints. In principle temporal constraints are applied so that all parameters are constrained to all other parameters, regardless of the timespan between them. The weight on a constraint equation is determined by equation (7.12) (shown in figure 7.2), and hence the weight on the constraint on a pair of parameters far from each other in time, is very small. Figure 7.5 shows the normalized weight on a constraint equation, as a function of the temporal distance \( t \), at \( d = 0 \) km. It is clear that the nearest three epochs (\( \sim \) 30 days) have a relatively big weight on the constraint equations. Mascon parameters that are further from each other than three epochs, generally have a weight lower than 5% of the maximum weight. This means that at least the first and last month of any solution should be discarded, due to insufficient temporal constraints. For the solutions presented in this thesis, a period of two months (6 epochs) was discarded in each end of the solution. Furthermore, an overlap of two months (6 epochs) was used to determine a potential offset between solutions. The offset was computed as the average difference of the six overlapping mascon parameters, for each location. As a result, an 18-months solution were made for each 12-months period in a final multi-year solution.

Sabaka et al. (2010) developed a regularized least squares inversion technique, based on the conjugate gradient method, that allows to solve for long (multiple years) time series in one step. This technique was not used in this study, but greatly improves the usability of the mascon method on global and long time scales.

### 7.6 Measure of solution fit

The simplest way to estimate the fit of a solution, is to look at the root mean square (RMS) of the daily KBRR residuals. The fit to the observation data (KBRR observations) is given for each observation \( j \) by the residual between the observed KBRR data \( KBRR_{obs,j} \) and the computed KBRR value \( KBRR_{comp,j} \) (equation 7.2):
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Figure 7.5: Normalized weight on the constraint equations as a function of temporal distance between two mascon parameters (equation 7.12). The spatial distance $d$ is zero, the correlation time $T$ is 10 days, and a correlation distance $D$ is 130 km.

$$y_j = KBRR_{obs,j} - KBRR_{comp,j}.$$  \hspace{1cm} (7.16)

As it was mentioned in the beginning of this chapter, the partial derivatives are computed with respect to a mean gravity field, and the partial derivative of the KBRR data with respect to the differential C and S coefficients in equation 8.3 is non-linear, so in principle the forward range rate computations in GEODYN should be done all over again, using the new mass distribution. This is however quite time consuming and not possible for me to do, so the next best thing is to compute the updated residuals from the estimated (mascon and hydrology) parameters, rewriting equation (7.2) by adding the transformation step:

$$y = APx.$$  \hspace{1cm} (7.17)

$A$ contains the partial derivatives of the KBRR data with respect to the mascon parameters, $P$ contains the partial derivatives of the mascon parameters with respect to the hydrology parameters and untransformed mascon parameters (see equations 7.1 and 8.3), and $x$ is the estimated parameter set consisting of hydrology and untransformed mascon parameters. The interesting thing is to compare the $RMS_{KBRR}$ before and after the inversion (the initial parameter set vs. the updated parameter set). The pre-inversion equation system however, contains arc parameters that have been forward computed by GEODYN using the global KBRR data. For the Southern Africa region we are only using a small fraction of the global data, and the fit of the arc parameters will automatically be improved as a reaction to this reduction in data (see section 6.5). Since the $RMS_{KBRR}$ is computed from all parameters (arc parameters and mascon parameters in the initial parameter set), the improvement of the arc parameters alone will cause the daily $RMS_{KBRR}$ values to improve compared to the globally adjusted arc parameters. Therefore, the $RMS_{KBRR}$ of the pre-inversion equation system, must have adjusted arc parameters to see the actual improvement in...
the $RMS_{KBRR}$ caused by the updating of the hydrology parameters and the mascon parameters. This is solved by inverting an equation system containing only the arc parameters, and then using the adjusted values of the arc parameters in the computation of the pre-inversion $RMS_{KBRR}$ (together with the a priori mascon parameter values). For the non-transformed mascon blocks, the a priori mascon values are always zero, whereas the transformed blocks has a non-zero a priori value (see section 8.4). This value is computed from the mass output of the hydrological model when using the a priori hydrology parameter values, re-sampled to mascon-sized blocks in time and space. The $RMS_{KBRR,i}$ for day $i$ is given by:

\[
RMS_{KBRR,i} = \sqrt{\frac{\sum_{j=1}^{n_{yi}} (y_{ij}^2)}{n_{yi}}} \tag{7.18}
\]

where $y_{ij}$ is the residual for the $j$'th KBRR observation on the $i$'th day, and $n_{yi}$ is the number of residuals (or KBRR observations) on the $i$'th day. The $RMS_{KBRR,i}$ for a single day may not improve after the inversion, since the least squares approach only ensures that the total fit is better after, not necessarily the fit on the individual days (equation 7.9). Therefore a total $RMS_{KBRR}$ is computed from the individual daily $RMS_{KBRR,i}$ for all days in the solution:

\[
RMS_{KBRR} = \sqrt{\frac{\sum_{i=1}^{n_{days}} (\sum_{j=1}^{n_{yi}} (y_{ij}^2))}{\sum_{i=1}^{n_{days}} (n_{yi})}} = \sqrt{\frac{\sum_{i=1}^{n_{days}} (RMS_{KBRR,i}^2 \cdot n_{yi})}{\sum_{i=1}^{n_{days}} (n_{yi})}} \tag{7.19}
\]

Since the model area is very small compared to the entire mascon setup (figure 6.4), it is more illustrative to look at the improvement in the fit to the KBRR data on the near vicinity of the model area. Figure 7.6 shows the area that was used to compute the KBRR residuals for the Okavango model. Furthermore, due to the limited temporal constraints on the first and last 6 epochs (see section 7.5), days belonging to those marginal epochs were not included in the computation of the $RMS_{KBRR}$. The program used to compute the daily $RMS_{KBRR}$ values was written by D. Rowlands.
Chapter 8

The mascon method III: Coupled hydro-geophysical least squares inversion

The chapter is the third and final chapter about the mascon method, describing the coupling of the mascon method with a hydrological model, and the transformation of mascon parameters into hydrology parameters. Appendix A provides a short list of expressions used in this chapter, and can be used as look-up.

8.1 Integration of the hydrology model

When solving equation system (7.13), no hydro- or geophysical information is involved in the parameter estimation. By integration of a hydrological model, the physics of the model will apply a physically based set of constraints to the mass variations that are recovered from the KBRR data. To be able to couple the model with the estimation of mass distribution, the hydrological model must describe the mass variations in a number of blocks, corresponding in size to the mascon blocks, \( j \in J \), where \( J \) are the blocks that can be described by the model (but not necessarily all mascon blocks in the solution), provided a number of hydrology input parameters:

\[
h_{j \in J}(t_i) = HM(j, t_i, p_1, p_2, ..., p_n) + b_j
\]  

(8.1)

where \( t_i \) is the epoch, \( j \) is the mascon block number (which is related to the location of the block), \( p_1, ..., p_n \) are the model parameters, and \( b_j \) is a bias parameter for block \( j \) (bias parameters will be described in section 8.3). Our hydrological model of the Okavango River (chapter 4) only covers a small number of mascon blocks in the Southern Africa region, so naturally the remaining mascon parameters for blocks \( j \notin J \) must be estimated like traditional mascon parameters. Even for small models, the number of spatial blocks that the model will replace, is usually larger than the number of parameters in the model. Furthermore, model parameters are constant in time, while mascon parameters are estimated every 10 days, reducing the number of parameters even further. The total number of parameters in the mascon only system
Chapter 8. The mascon method III: Coupled hydro-geophysical least squares inversion

\( n_{\text{parm, mascon only}} \) and the coupled system \( n_{\text{parm, coupled}} \) is given by

\[
\begin{align*}
n_{\text{parm, mascon only}} &= n_{\text{block}} \cdot n_{\text{epoch}} \\
n_{\text{parm, coupled}} &= (n_{\text{block}} - n_{\text{model block}}) \cdot n_{\text{epoch}} + n_{\text{bias parm}} + n_{\text{model parm}}
\end{align*}
\] (8.2)

respectively, where \( n_{\text{block}} \) is the total number of blocks (here: 644), \( n_{\text{epoch}} \) is the number of epochs (36 for one year), \( n_{\text{model block}} \) is the number of transformed blocks or the number of blocks that is covered by the model (here: 18), \( n_{\text{bias parm}} \) is the number of bias parameters \( (n_{\text{bias parm}} = n_{\text{model block}}) \), and \( n_{\text{model parm}} \) is the number of model parameters (here: 1). The new parameter set will contain a number of traditional mascon parameters (for the regions outside the model), as well as a relatively smaller number of hydrology parameters.

### 8.2 The new normal equation system

To estimate the new parameter set in a solution, we relate the new parameter set to the old parameters set through partial derivatives, just as it was done for the mascon parameter-KBRR data relation in equation (7.1), by applying the chain rule:

\[
AP_{ik} = A_{ij} \cdot P_{jk} = \frac{\partial \Delta\text{KBRR}_{\text{comp},i}}{\partial x_k} = \frac{\partial \Delta\text{KBRR}_{\text{comp},i}}{\partial \{\Delta C_{lm}, \Delta S_{lm}\}} \cdot \frac{\partial \{\Delta C_{lm}, \Delta S_{lm}\}}{\partial h_j} \cdot \frac{\partial h_j}{\partial x_k}. \quad (8.3)
\]

To transform the normal equation system from equation (7.13), pre- and post-multiplication of a transformation matrix \( P \) on the data matrix \( A \) is done prior to adding the constraints:

\[
\left( P^T \left( A^T VA \right) P + C^T WC \right) x = P^T \left( A^T Vy \right) + C^T Wz \quad (8.4)
\]

where \( P \) contains the partial derivatives of the traditional mascon parameters \( (h_j) \) with respect to the new set of parameters (hydrology parameters and remaining mascon parameters: \( x_k \)):

\[
P_{jk} = \frac{\partial h_j}{\partial x_k} \quad (8.5)
\]

for \( j = 1, ..., n_h \) and \( k = 1, ..., n_x \)

where \( n_x = n_h - n_b \cdot n_t + n_p + n_b \) and \( n_x < n_h \).

\( n_h \) is the number of parameters before the transformation (the mascon only system), \( n_x \) is the number of parameters after the transformation, \( n_p \) is the number of hydrology model parameters, \( n_b \) is the number of bias parameters, and \( n_t \) is the number of time steps in the solution. If the new parameter set is identical to the old one \( (x = h) \), \( P \) will be an identity matrix and the system would remain untransformed. For the mascon parameters that are effectively untransformed because of their location outside the modeled area \( (j \notin f) \), \( P \) will contain local identity matrices, allowing these
parameters to pass untouched through the transformation.

The partial derivatives of the old mascon parameters with respect to the hydrology parameters \(p_1, ..., p_n\) are computed numerically through \(n+1\) model runs for the \(n\) hydrology parameters that are to be estimated through the inversion. In every model run, one parameter at a time is perturbed from its original location in the parameter space, and the mass output in all mascon blocks covered by the model \((j \in J)\) is computed at all time steps \(t_i\):

\[
\frac{\partial h_j(t_i)}{\partial p_k} = \frac{\partial H(j, t_i, p_1, p_2, ..., p_n)}{\partial p_k} + \frac{\partial b_j}{\partial p_k} = \frac{\partial H(\ldots)}{\partial p_k} + 0 = \frac{\partial H(\ldots)}{\partial p_k}.
\] (8.6)

The overall structure of \(P^T\) is illustrated in figure 8.1 and 8.2.

The total number of parameters is reduced by replacing a number of mascon parameters with hydrology parameters, because mascon parameters are estimated every 10 days, whereas hydrology parameters are constant in time. Thus, the greater the number of mascon parameters that is replaced (longer time period, bigger area), the greater the reduction in the total number of parameters; and obviously the shorter the time to solve the equation system.

As it was the case with equation (7.13), equation (8.4) can be reduced to:

\[
E \cdot x = v
\] (8.7)

where \(E\), \(x\), and \(v\) have the sizes \((n_x \times n_x)\), \((n_x \times 1)\), and \((n_x \times 1)\) respectively, \(n_x\) is the number of parameters in \(x\) (which is smaller than the number of parameters in \(h\) of equation (7.14)),

\[
E = P^T \left( A^T VA \right) P + C^T WC, \quad \text{and} \quad v = P^T \left( A^T V y \right) + C^T W z.
\] (8.8)

Again, the complex system (8.4) is reduced to a simple normal equation system (8.7) that can be inverted by SOLVE to find the best least squares fit of the parameters in \(x\).

### 8.3 Bias parameters and bias parameter constraints

The output of the hydrological model is a function of the location \(j\), the epoch \(t_i\), and the hydrology parameters that was chosen for the model. The bias parameter \(b_j\) was introduced to account for the difference in level between the model mass output and the recovered mass output from the GRACE data in the mascon solution. There is one bias parameter pr. mascon region for \(j \in J\) (not one pr. mascon parameter) to describe this displacement in mass variations (figure 8.3). For the transformation matrix \(P\), the partial derivatives of the old mascon parameters with the respect to the bias parameters \(b_j\), are equal to 1, obtained by differentiation of equation (8.1):

\[
\frac{\partial h_j(t_i)}{\partial b_j} = \frac{\partial H(j, t_i, p_1, p_2, ..., p_n)}{\partial b_j} + \frac{\partial b_j}{\partial b_j} = 0 + 1 = 1.
\] (8.9)
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Figure 8.1: Schematic illustration of the structure of the transformation matrix $P$.

