Supplement of

Understanding terrestrial water storage variations in northern latitudes across scales

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**Supplement**

**S1 Detailed model description and formulas**

The model consists of three components: (1) a snow component that simulates accumulation and ablation of snow, (2) a soil water component to calculate soil moisture, evapotranspiration and land runoff, and (3) a runoff component that derives total runoff. All modelled fluxes and states correspond to the spatio-temporal resolution of the forcing data, which in this study is a 1° x 1° latitude/longitude grid and daily time steps.

The following describes all implemented processes and equations in detail.

**S1.1 Snow Component**

Snow storage is implemented as a simple accumulation and melt approach, which further is extended by consideration of sublimation and fractional snow cover. The snow storage as described by the snow water equivalent SWE [mm] at time t [d] is calculated as mass balance:

\[
S\text{WE}_t = S\text{WE}_{t-1} + SF_t - E\text{TSub}_t - M_t \\
\text{(S1)}
\]

where SWE\(_{t-1}\) [mm] is the snow water equivalent of the preceding time step which is increased by snowfall SF\(_t\) [mm d\(^{-1}\)] and reduced by the amount of sublimation ETSub\(_t\) [mm d\(^{-1}\)] and snow melt M\(_t\) [mm d\(^{-1}\)].

All precipitation P [mm d\(^{-1}\)] is assumed to fall as snow at temperatures below 0 °C. Since precipitation estimates, especially during the cold season, are known for biases due to substantial under-catch (Rudolf and Rubel, 2005; Seo et al., 2010), P is scaled using the parameter \(p_{sf}\) to derive SF at time t:

\[
SF_t = p_{sf} \cdot P_t \mid T < 0°C \\
\text{(S2)}
\]

In order to incorporate sub-grid variability, the fraction of the grid cell covered by snow is computed following the H-TESSEL approach (Balsamo et al., 2009; ECMWF, 2014):

\[
F\text{SC}_t = \min\left(\frac{S\text{WE}_{t-1}}{sn_c}, 1\right) \\
\text{(S3)}
\]

with fractional snow cover FSC [-] at time t being linearly dependent on SWE\(_{t-1}\) of the preceding time step and the parameter \(sn_c\) [mm] being the minimum SWE that ensures complete snow coverage of the grid cell.
Further, snow melt $M$ and sublimation $ET_{Sub}$ are assumed to only emerge from snow covered area by using FSC as scaling factor in the calculation of these fluxes.

Snow melt $M$ occurs when snow storage is present and temperature exceeds melting temperature. Based on the restricted degree-day radiation balance approach described by Kustas et al. (1994), melt $M$ [mm d$^{-1}$] at time $t$ depends on temperature $T_t[°C]$ and net radiation $R_n_t[\text{MJ m}^{-2} \text{d}^{-1}]$:

$$M_t = (m_t \cdot T_t + m_r \cdot R_{nt}) \cdot \text{FSC}_t$$  \hspace{1cm} | T > 0°C \hspace{1cm} (S4)$$

where the degree-day factor $m_t$ [mm °C$^{-1}$] and the radiation factor $m_r$ [mm MJ$^{-1}$] control the melt rate.

The derivation of snow sublimation $ET_{Sub}$ is adapted from the approach implemented in the GLEAM model. This technique is based on the Priestley and Taylor (1972) formula, which calculates evaporation rate as latent heat flux $LE$ [MJ m$^{-2}$ d$^{-1}$] based on the available energy $R_n$ [MJ m$^{-2}$ d$^{-1}$], ground heat flux $G$ [MJ m$^{-2}$ d$^{-1}$]) and a dimensionless coefficient $s_n$ that parameterizes evaporation-resistance. $LE$ at time $t$ is derived by

$$LE_t = \left( s_n \cdot \frac{\Delta s_{nt}}{\Delta s_{nt} + \gamma s_{nt}} \cdot (R_{nt} - G) \right) \cdot \text{FSC}_t$$ \hspace{1cm} (S5)$$

