23rd International Congress on Modelling and Simulation, Canberra, ACT, Australia, 1 to 6 December 2019
mssanz.org.au/modsim2019

Assimilating satellite soil moisture retrievals to improve operational water balance modelling

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Abstract: A simple and robust method for assimilating satellite soil moisture (SM) products into the Australian Water Resources Assessment (AWRA) model was developed and tested via the community modelling system, AWRA-CMS. The method requires time series of two satellite soil moisture products, along with AWRA simulations of upper-layer soil water storage for an offline determination of weights for use in the optimal merging of models and observations via the triple collocation (TC) technique. The candidate data sources were near real-time products from the Soil Moisture Active/Passive (SMAP), Soil Moisture and Ocean Salinity (SMOS), and Advanced Scatterometer on MetOp satellite (ASCAT) production systems.

Evaluation of AWRA model performance with and without data assimilation (DA) was conducted for key variables including upper-layer soil water storage, root-zone soil water storage, evapotranspiration and streamflow against in-situ networks. The comparisons demonstrated conclusively that the assimilation of satellite SM considerably improved the accuracy and representation of AWRA model surface soil moisture across Australia. The temporal correlation was increased by 0.2 correlation units on average after the assimilation compared to open-loop across in-situ SM monitoring sites. Positive impacts were found on the simulation of streamflow over majority of catchments with an increase in correlation by up to 0.4. The impact of SM assimilation on the other variables was not as significant, largely as a result of the indirect way SM assimilation imparts constraint on those variables.

Finally, an investigation into the impact of SM data assimilation on forecast accuracy was conducted through driving AWRA model with forecast meteorological forcing 9 days into the future. Improved skill in estimating surface soil moisture of AWRA were found to persist up to 4 days, and likely longer. Results of this study demonstrated the benefit of constraining model outputs with satellite soil moisture observation on improving model simulation, as well as the importance of accurate initial hydrological states on improving forecast skill. Improved SM is vital for assessing and predicting water availability and assisting policy making.

Keywords: *Data assimilation, soil moisture, water balance model*

1. INTRODUCTION

Soil moisture, a key variable in modulating climate variability and extremes through land-atmosphere interactions, is critical to climate and weather prediction as well as climate-sensitive socioeconomic activities. Soil moisture estimates from water balance models are largely dependent on the uncertainties of atmospheric forcing, model physics, model parameterization and initialization. Remotely sensed data can provide spatially and temporally varying constraint on the modelling of biophysical landscape variables that is often superior to that achieved by single static set of model parameters. Data assimilation merges models and observations in a way that compensates for the deficiencies in each (e.g. uncertainty, coverage), resulting in improved accuracy, coverage, and ultimately forecasting capability. Over the past decades, the assimilation of satellite soil moisture products derived from either passive or active microwave sensor has been shown to improve model estimates of soil moisture significantly (Draper et al. 2012; Renzullo et al. 2014; Tian et al. 2017; Tian et al. 2019).

Passive microwave sensor technology measures emissions emanating from the earth-atmosphere system in the microwave wavelengths of the electromagnetic spectrum. The dielectric constants of the various soil constituents (e.g. sand and clay) is known to respond dramatically to variations in soil water content which in turn influences the soil emissivity. The corresponding soil depth of microwave emission is related to the antecedent moisture status of the soil and sensing frequency (Jackson 1997), which for the typical passive microwave product is either top ~5 cm for L-band and ~2 cm for C-band frequencies. On the contrary, soil moisture products derived from active radar systems are based on the measurements of backscatter which is dependent on surface roughness and moisture condition (Choudhury et al. 1979). The soil wetness can be determined by examining its relative intensity between the weakest and strongest observed backscatter (Wagner et al. 1999). Most active systems are based on C-band microwave frequencies and as such their moisture estimates pertain to the upper ~2 cm of soil.

In this study, we evaluated three satellite soil moisture products from both active and passive microwave sensors over Australia continent with three in-situ soil moisture monitoring networks. Two of the satellite soil moisture products with best performance were assimilated into the Australian Water Resources Assessment (AWRA) Community Modelling system using a simple sequential state updating method. Soil water storage, evapotranspiration and streamflow from AWRA after the assimilation were evaluated with in-situ measurements and compared against model open-loop (without assimilation) outputs. Forecast meteorological data from the Bureau's Numerical Weather Prediction system were used to force AWRA model estimates 9 days into the future, with the upper layer soil water storage estimates from the assimilation as initial states, in order to assess the impact of data assimilation on forecasting skill.