Figure 8.2: Structure of the part of $P^T$ that involves the hydrology parameters (figure 8.1). Some parameters are traditional model parameters, while others are bias parameters.
Because of the very small block size used in this study, compared to the spatial resolution of GRACE data, bias parameters (much like regular mascon parameters) become unstable unless some spatial constraints are applied. This is reflected in parameters going from high negative values to high positive values in neighboring blocks, creating a checkerboard like pattern to balance each other out. To avoid this, spatial constraints on the bias parameters, similar to the ones used on the mascon parameters, are added to the system:

\[
\left( P^T \left( A^T V A \right) \right) P + C^T_m W_m C_m + C^T_b W_b C_b \right) \cdot x
\]

\[
= P^T \left( A^T V y \right) + C^T_m W_m z_m + C^T_b W_b z_b 
\]

(8.10)

The constraint matrix \( C \) from equation (8.4), is called \( C_m \) in equation (8.10), just like \( W \) and \( z \) are called \( W_m \) and \( z_m \) respectively. \( C_b \) is the constraints on the bias parameters, and \( W_b \) and \( z_b \) are the weights and residuals. These constraints do not affect the true model parameters, since they are added after the conversion (pre- and post-multiplication of \( P \)). The spatial constraints on the bias parameters are weighted just like regular mascon parameters, except for the time constraint (see equation 7.12):

\[
w_{ij,bias} = S_{bias} \cdot \exp \left( 1 - \frac{d_{ij}}{D_{bias}} \right) . \]

(8.11)

Equation (8.10) can be reduced to:

\[
F \cdot x = w
\]

(8.12)

where \( F \), \( x \), and \( w \) have the sizes \((n_x \times n_x)\), \((n_x \times 1)\), and \((n_x \times 1)\) respectively, \( n_x \) is
the number of parameters in $x$,

$$F = P^T \left( A^TVA \right) P + C^T_m W_m C_m + C^T_b W_b C_b,$$

and

$$w = P^T \left( A^T V y \right) + C^T_m W_m z_m + C^T_b W_b z_b.$$ (8.13)

While the mascon constraint equations and assigned weights are added internally in SOLVE, additional programs were needed for the coupled approach. These include an external program used to write the transformation matrix $P$ in e-matrix format (SOLVE format) and pre- and post-multiplying it on the data normal matrix, and a program used to add the bias parameter constraint equations to the normal equation system. Both were written by the author.

### 8.4 Updating the a priori mascon parameter values

When transforming mascon parameters to hydrology parameters, the entire normal equation system from equation (7.5) is changed. Before the transformation, the a priori values of the mascon parameters are all zero, meaning that the residuals (or the right hand side of the equation system, equation 7.3) are computed with respect to a priori mascon parameter values equal to zero. The transformation described in this chapter, transforms some of the mascon parameters to hydrology parameters. The partial derivatives $A$ and the data residuals $y$ are computed with respect to zero mass variation in $h$, but the baseline hydrological model does not have zero mass variation. In principle, the correct thing to do would be to recompute the partial derivatives in $A$ using the new mass distribution. In this new computation, the partial derivatives would be slightly different (because of the non-linearity of the $\partial \Delta KBRR / \partial \{ \Delta C, \Delta S \}$ relation), whereas the residuals $(\Delta KBRR_{obs} - \Delta KBRR_{comp})$ will change radically. An approximation of the new equation system can be made by using the partial derivatives $A$ to compute the change in the residuals $y$, using the new a priori parameters $h_{new}$:

$$y_{new} = Ah_{new}.$$ (8.14)

The updated a priori parameter values $h_{new}$ are computed from the hydrological model output, by re-sampling the total water mass to mascon sized spatial blocks and epochs. When a forward gravity model has some hydrology included, like the v.06 model described in section 6.4 that has GLDAS/Noah included, the background hydrology signal must be removed from the re-sampled model output $h_{new}$ prior to computation of the new residuals $y_{new}$.

The operations required to compute $y_{new}$ from equation (8.14) can be performed by SOLVE. The process is commonly referred to as "shifting" and results in an approximate set of normal equations that reflect the correct set of normal equations (which cannot be found without making a new forward GEODYN run).
Part III

Results, Analyses & Conclusions
Chapter 9

Sequential calibration & sensitivities

This chapter contains the results of the calibration (chapter 5) of the river basin model (chapter 4), as well as a one-at-a-time sensitivity analysis (section 5.5), performed for the parameter set that is used for the computation of partial derivatives for the coupled inversion. For the coupled mascon inversion (chapter 8), a relatively well calibrated model is needed. The coupled approach is quite time consuming, and a parameter set was chosen for the coupling before the work on the sequential calibration was actually finished. Therefore, the parameter set used to compute the partial derivatives for the coupled inversion, is different from the one presented here as the best parameter set, though the fit to both types of data is not much different.

9.1 Different calibration approaches

Calibration of the Budyko-type model of the Okavango River was performed. The model has eight parameters (described in section 4.3), and a simultaneous calibration of all eight parameters might not result in a unique best fitting parameter set. The information in the data may be insufficient for determination of all eight parameters, when strong parameter correlations occur.

A number of calibration runs was performed in order to find the best fitting parameter set. Different upper and lower bounds (UB and LB, respectively) on the parameters were tested in the attempt of keeping parameters within ranges that are realistic to the study area. Five different runs are presented here in tables 9.1 and 9.2, and figure 9.1 shows different components of the model output of each calibrated parameter set, given in mm of water. The discharge is given in m$^3$/s.

For the first calibration run (run no. 1), the mathematically defined UB and LB for the parameters (table 4.1) were used in the calibration, so that each parameter was allowed to adjust to any value within this interval. This run resulted in relatively narrow 95% confidence intervals (95CI) on the parameters $a_2$, $a_3$, $d$, $floss$, and $G_{min}$ (table 9.1). Furthermore, low correlation coefficients were found for all parameter pairs (table 9.2). Both $d$ and $floss$ however, adjust to values outside of the practically LB-UB range. For $floss$, the result is a very high flow loss of 92% of all water in
Table 9.1: Calibration details. LB and UB: Lower and Upper bound used in calibration. X: Adjusted values. 95CI: 95% confidence interval. Run no. 1 was made with the mathematically defined parameter bounds defined in section 4.3 (table 4.1), while run no. 2 was performed with the practical parameter bounds. Run no. 3 was made with a lower LB on \(d\) compared to run no. 2, while run no. 4 has a higher UB on \(f\) compared to run no. 2. Run no. 5 is the calibration run that was used for the coupled inversion in chapter 11. Large confidence intervals are marked in **bold**.
Table 9.2: Correlation coefficients from different calibration runs. Runs 1 to 4 have equal weight on both data types ($w = 0.5$ in equation 5.1), while run no. 5 was made with $w = 0.75$. Correlation coefficients larger/smaller than ±0.95 are marked in **bold**. $RMSE_w$ and $RMSE_Q$ are the root mean square of the errors (or misfits) with respect to the water storage (equivalent water layer thickness from GRACE) and the discharge, respectively.
the river (see figures 4.4 and 9.1). This is not a realistic result, and even though the parameter set provides a low objective function value and well defined parameter 95CI, the model should not be used like this.

The second calibration run was made with the practical UB and LB, defined in section 4.3 (table 4.1). In this run, both \(d\) and \(f\) adjust to their respective LB and UB, for \(f\) also resulting in a large 95CI relative to the parameter value. The remaining parameters, \(\alpha_1\), \(\alpha_2\), and \(S_{max}\) are not changed much, whereas \(\alpha_3\), \(K\), and \(G_{min}\) are significantly different. The 95CI on \(G_{min}\) is lower than for run no. 1, but for \(\alpha_1\) and especially \(S_{max}\) the 95CI is still very large. Furthermore, the objective function value is more than doubled from run no. 1 to run no. 2. The absolute correlation coefficients (CC) of \(\alpha_2-S_{max}\) and \(d-f\) are both larger than 0.95, showing that the parameters are highly correlated. For CC \(d-f\) the correlation is positive, meaning that high values of both parameters, will cause the same net objective function value as low values of the same parameters. Since a high \(d\) means high base flow and a high \(f\) means high flow loss; this makes perfect sense, as the higher discharge will be compensated by a higher flow loss. CC \(\alpha_1-S_{max}\) is found to be negative, and the parameter relationship is a bit more complicated. First of all \(S_{max}\) is a threshold parameter, hence it acts very non-linear. This means that the correlation CC \(\alpha_1-S_{max}\) is probably very different in other locations of the parameter space. Secondly, the retained water determined by \(\alpha_1\) is partitioned by \(\alpha_2\) into recharge, soil ET, and soil storage, and CC \(\alpha_1-S_{max}\) will also depend on the value of \(\alpha_2\).

Since run no. 2 has a high objective function value compared to run no. 1, attempts were made to find a parameter set that would result in realistic water balance components, but at the same time yield a better fit to the data, in the form of a lower objective function value. For run no. 3, the same UB and LB as in run no. 2 were used for all parameter, except \(d\) for which the LB was lowered by an order of magnitude from \(10^{-3}\) to \(10^{-4}\). This resulted in a lower \(d\) value, and all other parameters (except \(f\)) were also changed slightly. \(d\) was adjusted to a value that is not the defined LB, and the resulting objective function value is lower than for run no. 2. All parameters in run no. 3, except \(f\), have relatively narrow 95CI bounds (table 9.1) compared to run no. 2, also suggesting a better fit. For \(\alpha_1\), the parameter value is not much different but the confidence interval is smaller for run no. 3 compared to run no. 2. \(\alpha_2\) is found to be very different in run no. 3 compared to run no. 2. Run no. 3 predicts almost no evapotranspiration from the soil (\(\alpha_3\) and \(f\) will still produce some ET), and that all incoming water will go directly to recharge. This is a highly unrealistic scenario, and even though the objective function value is lower in run no.3, run no. 2 is found to perform better when taking the partitioning of water in the soil column into account.

For run no. 4, a high UB for \(f\) was tested. This run resulted in a higher \(f\) (equivalent to 92% of all water in the river, which is similar to run no. 1), a higher \(d\) value, and a \(G_{min}\) of zero. Furthermore, \(\alpha_1\) is adjusted to its LB, and 95CI on \(\alpha_1\), \(G_{min}\), and \(S_{max}\) are large. As it was argued in section 4.3, a low \(\alpha_1\) value is unrealistic since high \(\alpha_1\) values result in little direct runoff. It is interesting that at higher \(f\) values, \(d\) no longer adjusts to its LB of \(10^{-3}\), and \(f\) and \(d\) are no longer strongly correlated (CC \(d-f=0.7639\)). This same pattern was also seen for run no. 1. Again, the high flow loss is a problem in this calibration run. High parameter correlation is
Figure 9.1: Components of the water balance from the five calibration runs listed in tables 9.1 and 9.2 in mm or mm/day (except for discharge). Each curve is the weighted mean of the 7 sub-models. The discharge is the cumulated discharge, summed over all 7 sub-models and routed through the linear reservoir, and is hence comparable to the observed discharge at Mohembo (not shown). Since the soil storage is in general small compared to the groundwater, the groundwater storage is a good approximation of the total storage. For the flow loss, the total percentage of water lost from the river is written to the right of the figure. Runs 1 and 4 have the same big loss of 92%, while runs 2, 3, and 5 have a smaller loss of only 20%. While the calibration was performed on the entire 5-year period of September 2003 till August 2008, the figures show only the period from June 2004 till July 2005 for a better resolution of the individual components. The period shown is representative for the period prior to medio 2005, while the pattern is slightly different for flow loss and phreatic ET after 2005. The full time series can be found in appendix B.
only seen for $CC_{\alpha_1 - S_{\text{max}}}$.

All five calibration runs show similar levels for groundwater and discharge (figure 9.1). The total storage is computed as the sum of the soil water storage and the groundwater storage, and can be approximated by the groundwater storage since the amount of water in the soil is small relative to the groundwater. The total storage and the discharge was used for the calibration, and it is thus natural that both components are similar for all calibration runs. Calibration runs no. 1 (dark blue "o") and 4 (light blue ".") are very similar in output for all water balance components shown, which is no surprise since the parameters sets are very similar (table 9.2). Run no. 2 (green "+"), 3 (red "x"), and 5 (purple line) are also quite similar in recharge, flow loss, groundwater storage and discharge. They differ significantly on soil ET and soil water, which is caused by different values of $\alpha_2$. Soil storage and ET is biggest for run no. 5, intermediate for run no. 2, and smallest (zero) for run no. 3. The phreatic ET is also different for the three runs, being smallest for run no. 5, intermediate for run no. 2, and largest for run no. 3, caused by different $\alpha_3$ values. The precipitation input is naturally the same for all calibration runs.

In summary, calibration runs no. 1 and 4 have very high flow losses (92%) and are thus, in spite of low objective function values, not preferred parameter sets. Calibration run no. 3 have a $\alpha_2$ value of zero, resulting a no soil water and no soil ET. Run no. 2 has a higher objective function value than no. 1, 3, and 4, but the most realistic water storages and fluxes. Run no. 5 was made with a different weighting of storage data vs. discharge data, and the objective function value is thus not directly comparable. The objective subfunctions however are comparable, and we see a slightly better fit to the discharge ($\Phi_Q$) and a slightly worse fit to the storage ($\Phi_S$) compared to run no. 2. Nevertheless, run no. 5 was used in the coupled inversion, for which the results will be presented in chapter 11.

