Quantification of Drainable Water Storage Volumes in Both the Catchment and the River Network utilizing GRACE, River Discharge and their Phasing

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Abstract.

The knowledge of water storage volumes in catchments and in river networks leading to river discharge is essential for the description of river ecology, the prediction of floods and specifically for a sustainable management of water resources in the context of climate change. Measurements of water storage variations by the GRACE gravity satellite or by ground based observations of river or groundwater level variation do not permit the determination of the respective storage volumes, which could be considerably larger than the mass variations themselves. In addition mass variations measured by GRACE comprise all time variant storage compartments whether they are hydraulically coupled, contributing to river discharge, or uncoupled like soil moisture, isolated surface water or snow and ice.

The characterization of the Runoff-Storage relationship (Riegger and Tourian, 2014) revealed a linear relationship for hydraulically coupled storages with a phase shift. This allows to determine the hydraulic time constant and thus to quantify the total drainable storage directly from observed runoff, if the observed phase shift can be interpreted as a river system time lag. Global hydrological models describe a large number of different storages storage compartments yet the determination of the time lag and the related river network storage still means a huge effort. As a time lag can be described by a storage cascade a lumped conceptual model with cascaded storages for the catchment and river network is set up here with individual hydraulic time constants and mathematically solved by piecewise analytical solutions.

Tests of the scheme with synthetic recharge time series show that a parameter optimization either versus mass anomalies or runoff reproduces the time constants for both, the catchment and the river network τ_C and τ_R in a unique way, and hence permits an individual quantification of the respective storage volumes. The application to the full Amazon basin leads to a very good fitting performance for total mass, river runoff and their phasing (Nash-Sutcliffe for signals 0.96, for monthly residuals 0.72). The calculated river network mass highly correlates (0.96 for signals, 0.76 for monthly residuals) with the observed flood area from GIEMS and corresponds to observed flood volumes. This provides additional independent information for investigations on flood hydraulics.

The fitting performance versus GRACE permits to determine river runoff and Drainable storage volumes from recharge and GRACE exclusively i.e. even for ungauged catchments. An adjustment of the hydraulic time constants (τ_C, τ_R) on a training period facilitates a simple determination of Drainable storage volumes for other times directly from measured river discharge and/or GRACE and thus a closure of data gaps without the necessity of further model runs.

1 Introduction

In the context of water resources management and climate change there is an ongoing discussion on how to assess available water resources i.e. the storage volumes which can be used for water supply in a dynamic way beyond the limitations of sustainable extraction rates. The maximum average extraction rate for a sustainable use of water resources is limited by the long-term recharge of a catchment (Sophocleous, 1997, Bredehoeft, 1997), however, this rate based definition of groundwater stress only allows an assessment of water resources with respect to long-term sustainability and does not allow consideration of the volume of available water resources as a basis for short term groundwater management in order to satisfy specific demands. In addition, the knowledge of the storage volumes is essential for climate studies as it might lead to limitations in the water cycle.

Thus, the attempt was made by different authors to estimate available water resources by the volume of the respective groundwater storage (under the assumption that the contribution of surface water is comparably small). Korzun, 1978 and Nace, 1969 provide estimates of total storage volumes across the global land masses (except for Greenland and Antarctica) based on very coarse assumptions for aquifers with homogeneous thickness and porosity. As a consequence the uncertainties cover orders of magnitude as Shiklomanov, 1993 Alley, 2006 and Famiglietti, 2014 are warning. The revision of these estimates by the introduction of specific yield instead of porosity for dominant soil classes together with the assumption of different saturated thicknesses in order to obtain the "Extractable" storage (Richey et al., 2015a, Alley, 2006) does not solve the problem of missing information on the contributing soils or aquifers in general. Regional storage estimates for specific aquifers derived from groundwater models (Cao et al., 2013) or measured estimates of saturated thickness and porosity (Williamson et al.,1989) are considered to deliver more realistic estimates for storage volumes, yet are sparsely distributed over the globe. However, for semi-arid and arid climate zones with very low recharge and/ or deep aquifer systems with fossil water resources they deliver the best possible estimation at present. Richey et al., 2015b try to bypass the huge uncertainties in the quantification of total storage by the introduction of a "Total Groundwater Stress" indicator, which is defined by the time needed for the depletion of groundwater storage to a specified extent. It is determined by the ratio of an estimated total storage of a (sufficiently large) catchment and the measured trend in the mass anomalies given by GRACE.

Very little attention has so far been given to the storage volume of renewable water resources participating in the dynamic water cycle driven by precipitation P, actual evapotranspiration ET_a and river runoff R. The reason for this is seen in the problem that observations of time variant groundwater or river levels only permit the estimation of volume changes yet no absolute storage volumes, which could be considerably bigger. Natural systems consist of many different storage components like canopy, snow/ice, surface, soil, unsaturated/saturated underground, drainage system etc. Direct measurements of storage volumes from water or pressure levels are problematic as they are based on assumptions and approximations. Ground based measurements of storages for example are based on point measurements and quite rare on large spatial scales compared to the heterogeneity scale of the respective compartments. This leads to large interpolation errors. In addition, the storage coefficients for porous media describing the relationship between the measurable groundwater heads or capillary pressure on the one hand, and storage volume or absolute soil saturation on the other hand, are insufficiently known on large scales. Remote sensing data have been limited to near surface water storage (open water bodies, soil) up until now and are thus of limited benefit for the quantification of water storage with respect to accuracy and coverage due to methodological constraints (Schlesinger, 2007).

In contrast to discharge-less basins and/or arid areas, which are nearly exclusively driven by precipitation and evapotranspiration, the storage dynamics of catchments draining into a river system allows to address the hydraulically coupled storage compartments via their contributions to river discharge. These comprise groundwater, surface water, the river network and temporarily inundated areas. All storages draining into the river system by gravity are referred to as “Drainable” storage here. So aquifers or parts of them not draining into the river system without an energy input are not considered here.

For time periods with no recharge hydraulically coupled storage components with a linear runoff storage (R-S) relationship lead to an exponential decrease in river discharge or streamflow depending on the related hydraulic time constant τ:

$$Q(t) = Q(t_0) \cdot e^{-\frac{t-t_0}{\tau}} \quad (1)$$

The corresponding total Drainable Storage in terms of mass density $M_{Storage}$ for any given time t_0 is then given by an infinite temporal integration over river discharge Q(t) from the corresponding catchment area A - called river Runoff R(t) = Q(t)/A here - starting at time t_0 :

$$M_{storage}(t_0) = \frac{V_{tot}(t_0)}{A} = \frac{1}{A} \cdot \int_{t_0}^{\infty} Q(t)dt = \frac{Q(t_0)}{A} \cdot \int_{t_0}^{\infty} e^{-\frac{t-t_0}{\tau}} dt = \tau \cdot \frac{Q(t_0)}{A} = \tau \cdot R(t_0) \quad (2)$$

Contributions from several storage compartments (with individual time constants) superpose, if they drain in parallel and if there is no feedback from the river system. For this case, there is a wide range of time series analysis methods (Tallaksen, 1995), which allow to separate the flow components into fast, medium or slow and the corresponding surface, interflow or groundwater flow contributions according to their individual time constants. Thus, measurements of the different time constants allow to determine the Drainable Storage of the respective storage compartment and the corresponding mean Drainable Storage :

$$\overline{M}^{X} = \overline{R} \cdot \tau_X = \overline{N} \cdot \tau_X \ . \quad (3)$$

from mean runoff R or recharge N.

On global scales the absolute storage volume of the Drainable Storages can be determined from runoff time series directly, if there are distinct and long enough periods of negligible or even negative recharge (actual evapotranspiration > precipitation) as it occurs in seasonally dry regions (Niger, Mekong, some Amazon sub-catchments etc.). From the purely exponential decrease in river distcharge the time constant can be determined directly from a curve fit as shown in Fig.1b for Amazon sub-catchments. If the dry period is long enough the sequence of different time constants taken from the discharge curve even permits a discrimination between the fast response by overland flow and the slow response by the groundwater system. Catchments with permanent input i.e. no periods of negligible recharge, however, do not show an exponential behaviour for discharge (Fig.1a). For these cases the hydraulic time constant cannot be taken from discharge dynamics directly, but has to be estimated either from the R-S relationship or by hydrological models via an adaption to measured runoff, or – at least theoretically - to observed storage.

Since 2013 GRACE observations of the time-variable gravity field provide monthly distributions of mass density on large spatial scales >~ 200000km^2 (Tapley et al., 2004). However, as the water storage in different compartments (snow, ice, vegetation, soil, surface-, ground- water etc.) superposes with all other terrestrial (geophysical) masses, only the time variant part of the GRACE signal can be used to quantify the Terrestrial Water storage (TWS) anomalies (monthly mass signals minus long term average), but not the related absolute storage volumes. Nevertheless, this for the first time permits a direct comparison of measured TWS and river runoff R_o and an investigation of the R-S relationships on large spatial and monthly time scales. The R-S diagrams show hysteresis curves of distinct form and extent, which are characteristic for different climatic conditions like fully humid, seasonally dry or boreal (Riegger and Tourian, 2014).

Catchments in fully humid conditions (like the full Amazon basin upstream Obidos (295) and some of its sub-catchments like upstream Manacapuru (501)) with a permanent input i.e. only positive recharge (Fig.1a) show a counterclockwise hysteresis (Fig.1c), which can be interpreted as a phase shift caused by a time lag, as it is causal. River runoff and storage then behave like a Linear Time Invariant (LTI) system (Riegger and Tourian, 2014) i.e. the R-S relationship is linear, if the phase shift is adapted as shown in Fig.1c. For this case the slope in the R-S diagram corresponds to the hydraulic time constant via τ^{-1}. The time constant and the reasonable assumption of a proportional R-S relationship (no runoff for empty storage) then facilitates the quantification of the Drainable Storage, Eq. (3), i.e. the volume related to the hydraulically coupled storage compartment, which drains by gravity.

In contrast to this, catchments with distinct periods of zero or negative recharge (like Niger, Mekong or Rio Branco (504), Rio Jurua (506) in the Amazon basin (Fig.1b)) show a clockwise hysteresis in the R-S diagram (Fig.1d) and a form, which is determined by an increase in mass and runoff during wet periods, a decrease in mass and runoff with different slopes corresponding to different time constants and a possible mass loss without a related runoff (possibly from the soil zone by evapotranspiraton) during dry periods. This hysteresis cannot be explained by a time lag as it is not causal.

