On the Efficacy of Combining Thermal and Microwave Satellite Data as Observational Constraints for Root-Zone Soil Moisture Estimation

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ABSTRACT

Data assimilation applications require the development of appropriate mathematical operators to relate model states to satellite observations. Two such “observation” operators were developed and used to examine the conditions under which satellite microwave and thermal observations provide effective constraints on estimated soil moisture. The first operator uses a two-layer surface energy balance (SEB) model to relate root-zone moisture with top-of-canopy temperature. The second couples SEB and microwave radiative transfer models to yield top-of-atmosphere brightness temperature from surface layer moisture content. Tangent linear models for these operators were developed to examine the sensitivity of modeled observations to variations in soil moisture. Assuming a standard deviation in the observed surface temperature of 0.5 K and maximal model sensitivity, the error in the analysis moisture content decreased by 11% for a background error of 0.025 m$^3$ m$^{-3}$ and by 29% for a background error of 0.05 m$^3$ m$^{-3}$. As the observation error approached 2 K, the assimilation of individual surface temperature observations provided virtually no constraint on estimates of soil moisture. Given the range of published errors on brightness temperature, microwave satellite observations were always a strong constraint on soil moisture, except under dense forest and in relatively dry soils. Under contrasting vegetation cover and soil moisture conditions, orthogonal information contained in thermal and microwave observations can be used to improve soil moisture estimation because limited constraint afforded by one data type is compensated by strong constraint from the other data type.

1. Introduction

Increasingly, methods of data assimilation are being applied to both hydrological and hydrometeorological problems driven by prospects of better characterization of initial conditions and improved forecasting skill (Mecikalski et al. 1999; Reichle et al. 2001; Crosson et al. 2002; Reichle et al. 2002; Heathman et al. 2003; Merlin et al. 2006; Pan et al. 2008; Wang and Cai 2008; Barrett et al. 2008). The benefits afforded by the application of data assimilation approaches to hydrometeorological problems include better estimation of initial soil moisture and temperature in mesoscale climatological models (Jones et al. 2004; Huang et al. 2008), improved energy partitioning between latent and sensible heat fluxes (Pipunich et al. 2008), and a concomitant higher skill in quantitative precipitation forecasts (Koster et al. 2000). For example, it has been shown that updating soil moisture in a numerical weather model using passive microwave observations at daily intervals leads to an increase in precipitation forecast skill (Boussetta et al. 2008). In hydrologic applications, these methods have led to better estimation of antecedent soil moisture (Walker et al. 2001; Reichle et al. 2004; Reichle and Koster 2005; de Lannoy et al. 2007) with the potential for improved prediction of water availability, runoff, streamflow and flood discharge (Bach and MAuser 2003; Oudin et al. 2003; Scipal et al. 2005; Weerts and Serafy 2006), particularly in situations where stream hydrographs are sparse or non-existent (Barrett et al. 2008). Studies have demonstrated that combining observations of soil moisture with water budget models using data assimilation techniques on time scales of 1–3 days improves the prediction of modeled flows (Aubert et al. 2003; Pan et al. 2008). To capitalize on these benefits, it is necessary to develop and tailor...
methods for assimilating multiple types of observations into hydrological and hydrometeorological models.

Satellite observations in optical, thermal, and microwave wavelengths can provide indirect information on hydrologic “target” variables, such as profile soil moisture content and evapotranspiration. It is through “observation operators” that model target variables are transformed into the radiometric quantities observed by satellite sensors. The efficacy with which observations constrain model states depends on both the sensitivity of the observation to perturbation in the state and the magnitude of observation error. A yet untested assertion is that through the improved conditioning of model states by satellite observations, the evolution of a hydrologic model in time will more faithfully represent true system dynamics. A limited analysis of observation operators for satellite data and their sensitivity to the perturbation of model states has been completed (e.g., Jones et al. 2004).

Thermal observations from satellites provide information on the earth’s surface radiative properties via derived land surface temperature (LST). For over two decades, models of varying sophistication have been used to relate top-of-canopy LST to evaporative fluxes (Mecikalski et al. 1999; Boni et al. 2001; Caparrini et al. 2004; Sobrino et al. 2007). More challenging, however, is the diagnosis of profile soil moisture from LST using data assimilation methods (Crow et al. 2008), which requires explicit knowledge of the relationships between soil moisture, canopy resistance, and the partitioning of energy between the soil surface, vegetation canopy, and the atmosphere. In principle, these relationships can be exploited in data assimilation to provide information on profile soil moisture content (Entekhabi et al. 1994; Huang et al. 2008), but it remains uncertain as to the range of conditions under which these relationships hold.