2. DATA AND METHOD

2.1. Australian Water Resources Assessment Community Modelling system (AWRA-CMS)

The Australian Water Resources Assessment (AWRA) Community Modelling system (AWRA-CMS) has nearly10-year history of developments, starting with the landscape hydrology model (AWRA-L) (Van Dijk 2010), undergoing various revisions in the modelling structure (Hafeez et al. 2015; Vaze et al. 2013), to the operational version of today (Frost et al. 2018). The AWRA-CMS has been available since 2016 and the code accessible from github (https://github.com/awracms/awra_cms). The model runs at a daily time step with a 5km spatial resolution. It is a one-dimensional distributed water balance model that simulates the flow of water through the landscape from partitioning rainfall into vegetation, soil moisture and groundwater stores and out of grid cell through evapotranspiration, runoff and drainage. Hydrological processes are simulated separately for deep rooted vegetation and shallow rooted vegetation. The soil water storage has been partitioned into three layers (upper: 0–10 cm, lower: 10–100 cm, and deep: 1–6 m). The shallow rooted vegetation only has access to the upper and lower soil stores, while the deep rooted vegetation has access to all layers. The surface water storage and groundwater are simulated at each grid cell and conceptualized as a small unimpaired catchment.

2.2. Satellite near-surface soil moisture products

In this study we explore the use of soil moisture products derived from both passive and active systems. For the passive source, we have the Soil Moisture Active-Passive (SMAP) product from NASA (Entekhabi et al. 2010), and the product from the European Space Agency's (ESA's) Soil Moisture and Ocean Salinity (SMOS) mission (Kerr et al. 2001). Both SMAP and SMOS produce volumetric soil moisture estimates (units: m^3/m^3) of approximately the upper 5 cm of soil. The SMAP product used here is the level-2 enhanced radiometer half-orbit 9-km EASE-grid soil moisture (Chan et al. 2018), from the US National Snow and Ice Data Center (https://nsidc.org). The SMOS product we use is the level-2 soil moisture product on approx. 25-km grid from

ESA's SMOS online dissemination service (https://smos-diss.eo.esa.int/oads/access/). The active source of soil moisture product used in this study is from the Advanced Scatterometer (ASCAT) onboard the MetOp series of ESA polar orbiting meteorological satellites. The ASCAT soil moisture product is expressed as a degree of wetness (units: %, where 100% suggests saturated soil). The real-time level-2 data a resolution of 12.5 km are obtained from EUMETSAT Satellite Application Facilities (H-SAF), which are generated using change detection algorithm of Wagner et al. (1999).

2.3. Evaluation data

Model performance is evaluated against in situ measurements for four key AWRA-CMS outputs: namely, upper-layer soil water storage (S_0), lower-layer soil water storage (S_s), evapotranspiration (E_{tot}) and runoff (Q_{tot}). Evaluation of the soil water components of AWRA are against measurements from three soil moisture monitoring networks in Australia. The first are in situ measurements from the long-term, well-studied, moisture-monitoring network in Murrumbidgee catchment (Smith et al. 2012), known as the OzNet network; the second are from network of cosmic ray sensors known as CosmOz (Hawdon et al. 2014). In addition, the network of Flux Towers, OzFlux, contain as part of their suite of micrometeorological measurements of soil moisture, which will also be used in the evaluations. The model estimates of S_0 were compared with soil moisture measurements at 0-10 cm, whereas the modelled root-zone soil water storage ($S_0 + S_s$) were compared with measurements up to 100 cm. OzFlux sites are primarily used to evaluate AWRA E_{tot} estimates, which have been calculated from accumulated latent heat flux measurements at the sites. Streamflow data used to evaluate model estimates were obtained for each AWRA-L calibration and validation catchment (Zhang et al. 2013) from the Bureau's Water Data Online (http://www.bom.gov.au/waterdata/). Specifically the data were obtained for the Bureau's streamflow time series data management tool, Water Information System Kisters (WISKI). Data were converted from cumec (m^3/s) to mm per day using the catchment area provided by the Geofabric (http://www.bom.gov.au/water/geofabric/).