with $\Delta s_{nt}$ being the slope of the temperature/saturated vapor pressure curve [kPa K$^{-1}$] and $\gamma s_{nt}$ representing the psychrometric constant [kPa K$^{-1}$]. Both, $\Delta s_{nt}$ and $\gamma s_{nt}$, are modified for snow covered areas according to Murphy and Koop (2005). They calculate $\Delta s_{nt}$ as a function of $T_t[K]$ (Eq.(S6)), and $\gamma s_{nt}$ as a function of atmospheric pressure $Pair$ [kPa], specific heat of air at constant pressure $c_p$ [MJ kg$^{-1}$ K$^{-1}$], the ratio molecular weight of water vapor/dry air $MW$ and latent heat of sublimation of ice $\lambda s_{nt}$ [MJ kg$^{-1}$] (Eq.(S7)).

$$\Delta s_{nt} = \left( \frac{5723.265}{T_t^2} + \frac{3.53069}{T_t - 0.00728332} \right) \cdot e^{9.550426 - \frac{5723.265}{T_t} + 3.53068 \ln(T_t) - 0.00728332 \cdot T_t}$$ \hspace{1cm} (S6)$$

$$\gamma s_{nt} = \frac{Pair \cdot c_p}{MA \cdot \lambda s_{nt}}$$ \hspace{1cm} (S7)$$

In Eq.(S7), $Pair$ is assumed to be time- and space-invariant with a uniform value of 101.3 kPa and $c_p = 0.001$ MJ kg$^{-1}$ K$^{-1}$. $MA$ is a constant of 0.622 and $\lambda s_{nt}$ is defined by Murphy and Koop (2005) as a function of $T_t[K]$. With a molecular mass of water of 18.01528 g mol$^{-1}$, $\lambda s_{nt}$ can be calculated as:
\[ \lambda_{sn_t} = \left( 46782.5 + 35.8925 \cdot T_t - 0.07414 \cdot T_t^2 + 541.5 \cdot e^{-\left(\frac{t}{123.79}\right)^2} \right) \cdot \frac{0.001}{10.01528} \]  

(S8)

Since snow-covered ecosystems can be assumed to be unstressed due to the sufficient availability of water, LE corresponds to actual sublimation ETSub (Miralles et al., 2011). And ETSub [mm d\(^{-1}\)] can be converted from LE through division by \(\lambda_{sn}\):

\[ \text{ETSub}_t = \frac{\text{LE}_t}{\lambda_{sn_t}} \]  

(S9)

Altogether, the model calculates ETSub as a function of \(T_t\), \(Rn_t\), Pair, \(G\), \(sn_{ai}\) and FSC\(_t\). While \(T_t\), \(Rn_t\) and FSC\(_t\) are variable in time and space and depend on input data, the approach postulates constant Pair = 101.3 kPa and \(G = 0 \text{ MJ m}^{-2} \text{ d}^{-1}\).

### S1.2 Soil component

The central part of the model is the soil water component, which distributes input from rain fall and snow melt to soil water storage SM [mm], actual evapotranspiration ET [mm d\(^{-1}\)] and land runoff Qs [mm d\(^{-1}\)].

Like snow, the calculation of soil water storage as represented by soil moisture SM [mm] at time \(t\) follows the mass balance

\[ \text{SM}_t = \text{SM}_{t-1} + \text{In}_t - \text{ET}_t \]  

(S10)

with \(\text{SM}_{t-1}\) [mm] being the soil moisture of the preceding time step which is increased by infiltration \(\text{In}_t\) [mm d\(^{-1}\)] and reduced by actual evapotranspiration \(\text{ET}_t\) [mm d\(^{-1}\)].