### 9.2 Data weighting

The two data types, discharge (Q) and storage (S) in the form of equivalent water layer thickness derived from GRACE, where weighted equally in calibration runs 1 to 4 in the previous section. To explore different weights on the two data types, a number of calibration runs were performed with varying $w$ (equation 5.1). Only parameters with narrow 95CI and low correlation coefficients in the best parameter set (run no. 2) were calibrated. These include: $\alpha_2$, $\alpha_3$, $K$, and $G_{\text{min}}$. Initially $d$ was included as a variable parameters, but since the adjusted value was always the LB of $10^{-3}$, it was finally excluded. The same thing was tested for $floss$. Additionally the correlation between $floss$ and $d$ is very high (0.9928). The correlation coefficient of $S_{\text{max}}$ and $d$ is also large (-0.9692), and both parameters have a large 95CI, which eventually lead to the exclusion of both parameters from the calibration with varying weights. The parameters $\alpha_1$, $floss$, $d$, and $S_{\text{min}}$ were fixed at the adjusted values from calibration run no. 2.

Figure 9.2A shows the value of the objective functions ($\Phi$, $\Phi_Q$, and $\Phi_S$) as a func-
The objective function value $\Phi$ is lowest when $w = 0$, and has a maximum around $w = 0.95$ (figure 9.2A). The objective function value is a weighted average of the two objective sub-functions $\Phi_Q$ and $\Phi_S$. Each of these are again a function of the residuals of the simulated data with respect to the calibration data, the number of data points, and the uncertainty of each type of data (equations 5.3 and 5.2). Thus, the fact that $\Phi$ is smallest at $w = 0$, does not mean that this is necessarily the best weight for calibration. The Pareto front (figure 9.2B) shows that as $w$ goes from 0 to 1, there is a great improvement in $\Phi_S$, while the worsening of $\Phi_Q$ is relatively small, as long as $w < 0.75$ approximately. At $w > 0.75$ the improvement in $\Phi_S$ is smaller and the worsening of $\Phi_Q$ larger for the same change in $w$.

Figure 9.3 shows the optimal parameter values at each weight $w$, together with their 95% confidence intervals. All four parameters vary relatively smoothly when moving from low to high value of $w$ (figure 9.3). The confidence intervals are also relatively narrow at most $w$ values, except for parameter $K$ at high $w$. For parameters $\alpha_2$, $\alpha_3$, and $K$ the parameter values are not changed much between $w = 0.6$ and $w = 0.95$. The parameter $G_{\text{min}}$ shows a minimum around $w = 0.65$ and increases towards high values as $w$ approaches 1.

Figure 9.4 shows the correlation coefficients between all adjusted parameter pairs, as well as the average absolute correlation of all parameters pairs (black line). In figure 9.4, we can see that most of the correlation coefficients are getting smaller as $w$ gets closer to 1, except for $CC_{\alpha_3-G_{\text{min}}}$ and $CC_{\alpha_2-\alpha_3}$, which additionally are outside the $\pm 0.95$ interval for $0.4 < w < 0.99$. At $w < 1.5$, the correlation coefficients change

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A Pareto optimal set is a set of models in a multi-objective evaluation. For each model, no other model performs better on the evaluation measure and on another evaluation measure. A 2-dimensional Pareto front, presenting two evaluation measures like discharge and storage, is a curve that joins all models in the Pareto optimal set (Beven, 2008).
Chapter 9. Sequential calibration & sensitivities

Figure 9.3: Adjusted parameter values and confidence intervals as a function of \( w \). The red dot marks the parameter value associated with the smallest confidence interval.

Figure 9.4: Correlation coefficients \( CC \) for the parameters \( \alpha_2, \alpha_3, K, \) and \( G_{\text{min}} \) as a function of \( w \). The black line is the average absolute correlation, and the gray area is where the correlation is smaller than \( \pm 0.95 \).

rapidly with varying value of \( w \), while the variation is more smooth when \( w > 1.5 \), except for \( w \) close to 1. The average absolute correlation (black line) is also decreasing with increasing \( w \), except when \( w > 0.95 \).

At \( w = 0 \), only the discharge data is used for calibration, and for values of \( w \) close to 0 the equivalent water storage has very little weight in the calibration. At \( w = 0.1 \), \( \alpha_3 \) and \( G_{\text{min}} \) go from becoming lower with higher \( w \) at \( w < 0.1 \), to being relatively
stable with varying $w$ when $w > 0.1$. $\alpha_2$ goes from a relatively stable level at $w < 0.1$ to falling values with rising $w$ between $w = 0.1$ and $w = 0.6$. The value of $G_{min}$ falls smoothly from $w = 0$ to $w = 0.65$, after which it rises smoothly again.

When $w = 1$, only the equivalent water storage is used for calibration, and this clearly gives a very different calibration result, than if both storage and discharge are used. Besides a sudden change in correlation coefficients, the parameter $K$ adjusts to 1 day (the LB) instead of being around 15 days for intermediate values of $w$, and $G_{min}$ goes to 500 mm (the UB). $\alpha_2$ and $\alpha_3$ do not change radically at $w = 1$, but a small shift is seen.

To summarize, the optimal weight used for the calibration is between $w = 0.6$ and $w = 0.8$, since the parameters are relatively insensitive to small variations in $w$ in this interval, and the weight on the two types of data is well balanced. Calibration run no. 5 was made with $w = 0.75$. The correlation coefficients of table 9.2, cannot be recognized in figure 9.4 for reasons explained in the beginning of this chapter. The fact that multiple parameter sets perform equally well with respect to fitting the calibration data, and that the correlation coefficient differs significantly from run to run, underlines the difficulty of simultaneous calibration of many parameters.

Even though the model is relatively simple compared to other water balance models, the structure is still very non-linear, complicating the calibration further.

### 9.3 Sensitivity analysis

A one-at-a-time sensitivity analysis was performed on the eight parameters in the model. Since the model is non-linear, the sensitivities will vary depending of the parameters values, and the sensitivity was evaluated at the parameter set from calibration run no. 5 with a data weighting of 0.75, because this was the best parameter set and weighting value (section 9.1 and 9.2). The quadratic mean sensitivity ($S_{rms}$, equation 5.14) of each parameter with respect to total storage $S$, and discharge $Q$ are shown in table 9.3. Figure 9.5 shows $S_{rms}$ relative max sensitivity for all parameter with storage in green and discharge in red. Figure 9.6 shows the sensitivity for all eight parameters of each block (y-axis) at each time step (x-axis) with respect to storage (equation 5.11).

<table>
<thead>
<tr>
<th>Parameter no.</th>
<th>$\Delta S/\Delta P$ percentage of max</th>
<th>$\Delta Q/\Delta P$ percentage of max</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_1$</td>
<td>1.260 · 10$^{-3}$ 0.01%</td>
<td>3.770 2.18%</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>4.953 57.42%</td>
<td>85.54 49.47%</td>
</tr>
<tr>
<td>$\alpha_3$</td>
<td>8.626 100.00%</td>
<td>128.7 74.44%</td>
</tr>
<tr>
<td>$d$</td>
<td>2.698 31.28%</td>
<td>172.9 100.00%</td>
</tr>
<tr>
<td>$f_{loss}$</td>
<td>2.052 · 10$^{-3}$ 0.02%</td>
<td>45.56 26.35%</td>
</tr>
<tr>
<td>$K$</td>
<td>6.973 · 10$^{-4}$ 0.01%</td>
<td>15.65 9.05%</td>
</tr>
<tr>
<td>$G_{min}$</td>
<td>1.995 23.13%</td>
<td>34.58 20.00%</td>
</tr>
<tr>
<td>$S_{max}$</td>
<td>3.972 · 10$^{-1}$ 4.60%</td>
<td>7.190 4.16%</td>
</tr>
</tbody>
</table>

Table 9.3: Quadratic mean sensitivities ($S_{rms}$) of the eight parameters in the Budyko model, with respect to total storage $S$ and discharge at outlet $Q$. 
Chapter 9. Sequential calibration & sensitivities

Figure 9.5: Quadratic mean sensitivity ($S_{rms}$) relative to the highest $S_{rms}$ value for all parameters with respect to storage (green) and discharge (red). The parameter numbers (x-axis) corresponds to the numbers in table 9.3.

For both data types, the three most sensitive parameters are $\alpha_2$, $\alpha_3$, and $d$ (table 9.3 and figure 9.5). The most sensitive parameter with respect to storage is $\alpha_3$, while $\alpha_2$ is the second most sensitive parameter, with a $S_{rms}$ value that is 57% of the $S_{rms}$ of $\alpha_3$. With respect to discharge, $d$ is most sensitive while $\alpha_3$ has a $S_{rms}$ value that is 74% of the $S_{rms}$ for $d$. In conclusion, the most sensitive parameter is $\alpha_3$.

From figure 9.6, it is seen that the sensitivity varies with both time and location. The 18 mascon blocks that are included in the model (22, 27, 31, 86, 91, 92, 93, 94, 95, 96, 97, 98, 99, 210, 214, 217, 220, and 223) are shown on the y-axis with increasing block number from bottom to top. Some blocks have a high sensitivity, while some are hardly affected. The blocks with high sensitivities are 27, 31, 94, 95, 96, 97, 98, 99, 217, 220, and 223, which are located in the northern part of the catchment (figure 6.4), or primarily sub-catchments 1, 2, and 3 (figure 4.7). Furthermore, there seems to be a shift in the model regime in the fall of 2005, and sensitivities hereafter are smaller than prior to fall 2005, for all parameters except $\alpha_1$ and $K$, and partly $floss$. For the parameters $\alpha_2$, $\alpha_3$, $d$, $G_{miu}$, and $S_{max}$ the shift is very significant, especially in the northern blocks. From this figure it is also very clear that $\alpha_3$ is the most sensitive parameter with respect to discharge.

For the coupled hydro-geophysical inversion, which was described in chapter 8, only one parameter from the model will be adjusted in the project. Since the coupled calibration uses the level-1B tracking data from GRACE, this parameter must be sensitive to the storage changes $\Delta S$. The sensitivities of $\alpha_3$ far exceeds that of the other parameters, and $\alpha_3$ is thus a natural choice for adjustment in the coupled inversion.
Figure 9.6: Sensitivities of all eight parameters in all mascon blocks that are included in the model, at all time steps between January 2003 and November 2008. The mascon blocks are listed in rising order from the bottom and up (22, 27, 31, 86, 91, 92, 93, 94, 95, 96, 97, 98, 99, 210, 214, 217, 220, and 223, see figure 6.4 for locations). Note different color scales. Sensitivities are computed using equation (5.11).
Chapter 10

Mascon only solution

A 5-year terrestrial water storage product based on regular, isotropically constrained 18-month mascon solutions (see chapter 7), was produced for the period September 2003 to August 2008, and used to calibrate the regional model of the Okavango River (described in chapter 4, calibration results presented in chapter 9).

This chapter will shortly analyze the 5-year equivalent terrestrial water storage product (in the following referred to as mascon only water storage, GRACE MO TWS or simply GRACE MO). A comparison to GLDAS/Noah terrestrial water storage, as well as monthly UTCSR release 04 SH solutions (Bettadpur, 2007c), which at the time of writing was only available through February 2008 at the ftp download web site\(^1\), will be presented. An annual and semi-annual signal is fitted to each of the products for the period from September 2003 to August 2008, except for UTCSR which is used through February 2008. Since the TWS from GLDAS/Noah is used in the forward gravity model, some similarities are expected between GRACE MO and GLDAS (see section 6.4).

10.1 Inversion approach

The forward gravity model used to produce the mascon solutions is the v.06 model, which includes terrestrial water storage from GLDAS/Noah (see section 6.4 and table 6.1). The correlation time and distance on the mascon parameter constraints are \(T = 10\) days and \(D = 130\) km, respectively, and the scaling factor on the mascon parameter constraints is \(S = 2 \cdot 10^{-4}\) relative to the scaling of the data matrix (all in equation 7.12). Solving for long time series of mascon parameters, is computationally unfeasible with the methods used in Ph.D. project (see section 7.5), and a piece-wise patching approach was used instead. Hence, the final water storage product was patched from five individual 18-month mascon solutions which are overlapping by six months in each end. The first and last two months of each solution were removed to avoid marginal effects, and offsets between solutions were computed from the two remaining overlapping months. The piece-wise technique was initially tested with just one overlapping month (three 10-day epochs), and no removal of

\(^1\)Data web page: http://www.csr.utexas.edu/research/ggfc/datasources.html.
Data after February 2008 was not available at the time of writing.
Chapter 10. Mascon only solution

Figure 10.1: Average time series of the GRACE MO, GLDAS, and UTCSR signals as well as the fitted annual signals, computed from all blocks in the model of the Okavango River Basin. Location of the model blocks is shown in figure 6.4.

Marginal parameters due to insufficient time constraints. The patched time series was compared to a full two year solution for the same period, and a clear difference was seen for the second year where the patched solution was shifted according to the average difference between the two solutions over the three overlapping epochs. This lead to the approach over using a longer overlap, and discarding time-wise marginal parameters. It was found that when two marginal months are removed and the offset computed from two overlapping months, the patched solution was in accordance with the full two year solution.