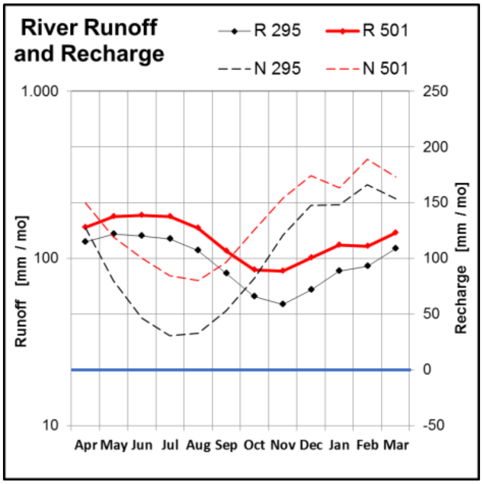

Fig.1a: Mean monthly Runoff R and Recharge N
for fully humid catchments (Log scale for R)

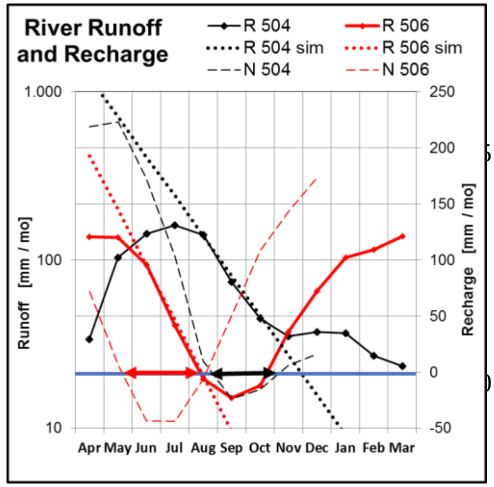

Fig.1b: Mean monthly Runoff R and Recharge N
for seasonally dry catchments (Log scale for R)
incl. exp. fittings for Runoff

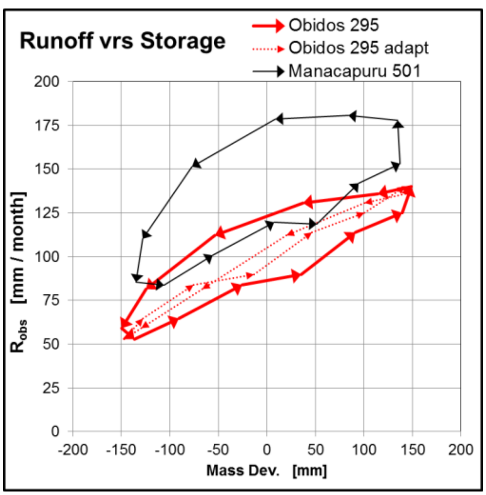

Fig.1c: R-S diagram with counter clockwise hysteresis for mean monthly runoff R vrs GRACE dM for fully humid catchments incl. a phase adaption for Amazon upstream Obidos

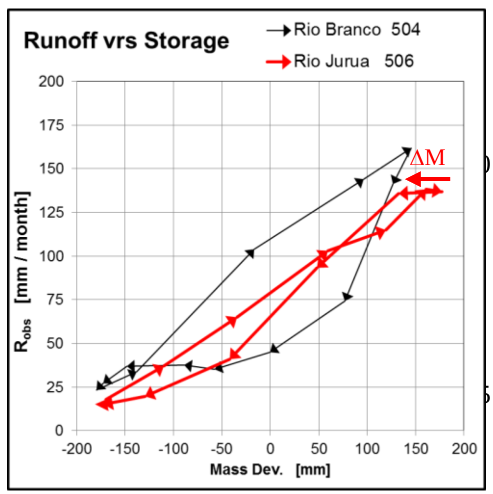

Fig.1d R-S diagram with clockwise hysteresis for mean monthly runoff R vrs GRACE anomaly dM for seasonally dry catchments

The accurate description and adequate adaption of the phase shift is the prerequisite for an accurate determination of the hydraulic time constant τ· and thus the Drainable storage volume. Different approaches are available for this purpose.

Recent developments on river routing schemes with hydrodynamic modelling of the flow in the river network system have successfully dealt with the description of phase shifts generated by the time lag in the river network (Paiva et al., 2013, Luo et al., 2017, Siqueira et al., 2018). Getirana et al., 2017a emphasize the importance of integrating an adequate river routing schemes not only for an improved phase agreement with observed river discharge but also for a better fit of the total mass amplitude with GRACE by the inclusion of the corresponding river network storage. Yet a hydrodynamic modelling of a complete river network system for the determination of the river network time lag and storage means a huge modelling effort (Getirana et al., 2017b).

A far more simple method is the Direct approach (Riegger and Tourian, 2014), in which the phase shift between the observations of GRACE and river runoff is adapted numerically (Eq.38 & 39) as shown in Fig.1c. This permits to determine the time constant of the whole system comprising catchment and river network storage from the slope in the R-S diagram without the need for modelling. Prerequisite for this method is that time dependent uncoupled storages are negligible, i.e. the hysteresis can be purely described by a time lag i.e. a positive phase shift. Tourian et al. (2018) apply an adaption of the phase shift using a Hilbert transform in order to determine the hydraulic time constants and the total Drainable water storage for the sub catchments of the Amazon basin. As shown in Fig1 this leads to reasonable results for the sub catchments with permanent input (Fig.1 a, c) for which the time dependent uncoupled storage is negligible. For Rio Branco (504) or Rio Jurua (506) this condition is not fulfilled as the hysteresis is determined by mass changes in the uncoupled storage and by runoff with different time constants (Fig.1b, d). For these catchments the exclusive adjustment of the phase shift leads to negative time lags (which are not physical) and to misleading time constants. This leads to considerable errors in the determination of Drainable storage volumes.

Another disadvantage of the above Direct approach is that it does not permit to quantify the individual Drainable storage volumes of both, the catchment and the river network separately, but only the total volume of the system. The information contained in the phase shift or time lag is not used for a quantification of the river network storage volume. Yet, as observations of inundated areas in river networks such as from the GIEMS “Global Inundation Extent from Multi-Satellites” project (Prigent et al, 2007, Papa et al., 2008, Papa et al., 2013) and hydrodynamic models of the river network (Paiva et al., 2013, Getirana et al., 2017b, Siqueira et al., 2018) indicate a considerable contribution of river network storage corresponding to a non negligible time lag, the river network storage should be considered in the integration of the total catchment water balance. As a sequence of storages (cascaded storages) leads to a time lag i.e. a phase shift (Nash, 1957), and storages draining in parallel (as for overland and groundwater flow) just lead to a superposition (with no time lag), a storage cascade is considered as an appropriate description to account for a time lag.

This paper explores the accuracy and uniqueness of a lumped top down approach called “Cascaded storage approach” based on the integration of given recharge in the water balance utilizing a cascade of a catchment and a river network storage for a simple description of the observed time lag and the individual storage volumes. This permits to describe the system with a minimum number of macroscopic observation data and an adaption of only two parameters, the hydraulic time constants of the catchment and the river network. These time constants then could be used for nowcasts or even forecasts (within the time lag) of river discharge and/or Drainable storage volumes directly from measurements without the need for further modelling.

The paper is structured as follows: Section 2 presents the mathematical framework of piecewise analytical solutions of the water balance equation for a cascade of catchment and river network storages. It also contains the description of observables, which permit the comparison of calculated and measured values. The Single Storage approach is handled as the specific case for a negligible river network time constant. In section 3, the properties of the Cascaded Storage approach and its impact on the performance of the parameter optimization are described for synthetic recharge data and compared to the “Single Storage” approach. In section 4 the approach is applied to data from the Amazon basin and evaluated versus measurements of GRACE mass, river runoff and flood area from GIEMS. Conclusions are drawn and discussed in section 5. In section 6 a purely data drive determination of Drainable storage volumes from observations of GRACE and river discharge is presented and an outlook on future investigations and possibilities is given in section 7.

2 Mathematical framework

In order to investigate the impact of a non negligible river water storage on the time lag in the river system, the water balance of the total system comprising both the catchment and river network storage has to be considered. A conceptual model corresponding to a Nash cascade (Nash, 1957), called “Cascaded Storage” approach here, is set up with individual time constants for the different storages and with the following properties:

- Surface and the groundwater storages both fed by recharge are summarized to one catchment storage M_C with time constant τ_C draining into the river network as overland and groundwater flow summarized as catchment runoff.
- Temporal variations of uncoupled storage compartments like soil or open water bodies are considered as negligible.
- The river network storage M_R with time constant τ_R is assumed to be instantaneously distributed within the river network system. Internal routing effects, which might lead to an additional delay in streamflow response, are not considered.
- Any possible hydraulic feedback from the river to the catchment system is assumed to be negligible.

These conditions are chosen for conceptual and mathematical simplicity in this first approach here regardless of the necessity to address several coupled storages with different time constants and different uncoupled storage compartments for the general applicability with a global coverage. Thus, applications of this first approach are limited to catchments for which the hysteresis can be fully described by a time lag.

The following abbreviations are used in the mathematical description (Table.1):

Abbreviation	**Description**	**Units:** general / for application
N	recharge = (precipitation - actual evapotranspiration)	volume $area^{-1}$ $time^{-1}$ [mm $month^{-1}$]
M_C	Storage mass catchment	mass density in equivalent water height [mm]
τ_C	Time constant catchment	time unit [month]
R_C	Runoff catchment	volume $area^{-1}$ $time^{-1}$ [mm $month^{-1}$]
ω_{MC}	Phasing catchment mass	time unit [month]
M_R	Storage mass river network	mass density in equivalent water height [mm]
τ_R	Time constant river network	time unit [month]
R_R	Runoff river network	volume $area^{-1}$ $time^{-1}$ [mm $month^{-1}$]
ω_{RR}	Phasing river network mass	time unit [month]
M_T	Storage mass total system	mass density in equivalent water height [mm]
τ_T	Time constant total system	time unit [month]
ω_{MT}	Phasing mass total system	time unit [month]
Ro	Observed river runoff	volume $area^{-1}$ $time^{-1}$ [mm $month^{-1}$]
GRACE	GRACE mass anomaly	mass density in equivalent water height [mm]
GIEMS	Flood area	area [km^2]
Prefix "d"	indicates signal anomalies from long term mean (anomalies)	
Suffix "m"	indicates mean values on the intervals	

Table.1: Abbreviations in the mathematical descriptions:

The total system behaviour is described by two balance equations :

1. catchment storage $\frac{\partial}{\partial t} M^C(t) = N(t) - R^C(t) = N(t) - \frac{1}{\tau_C} \cdot M^C(t)$ (4)

   with $R^C(t) = \frac{1}{\tau_C} \cdot M^C(t)$ (5)

2. river storage $\frac{\partial}{\partial t} M^R(t) = R^C(t) - R^R(t) = R^C(t) - \frac{1}{\tau_R} \cdot M^R(t)$ (6)

$$\text{with } R^R(t) = \frac{1}{\tau_R} \cdot M^R(t) \qquad (7)$$

with a proportional R-S relationship for hydraulically coupled storages. N denotes the recharge as input, R_C the catchment runoff from the catchment storage M_C, which cannot be measured directly on large spatial scales, and R_R the river runoff from the river network storage M_R which can be measured at discharge gauging stations.