2.4. Forecast meteorological forcing

The AWRA model were driven by forecast meteorological forcing to simulate water balance 9 days in advance. The forecast forcing data we used is from ACCESS-G APS2, which is the global version of ACCESS. ACCESS is an implementation of the UK Met Office's Unified Model for the Australian region which provides weather forecast variables, including rainfall, at a range of spatial scales and forecast lead times. Forecasts are provided globally at 0.25° resolution at hourly time steps for 10 days from the model start time. These data were resampled to 0.05° spatial resolution and daily temporal resolution, to match the resolutions of AWRA model.

2.5. Data assimilation

The method of data assimilation used here is the time sequential updating of model state(s) given observations of relevant model variables. Two key modelling components in data assimilation are the dynamics operator, which describes the time evolution of the system states and fluxes, and the observation operator, which provides the mathematical mapping from state to observation space (or vice versa). Here the dynamics operator is the AWRA-CMS. The role of the observation operator, denoted as H, is to perform a mapping between observation and state space, as often observations are not directly comparable to model states. In the case of satellite SM, for example, estimates are provided in volumetric (m^3/m^3), gravimetric and wetness (%) and can represent varying soil layer depths. However, AWRA's upper layer soil moisture is given in terms of storage, i.e. mm of water and simulated separately for 2 HRUs. The observation operator used in this study is to match the mean and variance between model and observations through a linear transformation. In this case, the observation operator also simultaneously removes systematic bias between AWRA S_0 and satellite soil moisture.

The state updating equation for sequential data assimilation is written generically as:

$$X_t^a = X_t^f + K_t\left(Y_t - H\left(X_t^f\right)\right)$$

which says that the best estimate of model state, known as analysis (X_t^a), is equal to the first guess or forecast estimate (X_t^f) plus a weighted difference between observations, Y_t, and the model equivalent to the observation ($H\left(X_t^f\right)$), for that time step. The multiplier, K_t, is known as the gain factor which contains information of the respective uncertainty in the model estimates and observations. The state variable of focus in this study is the storage in the upper soil layer, S_0.

The gain contains the information on the error variances of the model and observations. Error characterization in any field of research is a challenge mainly because there is rarely, a truth. Ensemble methods of data assimilation use random perturbations to the forcing data and model states to generate an empirical distribution of model estimates from which model error can be inferred. However these methods rely on an initial guess at what the magnitude of the error variance should be, and then *post hoc* correction to the ensemble are applied (e.g. inflation factors, Anderson (2009)) to ensure ensemble variance is a good approximation of the actual model error. Similarly the observation error variance, is often estimated through field campaigns (Panciera et al. 2014), but these rarely represent the spatial and temporal variability in errors. Alternatively, the data providers often specify an error estimates but can be overly optimistic in the magnitude of the errors.

Triple collocation (TC) was developed as a method of quantifying error characteristics in geophysical variables when the true error structure is elusive, first applied to near-surface winds (Stoffelen 1998) and later extensively applied, to soil moisture (McColl et al. 2014; Scipal et al. 2008) and rainfall (Massari et al. 2017). The basis of the approach is that under the assumption of linear Gaussian statics, three independent data sets of the same geophysical variable can be used to infer the error variances in each. Here we used TC as a way of inferring error variances needed to calculate K from time series of AWRA S_0 and each satellite SM products. To illustrate we consider the AWRA S_0, SMAP, and SMOS, as our three independent sources of soil moisture estimation. From the extended TC method of McColl et al. (2014), the correlation of each of the soil moisture estimates with the unknown truth is given by:

$$\rho_x^2 = \frac{Q_{x,y}Q_{x,z}}{Q_{x,x}Q_{y,z}},\ \rho_y^2 = \frac{Q_{x,y}Q_{y,z}}{Q_{y,y}Q_{x,z}},\ \text{and}\ \rho_z^2 = \frac{Q_{x,z}Q_{y,z}}{Q_{z,z}Q_{x,y}}$$

where x, y and z subscripts can denote AWRA, SMAP or SMOS soil moisture estimates, respectively, $Q_{x,x}, Q_{y,y}$ and $Q_{z,z}$ are the temporal variances and $Q_{x,y}$, $Q_{x,z}$ and $Q_{y,z}$ are the temporal covariance between data sets. The error variances can be calculated for AWRA, SMAP and SMOS respectively as follow:

$$\sigma_x^2 = (1-\rho_x^2),\ \sigma_y^2 = \left(1-\rho_y^2\right),\ \text{and}\ \sigma_z^2 = (1-\rho_z^2)$$