10.2 Time variable storage in the Okavango River Basin

Figure 10.1 shows the average storage variations of all blocks within the area of the Okavango River basin model. As expected, the GRACE MO solution and the terrestrial water storage from GLDAS are very similar in amplitude, with GRACE MO having slightly larger seasonal variations than GLDAS. The UTCSR solution on the other hand, has a significantly smaller amplitude than both GLDAS and GRACE MO. Furthermore, a phase discrepancy of approximately 20 days is seen, as GLDAS peaks earlier than both GRACE MO and UTCSR. Since the final GRACE MO solution was patched from five individual solutions, there might be a greater uncertainty in the long term trend in GRACE MO than for the other TWS products, while the seasonal variations are not affected. In figure 10.1, the 5-year trend of GRACE MO is very similar to that of GLDAS, which would be expected as GLDAS was used in the forward model, but this also indicates that the applied patching approach is giving a reasonable long term trend in the mass variation signal.
10.3 Seasonal variations in Southern Africa

Figure 10.2 maps the amplitude of the annual signal, and figure 10.3 the peak date in every $1.25^\circ \times 1.5^\circ$ mascon block, while table 10.1 lists the maximum and average amplitude, computed for all land blocks.

For all three solutions, the highest seasonal variation is found in the area of $11^\circ S$ to $17^\circ S$ and $15^\circ E$ to $35^\circ E$. The spatial distribution of amplitudes for GRACE MO is very similar to that of GLDAS, as expected. Comparison with the amplitude of the UTCSSR solutions however, show that this solution is quite different from the GRACE MO solution. UTCSSR in general has lower amplitudes, and a smoother spatial variation. From figure 10.2 it is clear that the GRACE mascon only solution has higher amplitudes and a greater level of spatial details than the monthly UTCSSR solutions. The UTCSSR solutions are characterized by a very smooth high amplitude area, while the mascon solution looks more like a realistic geophysical signal. Furthermore, the mascon solution GRACE MO and GLDAS, show locally lower annual amplitudes over the two lakes Lake Tanganyika (northern) and Lake Malawi (southern). In GRACE MO, this is most likely not a geophysical signal, but an artifact caused by the fact that surface water, like lake storages, are not included in GLDAS.
Table 10.1: Maximum and average amplitude of the annual signal, for the mascon only product (GRACE MO), the corresponding TWS from GLDAS/Noah, and the SH solution from UTCSR. Averages are computed for all 382 land blocks during September 2003 to August 2008 for GRACE MO and GLDAS, and during September 2003 to February 2008 for UTCSR.

<table>
<thead>
<tr>
<th>All land blocks</th>
<th>GLDAS</th>
<th>GRACE MO</th>
<th>UTCSR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum amplitude [cm]</td>
<td>17.25</td>
<td>21.45</td>
<td>15.51</td>
</tr>
<tr>
<td>Average amplitude [cm]</td>
<td>7.52</td>
<td>9.79</td>
<td>7.07</td>
</tr>
</tbody>
</table>

Figure 10.4: A) Peak-time for the 382 land blocks in the area, divided into monthly bins. B) Difference in peak-time between GRACE MO and GLDAS for the 382 land blocks. Five years of data was analyzed: September 2003 to August 2008. Reference date is 01/01/2006. 79% of all blocks have a delay in GRACE MO relative to GLDAS between 1 and 30 days, while this only the case for 58% of the blocks in UTCSR.

The peak date of the annual signal is mapped in figure 10.3. For the GRACE MO solution, the peak time varies from early March in the north-west and south-east, to late June towards the south-west. The central part of the area has peak times around April–May, and earlier or later peak times only occur along the coasts. For the GLDAS TWS signal, the pattern is a bit different. The central part have variations in peak time from early March to late May. Along the coast, peak times are found to be in December/January in the northern part, and in August/September in the southern part. For UTCSR we see a smooth shift in peak time from early February in the northern part, to August–September in the southern. In general, the signal peak occurs earlier for GLDAS than for GRACE MO and UTCSR. Figure 10.4A shows the number of land blocks that peak each month, while 10.4B shows the difference in days between peaks for all land blocks. From figure 10.4 it is clear that for most blocks (79%), the GRACE signal peaks between 1 and 30 days later than GLDAS. For UTCSR, this is the case for only 58% of all blocks.
Chapter 11

Coupled model-mascon solution

This chapter contains the results of the coupled hydro-geophysical inversion, described in chapter 8. Discussions and conclusions will be given throughout the chapter, and summarized in chapter 13.

The method of a coupled hydro-geophysical least squares inversion for estimation of model parameters from KBRR data have, to the best of my knowledge, not been applied before. For this reason, different approaches were tested to find the best way of implementing the method. First of all, varying weights on the mascon- and bias-constraint equations were tested. The weighting was changed by adjusting the scaling factor $S$ in equation (7.12) for the mascon constraints (from here on denoted $S_{\text{mascon}}$), and $S_{\text{bias}}$ in equation (8.11) for the bias constraints. All scaling factors discussed in this chapter, are given relative to the scaling factor on the data matrix. Experiments showed that the lowest scaling factor on the mascon constraints, which constrains the parameters sufficiently, is $10^{-4}$ relative to a scaling of 1 of the data matrix. Secondly, different correlation distances of the bias parameter constraints were explored, by adjusting $D_{\text{bias}}$ in equation (8.11).

11.1 Model perturbation

In chapter 9, the most sensitive model parameter was identified as $\alpha_3$ (see table 9.3), which is the parameter that controls the amount of water disappearing from the groundwater reservoir in the form of evapotranspiration (ET) or root uptake, also called the phreatic ET. Thus, $\alpha_3$ is the parameter that is chosen to be adjusted in the coupled solution. Partial derivatives of each mascon parameter with respect to the model parameter $\alpha_3$, were computed by running the model twice; one baseline model run and one run with a slightly perturbed $\alpha_3$ value. The difference in TWS between the two model runs, in each mascon block was computed using a 0.25°×0.25° grid (see figure 4.7). Figure 11.1 shows the equivalent water layer thickness from the baseline model run (top), the residual water layer thickness when TWS from GLDAS is subtracted (middle), and the difference between the baseline model run and the perturbed model run (bottom). Some blocks are found to be very sensitive, especially prior to 2006, whereas others have a more moderate sensitivity during the entire period, which was also seen in figure 9.6. The most sensitive blocks are located in the northern part of the river basin, more precisely sub-models 1 and 3.
Figure 11.1: Model output as equivalent water layer thickness from computation of partial derivatives of $a_3$. Each curve corresponds to one of the 18 mascon sized blocks in the model. Top: Equivalent water layer thickness in cm. Middle: Residual equivalent water layer thickness when terrestrial water storage from GLDAS has been subtracted. Bottom: Change in equivalent water layer thickness from baseline run to perturbed run.
11.2 Testing the coupled method

Table 11.1 (page 93) shows the summarized results from a number of different least squares inversion runs of the normal equation system, with different scaling factors in the constraint equations ($S_{\text{mascon}}$ and $S_{\text{bias}}$), while table 11.2 (page 94) summarizes the results for inversion runs with different correlation distances on the bias parameter constraints ($D_{\text{bias}}$). Both tables show the bias and model parameter adjustments, as well as the RMS of the KBRR residuals ($RMS_{\text{KBRR}}$) for the adjustments, and the RMS of the storage ($RMS_{S}$) and discharge ($RMS_{Q}$) residuals. The lower the RMS value, the better the fit to the respective data type.

The storage estimates used to compute the residuals is from the mascon only solution (GRACE MO), described in chapter 10. The solution was produced using a correlation distance of 130 km, a correlation time of 10 days, and a scaling of the mascon constraints of $2 \cdot 10^{-4}$. This solution is called "Mascon" in tables 11.1 and 11.2. A column of "A priori" values is also present in both tables. These are the parameter and RMS values, prior to the least squares adjustment. In both tables, any RMS-value smaller than the a priori value is marked in bold, indicating a better fit to the respective data type. The solutions are numbered from 1 to 18, and will be referred to in the text as #1 for solution no. 1 and so forth. Solutions #6 and #8 are shown in both tables for comparison.

In tables 11.1 and 11.2, the $RMS_{\text{KBRR}}$ value for the mascon only solution (Mascon), is much lower than the $RMS_{\text{KBRR}}$ for the coupled solutions, in which some mascon parameters were transformed to model parameters. The a priori RMS value for the mascon only solution (not shown in table) is also different from the a priori RMS values of the other solutions. The reason for this is, that all a priori mascon parameters are equal to zero in the mascon only solution, in contrast to the coupled solutions, in which the a priori mascon parameter values are computed from the model storage output, thus making the mascon only a priori fit ($RMS_{\text{KBRR}}$) different from the coupled a priori fit. The process of changing the a priori mascon parameters values, was previously referred to as "shifting" and is described in section 8.4. The obvious difference in KBRR residual RMS between the adjusted mascon only solution and the other solutions, is due to the different number of adjusted parameters. The mascon only solution has more parameters than the coupled solutions. For the model blocks, where mascon parameters have been transformed to model parameters, the hydrological model provides the temporal and spatial variations, whereas in the mascon only solution the mascon parameters are estimated individually (with constraints) at every block and for every epoch. Intuitively, it makes sense that a larger number of mascon parameters will be able to fit the KBRR data better than just one hydrology parameter, as it is the case in this study.

Furthermore, all of the adjusted $RMS_{\text{KBRR}}$ values are smaller than the a priori value, which is expected since the least squares inversion aims at minimizing those exact residuals (see chapter 7).
11.2.1 Scaling of bias- and mascon-parameter constraint weight

Finding the optimal scaling of the mascon parameter constraint equations is a trial and error process, and the optimal scaling factor might not be the same for different regions or different block sizes. Increasingly lower scaling factors are tested until the solution is found to be too noisy, and the last scaling factor to produce a good result is the best scaling factor. A number of different scaling factors on the mascon constraint equations were tested, but only two \( S_{\text{mascon}} = 10^{-4} \) and \( S_{\text{mascon}} = 2 \cdot 10^{-4} \) will be presented here, since they both produce good mascon solutions, with acceptable noise levels. In the following these are referred to as “low” and “high” weight, respectively, on the mascon parameters. Bias parameters were introduced to account for the difference between the absolute water storage from the model and the relative equivalent water storage estimated from GRACE. Spatial constraints on the bias parameters are applied to create stability in the adjusted bias parameter values, and the scaling of the weight on the constraints (equation 8.11) is tested here.

The fit to the KBRR data \( (RMS_{\text{KBRR}}) \) is in general better when a high weight is used on the mascon parameter constraints \( S_{\text{mascon}} \) (#1 to #5 vs. #6 to #10), except when the weight on the bias parameter constraints \( S_{\text{bias}} \) is also very low (#1 vs. #6). Secondly, the \( RMS_S \) and \( RMS_Q \) do not improve compared to the a priori values, for the solutions with high weight on the mascon constraints (#1 to #5), whereas some of the solutions with low weight on the mascon constraints show improved \( RMS_S \) and/or \( RMS_Q \) values also (#6, #8, #9, and #10). Solutions #1 and #6 provide a good fit to storage (small \( RMS_S \)), but a poor fit to the discharge (large \( RMS_Q \)), while solutions #8, #9, and #10 all provide a good fit (better than the a priori) to both storage and discharge. Regardless of the scaling factor used on the mascon constraints \( S_{\text{mascon}} \), the best scaling of the bias constraints is \( S_{\text{bias}} = 10^{-2} \) (#3 and #8), since this scaling provides the best simultaneous fit of both storage and discharge.

The magnitude of the bias parameter adjustments, as well as their standard deviations and the absolute sum of the bias parameters \( (\sum b_i) \), decrease with higher scaling of the bias constraints, as it is seen in table 11.1. This behavior is expected since the constraints are applied to dampen the variation. The bias parameters are in general positive towards the north-west, and negative towards the south-east (see a map of bias parameters for #8 in figure 11.3). For low \( S_{\text{bias}} \) values, the sum of all bias parameter values is positive, while it is negative for higher values of \( S_{\text{bias}} \).