The water balance equation, Eq.(4), for the catchment is generally solved by:

$$M^C(t - t_0) = M^C(t_0) \cdot e^{-\frac{t-t_0}{\tau_C}} + \int_{t_0}^{t} N(w) \cdot e^{\frac{w-t}{\tau_C}} \cdot dw \qquad (8)$$

where $M_C(t_0)$ is the initial condition and N(w) the time dependent recharge.

For recharge N(t) being given with a certain temporal resolution in time units or by periods of piecewise constant values and arbitrary length (stress periods) the recharge time series can be described as :

$$N(t) = \sum_{i=0}^{n-1} N_{i+1} \cdot \gamma_{i+1}(t) \quad \text{with} \quad \gamma_{i+1}(t) = \begin{cases} 1 \\ 0 \end{cases} \; for \; \begin{cases} t \in \lfloor t_i, t_{i+1} \rfloor \\ t \notin \lfloor t_i, t_{1+1} \rfloor \end{cases} \quad \text{for each interval } \lfloor t_i, t_{i+1} \rfloor \qquad (9)$$

For calculation convenience Eq. (8) can be solved successively for each stress period using the values at the end of the last period as starting value, which leads to the piecewise analytical solution for catchment mass for a time $t \in \lfloor t_i, t_{i+1} \rfloor$ in stress period $_{i+1}$:

$$M_{i+1}^C(t - t_i) = M_i^C(t_i) \cdot e^{-\frac{t-t_i}{\tau_C}} + N_{i+1} \cdot \tau_C \cdot \left(1 - e^{-\frac{t-t_i}{\tau_C}}\right) \; : \qquad (10)$$

The respective catchment runoff R_C based on Eq. (5) and M_C from Eq. (10) is used as input for the river network water balance, Eq.(6), and leads to the general solution for the river network storage M_R :

$$M^R(t - t_0) = M^R(t_0) \cdot e^{-\frac{t-t_0}{\tau_R}} + \int_{t_0}^{t} R^C(u) \cdot e^{\frac{u-t}{\tau_R}} \cdot du \qquad (11)$$

and the iterative solutions for time $t \in \lfloor t_i, t_{i+1} \rfloor$ in stress period $_{i+1}$:

$$M_{i+1}^R(t - t_i) = M_i^R(t_i) \cdot e^{-\frac{t-t_i}{\tau_R}} + N_{i+1} \cdot \tau_R \cdot \left(1 - e^{-\frac{t-t_i}{\tau_R}}\right) + \left[M_i^C(t_i) - N_{i+1} \cdot \tau_C\right] \cdot \frac{\tau_R}{\tau_C - \tau_R} \cdot \left(e^{-\frac{t-t_i}{\tau_C}} - e^{-\frac{t-t_i}{\tau_R}}\right) \qquad (12)$$

The total mass M_T is then given by : $$M_i^T = M_i^C + M_i^R \,. \tag{13}$$

The mixed term in Eq. (12) and thus the total mass are commutative in (τ_C, τ_R) and show a singularity at $\tau_C = \tau_R$ with an asymptotic value. For $\tau_R > \tau_C$ solutions also exist with analogous values in total mass M_T for $M_R > M_C$.

It has to be emphasized here, that the piecewise analytical solutions for time periods of constant recharge provide a mathematical solution for an arbitrary temporal resolution. Finite Difference solutions are limited by stability criteria $(t_{i+1}-t_i)<\tau$ and accuracy criteria $(t_{i+1}-t_i)<\tau/10$ for the smallest τ. Analytical solutions facilitate the calculation of the response of the river network on the time interval of constant recharge (though the time constant of the river network is much shorter than the time constant of the catchment), and thus avoid the very high temporal discretization, which otherwise would be needed for a Finite Difference scheme.

The observables related to measurements by GRACE and discharge from gauging stations are the total mass anomaly dM_T and the river runoff R_R. GRACE observations with acceptable error are still limited to monthly resolution. Discharge as well as some of the meteorological inputs like precipitation, evapotranspiration or moisture flux divergence are often measured in daily values, some of the products in monthly values. For an optimal adaption to the monthly resolution of GRACE products, the approach presented here is based on monthly values but could also be applied to daily data without problems.
The mass values used in the calculations here are assigned to the interval boundaries while the values for monthly recharge and measured runoff are constant over the interval and temporally assigned to the centre of the interval. Thus, for a comparison of the calculated mass and runoff values versus the observed monthly values of GRACE and discharge the calculated values have to be averaged over the interval. As the dynamics follow an exponential behaviour the mean values cannot be taken from arithmetic averages at the interval boundaries but instead from an integral average over the interval.

The mean storage mass for M_X is given for each interval $\lfloor t_i, t_{i+1} \rfloor$ by :

$$\overline{M}_{i+1}^X = \frac{1}{t_{i+1}-t_i} \int_{t_i}^{t_{i+1}} M_{i+1}^X (t-t_i) \cdot dt \tag{14}$$

leading to mean runoff $$\overline{R}^X(t) = \frac{1}{\tau_X} \cdot \overline{M}^X(t) \tag{15}$$

i.e. mean catchment mass and runoff :

$$\overline{M}_{i+1}^C = \left(M_i^C - N_{i+1}\cdot\tau_C\right)\cdot \frac{\tau_C}{(t_{i+1}-t_i)}\left(1-e^{-\frac{t_{i+1}-t_i}{\tau_C}}\right) + N_{i+1}\cdot\tau_C \tag{16}$$

and $$\overline{R}_i^C = \frac{1}{\tau_C} \cdot \overline{M}_i^C \qquad (17)$$

and mean river mass and runoff :

$$\overline{M}_{i+1}^R = \left(M_i^R - N_{i+1} \cdot \tau_R\right) \cdot \frac{\tau_R}{\left(t_{i+1} - t_i\right)} \cdot \left(1 - e^{-\frac{t_{i+1}-t_i}{\tau_R}}\right) + N_{i+1} \cdot \tau_R$$
$$+ \frac{\left[M_i^C - N_{i+1} \cdot \tau_C\right]}{\left(t_{i+1} - t_i\right)} \cdot \frac{\tau_R}{\tau_C - \tau_R} \cdot \left(\tau_R \cdot e^{-\frac{t_{i+1}-t_i}{\tau_R}} - \tau_C \cdot e^{-\frac{t_{i+1}-t_i}{\tau_C}} + \left(\tau_C - \tau_R\right)\right) \qquad (18)$$

The Observables, which allow a comparison to measured data are :

- average river runoff $\overline{R}_i^R = \frac{1}{\tau_R} \cdot \overline{M}_i^R$ corresponding to measured monthly runoff (19)
- average total mass $\overline{M}_i^T = \overline{M}_i^C + \overline{M}_i^R$ corresponding to monthly GRACE data (20)

The equations Eq. (10) - Eq. (20) are self-consistent, i.e. the corresponding balance equations are fulfilled with :

$$\frac{M_{i+1}^T\left(t - t_i\right) - M_i^T}{\left(t - t_i\right)} + \overline{R}_{i+1}^R\left(t - t_i\right) = N_{i+1} \qquad (21)$$

For the Single Storage approach the above piecewise analytical solutions of the Cascaded Storage approach, Eq. (8) - Eq. (21), are used for $\tau_R \ll \tau_C$ (here $\tau_R = 10^{-3}$ months). For this case the river network mass is negligible compared to the catchment mass.

3 Properties and optimization performance

For the evaluation of the parameter optimization performance of the Cascaded Storage approach an example with synthetic recharge as input is investigated. This permits the quantification of the uniqueness and accuracy of the parameter estimation undisturbed by noise. It also facilitates the discrimination of errors in the calculation scheme itself and impacts arising from undescribed processes when compared to real world data. For an application to GRACE measurements the main question is if and why the time constants τ_C and τ_R can be determined independently by an optimization versus anomalies in total mass and/or river runoff. Thus, in order to understand the optimization results with respect to uniqueness the general properties of the approach are presented and discussed first. For the synthetic case a recharge time series of sinusoidal form with a period of 12 arbitrary time units and length units with an amplitude and mean value of one is used as the driving force and the calculation is run until equilibrium is reached. The example in Fig.2 shows the effect of a non negligible river network time constant τ_R =2.5 time units for a catchment time constant τ_C = 3 time units which leads to an increase in total mass $M_T(t) = M_C(t)+M_R(t)$ with respect to the average level and signal amplitude and to a phase shift between total mass M_T and river mass M_R i.e. the corresponding river runoff R_R.

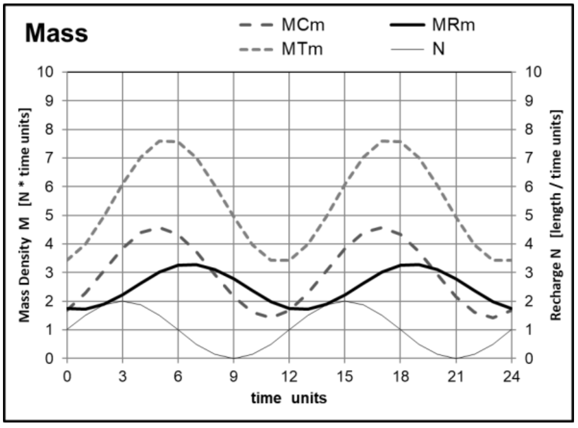

Fig.2: Time series of Recharge N, catchment mass M_C, river network mass M_R, and Total masses M_T for the synthetic case at equilibrium

In order to describe the general behaviour of the mass and runoff time series and their dependence on τ_C and τ_R, their properties are summarized here in the form of statistical values for the synthetic case with the sinusoidal recharge in equilibrium. This helps to understand why unique values for the time constants are achieved in the parameter optimization process. The values of time constants τ_C and τ_R used for the statistical description cover a wide range from 0.1 to 100 time units and are combined independently.