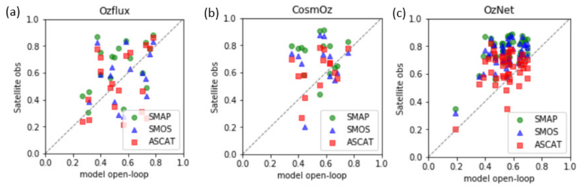

Figure 1. Comparison of Pearson correlation coefficients between surface soil moisture derived from SMAP, SMOS and ASCAT satellites and AWRA open-loop simulation against in-situ measurements from (a) Ozflux, (b) CosmOz and (c) OzNet network sites.

The reciprocal of these variances were used as indicators of the weight of influence that the respective source should have on the analysis estimate: i.e. low variances suggest more weighting than higher variances.

3. RESULTS

In order to assimilate satellite soil moisture, we first examined differences between three satellite soil moisture products, namely SMAP, SMOS and ASCAT. Understanding that the satellite, AWRA and in-situ data all represent soil moisture in different units, the Pearson correlation coefficient was the most relevant metric in evaluating performance. This statistic is summarized for each of the measurement networks in Figure 1 for the 2016-2017 period. Compared to AWRA model open-loop simulations, SMAP soil moisture generally showed better consistency with in-situ soil moisture measurements over a majority of CosmOz and OzNet sites. Overall ASCAT showed consistent poorer performance than the other satellite products. This is likely due to the comparative noisiness of the ASCAT product. The results demonstrated that satellite soil moisture products show great potential to improve model estimation of top-layer soil moisture.

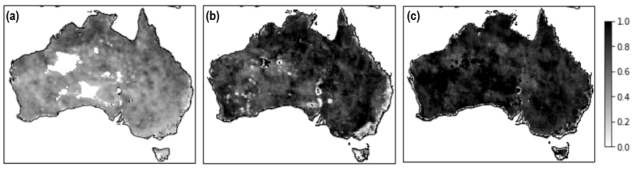

Figure 2. Triple collocation (TC) estimates of correlation with the truth for (a) AWRA-simulated upper layer soil water storage (b) SMOS soil moisture retrievals and (c) SMAP soil moisture retrievals.

Since SMAP and SMOS show overall better agreement with in-situ measurements with an average correlation of 0.71 and 0.64 comparing to ASCAT (0.58), we assimilated SMAP and SMOS into AWRA model to update the model simulated upper layer soil water storage. The error variances for AWRA, SMOS and SMAP were calculated using triple collocation method to ultimately weight the contribution of each data set in the data assimilation (Figure 2).

The AWRA model estimate driven by gauge-based rainfall analyses cannot properly simulate soil moisture patterns over regions with a lack of rain gauge coverage such as Western Australia (WA). The water storage simulations over these regions default to zero, thus no weights were given to the AWRA estimates (Fig. 2a). The assimilation of satellite SM introduces variability of surface SM through the direct updating of S_0. It largely mitigated the erroneous artefact of zero precipitation gaps over WA. Figure 3 shows the changes in model simulated S_0 after the assimilation during cyclone periods with heavy rainfall over those areas. Increasing soil moisture following the cyclone track was observed after the assimilation of satellite SM.

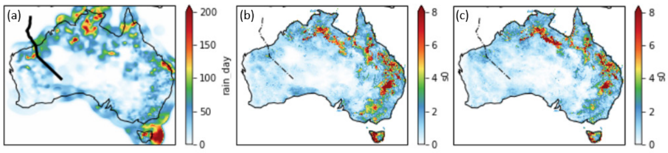

Figure 3. Cyclones track of (a) Stan overlaying accumulated rainfall for the period of 28 Jan - 03 Feb, 2016; average AWRA S_0 from open-loop (b) and analysis simulations (c) during cyclone Stan.