11.2.2 Bias parameter correlation distance

Since bias parameters are constant in time, the weight on the bias parameter constraints is a function of the distance between parameters, and thus different correlation distances (equation 8.11) are tested. The bias parameter correlation distance \( D_{\text{bias}} \) is different for the individual solutions listed table 11.2. Furthermore, the different correlation distances were tested at two different scaling factor values on the bias constraint equations \( S_{\text{bias}} = 10^{-4} \) in #6, #11 to #13, and \( S_{\text{bias}} = 10^{-2} \) in #8, #14 to #18). Figure 11.2 shows the correlations between \( D_{\text{bias}}, RMS_{\text{KBRR}}, RMS_S, \) and \( RMS_Q \) for the two \( S_{\text{bias}} \) values used. It is clear the a simultaneous good fit to discharge (low \( RMS_Q \)) and storage (low \( RMS_S \)), is only obtained when \( S_{\text{bias}} = 10^{-2} \) (figure 11.2B).
Solution no. | A priori Mascon | S_mascon | T_mascon (days) | D_mascon (km) | S_obs | D_obs (km) |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Σ</td>
<td>-</td>
<td>2.10^{-4}</td>
<td>2.10^{-4}</td>
<td>2.10^{-4}</td>
<td>2.10^{-4}</td>
<td>2.10^{-4}</td>
</tr>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
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<td>1</td>
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</tr>
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<td>1</td>
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<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
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<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
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<td>1</td>
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<td>1</td>
</tr>
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<td>1</td>
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<td>1</td>
</tr>
<tr>
<td>9</td>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>10</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

| RMSKBR (m/s) | 0.29276 |
| RMS_c (cm) | 2.9330 |
| RMS_c (m^2/s) | 134.77 |
| Bias parameter adjustments | |
| b_2 (cm) | -32.16 ± 0.860 |
| b_2 (cm) | -27.55 ± 0.993 |
| b_3 (cm) | -79.04 ± 0.700 |
| b_3 (cm) | -81.77 ± 0.589 |
| b_4 (cm) | -23.42 ± 0.837 |
| b_4 (cm) | -71.90 ± 0.680 |
| b_5 (cm) | -19.78 ± 0.737 |
| b_5 (cm) | 94.75 ± 0.861 |
| b_6 (cm) | 44.36 ± 0.730 |
| b_6 (cm) | 157.72 ± 0.919 |
| b_7 (cm) | 78.16 ± 0.919 |
| b_8 (cm) | 11.46 ± 0.775 |
| b_9 (cm) | -83.75 ± 0.682 |
| b_10 (cm) | 56.17 ± 0.672 |
| b_11 (cm) | 64.55 ± 0.764 |
| b_12 (cm) | 38.28 ± 0.656 |
| b_13 (cm) | 77.29 ± 0.667 |
| b_14 (cm) | 35.09 ± 0.650 |
| b_15 (cm) | 278.01 |
| b_16 (cm) | 0.0000 |
| b_17 (cm) | 0.1689 |

| Model parameter adjustment | |
| b3 | -0.862 ± 0.004 |
| b3 | -0.3663 ± 0.003 |
| b3 | -0.0639 ± 0.001 |
| b3 | -0.0781 ± 0.001 |
| b3 | -0.0849 ± 0.001 |
| b3 | -0.6800 ± 0.003 |
| b3 | -0.1836 ± 0.002 |
| b3 | 0.0545 ± 0.001 |
| b3 | 0.0247 ± 0.001 |
| b3 | 0.0171 ± 0.001 |

Table 11.1: Summary of inversion results from different coupled solutions with varying weight on the bias and mascon parameter constraints. S_mascon is the scaling factor on the mascon constraint matrix relative to the data matrix, S bias is the scaling factor on the bias parameter constraint matrix relative to the data matrix, and D bias is the correlation distance of the bias parameters. The correlation distance and time of the mascon parameters are: D_mascon = 130 km and T_mascon = 10 days respectively for all solutions. RMS_KBR is the RMS of the KBR residuals, RMS_c is the RMS of the residuals with respect to storage from the GRACE mascon only solution used for the calibration presented in chapter 9, and RMS_c is the RMS of the residuals with respect to discharge. A priori values are listed in the second column, b_i is the bias parameter value for block i, and Σ b_i is the sum of the bias parameter values. b3, is the scaling factor on the model parameter (see section 5.5), and a3 is the absolute parameter value. The adjusted bias and model parameter values are listed ± their standard deviation. RMS values smaller than the a priori RMS value are marked in bold, since these represent an improved fit to the respective data type.

[1] The a priori RMS_KBR of the mascon only solution, is based on all mascon parameters being equal to zero, and is thus different from the a priori values of the rest of the solutions: RMS_KBR_a_prio_mascos = 0.30129 m/s.
### Chapter 11. Coupled model-mascon solution

#### Table 11.2: Summary of inversion results from different coupled solutions with varying bias parameter correlation distance. $S_{\text{mascon}}$ is the scaling factor on the mascon constraint matrix relative to the data matrix, $S_{\text{bias}}$ is the scaling factor on the bias parameter constraint matrix relative to the data matrix, and $D_{\text{bias}}$ is the correlation distance of the bias parameters. The correlation distance and time of the mascon parameters are: $D_{\text{mascon}} = 130$ km and $T_{\text{mascon}} = 10$ days respectively for all solutions. $RMS_{\text{KBRR}}$ is the RMS of the KBRR residuals, $RMS_{S}$ is the RMS of the residuals with respect to storage from the GRACE mascon only solution used for the calibration presented in chapter 9, and $RMS_{Q}$ is the RMS of the residuals with respect to discharge. A priori values are listed in the second column. $b_{i}$ is the bias parameter value for block $i$, and $\Sigma_{b_{i}}$ is the sum of the bias parameter values. $s_{x_{3}}$ is the scaling factor on the model parameter (see section 5.5), and $a_{3}$ is the absolute parameter value. The adjusted bias and model parameter values are listed ± their standard deviation. RMS values smaller than the a priori RMS value are marked in bold, since these represent an improved fit to the respective data type.

<table>
<thead>
<tr>
<th>Solution no.</th>
<th>A priori</th>
<th>Mascon</th>
</tr>
</thead>
<tbody>
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<td></td>
<td>$S_{\text{mascon}}$</td>
<td>$T_{\text{mascon}}$ (days)</td>
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<tr>
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</tr>
<tr>
<td>4</td>
<td>130</td>
<td>130</td>
</tr>
</tbody>
</table>

#### Bias parameter adjustments

<table>
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<tr>
<th>$b_{x_{1}}$ (cm)</th>
<th>$b_{x_{2}}$ (cm)</th>
<th>$b_{x_{3}}$ (cm)</th>
<th>$b_{x_{4}}$ (cm)</th>
<th>$b_{x_{5}}$ (cm)</th>
<th>$b_{x_{6}}$ (cm)</th>
<th>$b_{x_{7}}$ (cm)</th>
<th>$b_{x_{8}}$ (cm)</th>
<th>$b_{x_{9}}$ (cm)</th>
<th>$b_{x_{10}}$ (cm)</th>
<th>$b_{x_{11}}$ (cm)</th>
<th>$b_{x_{12}}$ (cm)</th>
<th>$b_{x_{13}}$ (cm)</th>
</tr>
</thead>
</table>

#### Model parameter adjustment

<table>
<thead>
<tr>
<th>$s_{x_{3}}$</th>
<th>$a_{3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0000</td>
<td>0.1689</td>
</tr>
</tbody>
</table>

**Footnote:** The a priori $RMS_{\text{KBRR}}$ of the mascon only solution, is based on all mascon parameters being equal to zero, and is thus different from the a priori values of the rest of the solutions: $RMS_{\text{KBRR,a priori,mascon}} = 0.30129$ m/s.
11.2.3 Bias parameter adjustments

A map of the bias parameters for solution #8 is shown in figure 11.3. The bias parameter values are positive in the western and north-western part of the model area, and negative in the eastern and south-eastern part. The vary in value from -13.44 cm to 6.29 cm (table 11.1, figure 11.3).

Though bias parameters represent the difference the model derived storage and GRACE derived equivalent water height, bias parameters can not be thought of as the absolute difference between the model storage output and a GRACE solution. First of all, the mean of the TWS from GLDAS/Noah (minus snow and canopy water) over a certain period was removed prior to the inclusion in the forward gravity model (section 6.4). Secondly, GLDAS/Noah might have problems in extreme hydrological conditions like drought and during large precipitation events. During a drought, the model may be completely drained, reaching a zero water level. During large rainfall events, the soil column may reach full saturation, leading the incoming water directly to runoff. Altogether, this causes a smaller amplitude of the hydrology signal from GLDAS/Noah, compared to the truth, and can possibly create biases in the model. Finally, the bias parameters will act as an "absorber" of errors in the mean gravity field (pers. com. J.-P. Boy and D. Rowlands). In summary, it is unlikely that the bias parameters should have a physical meaning.

11.2.4 Model parameter adjustment

The adjustment of the model parameter $a_3$, is negative for #1 to #7 and #11 to #14 and positive for the others. Figure 11.4 shows the magnitude of the parameter ad-
Chapter 11. Coupled model-mascon solution

Figure 11.3: Value of bias parameters for solution #8. Western coast line of Africa and model blocks are outlined in black.

Figure 11.4: Model parameter adjustments as a function of A) $S_{bias}$ (from table 9.1) and B) $D_{bias}$ (from table 11.2).

Adjustment as a function of the scaling of the bias parameter constraint ($S_{bias}$, 11.4A) and the bias parameter correlation distance ($D_{bias}$, 11.4B). There seems to be no obvious correlation between the sign of the adjustment and the scaling factors or correlation distance. However, positive adjustments are only seen when $S_{mascon} = 10^{-4}$, $S_{bias} \geq 10^{-2}$, and $D_{bias} \geq 100$ km. Additionally, the magnitude of the parameter adjustment is inversely proportional to the bias constraint scaling, when $S_{mascon} = 10^{-4}$ (#6 to #10), but not when $S_{mascon} = 2 \cdot 10^{-4}$ (#1 to #5) (see figure 11.4A).

11.3 Seasonal variations in Southern Africa

Description of the spatial distributions of amplitudes, and peak dates of the annual signal for the entire 5-year mascon solution (GRACE MO) was given in chapter 10. This section will focus on the terrestrial water storage from the coupled mascon so-
Figure 11.5: Amplitude of annual signal for the GRACE CO, GRACE MO solutions, as well as GLDAS and monthly SH solutions from UTCSR. Model area is marked in white.

The annual and semi-annual amplitude was fitted to all four TWS products for the period June 2004 to July 2005, a total of 14 months. Figure 11.5 shows the amplitudes of the annual signal, while figure 11.6 maps the peak date of the signal. The maximum and average annual amplitudes are listed, for the entire land area in table 11.3, and for the model area only in table 11.4.

Regarding the amplitude of the annual signal (figure 11.5), the GRACE CO solution outside the modeled area is similar to the GRACE MO solution and GLDAS, where amplitudes up to 21 cm are found for this particular year. Like for the 5-year analysis, the UTCSR solution shows a maximum amplitude which is approximately 25% lower, compared to the other three. It is also seen that UTCSR pattern is more smooth than the others. In the modeled area (marked in white), annual amplitudes are larger for GRACE CO compared to GRACE MO, GLDAS, and UTCSR. This is
Chapter 11. Coupled model-mascon solution

<table>
<thead>
<tr>
<th>All land blocks</th>
<th>GLDAS</th>
<th>GRACE CO</th>
<th>GRACE MO</th>
<th>UTCSR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum amplitude [cm]</td>
<td>20.16</td>
<td>20.73</td>
<td>20.92</td>
<td>14.01</td>
</tr>
<tr>
<td>Average amplitude [cm]</td>
<td>7.81</td>
<td>8.06</td>
<td>8.04</td>
<td>6.38</td>
</tr>
</tbody>
</table>

Table 11.3: Maximum and average amplitude of the annual signal for the coupled solution (GRACE CO), the mascon only product (GRACE MO), the monthly UTCSR solutions, and the corresponding TWS from GLDAS/Noah. Averages are computed for all 382 land blocks.

Figure 11.6: Phase of the annual signal from the GRACE CO, GRACE MO and GLDAS. Model area is marked in black.

mostly valid for the northern part of the model (north of 16°S). As seen in chapter 10, the two mascon solutions (GRACE CO and GRACE MO), show locally lower annual amplitudes over lakes Tanganyika and Malawi, probably caused by a zero surface water storage in GLDAS.

The peak time for the annual signal is shown in figure 11.6. The spatial distribution of timing of the signal peak for the two GRACE mascon solutions (MO and CO) are similar. Figure 11.7A shows the number of land blocks that peak each month, while 11.7B shows the difference in days between peaks in each of the GRACE solutions relative to GLDAS, for all land blocks. Though all four signals have most blocks peak within the same month (March) for this 1-year comparison (figure 11.7A), the delay of about 70% of the blocks in GRACE CO and GRACE MO is between 1 and 30 days, while this is only seen for 57% of all blocks in the UTCSR solution (figure 11.7B).
Figure 11.7: A) Peak-time for the 382 land blocks in the area, divided into monthly bins. B) Difference in peak-time between GRACE and GLDAS for the 382 land blocks. Data from 14 months were analyzed: June 2004 to July 2005, and the reference date is 01/01/2005. 71% and 73% of all land blocks in GRACE CO and GRACE MO respectively, have a delay between 1 and 30 days relative to the fitted GLDAS signal.

<table>
<thead>
<tr>
<th>Model blocks only</th>
<th>GLDAS</th>
<th>GRACE CO</th>
<th>GRACE MO</th>
<th>UTCSR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum amplitude [cm]</td>
<td>16.79</td>
<td>20.00</td>
<td>17.92</td>
<td>11.01</td>
</tr>
<tr>
<td>Weighted average amplitude [cm]</td>
<td>11.39</td>
<td>14.79</td>
<td>12.09</td>
<td>7.73</td>
</tr>
<tr>
<td>Weighted average peak date</td>
<td>20-Mar</td>
<td>12-Apr</td>
<td>08-Apr</td>
<td>08-Apr</td>
</tr>
</tbody>
</table>

Table 11.4: Maximum amplitude, average amplitude, and phase of annual signal the coupled solution (GRACE CO), the mascon only product (GRACE MO) and the corresponding TWS from GLDAS/Noah. Averages are computed only for the model blocks, weighted according to the number of modeled cells in each block (figure 4.7).

11.4 Time variable storage in the Okavango River Basin

A time series of the weighted average storage for all blocks in the model area, is shown in figure 11.8, and the maximum and average amplitudes are listed in table 11.4. The mean value of the signal was subtracted in figure 11.8. The two mascon solutions (GRACE MO and GRACE CO) are similar in both average amplitude and phase, while GLDAS differs by having an earlier peak date and UTCSR by having lower amplitudes (table 11.4).