3.1 Catchment and river mass

Based on the mean mass values, Eq.(14), (16), (18), of each stress period the long term averages for the storage compartments are given by :

$$\overline{M}^C = \overline{N} \cdot \tau_C \qquad \overline{M}^R = \overline{N} \cdot \tau_R \qquad \overline{M}^T = \overline{N} \cdot (\tau_C + \tau_R) \qquad (22a,b,c)$$

For $\tau_R \ll \tau_C$ (here $\tau_R = 10^{-3}$) the river network mass is negligible and the solution corresponds to a Single Storage approach. For a non negligible river network storage the given average values for total mass M_T mean that the effective "total" time constant is given by the sum of the catchment and river time constants $\tau_T = \tau_C + \tau_R$, which means that the total mass M_T observed by GRACE is bigger than the mass M_C calculated for the catchments alone. However, Equation (22c) cannot be used for the determination of $\tau_T = \tau_C + \tau_R$ from GRACE measurements directly as GRACE only provides mass anomalies.

The relative signal amplitudes (standard deviations normalized with those of the respective input) of both the catchment mass M_C or river mass M_R show the same functional form $\sigma_{MC} / \sigma_N \sim \sigma_{MR} / \sigma_{RC} = stdev(M_C) / N$ for the respective time constants τ_C or τ_R (Fig.3, $\tau_R = 10^{-3}$) with a monotonous increase to an asymptotic value $\sigma_{MC} / \sigma_N \sim \sigma_{MR} / \sigma_{RC} = 2$ which is reached at about one full period of the input. The superposition of the signal amplitudes for the observable total mass $M_T(t) = M_C(t) + M_R(t)$ leads to a complex behaviour for $\sigma_{MT} / \sigma_N (\tau_C, \tau_R)$ (Fig.3), if the river time constant τ_R is not negligible ($\tau_R = 10^{-3}$) and especially if it gets close to τ_C.

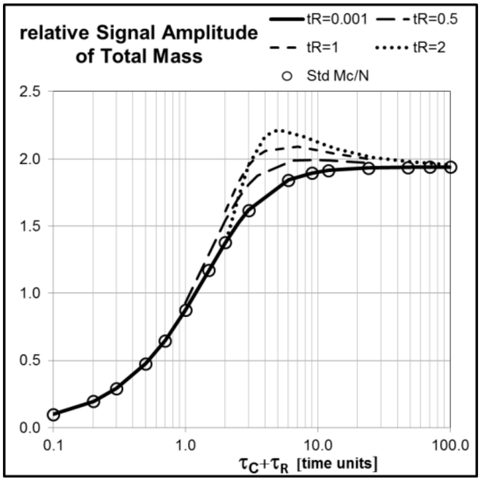

Fig.3: Signal Amplitudes of Total mass normalized by recharge: σ_{MT} / σ_N versus total mass time constant $\tau_T = \tau_C + \tau_R$ for different river time constants τ_R

3.2 Catchment and river runoff

The calculated long term averages of the runoff contributions R_C and R_R correspond to the ones of the water balance equations, Eq.(4), (6), given by the mean recharge and thus are not dependent on the time constants.

$$\overline{R}^R(t) = \overline{R}^C(t) = \overline{N} \tag{23}$$

Thus, an observed long term average of runoff does not permit the determination of the time constant and hence the storage volume, Eq. (22).

The relative signal amplitudes of both, catchment and river runoff (normalized with the respective input σ_{RC} / σ_N and $\sigma_{RR} / \sigma_{RC}$ show the same functional form corresponding to a Single Storage approach (Fig.4, $\tau_R = 10^{-3}$) and decrease monotonously with the respective time constants τ_C and τ_R to an asymptotic zero. However, the signal amplitude of the observable river runoff $\sigma_{RR} / \sigma_N (\tau_C + \tau_R)$, normalized with recharge N, shows a deviations for different τ_C and τ_R with the same $\tau_C+\tau_R$ (Fig.4).

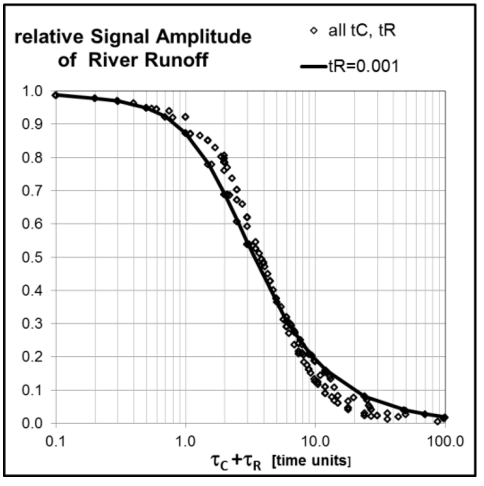

Fig.4: Signal Amplitudes for river runoff normalized by recharge: σ_{RR} / σ_N versus total mass time constant $\tau_T = \tau_C + \tau_R$ for combinations in (τ_C, τ_R)

Both observables, total mass and river runoff, show a non unique behaviour with respect to combinations in (τ_C, τ_R) for the same $\tau_T = \tau_C + \tau_R$ and considerable deviations from the Single Storage approach ($\tau_R = 10^{-3}$). Measurements of the signal amplitudes thus only provide coarse estimates of the total time constant τ_T, yet do not perrmit distinction betweenτ_R and τ_C and betweeen catchment and river network storage.

However, so far, only the signal amplitudes are examined, but not the specific properties of the time series, i.e. the dynamic response to input signals in form and phase. The convolution in the solution of the balance equation, Eq.(8) and (11), leads to a different phasing with respect to the input N(t), which can be utilized for a separation of the respective time constants.

3.3 Phasing

For the synthetic example with a sinusoidal recharge time series N(t) as input the phasing ω of the different response signals is determined by the fit of a sinusoidal function (Fig.5). This facilitates the easy determination of the phasing and thus the relative phase shift $\Delta\omega$ between the signals. Masses and the related runoffs are in phase for the same storage compartments, Eq.(15). For a negligible river network time constant ($\tau_R = 10^{-3}$) river runoff R_R is in phase with the catchment storage M_C.

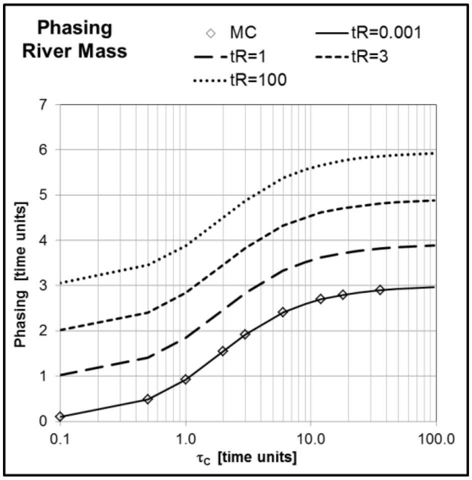

Fig.5: Phasing of river network mass with respect to recharge time series displayed versus τ_C for different τ_R

The functional form of the phasing ω_{MC} for the catchment mass M_C or the corresponding runoff R_C relative to recharge N(t) (Fig.5) can be empirically described by the monotonous function :

$$\omega_{MC}(\tau_C) = \omega_{\max}\left(1 - e^{-\frac{\tau_C}{\lambda}}\right) \tag{24}$$

with the empirical parameters $\omega_{\max} = 2{,}8$ and $\lambda = 2.7$ and an error $\varepsilon < {}_{\sim}2\%$ relative to the maximum.

As the catchment runoff R_C with the phasing ω_{MC} serves as input into the river system, the phasing of the river system with respect to to catchment runoff R_C, which has the same functional form as Eq. (24), is added on top of it (Fig.5). The resulting phasing of the river network storage or river runoff is thus given by a superposition in the form:

$$\omega_{RR}(\tau_C, \tau_R) = \omega_{\max}\left(1 - e^{-\frac{\tau_C}{\lambda}}\right) + \omega_{\max}\left(1 - e^{-\frac{\tau_R}{\lambda}}\right) \tag{25}$$

for any combination (τ_C, τ_R) and with the same empirical parameters as in Eq. (24).

As total mass M_T (t) = M_C (t) + M_R (t) is the superposition of the signals with the respective amplitudes and phasing, the phasing of total mass M_T(t) is situated between catchment and the river system mass according to τ_R. This means that for non negligible river network mass ($\tau_R > 0$) a phase shift between total mass (GRACE) and observed river discharge and also between total mass and modelled catchment mass must occur. The phasing of total mass M_T(t) for all combinations (τ_C, τ_R) Fig.6 shows the same functional form as ω_{MC} and ω_{MR}, Eq.(24), (25) if displayed versus the total time constant $\tau_T = \tau_C + \tau_R$.

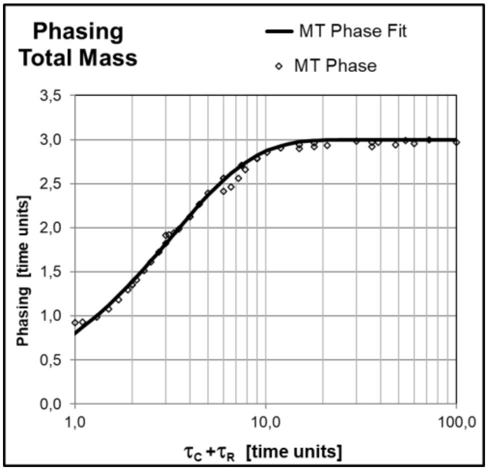

Fig.6: Phasing of Total mass versus total time constant $\tau_T = \tau_C + \tau_R$

It can be approximated by the fitting function M_T fit :

$$\omega_{MT}(\tau_C, \tau_R) = \omega_{\max}\left(1 - e^{-\frac{\tau_C + \tau_R}{\lambda}}\right) \tag{26}$$

with the empirical parameters $\omega_{max} = 2{,}95$ and $\lambda_T = 3.2$

The phase shift between GRACE total mass and river runoff is thus given by :

$$\Delta\omega(\tau_C, \tau_R) = \omega_{RR} - \omega_{MT} = \omega_{\max}\left(1 - e^{-\frac{\tau_C}{\lambda}}\right) + \omega_{\max}\left(1 - e^{-\frac{\tau_R}{\lambda}}\right) - \omega_{\max}\left(1 - e^{-\frac{\tau_C + \tau_R}{\lambda}}\right) \tag{27}$$

The empirical phase shift $\Delta\omega$ from Eq.27 corresponds to the one determined by a phase adaption $\Delta\omega_{adapt}$ (Eq. 38 & 39) of total mass and runoff within <~5% (see supplement). This in principle allows for a determination of τ_C and τ_R separately from the adapted phase shift $\Delta\omega_{adapt}$ and the total mass time constant $\tau_T = \tau_C + \tau_R$ according to Eq. (27). However, errors introduced by the linear interpolation used for the adaption of the phase shift lead to a much lower accuracy than the parameter estimation via the time series.