On the one hand, the amount of infiltration \(\text{In}\) [mm d\(^{-1}\)] depends on the possible inflow \(\text{IW}\) [mm d\(^{-1}\)], which is the sum of rain fall RF (precipitation \(P\) if \(T \geq 0^\circ\text{C}\)) and snow melt \(M\) at time \(t\):

\[ \text{IW}_t = \text{RF}_t + \text{M}_t \]  

(S11)

On the other hand, a part of \(\text{IW}\) may not infiltrate due to current soil moisture conditions but contribute to (direct) land runoff \(\text{Qs}\) [mm d\(^{-1}\)]. To estimate the partitioning of \(\text{IW}\) into \(\text{SM}\) and \(\text{Qs}\), \(\text{Qs}\) at time \(t\) is calculated after Bergström (1995) as:

\[ \text{Qs}_t = \text{IW}_t \cdot \left( \frac{\text{SM}_{t-1}}{s_{\text{max}}} \right)^{s_{\exp}} \]  

(S12)
In Eq. (S12) $Q_s_t$ depends on the inflow $IW_t$, the runoff coefficient $s_{exp}$ and the actual soil moisture $SM_{t-1}$ compared to its maximum water holding capacity $s_{max}$. Thus, no land runoff occurs if the soil water storage is empty and all IW is allocated to land runoff if the soil is completely saturated. Between these points, $s_{exp}$ determines the amount of inflow that converts to $Q_s$. While low values of $s_{exp}$ lead to a high amount of $Q_s$ even if the soil moisture deficit is low (e.g. low $SM/s_{max}$ ratio), higher values of $s_{exp}$ increase the proportion of IW that infiltrates.

Infiltration $In$ at time $t$ is derived in accordance to the law of conservation of mass as:

$$In_t = IW_t - Qs_t$$ (S13)

Potential evapotranspiration $potET$ [mm d$^{-1}$] at time $t$ is derived from net radiation $Rn$ [MJ m$^{-2}$ d$^{-1}$] and air temperature $T$ [°C] according to the Priestley-Taylor formula (Priestley and Taylor, 1972), where $e_{t0}$ is the alpha coefficient:

$$potET_t = e_{t0} \cdot \left( \frac{\Delta_t}{\Delta_t + \gamma_t} \cdot \frac{Rn_t}{\lambda_t} \right)$$ (S14)

where $\Delta_t$ is the slope of the temperature/saturated vapor pressure curve [kPa K$^{-1}$], $\lambda_t$ the latent heat of vaporization [MJ kg$^{-1}$] and $\gamma_t$ the psychrometric constant [kPa K$^{-1}$].

The slope of the saturated vapor pressure curve $\Delta_t$, as well as the latent heat of vaporization $\lambda_t$ are functions of $T$ at time $t$:

$$\Delta_t = \frac{4098 \cdot 0.611 \cdot e^{17.27 \cdot T_t}}{(T_t \cdot 237.3)^2}$$ (S15)

$$\lambda_t = 2.501 - (2.361 \cdot 10^{-3}) \cdot T_t$$ (S16)

Analogue to Eq.(S7), $\gamma_t$ depends on a constant atmospheric pressure $Pair$ of 101.3 kPa, the specific heat of air at constant pressure $c_p$ [MJ kg$^{-1}$ K$^{-1}$], the constant $MA$ and the latent heat of vaporization $\lambda_t$:

$$\gamma_t = \frac{Pair \cdot c_p}{MA \cdot \lambda_t}$$ (S17)

In order to avoid complete depletion of the soil water storage and to account for cohesion of water in the soil matrix, only a fraction of soil moisture after infiltration is assumed to be available for evapotranspiration. We express the sensitivity of evapotranspiration to available water similar to Teuling et al. (2006) by the parameter $et_{sup}$. Thus, $et_{sup}$ determines the portion
of the sum of infiltration $I_n$ [mm d$^{-1}$] and soil moisture $SM_{t-1}$ [mm], that represents evapotranspiration supply $supET$ [mm d$^{-1}$] at time $t$:

$$supET_t = et_{sup} \cdot (SM_{t-1} + I_n)$$  \hspace{1cm} (S18)

Finally, actual evapotranspiration $ET$ [mm d$^{-1}$] at time $t$ is derived by comparing $potET_t$ [mm d$^{-1}$] and $supET_t$ [mm d$^{-1}$]:

$$actET_t = \min(potET_t, supET_t)$$  \hspace{1cm} (S19)