11.5 Model performance after July 2005

The GRACE CO solution was produced using just 18 months of GRACE level-1B data (April 2004 to September 2005). The reason that the entire GRACE time series was not used, is that the computational time would be tremendous. The model was initially calibrated against 5 years (September 2003 to August 2008) of discharge and
Chapter 11. Coupled model-mascon solution

Figure 11.8: Weighted average time series of the GRACE MO, GRACE CO, GLDAS, and UTCSR signals as well as the fitted annual signals for all, computed from all blocks in the model of the Okavango River Basin. Model area location is shown in figures 11.5 and 11.6, and on figure 6.4. The average is weighted according to the number of cells in each block that is included in the model (figure 4.7).

<table>
<thead>
<tr>
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<th>14 months</th>
<th>5 years</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$RMS_Q$ [m$^3$/s]</td>
<td>$RMS_S$ [cm]</td>
</tr>
<tr>
<td>Pre-inversion</td>
<td>134.77</td>
<td>2.9330</td>
</tr>
<tr>
<td>Post-inversion</td>
<td>124.03</td>
<td>2.9183</td>
</tr>
<tr>
<td>Improvement</td>
<td>8.0%</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

Table 11.5: RMS of data residuals pre and post the least squares inversion, for the calibration period (14 months) and for a 5-year period. Improvement is given in percentage relative to the pre-inversion RMS value.

equivalent water storage from GRACE (chapter 9), so the fit is already good for the entire period, even though only part of it was used for the coupled least squares inversion. It has already been explored how much the improvement in the RMS of the data residuals are for the 14 months\(^1\) (June 2004 to July 2005) used in calibration, but here the RMS values are presented for the entire 5 year period. Table 11.5 shows the $RMS_Q$ (fit with respect to discharge) and $RMS_S$ (fit with respect to storage from GRACE MO) values before (pre-) and after (post-) the inversion for the 14-month period (also shown in table 11.1 and 11.2), and for the 5-year period. The table also lists the improvement in percentage relative to the pre-inversion fit. Figure 11.9 shows the observed and pre- and post-inversion simulated equivalent water storage in cm, and the discharge at Mohembo gaging station in m$^3$/s.

Like it was seen in tables 11.1 and 11.2, the post-inversion fit is improved compared to the pre-inversion fit for the 14-month period. The improvement is 8% for the discharge and 0.5% for the equivalent water storage. For the 5-year period, the fit to discharge is improved by 4.6%, while the fit to equivalent water storage is worsened by 2.3%. As expected, the overall fit is still relatively good, and as figure 11.9 shows, there is not much difference in the output from the two model runs.

\(^1\)The first and last two months were removed due to marginal effects (see section 7.5).
Figure 11.9: 5-year fit of equivalent water height (top) and discharge at Mohembo gaging station (bottom), for the adjusted parameter $a_3$ before and after the least squares inversion.
Chapter 12

Summary of Krogh et al. (2010)

This chapter provides a short summary of the work published in Krogh et al. (2010), which is also a part of this Ph.D. project. The article explores the use of regional constraints on small hydrological sub-catchments in Southern Africa.

Regional constraints vs. isotropic constraints were tested on 19 sub-catchments of the four river basins: Zambezi, Okavango, Limpopo, and Orange, for a 13-month period: July 2003 through July 2004. The block size used is 1.25°×1.5°, and the smallest regions consist of only four mascon blocks, while the largest cover as many as 16 mascon blocks. The correlation time and distance used was 10 days and 130 km, and the forward gravity model was v.02, which has no hydrology signal included (see section 6.4). Comparisons of annual amplitude were made with other 10-day terrestrial water storage products, like GLDAS/Noah, 4°×4° global mascons, and CNES/GRGS storage from GRACE. It was found that the regional solution in general had a maximum amplitude that was 40-80% larger (up to ~31 cm of water) than all other products in the comparison (see table 12.1).

The Noah land surface model is a soil moisture model, which does not include surface water bodies like Lake Malawi in the Zambezi Basin, and a correction of GLDAS/Noah with altimetry lake levels of Lake Malawi from Jason-1 and TOPEX/POSEIDON, was made for comparison with the regional solution. Under the assumption of vertical banks of the lake, the equivalent water level from GLDAS/Noah of the region where Lake Malawi is located, was brought from 11.1 cm to 18.9 cm when including the lake level variations from altimetry. This water level was found to compare well with the average storage from the regional mascon solution in the area, of 17.4 cm of water.

The study shows that there are more details to be recovered from the GRACE data, than what had previously been achieved with spherical harmonic solutions and

<table>
<thead>
<tr>
<th></th>
<th>1.25°×1.5° mascons</th>
<th>4°×4° mascons</th>
<th>CNES/GRGS</th>
<th>GLDAS/Noah</th>
</tr>
</thead>
<tbody>
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<td>Regional constraints</td>
<td>31 cm</td>
<td>19 cm</td>
<td>17 cm</td>
<td>22 cm</td>
</tr>
<tr>
<td>Isotropic constraints</td>
<td>19 cm</td>
<td>20 cm</td>
<td>22 cm</td>
<td>20 cm</td>
</tr>
</tbody>
</table>

Table 12.1: Maximum amplitude of annual signal for five comparable continental water storage products. From figures 3 and 4 in Krogh et al. (2010).
4°×4° mascons. While the regional approach may be a little overoptimistic in the sense that the resolution of the GRACE data is not nearly good enough to resolve mass variations in regions this small, the idea of using hydrological regions, either larger in size or with some (weaker) constraints across regions, is certainly feasible.

Recently, Boy et al. (2011) used the regional approach on 2° equal area mascons over the entire African continent and surrounding areas, testing both a seven (land vs. ocean) and a 17 (individual river basins defined in Africa) region setup. The smallest region, being the Red Sea, consists of 13 (2°) blocks, which is probably a better choice of region size than what was tested in Krogh et al. (2010). With both setups, they obtain good solutions with approximately the same maximum amplitude as an isotropically constrained solution in the African continent, while Southern Europe shows larger amplitudes in the regional solutions, which is consistent with precipitation data. In particular, they find that when ocean and land blocks are evaluated separately, the variations over the oceans are closer to zero, and small areas with large seasonal variations, like Europe and the Red Sea, are better resolved with the regional approach.
Chapter 13

Summary & conclusion

In this thesis, a novel approach for calibration of a large scale hydrological models by using Gravity Recovery And Climate Experiment (GRACE) data, is presented. The study areas is the Okavango River basin in Angola, Namibia, and Botswana.

A joint sequential calibration of a regional Budyko-type model, against discharge and terrestrial water storage variations from GRACE mascon only solutions, was performed on eight different model parameters.

Two types of data, discharge and total water storage, were used in the calibration. High correlation coefficients and large 95% confidence intervals were found on some parameters, and a number of different parameter sets were found to fit the calibration data well. Two calibrations runs however, provided the best least squares fit to both discharge and storage. An evaluation of the individual water fluxes and storages (evapotranspiration from the soil, preatic evapotranspiration, flow loss, recharge, soil storage, groundwater storage, and discharge) was performed, in order to assess how realistic these “best fitting” models were. It was found that the two parameter sets that provided the best joint least squares fit to discharge and storage, produce an unrealistic high flow loss and low (zero) soil storage/evapotranspiration.

The conclusion drawn from this is that the model lacks complexity, to accurately simulate both storage and discharge, and that the parameters which produce the best least squares fit to the calibration data, is not always the best parameter set to produce realistic storage and flux components. Another problem is that precipitation products, that are used as input in the hydrological model, vary greatly over Southern Africa, which introduces a great uncertainty.

Experiments with different weights on the two data types revealed a typical Pareto front, balancing the fit to discharge with the fit to storage. The “break” in the Pareto front was found to occur when the weight on the storage data is between 0.5 and 0.9. Furthermore, most of the variable parameters were found to be relatively insensitive to small changes in the data weighting, when the weight on storage was between 0.6 and 0.8. The weighting of storage data chosen for the final calibration was 0.75, since this weight balances the information from the terrestrial water storage and discharge well.
The terrestrial water storage product used for the sequential calibration, is a 5-year (September 2003–August 2008) GRACE mascon product assembled from five overlapping 18-month mascon solutions. Compared to the terrestrial water storage from GLDAS/Noah for the same time period, the seasonal variations from GRACE are found to be similar, but the timing of the signal peak is approximately 20 days earlier in GLDAS/Noah than in the GRACE mascon only solution. The similarity to GLDAS/Noah was expected since the TWS from GLDAS/Noah was used in the forward gravity model applied in the least squares inversion to generate the mascon solutions.

Comparison with monthly UTCSR spherical harmonic solutions, show that the mascon solutions provide a higher resolution, since more spatial variations are seen. Also, the UTCSR underestimates the amplitude of the annual signal, compared to both GLDAS/Noah and the GRACE mascon only solution.

In a coupled approach, a number of mascon parameters were replaced by one hydrology parameter, thus reducing the total number of parameters. The transformation from one type of parameter to another, was done through chaining of partial derivatives. In the least squares inversion of the normal equation system, different scaling factors on the mascon parameter constraints, and on the bias parameter constraints, were tested. Additionally, different correlation distances on the bias parameters were tried.

Results showed that the best correlation distance for the bias parameter constraints, is equal to one block spacing (∼130 km), and that the best scaling of the bias parameter constraints was $10^{-2}$ relative to a scaling factor of 1 on the data matrix. The best scaling of the mascon constraint equations was found to be $10^{-4}$.

The use of regional constraints instead of isotropic, showed that improvement of the resolution of GRACE data is possible by the use of regional constraints. For small regions some constraints should still be applied across region boundaries, while larger regions will not need additional constraints.

The novel approach of calibrating large scale hydrological models presented here, show great potential. Within the time frame of this Ph.D. project, application of the method on larger models and longer time scales was not possible, but should be performed in order to explore and outline the possibilities of the coupling method.

In this thesis, 18-month mascon solutions where the first and last two months are removed due to insufficient temporal constraints, are used. Already, for the 18-month solutions, the computation time for the least squares inversion is long (∼20 hours). Sabaka et al. (2010) introduced a more efficient inversion algorithm than the method used in this study, based upon the conjugate gradient method, reducing the computation time and storages requirements, and thus making inversion of longer time series possible. Another problem in the coupling method, is the problem of patching time-wise overlapping solutions, like for the mascon only solution, when the hydrology parameters are constant in time. This problem could be solved by application of the more efficient inversion method, if the entire time period could be inverted in one step.
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Appendices
Appendix A: Mascon terminology

**Coupled solution**
A mascon solution where the parameters in $x$ are both mascon parameters and model parameters.

**Isotropic constraints**
Spatial constraints applied so that all mascon parameters are constrained to all other mascon parameters, regardless of location. Note: For the work done in this Ph.D. project, the term "isotropic constraints" are used even though land and ocean blocks are constrained separately, which is in principle a regional approach. The word "isotropic" refers to the fact that all land blocks are constrained together.

**Isotropic solution**
A mascon solution made with isotropic constraints.

**Mascon block**
A predefined spatial area for which the mascon parameters are evaluated. The study area is divided into 644 mascon blocks of the size $1.25^\circ \times 1.5^\circ$ and $1.5^\circ \times 1.5^\circ$.

**Mascon parameter**
The equivalent terrestrial water storage in cm of water, in a certain mascon block at a certain 10-day epoch. For the study area of 644 mascon blocks, the number of mascon parameters is $644 \cdot n_t$, where $n_t$ is the number of epochs.

**Mascon solution**
A set of mascon parameters ($x$), which are the result of a least squares inversion of a normal equation system containing as minimum a data matrix ($A$), and data residuals ($y$) on the right-hand-side:

\[ A \cdot x = y \]

Sometimes also called **mascon only solution**, referring to the fact that $x$ contains only mascon parameters.

**Regional constraints**
Spatial constraints applied on a regional level, where mascon blocks are divided into separate areas. Each mascon parameters is constrained only to other mascon parameters that are located in the same region. The time constraining is the same as for isotropic constraints.

**Regional solution**
A mascon solution made with regional constraints.
Appendix B: 
Water balance components from calibration runs

In chapter 9, five calibration runs were presented. Figure 9.1 shows the water balance fluxes: soil evapotranspiration, pheatic evapotranspiration, flow loss, recharge and discharge, as well as the storages: soil water and groundwater, for the five runs in the period June 2004 till July 2005. This appendix shows the entire calibration period, which is September 2003 till August 2008.
Figure B.1: Components of the water balance from the five calibration runs listed in tables 9.1 and 9.2 in mm or mm/day (except for discharge). Each curve is the weighted mean of the 7 sub-models. The discharge is the cumulated discharge, summed over all 7 sub-models and routed through the linear reservoir, and is hence comparable to the observed discharge at Mohembo (not shown). The calibration period is September 2003 till August 2008, while model output is shown for January 2003 till December 2008.
Appendix C: Published work

The following article was published as a part of this Ph.D. project. The article is included on the pages hereafter.

Evaluating terrestrial water storage variations from regionally constrained GRACE mascon data and hydrological models over Southern Africa – preliminary results

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A concentration of surface mass has a distinct, localized signature in Gravity Recovery and Climate Experiment (GRACE) K-band range rate (KBRR) data. This fact is exploited in the regional solutions for mass concentration parameters (mascons) made at the Goddard Space Flight Center (GSFC). In this paper we explore an experimental set of regionally constrained mascon blocks over Southern Africa where a system of 1.25° × 1.5° and 1.5° × 1.5° blocks has been designed. The blocks are divided into hydrological regions based on drainage patterns of the largest river basins, and are constrained in different ways. We show that the use of regional constraints, when solving mascon parameters of different hydrological regions independently, yields more detail and variation than comparable spherical harmonic solutions and mascon solutions using isotropic constraints. We validate our results over Lake Malawi with water level from altimetry. Results show that weak constraints across regions in addition to intra-regional constraints are necessary, to reach reasonable mass variations.