3.4 Parameter estimation

The analytical solutions for synthetic recharge time series permit the evaluation of the uniqueness and accuracy of the parameter optimization for given observables independent from limitations in the accuracy of numerical schemes and independent from noise in real world data sets. For given combinations (τ_C, τ_R) the analytical solutions are used as synthetic measurements and are fitted with the same algorithm in order to retrieve the fit parameters ($\underline{\tau}_C$, $\underline{\tau}_R$).

As the total mass M_T, Eq.(20), and the phasing, Eq.(25-27), are commutative in (τ_C, τ_R), either the data range $\tau_R < \tau_C$ or $\tau_R > \tau_C$ has to be used for a unique optimization. This is realized via an additional constraint in the optimization. For the discussion here the condition $\tau_R < \tau_C$ is used, which hydrologically reflects the more frequent situations that the inundation volume is smaller than the catchment storage but the results can also be applied to $\tau_R > \tau_C$, which might be the case in flat areas with a dense river network (such as the Amazon), which typically leads to temporarily inundated areas.

As absolute signal values are not relevant for the determination of the time constant from runoff or not available for GRACE data, the optimization versus the respective time series is based on signal amplitudes and the phasing. Thus, for a unique determination of ($\underline{\tau}_C$, $\underline{\tau}_R$) the following conditions have to be fulfilled:

a) Optimization versus runoff

$$\sigma_{RR} / \sigma_N (\hat{\tau}_C, \hat{\tau}_R) = \sigma_{RR} / \sigma_N (\tau_C + \tau_R) \tag{28}$$

$$\omega_{RR}(\hat{\tau}_C, \hat{\tau}_R) = \omega_{\max}\left(1 - e^{-\frac{\tau_C}{\lambda}}\right) + \omega_{\max}\left(1 - e^{-\frac{\tau_R}{\lambda}}\right) \tag{29}$$

b) Optimization versus mass anomalies

$$\sigma_{MT} / \sigma_N (\hat{\tau}_C, \hat{\tau}_R) = \sigma_{MT} / \sigma_N (\tau_C, \tau_R) \tag{30}$$

$$\hat{\omega}_{MT}(\hat{\tau}_C, \hat{\tau}_R) = \omega_{MT}(\tau_C + \tau_R) = \omega_{\max}\left(1 - e^{-\frac{\tau_C + \tau_R}{\lambda}}\right) \tag{31}$$

With the constraints $\tau_R < \tau_C$ or $\tau_R > \tau_C$ there is only one ($\underline{\tau}_C$, $\underline{\tau}_R$) fulfilling the respective conditions, thus leading to unique solutions. The optimization delivers RMSE errors for the time series in the range 10^{-8} - 10^{-7} and estimated time constants ($\underline{\tau}_C$, $\underline{\tau}_R$) with a relative error $\varepsilon(\underline{\tau}_X)/\tau_X$ which does not depend on absolute values of (τ_C, τ_R) but on their ratio τ_R / τ_C (Fig.7).

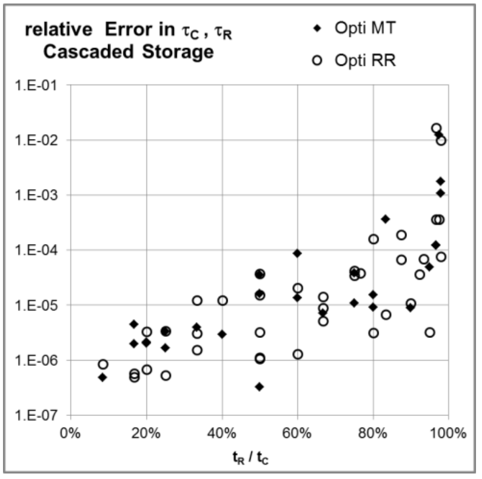

Fig.7: Relative error $\varepsilon(\underline{\tau}_X)/\tau_X$ of the time constants τ_C and τ_R for the Cascaded Storage approach with an optimizations versus Total mass M_T or versus river runoff R_R.

For the synthetic case relative errors $\varepsilon(\tau_X)/\tau_X$ are very small (~10^{-7} at $\tau_R / \tau_C \sim 0$) and show an exponential increase to a maximum of ~ 1% at $\tau_R \sim \tau_C$. The error for $\tau_R < \tau_C$ is analogous to $\tau_R > \tau_C$ and equal for an optimization versus runoff or mass anomalies .

For catchments showing a phase shift between total mass and runoff the description of the system by a Single Storage approach ($\tau_R = 10^{-3}$) leads to a considerably higher relative error $\varepsilon(\underline{\tau}_X)/\tau_X$ in the estimated time constant $\underline{\tau}_C \sim (\tau_C + \tau_R)$ and thus also in Drainable Storage volume. It follows a power function and corresponds to $\varepsilon < 10\%$ for $\underline{\tau}_C < 3$ and $\varepsilon > 40\%$ for $\underline{\tau}_C > 6$. For this case the optimization versus river runoff or mass anomalies leads to different total time constants (rel. Diff. $\varepsilon > 7\%$ for $\underline{\tau}_C > 5$). Even though this might look like an acceptable result for $\underline{\tau}_C < 3$, there are still inevitable deviations in signal amplitudes (10-20%) and phasing between the modelled and measured signals for both total mass and river runoff time series.

It can be summarized that in contrast to the Single Storage approach the Cascaded Storage approach permits the determination of both time constants (τ_C, τ_R) independently in a unique, highly accurate way for optimizations with respect to either total mass anomalies or river runoff. However, it has to be mentioned that even though the theoretical error in time constants remains below 1% for $\tau_R \sim \tau_C$, the ambiguity for $\tau_R < \tau_C$ or $\tau_R > \tau_C$ cannot be solved without further information on the volume of the river network.

4 Application to the Amazon catchment

The R-S diagram of the full Amazon basin shows a hysteresis (Fig.1b, d) corresponding to a phase shift, which can be interpreted as the time lag of river discharge. The Amazon basin upstream Obidos is situated in a fully humid tropic environment with permanent, yet variable recharge and is large enough (4704394km^2) for low noise levels in the signals of GRACE and moisture flux divergence. With permanent recharge flow contributions from overland flow and groundwater cannot be distinguished in the discharge curve. Also, on a spatial average over the full Amazon basin, with permanent recharge the uncoupled storages (like soil water storage, open water bodies etc.) are not time variant, i.e. there is no dry out effect. Any contribution from time dependent, uncoupled storages could be recognized in the R-S diagram as it would appear as a hysteresis, which does not correspond to a time lag. This is not the case.

Generally recharge from different approaches and products can serve as input to the system such as :

1. $$N(t) = P(t) - ET(t) \tag{32}$$

   from the hydrometeorological products precipitation P and actual evapotranspiration ETa

2. $$N(t) = -\nabla \cdot \vec{Q} \tag{33}$$

   from atmospheric data, with monthly vertically integrated moisture flux divergence viMFD

3. $$N(t) = \frac{\partial}{\partial t} M(t) + R(t) \tag{34}$$

   from the terrestrial water balance with monthly temporal derivatives of GRACE measurements and measured river runoff R_o of the catchment.

Here recharge [mm/month] is taken either from the water balance, Eq.(34), or from moisture flux divergence, Eq.(33), provided by ERA-INTERIM of ECMWF and processed by the Institute of Meteorology and Climate Research, Garmisch, Germany. For GRACE mass anomalies data from GeoForschungsZentrum GFZ Potsdam Release 5 are used in mm equivalent water height. Both are handled as described in detail in Riegger and Tourian, 2014. Their spatial resolution limits the application of the approach to global scales >>200000km^2. River discharge is taken from the ORE HYBAM project (http://ore-hybam.org) and converted to runoff [mm/month] by normalization with the catchment area. For a comparison of the calculated river network storage with observations from the “Global Inundation Extent from Multi-Satellite GIEMS (Prigent et al., 2001) flood area [km^2] is used. As GRACE mass anomalies are most accurate for a monthly time resolution at present, the other data sets are aggregated to a monthly resolution as well. For the parameter optimization time series of river runoff and GRACE mass anomalies are used for the time period from January 2004 until January 2009. Monthly runoff and the storage volume of the catchment and river network are calculated for Amazon based on different recharge products here and optimized either versus runoff or GRACE mass anomalies . The results calculated with recharge from the terrestrial water balance optimized versus GRACE are shown in Figures 8-10 for both (a) the monthly signal and (b) the monthly residual (monthly value minus mean monthly value) for January 2003-2009 .