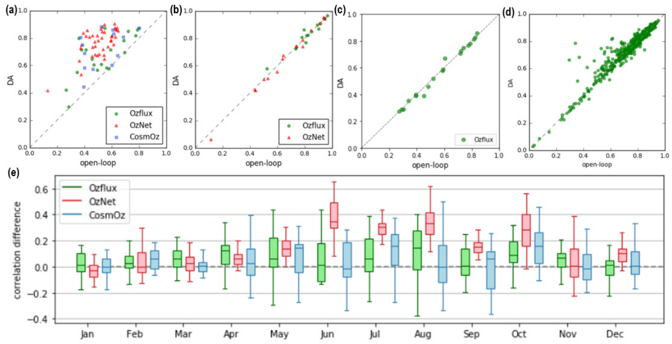

Figure 4. Temporal correlation of model-simulation and in-situ measurements at daily time step for (a) S_0, (b) root-zone soil water storage, (c) E_{tot} and (d) Q_{tot} during 2016 to 2018. (e) Changes in correlation of S_0 after the assimilation for individual months.

Consistent improvements against model open-loop were found after the assimilation for S_0 over all the in-situ sites (Figure 4a). In particular, the sites where satellite SM shows less correlation with model open-loop (Fig. 1) were also improved. Thus, the assimilation optimally combined the information from both model and observations to reduce the model uncertainties. The assimilation improved the daily correlation between in-situ surface SM measurements by 0.14, 0.26 and 0.18 on average for OzFlux, OzNet and CosmOz sites respectively. Overall, there is no degradation on estimates of root-zone soil water storage, E_{tot} and Q_{tot} (Fig. 4 b-d). This result is not surprising since those variables were not directly updated with the assimilation. The model S_0 for individual month over OzNet sites were improved most in terms of correlation among the three surface soil moisture networks (Fig. 4e). The improvements were mainly found in rainy seasons from May to October with a median correlation improvement of over 0.3. The assimilation shows positive impacts on the simulation of temporal variability of streamflow for majority of catchments (Fig. 4d). Figure 5 shows the simulation of streamflow dynamics compared to in-situ measurements. The increasing soil water storage in the upper layer resulted in the increasing streamflow and better agreement with in-situ measurements during wet seasons.

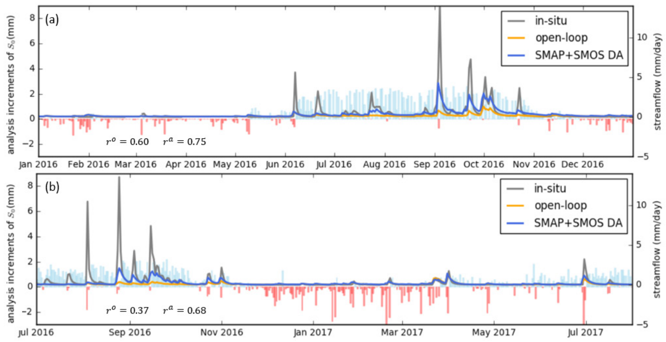

Figure 5. Analysis increments (difference between analysis

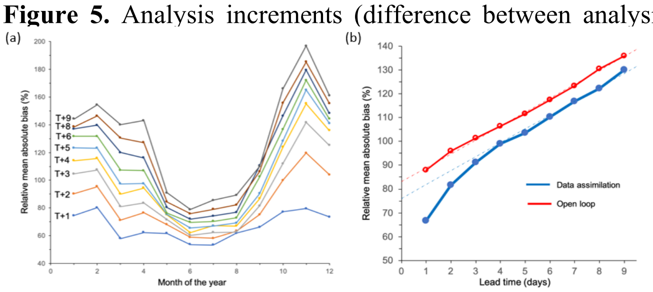

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Figure 6. (a) Australia-wide median MRB for each month of the year for forecast S_0 at lead times 1- to 9-days. (b) Australia-wide median MRB as a function of lead time for forecasts from open-loop (red) and analyzed (blue) S_0.