1. Introduction

Hydrological models have traditionally been calibrated using in situ surface water and groundwater levels as well as river discharge data from local gauges. However, the spatio-temporal resolution and coverage of this data is very often inappropriate for regional-scale water resources applications. In many regions of the planet, few reliable point observations of water level and discharge are available, and a number of drainage basins on the African continent are un-gauged, making other ways of calibrating hydrological models necessary.

The focus of this study is on the southern part of Africa where water availability is strongly seasonal, and open water bodies are often found in the wet periods, especially in the north of the area. The four river basins covering the study region are the Zambezi, the Okavango, the Limpopo, and the Orange River basin. The results presented here are mainly from the Zambezi region.

The Zambezi River basin is situated south of the large Congo River basin, where very intense rainfall occurs in the summer months. The outlet of the Zambezi basin is

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to the east, into the Indian Ocean. The Okavango delta lies south-west of the Zambezi and drains the wet highlands of Angola. The Okavango basin is an endorheic river basin; at its downstream end the water spreads out to form a huge inland delta, the Okavango Delta, in northern Botswana, where it infiltrates or evaporates during the fall and winter months. South of the Zambezi and south-east of the Okavango, the smallest of the four rivers, the Limpopo, drains the eastern highlands of the region into the Indian Ocean. Further south, the large catchment area of the Orange River, where precipitation is sparse compared to the northern part of the area, drains towards the south-west into the Atlantic Ocean. Generally, precipitation is strongly seasonal and the amount decreases towards the south and east. The Kalahari Desert takes up a large part of the Okavango and northern Orange basins. The rainy season takes place in the summer months (December–February) and the peak in terrestrial water storage is in the fall (March–April) whereas the dry season peaks in late spring (November). Large seasonal wetlands, which are hydrologically complex and scarcely monitored, are located in the northern part of the area (mainly in the Zambezi and Okavango drainage basins).

The Gravity Recovery and Climate Experiment (GRACE) satellites capture the gravity signal from the change in total mass of water in an area (e.g. Tapley et al. 2004, Wahr et al. 2004, Han et al. 2005, Crowley et al. 2006). The inherent spatial and temporal resolution of GRACE data is around 200–400 km and 10 days (Rowlands et al. 2005), which enables the use of GRACE data for calibration of large-scale hydrological models on both global and regional scales (e.g. Niu and Yang 2006, Günther 2008, Werth et al. 2009). In the following we present a system design of regionally constrained mass concentration blocks (mascons) over Southern Africa and compare these with 10-day GRACE solutions and output from the Global Land Data Assimilation System (GLDAS)/National Centers for Environmental Prediction/Oregon State University/Air Force/Hydrologic Research Lab Model (Noah) land surface model with observation based forcing (for precipitation, Climate Prediction Center Merged Analysis of Precipitation (CMAP) is used) (Rodell et al. 2004; see http://disc.sci.gsfc.nasa.gov/hydrology/data-holdings), which has previously been used to validate GRACE observations of terrestrial water storage change on inter-annual scales (e.g. Andersen and Hinderer 2005). Finally, we validate our results for the Lake Malawi region in the eastern Zambezi basin where ground truth in the form of lake level changes is available from satellite altimetry.

2. Regionally designed mascons for the Southern Africa drainage regions

We explore the use of mascons which enable the study of sub-monthly terrestrial water storage (TWS) variations, at a higher resolution than most global GRACE solutions. The advantage of using the mascon approach lies in the fact that the signature in the GRACE K-Band Range-Rate (KBRR) observations associated with each mass concentration manifests itself directly over the area of excess mass, because both GRACE satellites are subject to the same perturbation by the excess mass, only displaced in time, as they pass over the mascon (Rowlands et al. 2010). Consequently, regional solutions can be derived using only the data from directly overflying the region of interest for each specific mascon (Han et al. 2008).

Currently available mascon solutions (http://grace.sgt-inc.com/) use a block size of $4^\circ \times 4^\circ$, and a temporal resolution of 10 days (Rowlands et al. 2005). To increase the
spatial resolution and evaluate mascons in specific regions, we have designed a system of $1.25^\circ \times 1.5^\circ$ and $1.5^\circ \times 1.5^\circ$ blocks over the target area, and assigned each block to a hydrological region, in order to make use of the shape of the individual drainage basins in evaluating the mascon solutions. The entire Southern Africa region has been divided into 644 small blocks, $1.25^\circ \times 1.5^\circ$ north of $26^\circ$ S and $1.5^\circ \times 1.5^\circ$ south of $26^\circ$ S (figure 1). All central land blocks (165 blocks in total) have been assigned to one of the afore-mentioned four river basins, according to their location (figure 1: thick grey lines). The ocean blocks and the marginal land blocks that could not be assigned to one of the four river basins were arranged into marginal regions. Furthermore, river basin blocks have been grouped in smaller drainage regions (figure 1: black outlines) in order to separate the hydrological signal of each sub-catchment from the others. The sub-catchments are derived from Shuttle Radar Topography Mission (SRTM) data (http://seamless.usgs.gov/index.php), and the Watershed Delineator tool in ArcSWAT 2.0.0 (Gassman et al. 2007, Arnold and Fohrer 2005). They are shown in figure 1 as light grey irregular lines.

The exceptional spatial and temporal (10-day) resolution of this GRACE solution procedure is attained by preserving the gravity information contained within the GRACE inter-satellite range-rate measurements, and by parameterizing local mass variations as mass concentrations (mascons) (Rowlands et al. 2005, Luthcke et al. 2006).

Figure 1. Overview of the system design. The coastline outlines the southern part of Africa. Light grey irregular lines show the sub-catchments of the river basins, derived from SRTM data. Dotted north–south and east–west going lines are the mascon blocks and the solid straight lines show the hydrological regions we have chosen for constraining the mascons. Regions 1–7 correspond to the Zambezi River basin with Lake Malawi in region 4. Regions 8–10 correspond to the Okavango River basin. Regions 11–14 correspond to the Limpopo River basin. Regions 15–19 correspond to the Orange River basin.
In order to keep the inversion stable, mascon parameters are constrained to one another. For each pair of mascons a constraint equation is written to force the parameter values (which are the equivalent water height of the mascon block) of the pair to be equal to each other. If equal weights are assigned to all constraint equations, no temporal or spatial variation would be visible, and therefore the assigned weight depends on the distance between a pair of mascon parameters in time and space. The following weighting formula is used on the constraint equations

\[ w_{ij} = S \exp \left( 2 - \frac{d_{ij}}{D} - \frac{|t_{ij}|}{T} \right), \]  

where \( w_{ij} \) is the weight assigned to the constraint between mascon \( i \) and \( j \), \( S \) is a scaling factor on the constraints used to adjust the weight on the constraints relative to the weight on the data, \( D \) and \( T \) are the correlation distance and time, and \( d_{ij} \) and \( t_{ij} \) are the distance between mascon \( i \) and \( j \) in space and time respectively (Rowlands et al. 2010). The correlation constants \( (D \) and \( T) \) have to be large enough to effectively constrain a mascon parameter to neighbouring parameters, but also small enough for spatial and temporal variation to show in the solution. For monthly solutions, temporal constraints are generally not needed and spatial constraints can be smaller than for sub-monthly solutions. Rowlands et al. (2005, 2010) found that a correlation distance \( D \) equal to one block spacing works well, and used a correlation time \( T \) of 10 days for 10-day solutions. In this study, we have gradually decreased \( D \) to observe the effects, and have found that \( D = 130 \) km is appropriate. For the correlation time we have used \( T = 10 \) days. Additional information about mass anomalies, mascons and constraints can be found in Rowlands et al. (2005, 2010) and Han et al. (2008). Traditionally, isotropic constraints are applied so that all blocks are constrained to all other blocks using the weighting of equation (1) (figure 2(a)). In a regional set-up however, each block is constrained only to other mascon blocks within the same hydrological region and there are no constraints across regional boundaries (figure 2(b)), making the overall constraints anisotropic.

Figure 2. Value of the weighting function (equation (1)) of traditional, isotropic constraints (IC) versus regional constraints (RC) with correlation distance \( D = 250 \) km and a zero difference in time \( (t_{ij} = 0 \) days), as a function of inter-block distance \( d_{ij} \). (a) Isotropic constraints where each block is constrained with isotropic weights. (b) Regional constraints where one block is constrained only to other mascon blocks in the same hydrological region.
This allows the individual regions to vary independently of neighbouring regions, and thus makes sure that local highs and lows are not smeared over a large area.

3. Comparison between GRACE and hydrological models on annual scales

We have investigated data from one year (July 2003–July 2004) and are using two new mascon solutions: an isotropically constrained solution (IC), and a solution constrained with a regional weighting principle (RC); see figure 2(b). Both are constrained with a correlation distance and time of 130 km and 10 days respectively. The final solution is given to order and degree 120 and has a temporal resolution of 10 days. In the following, these will be compared on an annual scale to both mascon and spherical harmonic GRACE solutions with a 10-day temporal resolution, as well as with the GLDAS/Noah output.

The GLDAS/Noah 3-hour temporal and $0.25^\circ \times 0.25^\circ$ spatial resolution soil-moisture fields were integrated over each 10-day GRACE interval and $1.25^\circ \times 1.5^\circ/1.5^\circ \times 1.5^\circ$ blocks in order to mimic the temporal and spatial resolution of the new GRACE mascon solutions (figure 3(a)).

Joint NASA/Goddard Space Flight Center (GSFC) and SGT-Inc Access Mascons are available via WEB2 as $4^\circ \times 4^\circ$ blocks. They have a temporal resolution of 10 days, are supplied for all non-polar land areas, and have been computed using isotropic constraints with a correlation distance of 250 km and a correlation time of 10 days (figure 3(b)).

This study uses 10-day Groupe de Recherche de Géodésie Spatiale/Centre National d'Etudes Spatiales (GRGS/CNES) spherical harmonic (SH) solutions (Lemoine et al. 2007, http://bgi.cnes.fr:8110/geoid-variations/README.html) as normalized SH geopotential coefficients of equivalent water storage variations, up to degree and order 50. A constraint towards the mean field is applied to stabilize and de-stripe the solutions, mainly from degree and order 30 and up. Data are given every 10 days as monthly means, centred on 10 days based on the running average of three 10-day data periods with weights 0.5/1.0/0.5. The $1^\circ \times 1^\circ$ grids have been re-sampled to the resolution of our system ($1.25^\circ \times 1.5^\circ/1.5^\circ \times 1.5^\circ$ in the southern part) for comparison (figure 3(c)).

The access mascons ($4^\circ \times 4^\circ$) and the spherical harmonic solution from GRGS/CNES are given only to degree and order 60 and 50 respectively, which is not comparable with the new mascon solutions given to order and degree 120. In order

Figure 3. Amplitude of the annual signal for comparable 10-day GRACE solutions and GLDAS. (a) GLDAS/Noah hydrological model. (b) $4^\circ \times 4^\circ$ access mascons. (c) Spherical harmonic solution from GRGS/CNES to degree and order 50. GRGS/CNES and GLDAS/Noah have been re-sampled from $1^\circ$ arc-degree resolution to the resolution of our system ($1.25^\circ \times 1.5^\circ/1.5^\circ \times 1.5^\circ$). All data used are from the period July 2003–July 2004. The colour scale is the same for (a), (b) and (c) and the unit is eq. water height in cm.
to compare the amplitudes of the new RC regional solution with these, we have truncated the solution at order and degree 50. Figure 4 shows the annual signal of the new mascon solutions for the period July 2003–July 2004. Figure 4(a) shows the solution with traditional isotropic constraints (IC) and figure 4(b) with regional constraints (RC). Figure 4(c) is the truncated regionally constrained solution (RC50).

The regional solution (RC) (figure 4(b)) shows much more variation from region to region, and hence gives more information about the variation in the hydrology of the area than the isotropically constrained solution (IC) (figure 4(a)). In the truncated version of the RC solution (RC50) the amplitudes are damped and the boundaries are smoother compared to the full RC solution. This is due to the use of fewer spherical harmonic coefficients. Table 1 shows the average amplitude of both solutions for each region, as well as the difference between them. The rows have been sorted by river basin and amplitude of the RC solution. The general trend is that the northernmost part of the area (regions 3–7 and 10) show the largest differences between the two solutions. Here the RC amplitudes are higher (for some regions considerably) than the IC amplitudes. Exceptions are region 6 in the north where the RC amplitude is lower than the surroundings; and regions 15 and 18 in the south, where the RC amplitudes are higher than the surroundings (figure 4(b) and table 1 (italicized)). Moreover, there seems to be a correlation between the RC amplitudes and the IC–RC difference for all four basins.

Annual equivalent water storage variations are significantly higher in the new regionally constrained mascon solution (RC) (more than 30 cm of water) (figures 4(b) and 4(c)) compared to the isotropically constrained solution (IC) (up to about 17 cm of water) (figure 4(a)), and the other GRACE solutions (up to approximately 15 cm for the access mascons and 23 cm for the GRGS/CNES SH solution) (figures 3(b) and 3(c)). The IC solutions (figure 4(a)) and the access mascon solution (figure 3(b)) are both fully constrained solutions, in the sense that all blocks are constrained to each other, which does not allow for a lot of variation, and hence dampens the amplitude of the signal. The spherical harmonic solution (GRGS/CNES) (figure 3(c)) has been derived using constrained inversion, and we can therefore also expect the amplitudes of this solution to be slightly damped. The GLDAS/Noah version used for this comparison uses the CMAP precipitation input, the reliability of which might be questionable over Southern...
Table 1. The average amplitude (cm of water) of the annual signal for all regions in both solutions and the difference between them, listed according to river basin and amplitude in the regional solution (RC). Italicized regions stand out compared to the surrounding regions (see text in §3).