Passive microwave observations are used to infer surface soil moisture content from space by exploiting the relationship between brightness temperature and water content via the dielectric properties of the soil mixture (Entekhabi et al. 1994; Njoku et al. 2003; Gao et al. 2006). Experiments have shown (Crow et al. 2001; de Jeu and Owe 2003; Moran et al. 2004; McCabe et al. 2005; Prigent et al. 2005) that inversion schemes based on relatively simple microwave radiative transfer (MRT) theory can yield reliable estimates of volumetric soil moisture content for soil layers 1–5 cm depth, depending on whether C-, X-, or L-band radiation is used. Accurate soil moisture retrieval requires information on surface emissivity, canopy optical thickness, vegetation and soil temperatures, and proportions of soil clay and sand contents. However, the quality of the retrieval may be compromised by radio frequency interference (RFI), standing water, scattering by dense woody vegetation, and liquid water droplets in overlying clouds (Njoku et al. 2003; de Jeu and Owe 2003; Wagner et al. 2007).

In data assimilation, it is of interest to know whether observations, such as thermal and microwave satellite data, are effective “constraints” on the model states and, conversely, under which conditions these observations contribute little to the analysis. We define “observational constraint” as the degree to which an additional observation of specified standard deviation reduces error in the initial model estimate of state variables (i.e., “background” state).

An important component of an assimilation scheme is the observation operator $H$, which comprises model code that defines the relationship between an observation and the relevant model state. Where $H$ is continuous and differentiable, it is possible to generate the first derivative of the operator known as the Jacobian. The Jacobian is required in variational data assimilation applications to efficiently compute optimal values of state variables and their errors. The most efficient way to calculate the Jacobian is to first determine the tangent linear model (TLM) of the observation operator. The TLM is model code that computes the action of the Jacobian on the state vector (Giering 2000) and can also be used to efficiently analyze the effect of perturbations in state variables on model output at any point on the model trajectory (Giering and Kaminski 1998). Thus, the TLM has intrinsic value as an efficient tool for examining model sensitivity (Errico 1997).

In this paper, we use TLMs to assess the sensitivity of satellite thermal and microwave observations to perturbation in soil moisture. From this analysis, the efficacy of combining these satellite observations in data assimilation as constraints on profile average soil moisture content $\tilde{\theta}$ and surface layer soil moisture content $\theta_{sl}$ can be determined. First, we establish observation operators, $H$, as model code, then we develop the TLM by differentiating the code in $H$ line by line. Using both the observation and TLM, we explore the sensitivity of temperature to variation in soil moisture under a variety of soil, vegetation, and climatic conditions experienced in a study area in southeastern Australia. With the range of sensitivities observed for this real case, we can determine under which conditions the satellite thermal and passive microwave observations are capable of providing effective constraint on the analysis of soil moisture and under which conditions model states are effectively independent of observations (i.e., the model trajectory is only determined by the previous state, model parameters, and forcing). We also examine the effect of current and future errors in satellite observations on the resulting analysis error.
2. Observation operators and tangent linear models

Two observation operators are developed in this work as well as their respective TLMs. In the context of this paper, \( H \) can be written as

\[
H^t(\theta_z) \rightarrow T_s \quad \text{and} \\
H^m(\theta_z) \rightarrow T_b,
\]

where the superscripts \( t \) and \( m \) distinguish the thermal and microwave observation operators, \( T_s \) is land surface temperature, and \( T_b \) is surface microwave brightness temperature. We briefly describe each observation operator in the following subsections, but details of the underlying models are found in the references. The soil profile water balance (the “forward model”) was simulated using a simple six-layer “bucket” model with Green–Ampt infiltration (Mein and Larson 1973) and Penman–Monteith evapotranspiration (Monteith 1965) coupled with the root depth distribution functions of Jackson et al. (1996).

a. Land surface temperature observation operator

The starting point for both observation operators is the two-layer surface energy balance (SEB) model of Shuttleworth and Wallace (1985), Friedl (1995), Norman et al. (2003), Anderson et al. (1997), and Friedl (2002). In a two-layer SEB, the soil and vegetation layers are sources of latent and sensible heat fluxes mediated by aerodynamic, canopy, boundary layer, and soil surface resistances. The fluxes are driven by gradients in temperature and water vapor between the sources, air in the canopy volume, and the overlying turbulent atmosphere. The canopy conductance function relates the transfer of water vapor across the resistance network to soil moisture, atmospheric vapor pressure deficit, and light availability by means of scaling functions (e.g., Cox et al. 1998). Six nonlinear equations describing the energy partitioning between vegetation, canopy, soil surface, and the overlying atmosphere are solved numerically to yield vegetation, soil and aerodynamic temperatures, and water vapor pressures (Friedl 1995, 2002). The top-of-canopy land surface temperature is determined by the canopy and soil temperatures derived from the SEB model and also from the sensor view zenith angle, which determines the proportion of soil visible to an orbiting satellite sensor.