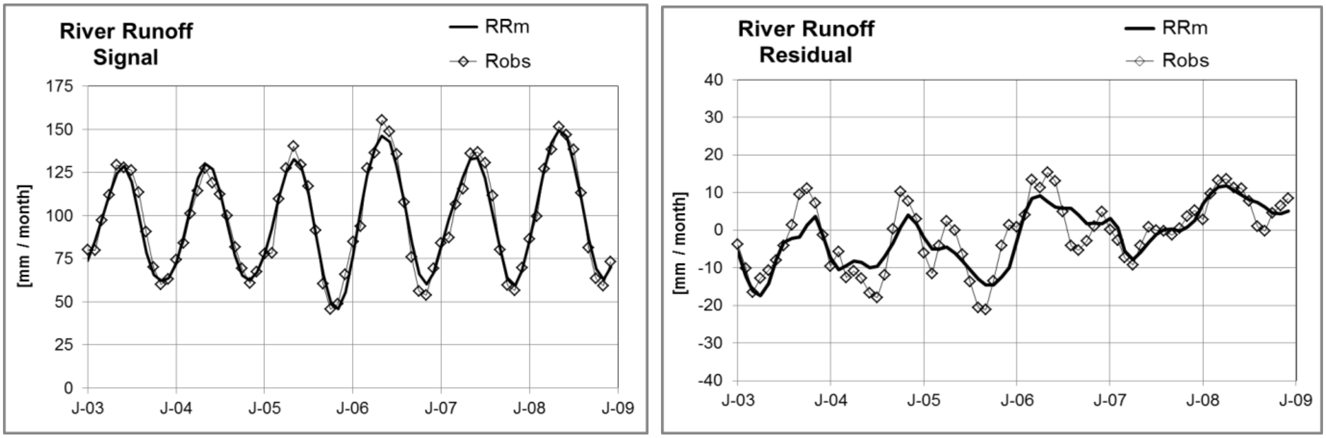

Fig.8: Time series of river runoff for the Amazon basin (Obidos) and optimization versus GRACE (a) for the signal (b) for the residual

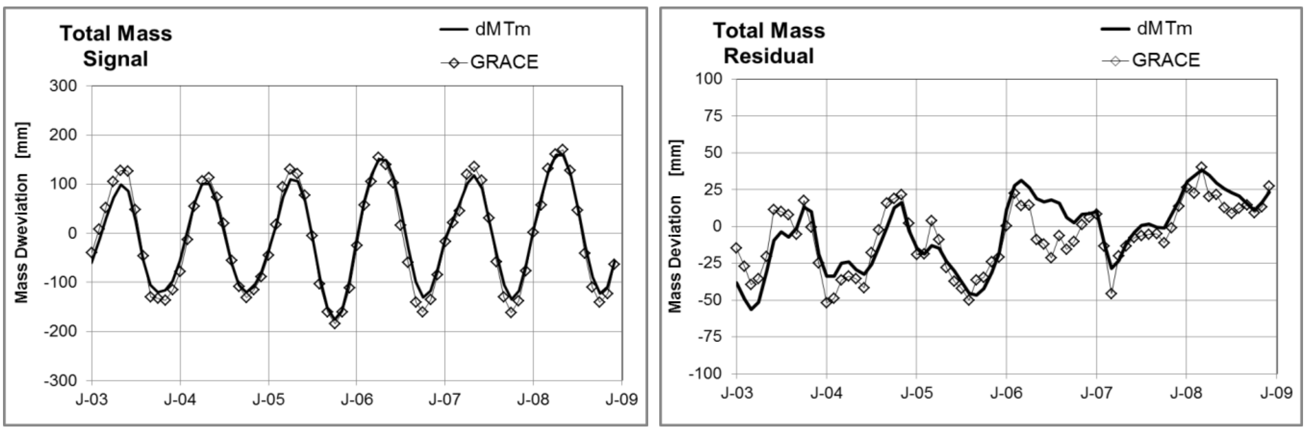

Fig.9: Time series of Total mass anomalies for the Amazon and optimization versus GRACE (a) for the signal (b) for the residual

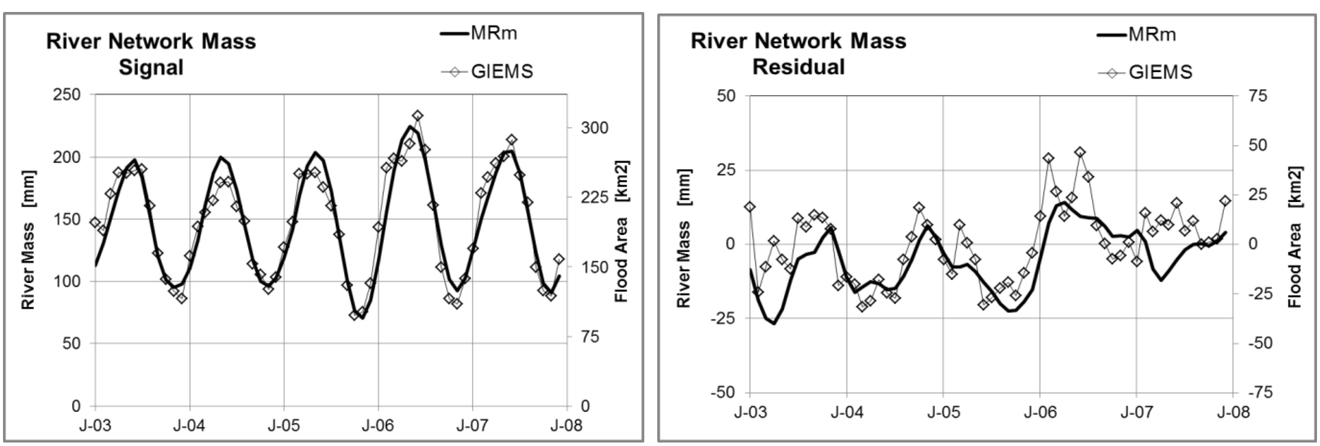

Fig.10: Time series of River network storage and inundated area from GIEMS for the Amazon (a) for the signal (b) for the residual

The calculated river runoff R_R, total mass anomaly dM_T and river network mass M_R fit very well with the measured river runoff, GRACE and the flooded area from GIEMS both with respect to the signal and the de-seasonalized monthly residual. The Cascaded Storage approach reproduces the phase shift between measured runoff R_o and total mass dM_T (or GRACE respectively). The calculated river network mass M_R of about 50% of the total mass M_T for Amazon is proportional to observed runoff R_o without any phase shift (Fig.11)!

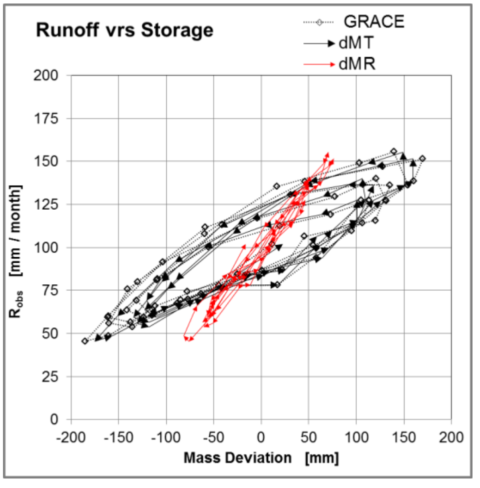

Fig.11: R-S relationships for observed runoff versus the mass anomalies of GRACE, calculated Total mass dM_T and river network mass dM_R

Calculated hydraulic time constants, mean values and signal amplitudes for the absolute storage volumes are provided in Table.2 for the full Amazon basin upstream Obidos. In addition the performance of optimizations either versus river runoff (Column A) or versus GRACE (Column B) and for different recharge products (Column D, E) is displayed. This shows that the optimization versus different references leads to a very similar results while the fitting performance for the two recharge products (Columns A, B and D, E) is quite different. For recharge from water balance, Eq.(34), the resulting time constants and thus the storage masses differ in a range of ~5% for the different references while they vary ~10% for recharge from moisture flux divergence.

In order to illustrate the benefits of the Cascaded versus a Single Storage approach even in the fitting quality, results for a fixed $\tau_R = 10^{-3}$, which correspond to a Single Storage, are shown (Column C, F) for different recharge products. With the Single Storage approach - beside the much worse fitting performance - the resulting time constant $\tau_T = \tau_C + \tau_R$ is overestimated (corresponding to the investigations in section 3) and the modelled signal amplitude is about 20% less than that measured from GRACE. In addition a non negligible phase shift remains between the modelled runoff and measured discharge.

	A	B	C	D	E	F
Approach	**Cascaded**	**Cascaded**	**Single**	**Cascaded**	**Cascaded**	**Single**
Recharge	R+dM/dt	R+dM/dt	R+dM/dt	-divQ	-divQ	-divQ
Optimization	RR	dMT	dMT	RR	dMT	dMT
τ_C [month]	1.53	1.62	3.55	1.68	1.87	3.95
τ_R [month]	1.53	1.62	0.001	1.68	1.87	0.001
Avg M_T [mm]	304.81	321.77	353.29	333.00	370.93	392.02
Avg M_C [mm]	152.17	160.58	353.19	166.23	185.12	391.92
Avg M_R [mm]	152.64	161.18	0.10	166.77	185.81	0.10
Avg R_R [mm month^{-1}]	99.53	99.59	99.39	99.35	99.49	99.34
Avg N [mm month^{-1}]	98.80	98.80	98.80	99.07	99.07	99.07
Stdev M_T [mm]	98.46	100.38	84.09	101.73	105.34	87.83
Stdev M_C [mm]	58.49	60.40	84.06	61.22	65.05	87.80
Stdev M_R [mm]	45.48	46.02	0.02	46.70	47.55	0.02
RMSE R_R-R_o [mm month^{-1}]	5.76	6.08	12.13	11.99	12.57	18.08
RMSE M_T- GRACE [mm]	15.28	14.73	28.93	35.45	34.54	42.31
NS_S R_R-R_o	0.96	0.96	0.84	0.85	0.83	0.65
NS_R R_R-R_o	0.74	0.72	0.73	-0.09	-0.08	-0.10
$corr_S$ R_R-R_o	0.98	0.98	0.94	0.92	0.92	0.82
$corr_R$ R_R-R_o	0.86	0.85	0.87	0.48	0.46	0.41
NS_S dM_T- GRACE	0.98	0.98	0.92	0.89	0.89	0.84
NS_R dM_T- GRACE	0.74	0.72	0.71	-0.57	-0.81	-0.71
$corr_S$ dM_T- GRACE	0.99	0.99	0.98	0.94	0.94	0.93
$corr_R$ dM_T- GRACE	0.90	0.90	0.88	0.58	0.56	0.51
$corr_S$ dGIEMS- GRACE	0.92	0.92	0.92	0.92	0.92	0.92
$corr_S$ GIEMS-M_T	0.93	0.94	0.95	0.82	0.84	0.82
$corr_S$ GIEMS-M_R	0.96	0.95	0.95	0.88	0.86	0.82
$corr_R$ dGIEMS- GRACE	0.65	0.65	0.65	0.65	0.65	0.65
$corr_R$ GIEMS-M_R	0.76	0.75	0.78	0.04	-0.01	0.01

Table.2: The statistical characteristics are listed for calculated river runoff R_R, total mass M_T, catchment mass M_C and river network mass M_R and observed river runoff R_o, GRACE mass anomalies and flood areas from GIEMS using: RMSE: Root-mean-square error of simulated versus measured, NS_S: Nash Sutcliffe coefficient of the signal (simulated values versus long-term mean of measured), NS_R: Nash Sutcliffe coefficient of monthly residuals (simulated values versus monthly mean of measured), $corr_S$: correlation of simulated versus measured signals, $corr_R$: correlation of simulated versus measured monthly residuals, Avg and Stdev are the long term mean and standard deviations, prefix "d" used for anomalies related to the long term mean.
Results are compared for the different optimization references runoff R_o or GRACE for recharge from water balance R+dM/dt (A, B) and for atmospheric input -divQ (D, E). The Cascaded storage approach is compared to Single storage approach in (C, F).