<table>
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<th>Difference</th>
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<td>9</td>
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<tr>
<td></td>
<td>8</td>
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Africa. Additionally, Noah is a grid-based soil moisture model that does not include groundwater storage and surface water bodies. The GLDAS output is therefore not expected to replicate the true amplitude of the total TWS (figure 3(a)), and lower amplitudes in GLDAS than in GRACE are not surprising. While the new regional solution may have questionably high amplitudes and variability, we do not have any other GRACE solutions or models that are fully comparable in order to reject or validate the results. Even though it is hard to argue for such large variations from region to region from a hydrological point of view, as most of the annual signal is driven by storage in the soil column and in shallow aquifers (Leiriao 2007, Michailovsky 2008), there are still some interesting things about the RC solution:

1. When comparing the IC and the access mascon solution we see very little difference, which indicates that we are not gaining much new information by using smaller blocks. This is not the case for the RC solutions which provide new information.

2. Region 8 is located in the Kalahari Desert and hence a particularly dry region with little or no precipitation, and only rarely inflow from region 9. Region 9, on the other hand, though also located at the rim of the desert, has quite a large seasonal input of water from region 10, which contains the highlands of Angola. In region 9 the water from the rivers Cuito and Cubango joins to form the Okavango River, which empties its water into the wetlands of the Okavango Delta just north of the Kalahari Desert, where it evaporates or infiltrates. This difference between regions 8 and 9 is clearly seen in the new RC solution (RC) (figure 4(b)), because regional constraints are used, while the IC solution, due to isotropic constraints, shows almost no variation (figure 4(a)).
4. Evaluation in the Lake Malawi region

To validate the relatively large amplitudes in the regionally constrained mascons, we have carried out an investigation in the region around Lake Malawi in the northern Zambezi basin. This region was chosen for validation because of its large surface water body, which is not included in GLDAS. Furthermore, the lake’s water level is available from altimetry data. Lake Malawi takes up about 13% of the surface area of the region, and a variation in the lake’s water level will certainly have an effect on the GRACE data. All of the GRACE solutions presented include the signal from the lake, but since the GLDAS/Noah land surface model (LSM) is a one-dimensional column soil moisture and canopy model, it does not account for overland water bodies or oceans, and the annual signal thus has zero amplitude in the lake area (figure 5).

We have applied a correction to the average amplitude of the GLDAS output in the region to account for water storage variations in Lake Malawi, in order to compare water storage from GLDAS to the regional mascon solution for this region. For this we use satellite altimetry, made available by the Earth and Planetary Remote Sensing (EAPRS) laboratory via the ESA river and lake website (http://www.cse.dmu.ac.uk/EAPRS/projects_riverlake_overview.html). All standard range and geophysical corrections applicable to lake data have been applied and outliers have been removed. Lake level variations from Envisat (medium grey) and Jason-1 (black) are shown in figure 6. Data from Topography Experiment for Ocean Circulation (TOPEX)/POSEIDON (dark grey) and ERS-2 (light grey) up to 2002 are also shown in the figure along identical passes to confirm the amplitude found by Jason-1 and Envisat.

In the period of interest for this project (July 2003–July 2004), the peak-to-peak water level variation measured by Envisat is 1.4 m. Jason-1 data (black) is only available for the first 3/4 of this period, and the amplitude of the annual variation according to Jason-1 seems to be a little lower (closer to 1 m) than what is found by Envisat, since Jason-1 does not capture the peak values as well as Envisat. This can be due to the different sampling times and ground track locations of the two satellites, and gives us an idea of the uncertainty in the measurements. In the following we use an average of the observed variation from Envisat and the estimated variation from Jason-1: 1.2 m. In order to estimate the total water volume in Lake Malawi, we assume the lake to have vertical
banks. Calculations show that the maximum error in volume when using this approximation, compared to a situation with leaning banks, is small relative to the additional water volume in the lake caused by a 1.2 m rise in water level. Furthermore, thermal effects have been interpreted as mass change signals. Calculations are presented in table 2.

Table 2. Calculations of Lake Malawi-correction applied to GLDAS/Noah.

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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>A</td>
<td>Region 4 surface area</td>
<td>227 000 km²</td>
</tr>
<tr>
<td>B</td>
<td>Lake Malawi surface area</td>
<td>29 600 km²</td>
</tr>
<tr>
<td>C</td>
<td>Variation in water level (July 2003–July 2004)</td>
<td>Figure 6† 1.20 m</td>
</tr>
<tr>
<td>D</td>
<td>Extra water volume equivalent to variation in water level</td>
<td>(C × B) 35.5 km³</td>
</tr>
<tr>
<td>E</td>
<td>Uniform layer of water over reg. 4 equivalent to extra water volume</td>
<td>D/A 15.6 cm</td>
</tr>
<tr>
<td>F</td>
<td>Amplitude of annual signal equivalent to uniform layer of water</td>
<td>E/2 7.82 cm</td>
</tr>
<tr>
<td>G</td>
<td>Average amplitude of GLDAS over region 4 including unmodelled lake area</td>
<td>Figure 3(a)‡ 11.1 cm</td>
</tr>
<tr>
<td></td>
<td>Average amplitude of GLDAS (incl. Lake Malawi-correction) over region 4</td>
<td>G + F 18.9 cm</td>
</tr>
<tr>
<td></td>
<td>Average amplitude of regionally constrained mascons over region 4</td>
<td>Figure 4(b)‡ 17.4 cm</td>
</tr>
<tr>
<td></td>
<td>Lake Malawi-correction in percentage for scaling of GLDAS</td>
<td>F/G +70%</td>
</tr>
</tbody>
</table>

†Average amplitude estimated from figure 6.
‡Average amplitude calculated from the data shown in figure.
The volume of water that corresponds to an annual lake level variation of 1.2 m is equivalent to adding a 7.82 cm thick layer of water over all of region 4, which is equal to 70% of the GLDAS/Noah signal. Therefore, our Lake Malawi correction (LM-correction) to GLDAS/Noah will be an up-scaling of the signal by 70%. This brings the average annual water storage amplitude of region 4 up to 18.9 cm, relative to which the average estimated amplitude of 17.4 cm for the new regionally constrained solution (RC) is 7.9% lower. The high amplitudes of Lake Malawi region are therefore in agreement with the hydrology. The fact that the amplitude of the LM-corrected GLDAS values are even higher than the GRACE solution might be explained by horizontal water transport from the surroundings to Lake Malawi, which potentially will cause the water to be ‘counted’ twice in the calculations.

In order to investigate a hydrological model that includes Lake Malawi, we introduce a model of the Zambezi Basin by Michailovsky (2008). A catchment based semi-distributed model of the Zambezi River basin was built using SWAT (Soil and Water Assessment Tool) (Arnold and Fohrer 2005, Gassman et al. 2007), and calibrated manually using discharge data from local gauging stations supplied by the Global Runoff Data Centre (GRDC, http://www.bafg.de/GRDC/Home). Comparison with the GRACE access mascon data points to a problem in the hydrological model. The error may be in the model structure, or in the input data, or both (Michailovsky 2008).

The average annual signal in region 4 for the different GRACE solutions and hydrological models are shown in figure 7. Figure 7(a) shows the GRGS/CNES spherical harmonic solution (grey dashed) and the access mascon solution from GSFC (grey solid), which are given to order and degree 50 and 60 respectively. In this figure the truncated regional solution (RC50) is also shown (black solid). Figure 7(b) shows the average annual signal of the LM-corrected GLDAS (grey dashed), the two new mascon solutions (IC (grey solid) and RC (black solid)), and the Zambezi River basin SWAT model (black dotted), over the area of region 4 where Lake Malawi is situated. Table 3 shows the amplitudes and phases of the curves shown in figure 7.

The phases of the annual signal for most solutions are rather similar, peaking around mid April. The GRGS/CNES and the GLDAS solutions deviate from this by peaking approximately two weeks earlier. The regional SWAT model, however,

![Figure 7](image_url)

**Figure 7.** Average annual signal of region 4, which include Lake Malawi, from different GRACE solutions, the GLDAS/Noah global model output, and the regional SWAT model. (a) GRACE solutions to order and degree 50. (b) GRACE solutions to order and degree 120, GLDAS/Noah (corrected for Lake Malawi water level variations) and the SWAT model.
is closer to the mid April peak. Discrepancies in phase between the LM-corrected GLDAS and GRACE can be explained by the fact that groundwater and surface water storages are not represented in GLDAS land surface models. Water that drains from the bottom of the modelled soil column (2 m below the surface, in the case of the Noah LSM) exits the model world as run-off. In the real world, that water would become groundwater, then base flow, then river channel storage before leaving the region as run-off. This results in a phase lag between GLDAS soil moisture and GRACE terrestrial water storage. In this case the phase lag was about two weeks, which is consistent with previous studies (e.g. Rodell and Famiglietti 2001). The regional SWAT model has groundwater storage and some surface water included, and thus does a better job in estimating the phase of the annual signal.

In figure 7(a) all solutions are truncated at order and degree 50, and the new regional mascon solution (RC50) shows a higher amplitude (16.0 cm) than both the SH solution from GRGS/CNES (14.5 cm) and the access mascons (11.7 cm) from GSFC (see table 2). These lower GRACE amplitudes are mainly due to the limited spatial resolution of order and degree 50, and the solutions will only recover wavelengths longer than 400 km. Consequently the impact of Lake Malawi’s annual water storage variations will be smaller on these solutions.

In figure 7(b) the LM-corrected GLDAS and the new regional mascon solution (RC) show very similar amplitudes of around 18.9 and 17.4 cm respectively, whereas the traditionally constrained solution (IC) and the regional SWAT model show lower amplitudes of 11.8 and 12.1 cm (table 2). The fact that the LM-corrected GLDAS signal shows an amplitude very close to that of the new regionally constrained mascon solution indicates that this very high amplitude is not completely off. The solution with the isotropic constraints however has a very low amplitude compared to the LM-corrected GLDAS, which is due to the isotropic constraints linking wet and dry regions. The amplitude of the regional SWAT model is also very low compared to the LM-corrected GLDAS output.

5. Conclusions

A system of regionally constrained mascon blocks over Southern Africa was presented in order to improve the spatial resolution of GRACE data and the relevance of GRACE data for use in hydrological modelling.
Two new mascon solutions were presented, one using isotropic constraints and one using regional constraints. Interesting observations on the regional solution are:

- More information is gained compared to the isotropic solution, the access mascons and the spherical harmonic solution from GRGS/CNES.
- Regions 8 and 9 are clearly separated, as they should be, and have very different amplitudes; region 8 being dry and region 9 wet.

The comparison of the regional solution in the Lake Malawi region to the GLDAS/Noah output in the same area shows that the relatively high annual amplitudes (17.4 cm) are not unrealistic for this region. In fact, when we add the expected signal from the varying lake level to the GLDAS/Noah signal, the amplitude of the regional mascon solution is 7.9% lower than the scaled GLDAS/Noah amplitude (18.9 cm). Thorough validation in other areas could not be done for the current solution, except for visual examination, because of lack of in situ data.

Altogether comparison of the regional mascon solution with hydrological models has pointed out the following:

- The phase of GLDAS is approximately two weeks ahead of the GRACE solutions.
- When including the water level variation in Lake Malawi, GLDAS/Noah amplitudes show a better match to the regional mascon solution.
- The SWAT model estimates the phase of the GRACE signals quite well, but the amplitude is too low, probably due to improperly modelled surface water.

The experimental constraints we have applied in our new solution (regional constraints) yield a higher level of detail, but also very high amplitudes (up to 32 cm of water) compared to other 10-day GRACE solutions (up to 23 cm for the GRGS/CNES solution and only 15.5 cm for the access mascons) and hydrological models (up to 19 cm for GLDAS/Noah) (figures 3 and 4). Based on the spatial jumps in annual amplitude we see in the regionally constrained solutions (figure 4(b)), we conclude that these constraints are questionable and must be augmented with intra-basinal constraints. The initial approach of assuming that one sub-catchment (or hydrological region) is independent of all its neighbours is also questionable from a hydrological point of view since investigations have shown that the majority of the signal originates from storage in the soil column and shallow aquifers, and not from the lateral redistribution of water (Leiriao 2007, Michailovsky 2008). However, the solutions demonstrate the possible design of regional mascons that in turn can be used to constrain hydrological models.

We chose to use a CMAP forced GLDAS/Noah simulation for validation because it is a global dataset that has previously been used for GRACE validation. However, it would be interesting to test other models, such as the Watergap Global Hydrological Model (WGHM) (Döll et al. 2003), which includes both surface and ground water and has also been used for comparison with GRACE (e.g. Werth et al. 2009), to see how the modelled storage variation in Southern Africa compares to our regional solution.

In order to improve the solution, we intend to continue using the regional approach, but instead of applying no constraints at all across regions, weak constraints should be applied to realistically mimic the inter-regional relations. Moreover we want to use an iterative process of alternately calibrating our hydrological model with the GRACE data and constructing new constraints based on the hydrological model.
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