### S1.3 Runoff component

As total runoff comprises fast direct runoff as well as delayed interflow and base flow, it’s appropriate to consider retardation (Orth et al., 2013). Accordingly, total runoff $Q$ [mm d$^{-1}$] at time $t$ results from the accumulated effects of all land runoff $Qs$ [mm d$^{-1}$] generated during the preceding 60 time steps:

$$Q_t = \sum_{i=0}^{60} Qs_{t-i} \cdot \left[ e^{-\frac{i}{q_t}} - e^{-\frac{i+1}{q_t}} \right]$$  \hspace{1cm} (S20)

where the recession time scale $q_t$ [d] determines how quickly land runoff is transformed into streamflow. In theory, an infinite number of time steps would be necessary to ensure that all generated $Qs$ is transformed into $Q$. However, the arbitrary number of 60 days allows accounting for > 99 % of $Qs$ (Orth et al., 2013), as long as $q_t$ is below 13 days. To allow longer recession times when calibrating the model and still account for > 99 % of $Qs$ within the 60 days-window, the delay component of Eq.(S20) is scaled with its sum.

Introducing temporal delay leads to retention of a portion of $Qs$, and thus to an additional, temporal storage of retained water $RW$ [mm]. The change of retained water storage $\Delta RW$ [mm d$^{-1}$] at time $t$ can be inferred using the water balance:

$$0 = P_t - actET_t - Q_t + \Delta TWS_t$$ \hspace{1cm} (S21)

with the change of total water storage $\Delta TWS$ [mm d$^{-1}$] resulting from

$$\Delta TWS = (SWE_t - SWE_{t-1}) + (SM_t - SM_{t-1}) + W_t$$ \hspace{1cm} (S22)

so that solving Eq.(S21) and Eq.(S22)
\[
\Delta RW_t = \text{actET}_t + Q_t - P_t - (\text{SWE}_t - \text{SWE}_{t-1}) - (\text{SM}_t - \text{SM}_{t-1})
\]  

(S23)

The amount of retained water RW [mm] at time t then results from

\[
RW_t = RW_{t-1} + \Delta RW_t
\]  

(S24)

Finally, the integrated terrestrial water storage TWS [mm] at time t represents the sum of all storage components:

\[
TWS_t = \text{SWE}_t + \text{SM}_t + RW_t
\]  

(S25)

**S2 Uncertainty of the observational constraints**

Maps of the temporal average uncertainties of observed TWS, ET and Q that are used for model calibration are shown in Fig. S1. For observed SWE a constant average uncertainty of 35 mm is applied.

![Maps of temporal average uncertainties](image)

**Figure S1.** Mean uncertainty of monthly TWSobs [mm], and of the mean seasonal cycle of ETobs [mm d^{-1}] and Qobs [mm d^{-1}] used for model calibration. Values are truncated to 50 mm resp. 10 mm.
S3 Cost terms

Table S1 shows the cost terms achieved with the default and the optimized parameter set. Compared to the default parameter values, total costs clearly improve after calibration. The shown optimized values represent a weighted Nash-Sutcliff efficiency of 0.37 (TWS), 0.44 (SWE), 0.57 (Q) and 0.80 (ET) (weighted Nash-Sutcliff = 1 – cost value).

Table S1. Cost values obtained with the default and the optimized model parameters using Eq. (1).

<table>
<thead>
<tr>
<th>parameter values</th>
<th>TWS</th>
<th>SWE</th>
<th>ET</th>
<th>Q</th>
<th>total</th>
</tr>
</thead>
<tbody>
<tr>
<td>default</td>
<td>0.84</td>
<td>0.54</td>
<td>0.15</td>
<td>1.00</td>
<td>2.55</td>
</tr>
<tr>
<td>optimized</td>
<td>0.63</td>
<td>0.56</td>
<td>0.20</td>
<td>0.43</td>
<td>1.82</td>
</tr>
</tbody>
</table>

S4 Model performance regarding evapotranspiration and runoff

Figure S2. Spatially averaged mean seasonal cycle (MSC) of the period 2002–2012 and inter-annual variability (IAV, difference between monthly values and the MSC) for ETmod and FLUXCOM based ETobs.
Figure S3. Spatially averaged mean seasonal cycle (MSC) of the period 2002–2012 and inter-annual variability (IAV, difference between monthly values and the MSC) for Qmod and EU-grid runoff Qobs. Qmod\textsubscript{consistent} solely considers grid cells that coincide with Qobs, while Qmod\textsubscript{all} is based on modelled runoff for all grids of the study domain.