The Cascaded Storage approach with recharge from the water balance, Eq. (34), leads to high accuracy fits between calculated and measured river runoff and total storage mass for the signals (NSS R_R-R_o=0.96, NSS dM_T- GRACE = 0.98) and for the residuals (NSR R_R-R_o = 0.74, NSR dM_T- GRACE = 0.74, the respective calculations are available in the xls-workbook provided in the supplement). The comparison of the water budgets for 14 different LSMs (Getirana et al. (2014)) permit to sort in the results of the Cascaded Storage Approach into those of the LSMs (Getirana et al. (2014), Fig. 14). With a Nash-Sutcliffe (NS) coefficient of 0.74 and a correlation of 0.90 (with respect to the mean seasonal cycle) compared to an NS of 0.58 and a correlation of 0.84 for the best LSM, the Cascaded Storage approach outperforms the LSMs for Amazon. This is mainly seen as the result of the quality of recharge data taken from the water balance using GRACE and river runoff, as the use of moisture flux divergence for this purpose leads to much worse results.

The calculated river network mass M_R of the Amazon varies in the range of 40-65% of total mass M_T with an average ~50%, corresponding to the values found by Paiva et al., 2013 and Papa et al., 2013 or ~41% by Getirana et al., 2017a. The correlation versus the observed flood area from GIEMS is higher for the calculated river network mass M_R (0.96 for the signal and 0.76 for the monthly residual) than for GRACE (0.92 and 0.65 respectively). The consistency of the calculated river network mass (and the corresponding observed river runoff $R_R = M_R \tau_R^{-1} = 0.742\ M_R$) with the flood areas is seen much more clearly in the phasing (Fig.12), which shows a clear phase shift for GRACE versus GIEMS (see also Papa et al., 2008), yet none for calculated M_R. As already Getirana et al., 2017a emphasized, only an appropriate description of the river network storage permits a correct description of the total storage in amplitude and phasing for a comparison with GRACE.

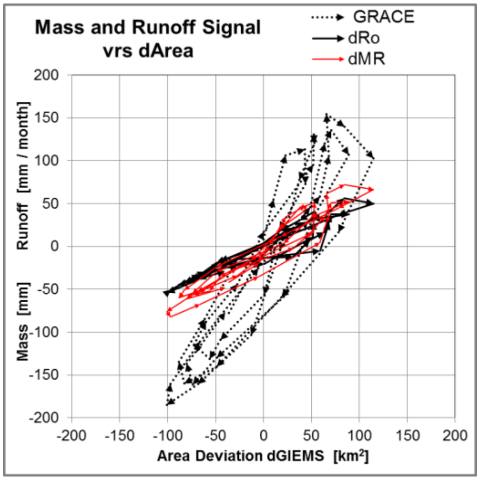

Fig.12: GRACE mass, calculated river network mass dM_R and observed river runoff dR_o versus Flood Area dGIEMS; all displayed as anomalies (please consider $dM_R = dR_R\ \tau_R = 1.53\ dR_R$)

6 Conclusions and Discussion

The test of the Cascaded storage approach with synthetic recharge data has shown that the parameter optimization either versus mass d anomalies or runoff reproduces the time constants (τ_C, τ_R) for both, the catchment and the river network in a unique way with high accuracy, yet with an ambiguity for $\tau_R < \tau_C$ or $\tau_R > \tau_C$, and thus in the related storage volumes. This problem can only be solved by reasonable assumptions or better by additional information on the volume of river network or flood areas, which can be taken from ground based observations or remote sensing. In principle, river network storage could be directly used for the parameter optimization. It could be provided by GIEMS flood areas and water levels from altimetry. This might also help to decide whether the catchment storage is clearly bigger than the river network storage, even if these data are not too accurate. Close to $\tau_R \sim \tau_C$, the generally high accuracy of ~1% RMSE is limited as the separation of the storages depends on the quality of the respective additional information on the volume of the river network. In contrast to this, the description of a system (showing a phase shift) by a Single Storage approach can only address the total Drainable storage and leads to phasing differences between the calculated and measured runoff or storage and to considerable errors in the time constant of the total system.

The application to the full Amazon catchment shows that the system behaviour including the time lag can be described by a simple conceptual model with a catchment and a river network storage in sequence and an adjustment of only two parameters, the time constants. The storage amplitudes for the total Drainable water storage and the time lag to runoff are described with high precision. Calculated river network volume and the observed flood area are in phase with river discharge.

The accuracy of the Drainable storage volume mainly depends on the quality of recharge data. The use of recharge from water balance with data from observed river discharge and GRACE is preferable to the use of moisture flux divergence, yet, it limits the approach to a lumped description of basins on global scales (>> 200000km^2) due to the resolution of GRACE. This means that the simplicity and accuracy of this approach is payed by the lack of the spatial information, regardless of the difficulty to evaluate storages volumes locally.

The Cascaded storage approach, if it is based on one catchment and one river network storage only, is limited to climatic and physiographic conditions for which the hysteresis is completely explained by a time lag. This prerequisite is fulfilled if the R-S diagram shows a counter clockwise hysteresis and if a phase shift adaption leads to positive values and a linear relationship. If any contributions from time dependent, not drainable i.e. uncoupled storage compartments occur, which could result from processes like freezing, melting, evapotranspiration etc., these can be recognized in the R-S diagram (Fig.1d) or by the respective deviations in the scatter plots of calculated versus measured runoff or storage volumes (see supplement). For this case both, the time dependent coupled and uncoupled storage components have to be addressed explicitly in the lumped model description of the system. The uncoupled storage components then have to be quantified either with their absolute storage volume or by their relative contribution to total storage.

As Riegger and Tourian, 2014, have shown for boreal catchments, this can be done by means of remote sensing and a conceptional description. Boreal catchments are temporarily dominated by snow leading to a huge hysteresis due to a superposition of masses from fully coupled (liquid) and uncoupled (solid) storage compartments. Remote sensing of the catchments snow coverage by MODIS facilitates the separation of the coupled liquid storage (proportional to river runoff) and the uncoupled frozen part. The coupled liquid storage determined in this way actually constitutes a LTI system, i.e. the hysteresis can be fully explained by a phase shift. This fulfils the prerequisites for the Cascaded storage approach and thus permits an application to boreal catchments as well. In consequence, the principle of the Cascaded storage approach is not limited to fully humid climatic conditions. It permits an application to other climatic regions as well provided that the coupled and uncoupled storage can be quantified, which of course is a major task.

As the optimization performance is comparable for either reference, the observed river runoff or GRACE anomalies, a calculation with given recharge and an optimization versus measured GRACE data can be used to determine both, the river discharge as well as the Drainable storage volumes even for ungauged basins. For these cases the availability of accurate recharge data limits the accuracy of runoff and storage calculations at present. However, for ungauged basins the use of moisture flux divergence still provides quite acceptable results based on remote sensing and atmospheric data exclusively.

Where river discharge is available the Cascaded storage approach facilitates a simple determination of the Drainable water storage volumes both for the catchment and for the river network directly from observations without the necessity of new model runs.

6 Data driven Determination of Drainable Storage volumes

The two time constants (τ_C, τ_R) adapted during a training period permit to quantify the Drainable water storage volumes M_T, M_C and M_R at other times directly from observation data of GRACE and river discharge. With a simple numerical adaption of the phase shift $\Delta\omega$ resulting from the time constants (τ_C, τ_R) a quite accurate determination of the total Drainable storage volume from measured river discharge exclusively or the other way round of runoff from GRACE is possible.

These can be determined by the following calculations :

1. Long term averages of Drainable storage volumes from observed runoff R_o :

   $\overline{M}^{C}_{sim} = \tau_C \cdot \overline{R}_o$ $\quad$ $\overline{M}^{R}_{sim} = \tau_R \cdot \overline{R}_o$ $\quad$ $\overline{M}^{T}_{sim} = \tau_T \cdot \overline{R}_o$ $\quad$ with $\overline{R}_o = \overline{N}$ and $\tau_T = \tau_C + \tau_R$

   according to Eq. (22a,b,c) and Eq. (23) :

2. Time series of Drainable storage volumes from GRACE and observed runoff R_o without the need for a phase adaption:

$$M_{sim}^{R}(t) = \tau_R \cdot R_o(t) \quad (35)$$

(NSS 0.961, NSR 0.576, corrR 0.859 vs M_R from Eq.18)

$$M_{sim}^{T}(t) = dM^{T}(t) + \overline{M}^{T} = GRACE(t) + \overline{M}^{T} = GRACE(t) + \tau_T \cdot \overline{N} \cdot = GRACE(t) + \tau_T \cdot \overline{R}_0 \quad (36)$$

(NSS 0.973, NSR 0.751, corrR 0.901 vs M_T from Eq.20)

$$M_{sim}^{C}(t) = M^{T}(t) - M^{R}(t) = GRACE(t) + \tau_T \cdot \overline{R}_o \; - \; \tau_R \cdot R_o(t) \quad (37))$$

(NSS 0.906, NSR -0.065, corrR 0.607 vs M_C from Eq.16)

The simplified calculations directly from observations lead to accurate equivalences to the fully calculated time series of total and the river network storage volumes M_T and M_R and to a reasonable description of the catchment storage volumes M_C.

3. Time series of total Drainable storage volumes M_T, from observed runoff R_o or simulated river runoff R^R_{sim} from GRACE with a numerical phase adaption of $\Delta\omega$.

Use of the phase shift $\Delta\omega$ between GRACE and observed river runoff for a linear temporal interpolation (Riegger and Tourian, 2014) permits a simple description of river runoff directly from GRACE (Eq.38) or of total Drainable water storage MT directly from observed runoff (Eq.39). The phase shift $\Delta\omega_{adapt}$ can also be adapted directly (Eq.38, Eq.39) and corresponds to $\Delta\omega$ from Eq.27 within <~10%. Both lead to very similar fitting performances.

$$R_{sim}^{R}(t_i) \;=\; \frac{1}{\tau_T} \cdot \left[\; (1-\Delta\omega) \cdot GRACE(t_i) \;+\; \Delta\omega \cdot GRACE(t_{i-1}) \;+\; \tau_T \cdot \overline{R}_o \right] \quad (38)$$

(NSS 0.943, NSR 0.698, corrR 0.864 vs measured R_o,)

$$M_{sim}^{T}(t_i) = \tau_T \cdot \left\lfloor\; (1-\Delta\omega) \cdot R_o(t_i) \;+\; \Delta\omega \cdot R_o(t_{i+1}) \;\right\rfloor \quad (39)$$

(NSS 0.946, NSR 0.483, corrR 0.859 vs GRACE))

This facilitates a simple determination of Drainable storage volume or runoff time series directly from measurements and thus a closure of data gaps with high accuracy comparable to the best performances in the LSM test by Getirana et al. (2014). The related calculations are accessible in the xls-workbook provided in the supplement.