Forecast forcing meteorology were used to drive AWRA model estimates 9 days into the future. Given that the evaluation above shows soil moisture assimilation has the strongest impact on S_0, our exploration of the impact of forecasting is limited to this variable. Figure 6a illustrates the temporal behavior of mean relative absolute bias (MRB) for each month in terms of median value across the country for each forecast lead time. We see that MRB increase with lead time over the year, with 1-day lead time forecast median MRB ranging from 55-80%, while 9-day MRB considerably more variable ranging from 80-200%. We also observe that that June and July have lower MRB than other months, particularly November, December and January. This temporal pattern in MRB is typical of what we see in rainfall error statics (e.g. Chappell et al. (2013)), where the broad extent of monsoon rainfall across northern Australia dominates the nation-wide statistics in the summer months. Finally, to assess how long the improvements in AWRA forecasts persist due to soil moisture assimilation, we compared the Australia-wide median MRB for the forecasts made from open-loop with analyzed S_0 states (Figure 6b). Note that MRB values for forecasts made from the open-loop S_0 states were evaluated against analyzed states (as the reference). We see in Fig. 6b that MRB plotted as a function of lead time increases with lead time (as expected), but that the open-loop MRB's are always higher than those based on analyzed S_0. A direct comparison between open-loop and analysis forecasts skill is unfair since analysis soil moisture were used to calculate the skill metric (MRB). Instead we could compare the respective asymptotic behavior of skill with lead time of both. The red dashed lines in Fig. 6b is a line of best fit to the open-loop MRB. It is included here to highlight the oblique asymptotic behavior. The blue dash line is parallel to the red (shifted only vertically by an offset). The figure suggest that improvements in the analyzed S_0 can persist up to 4 day, but possibly longer, until improvements in forecasts performance resembles that of open-loop simulations.

4. DISCUSSION AND CONCLUSION

In this study, we proposed a simple and robust method for assimilating satellite SM products into AWRA as a first step towards a new data assimilation (DA) capability for the operational system. The method involves the sequential (daily) updating of AWRA model's upper layer soil water storage with satellite SM observations through a linear combination with weights determined through triple collocation.

Despite the model estimates of upper layer soil water storage performing better at some locations than the satellite products, we have conclusively demonstrated using AWRA-CMS version 6.1 that the method improves both the accuracy (assessed against in-situ data) and representation (e.g. in areas of sparse rain gauge coverage) of upper layer soil water storage estimates in comparisons with AWRA open-loop (i.e. without DA) simulations. The biggest improvements occurred over the winter rain months of the year. The proposed method, with weightings determined a priori (offline) through triple collocation is fast to implement and unlikely to require significant modifications to the current operational workflow of Bureau's AWRA-L modelling system.

The analyzed upper layer soil water storage imparts constraint on the other states at the following time step of the AWRA model through the dynamic operator. It is the relationships between upper layer soil water storage and the other soil water stores, evapotranspiration and streamflow in the model that determines what impact the improved upper-layer soil water storage may have on them. Given the order of magnitude difference in the respective sizes of the water storages of the upper-layer (10 cm thick) and the subsequent lower-layer making up the root-zone (90 cm thick), it perhaps is not too unexpected to see little impact on the root-zone. For a more direct, faster constraint on all model states, a simultaneous updating of all model states would need to be developed. Overall improvements were found in streamflow simulation in the rain months and this is because the assimilation of SM adds moisture to the system where the model on its own under-estimates it, leading to better representation of flow during this time.

Our assessment of the impact of soil moisture data assimilation revealed that forecast accuracy persists in the upper layer soil water storage for up to 4 days lead time. This was based on a comparison of the behavior of the open-loop and analysis-based mean relative absolute bias (MRB) curves. Both showed MRB increasing with increasing lead time, as one would expect, but it took 4 days for the analysis-based results to exhibit the same asymptotic behavior as the open-loop results. From this we may conclude that the improvements from SM assimilation can last up to 4 days longer in S_0 forecasts than without assimilation. While this is a valid approach to forecasts verification, and quantifies the theoretical skill, an objective analysis would involve evaluation against independent ground-based data. An obvious next step in this component of the investigation would be to evaluate the open-loop and analysis-derived forecasts against the in-situ surface soil moisture monitoring networks.

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