Figure S4. RMSE of the mean seasonal cycle of simulated and observed a) ET [mm month\textsuperscript{-1}] and b) Q [mm month\textsuperscript{-1}]. RMSE values have been truncated to the range 0–30 (a) resp. 0-50 (b).
Figure S5. Grid wise phase lag [months] between mean seasonal TWSobs and TWSmod. Negative values indicate preceding of the model compared to GRACE TWS.
Figure S6. Comparison of spatially averaged observed (obs) a) SWE (GlobSnow) and b) TWS (GRACE) to simulations of this study (mod) and earth2Observe models (incl. ensemble mean) in terms of average mean seasonal cycle (MSC) and inter-annual variability (IAV). MSC is calculated for the period 2002–2012, and IAV represents the difference of monthly values from the MSC. Only data points consistent between all models and the respective observational data are considered.
Figure S7. RMSE for the spatially averaged SWE (left) and TWS (right) achieved by our model compared to the model ensemble of eartH2Observe models and the ensemble mean across temporal scales.

Figure S8. Comparison of a) RMSE and b) Pearson correlation $r$ for monthly SWE and TWS time series simulated with the eartH2Observe models, the model ensemble mean (model mean) and by our model (mod).
S7 Uncertainty due to forcing and calibration data

S7.1 Comparison to WFDEI precipitation forcing

To assess the uncertainty in TWSmod and SWEmod that emerges from the choice of precipitation forcing, we calibrated our model in the same manner as before, yet used rain fall and snow fall estimates from the reanalysis based WFDEI product (Weedon et al. 2014) instead of GPCP-1DD precipitation data. Since precipitation is likely the most uncertain input data (Herold et al. 2015, Schellekens et al. 2017), we did not change the temperature and net radiation data sets. The global meteorological WFDEI data for land area is generated by applying the Water and Global Change (WATCH) forcing data methodology to ERA-Interim reanalysis data (Dee et al. 2011). The advantage of the WFDEI product is that it already provides separate values for snow and rain fall, as diagnosed by the reanalysis (Weedon et al. 2014). Therefore, it is not necessary to partition precipitation based on a temperature threshold within the model. We rather applied the provided rain and snow fall estimates directly, and also desisted from scaling snow fall.

Regarding the MSC, we obtained similar model performance in terms of SWE and TWS for both, the spatially averaged dynamics (Fig. S9, Fig. S10) and the spatial pattern (not shown). Although the dynamics and thus the correlation coincidence, we obtain a higher amplitude in TWSmod when using WFDEI as forcing compared to the original TWSmod (and TWSobs). This higher amplitude relates to larger seasonal snow accumulation in SWEmodWFDEI, because the scaling parameter for snow fall is not calibrated. In terms of IAV, the correlation between observation and WFDEI forced model is comparable for both, TWS and SWE. However, the key findings (Fig. S11) remain the same as with GPCP precipitation forcing.

Figure S9. Comparison of the spatially averaged mean seasonal cycle (MSC) and inter-annual variability (IAV, difference between monthly values and the MSC) of observed SWE (SWEobs), modelled SWE (SWEmod), and modelled SWE based on WFDEI precipitation forcing (SWEmodWFDEI). SWEmod consistent and SWEmodWFDEI consistent refers to modelled SWE considering only data points with available SWEobs, while SWEmod all and SWEmodWFDEI all incorporates all time steps for all grids of the study domain.
Figure S10. Comparison of the spatially averaged mean seasonal cycle (MSC) and inter-annual variability (IAV, difference between monthly values and the MSC) of observed TWS (TWSobs), modelled TWS (TWSmod), and modelled TWS based on WFDEI precipitation forcing (TWSmodWFDEI). For IAV, TWSobsmonthly value shows the original IAV of individual TWSobs months, while TWSobs, TWSmod and TWSmodWFDEI are smoothed using a 3-month average moving window filter. Pearson correlation r refers to the smoothed values. For the MSC no smoothing is applied.