7 Summary and Outlook

The lumped description of the water storages in catchment systems by a cascade of catchment storages and a river network storage facilitates the quantification of their individual Drainable storage volumes and their phasing directly from large scale observations of GRACE, remote sensing and river discharge. No detailed information on vegetation, soil etc., complex flow processes nor hydrodynamic modelling with detailed hydraulic information on river roughness, cross section, gradient or backwater effects is needed. An optimization versus GRACE measurements permits a determination of river runoff and Drainable storage volumes from recharge and GRACE exclusively, and thus provides reasonable results for ungauged catchments. The piecewise analytical solutions for time periods of constant recharge provide accurate calculations even for the much shorter time constants of the river network without numerical limitations.

The fact, that river network and flood volumes can be quantified by this approach independently, permits an investigation of the relationship between flood areas, flood volumes, river runoff and calculated river network with additional information and might provide insights into river hydraulics i.e. routing times and the mass- area- and level- relationships of flooded areas.

The individual adjustment of the hydraulic time constants for the catchment and the river network (τ_C, τ_R) on a training period facilitates a determination of Drainable storage volumes M_C, M_R and M_T at other times directly from measurements of river discharge and GRACE without the necessity of further model runs. River runoff can also be determined directly from GRACE and vice versa by an adaption of the time lag. This permits to close data gaps in river discharge or GRACE time series and even provides the possibility for operational forecasts within the period of the time lag.

For a global coverage the Cascaded storage approach has to be extended for an implementation of the uncoupled storage components according to the regional climatic and physiographic conditions. For boreal catchment MODIS snow coverage can be used for a quantification or coupled and uncoupled storage components. The description of monsoonal regions, which play an important role in the global water budget, remains a major challenge. For these regions with seasonally dry periods high precipitation events during the wet season lead to distinct runoff in parallel from overland and groundwater with different time constants τ_S and τ_{GW} and to time dependent uncoupled storage compartments like soil or isolated open water bodies, which do not contribute to discharge. All these storages have to be addressed for an adequate description of the

Drainable Storage Volumes. The uncoupled storage compartments have to be quantified by remote sensing (soil moisture and open water body altimetry from satellites) and subtracted from the total catchment mass measured by GRACE.

As the spatial resolution of GRACE and the accuracy of moisture flux divergence is limiting the Cascaded storage approach to global scale catchments at the moment, any improvement in the spatial / temporal resolution and accuracy of GRACE and hydrometeorological data products will tremendously increase the number of catchments which can be described by this approach in future.

Data availability

In the supplement calculations and data are provided in an EXCEL workbook for the synthetic case and for the Amazon catchment.

Acknowledgements

The author would like to thank Nico Sneeuw and Mohammad Tourian from the Institute of Geodesy, Stuttgart, for the handling of GRACE data , Harald Kunstmann and Christof Lorenz from the Institute of Meteorology and Climate Research, Garmisch, for the provision of moisture flux data and Catherine Prigent, Observatoire de Paris, for the provision of Flood areas from the GIEMS project.

References

Alley, W. M.: Tracking U.S. groundwater reserves for the future?, Environment, 48(3), 10–25, 2006.

Bredehoeft, J.: Safe yield and the water budget myth, Ground Water, 35(6), 929–929, doi:10.1111/j.1745-6584.1997.tb00162.x, 1997

Cao, G., Zheng, C., Scanlon, B. R., Liu, J., and Li W.: Use of flow modeling to assess sustainability of groundwater resources in the North China Plain, Water Resour. Res., 49, doi:10.1029/2012WR011899, 2013

Famiglietti, J. S.: The global groundwater crisis, Nat. Clim. Change, 4(11), 945–948, doi:10.1038/nclimate2425, 2014

Frappart, F., Papa, F., da Silva, .,J.S., Ramillien, G., Prigent, C., Seyler, F., Calmant, S.: Surface freshwater storage and dynamics in the Amazon basin during the 2005 exceptional drought, Environ. Res. Lett. 7, doi: 10.1088/1748-9326/7/044010, 2012

Getirana, A. et al.: Water Balance in the Amazon Basin from a Land surface Model Ensemble, Journal of Hydrometeorolgy, 2586-2614,doi:10.1175/JHM-D-14-0068.1, 2014

Getrirana, A., Kumar, S., Girotto, M., & Rodell, M.: River and Floodplains as Key Components of Global Terrestrial Water Storage Variability, Geophysical Research Letters, 44-50, doi: 10.1002/2017GL074684, 2017a

Getirana, A., Peters-Lidard, Ch., Rodell, M., Bates, P. D., Tradoff between cost and accuracy in large-scale surface water dynamic modeling, Water Resour. Res., 53, doi:10.1002/2017WR020519 , 2017b

Korzun, V. I.: World Water Balance and Water Resources of the Earth [in Russian], 638 pp., Hydrometeoizdat, Leningrad, 1974

Luo, X., Li, H.-Y., Leung, L. R., Tesfa, T. K., Getirana, A., Papa, F., and Hess, L. L.: Modeling surface water dynamics in the Amazon Basin using MOSART-Inundation v1.0: impacts of geomorphological parameters and river flow representation, Geosci. Model Dev., 10, 1233-1259, https://doi.org/10.5194/gmd-10-1233-2017, 2017

Nace, R. L.: World water inventory and control, in Water, Earth, and Man, edited by R. J. Chorley, pp. 31–42, Methuen, London, U. K., 1969

Nash, J.E.: The form of the instantaneous unit hydrograph, Proc. I.A.S.H. Assem. Gen., Toronto, Ont., 3: 114-131, 1957

Paiva, R.C., Buarque, D.C., Collischonn, W., Bonnet, M. P., Frappart, F., Calmant, S., Mendes, C.A.B.: Large scale hydrologic and hydrodynamic modelling or the Amazon river Basin, Water Resour. Res., 49, doi: 10.1002/wrcr.20067, 2013

Papa, F., Güntner, A., Frappart, F., Prigent, C., Rossow, W.B.: Variations of surface water extent and water storage in large river basins: A comparison of different global sources, Geophysical Research Letters, 35, doi: 10.1029/2008GL033857, 2008

Papa, F., Frappart, F., Güntner, A., Prigent, Aires, F., Getirana, A.C.V., Maurer, R.: Surface freshwater storage and variability in the Amazon basin from multi-satellite observation, 1993-2007, J. Geophys. Res.: Atmos., *118*, 11,951-11,965, doi: 10.1002/2013JD020500, 2013

Prigent, C., E. Matthews F. Papa, F. Aires, Rossow, W. B.: Remote Sensing of global wetland Dynamics with multiple satellite data sets, Geo. Res. Lett., 28, 4631-4634, 2001

Prigent, C., F. Papa, F. Aires, F., Rossow, W. B. , and Matthews E.: Global inundation dynamics inferred from multiple satellite observations, 1993 – 2000, J. Geophys. Res., 112, D12107, doi:10.1029/ 2006JD007847, 2007

Richey, A. S., Thomas, B. F., Lo, M.-H., Famiglietti, J. S., Swenson, S., and Rodell M.: Uncertainty in global groundwater storage estimates in a Total Groundwater Stress framework, Water Resour. Res., 51, 5198–5216, doi:10.1002/2015WR017351, 2015a

Richey, A. S., Thomas, B. F., Lo, M.-H., Reager, J. T., Famiglietti, J. S., Voss, K., Swenson, S., and Rodell M.: Quantifying renewable groundwater stress with GRACE, Water Resour. Res., 51, 5217–5238, doi:10.1002/ 2015WR017349, 2015b

Riegger, J., Tourian, M., Devaraju, B., Sneeuw, N., Analysis of grace uncertainties by hydrological and hydro-meteorological observations, Journal Geodyn., 5960, 16-27, doi:10.1016/j.jog.2012.02.001, 2012

Riegger, J., and Tourian, M. J.: Characterization of runoff-storage relationships by satellite gravimetry and remote sensing. Water Resour. Res., 50, doi:10.1002/2013WR013847, 2014

Schlesinger, M.E.: Human-induced climate change : an interdisciplinary assessment, xviii, Cambridge University Press, 2007

Tapley, B. D., Bettadpur, S., Ries, J. C., Thompson, P. F., and Watkins M. M.: GRACE measurements of mass variability in the Earth system, Sciences N. Y., 305(5683), 503–505, doi:10.1126/science.1099192, 2004

Tourian, M. J., Reager, J. T. and Sneeuw, N.: The Total Drainable Water Storage of the Amazon River Basin: A First Estimate Using GRACE, Water Resources Research, 54(5), 3290–3312, doi:10.1029/2017WR021674, 2018.

Williamson, A. K., Prudic, D. E., and Swain L. A.: Ground-water flow in the Central Valley, California, U.S. Geol. Surv. Prof. Pap. 1401-D, 225 pp, 1989

Shiklomanov, I. A.:World freshwater resources, in Water in Crisis: A Guide to the World's Fresh Water Resources, edited by P. H. Gleick,,pp. 13–24, Oxford Univ. Press, N. Y., 1993

Siqueira, V. A., Paiva, R. C. D., Fleischmann, A. S., Fan, F. M., Ruhoff, A. L., Pontes, P. R. M., Paris, A., Calmant, S., and Collischonn, W.: Toward continental hydrologic–hydrodynamic modeling in South America, Hydrol. Earth Syst. Sci. Discuss., https://doi.org/10.5194/hess- 2018-225, in review, 2018

Sophocleous, M.: Managing water resources systems: Why ‘‘safe yield’’ is not sustainable, Ground Water, 35(4), 561–561, doi:10.1111/ j.1745-6584.1997.tb00116.x, 1997

Tallaksen, L.M.: A review of baseflow recession analysis, Journal of Hydrology, No. 165, S. 349-370, 1995