Figure S11. Relative contribution (based on CR (Eq. Fehler! Verweisquelle konnte nicht gefunden werden.)) of snow (SWE) and liquid water (W) to TWS variability on different spatial (local grid scale, spatially integrated) and temporal (mean seasonal MSC, inter-annual IAV) scales when forced with WFDEI rain and snow fall. The boxplots represent the distribution of grid cell CR, with the dashed line marking the corresponding average. The star represents the CR calculated for the spatially integrated values.
S7.2 Comparison to other GRACE solutions

In this study we used TWS estimates from the JPL mascon RL05 product for model calibration and evaluation (Watkins et al., 2015; Wiese, 2015). However, various GRACE solutions for TWS from different institutions and using different processing approaches exist. To assess the potential uncertainty resulting from the choice of TWS solution, we compared modelled TWS (mod) and the JPL mascon solution (JPLmasc) with other solutions based on different processing approaches. They include the mascon product from the Center of Space Research (CSR at the University of Texas) (CSRmasc) (Save et al., 2016), as well as three RL05 solutions based on spherical harmonics provided by JPL, CSR and GeoforschungsZentrum (GFZ) (Swenson and Wahr, 2006; Landerer and Swenson, 2012; Swenson, 2012). As recommended, we also considered the average of the latter three (AvgJPL/CSR/GFZ). All TWS estimates were taken as anomalies to the respective time-mean of 2002–2012, and scaled with the provided gain factors (except for CSRmasc that does not require scaling (Save et al., 2016). For comparison, we calculated the spatial average mean seasonal cycle (MSC) and inter-annual variability (IAV) across all grid cells of the study domain (Fig. S12).

Thereby, we find that the spatial average MSC of all GRACE TWS estimates agrees in its dynamics, albeit minor differences in the solutions’ amplitudes exist (by ±15 mm). This results in comparable correlation and RMSE with modelled TWS. As the signal itself is noisier on IAV scales, the GRACE solutions show broader variability for IAV than at MSC scales as well. However, the qualitative pattern between the solutions remains, and modelled TWS is not closer to one specific solution or another during the entire time period. Therefore, the uncertainty evolving from the choice of GRACE solution used for model calibration can be assumed to be minor.

Figure S12. Comparison of the spatially averaged mean seasonal cycle (MSC) and inter-annual variability (IAV, difference between monthly values and the MSC) of modelled TWS (mod) and observed TWS of different GRACE solutions.
S8 Covariances between SWE and W

Figure S13 and Fig. S14 compare the contribution of the combined SWE and W variances and the covariance of both storages to the total variance of the spatially aggregated TWSmod. On the interannual and spatially aggregated scale, 81% of TWS variability is explained by the variances in SWE and W, suggesting that the covariance between SWE and W only has minor effect. This is underlined by high percentage of SWE and W variance on total TWSmod variance for all grids of the study domain (Fig. S14). On mean seasonal scales, the majority of spatially aggregated TWS variability is still explained by variances in SWE and W, but the contribution of the covariance increases. This can be expected, as the seasonal variation of snow storage affects the subsequent availability of liquid water storages through the snowmelt process. At the local scale, though, the percentage of SWE and W variance on total TWSmod variance remains high in regions where the dominance of either snow or liquid water components are clear (Fig. 7 of the manuscript). In regions where covariances of two storage components is larger, the contribution of two storage components to TWS variability are similar resulting in a CR value of around 0. Therefore, we conclude that while the covariances of snow and liquid water can be remarkable on the seasonal scale over a large spatial domain, it does not affect or change the dominant components on the TWS.

Figure S13. Percentage of SWE and W variance on total TWSmod variance on mean seasonal (MSC) and interannual (IAV) scales.
Figure S14. Percentage composition of spatially aggregated TWSmod variance from the combined variances of SWE and W, and two times the covariance of SWE and W on mean seasonal (MSC) and interannual (IAV) scales.
References


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