b. Microwave brightness temperature observation operator

A coupled SEB–MRT model was used to generate the microwave observation operator. This coupled model used all of the equations from the previous subsection to provide soil and vegetation temperatures \( T_s \) and \( T_v \) to the MRT model of Mo et al. (1982), which itself has widespread use for retrieving land surface layer soil moisture content (Njoku et al. 2003; Owe et al. 2001; de Jeu and Owe 2003). Microwave brightness temperature \( T_b \) at a given frequency is related to canopy and soil temperatures, soil emissivity, vegetation optical thickness, and soil dielectric properties. The soil dielectric constant is strongly sensitive to the variation in soil moisture, and this provides the basis for the estimation of surface moisture content from passive microwave emissions.

c. The tangent linear models and model sensitivity

To generate the tangent linear models, each equation in each of the observation operators was differentiated with respect to specified “active” variables (Giering and Kaminski 1998). The active variables comprised all the variables in each operator that were directly a function of the target variables, \( \theta_z \) or \( \theta_s \), or any intermediate assignments that depended on the target variables in the computation of \( T_s \) and \( T_b \). Constants, parameters, and other variables that have no dependency on \( \theta_z \) or \( \theta_s \) were therefore excluded from the TLM. The derivation of TLMs is illustrated for the key operator equations in the appendix. The equations displayed are the components of both models that link the active variables to the modeled \( T_s \) and \( T_b \). In the case of the SEB model, LST is related to profile average soil moisture content \( \theta_z \) by the canopy resistance to transpiration \( r_c \). For MRT the microwave brightness temperature is related to \( \theta_s \) by the complex dielectric constants of the soil water mixture via the rough surface emissivity \( e_r \). Additional symbols and variables are defined in the appendix.

The TLMs were used to calculate the variations \( \delta T_s \) and \( \delta T_b \) based on the perturbations \( \delta \theta_z \) or \( \delta \theta_s \). A one-to-one relationship was established between the observation operator variables and the associated TLM variables, including those within the loop construct and conditional statements. This was achieved by ensuring that an equivalent tangent linear statement was constructed in the TLM for each statement in the observation operator (Giering and Kaminski 1998). Because each operator, \( H^t \) and \( H^m \), had different target variables, the SEB equations were differentiated twice, once for each target variable, \( \theta_z \) and \( \theta_s \). Given that the estimation of \( T_s \) and \( T_b \) required the evaluation of a loop construct where each pass relied on results of a previous pass, it was necessary to retain the interim values of \( T_s \) and \( T_b \) to calculate the perturbations \( \delta T_s \) or \( \delta T_b \). In the present work, both the observation operator and TLM code were evaluated inside the same loop construct and thus
interim values for \( T_s \) and \( \delta T_s \) or \( T_b \) and \( \delta T_b \) were stored in memory during each iteration.

d. Efficacy of satellite observations as constraints

Our mathematical treatment of the efficacy of thermal and microwave observations as constraints on a soil moisture modeling begins by considering the “gain” matrix \( K \), common to sequential data assimilation schemes. Recall the form of the gain matrix from the optimal least squares solution of the variational assimilation problem (Bouttier and Courtier 1999):

\[
K = B H^T (H B H^T + R)^{-1},
\]

where \( B \) is the background error covariance, \( R \) is the observation error covariance, and \( H \) is the Jacobian of the observation operator (i.e., known as the differential of \( H \)) derived from the TLM. A measure of the accuracy of the analysis (i.e., the updated state variable) is provided by the analysis error covariance matrix \( A \),

\[
A = (I - KH)B.
\]

Matrix \( H \) contains information on the effects of perturbations of the state variable on the modeled observation. Here we denote perturbations on the soil moistures, \( \delta z \) and \( \theta_{soil} \), collectively as \( \delta \theta \), and the resulting variation in modeled temperatures, \( T_s \) and \( T_b \), as \( \delta T \). We therefore write \( H = \delta T / \delta \theta \).

From Eqs. (1) and (2), a scalar expression for the analysis error variance, \( \sigma_a^2 \), can be determined for a given single observation of \( T_s \) or \( T_b \) as

\[
\sigma_a^2 = \frac{\sigma_o^2 \sigma_b^2}{(\delta T / \delta \theta)^2 \sigma_b^2 + \sigma_o^2},
\]

where subscripts \( o \) and \( b \) refer to observation and background error variances. From Eq. (3), the degree to which an observation constrains the model given a background error is a function of both the operator sensitivity to the perturbation in state and the magnitude of observation error. In tightly constrained assimilation, the analysis error will be significantly less than either the observation or background errors. The measure of the efficacy adopted in this work is the proportional constraint,

\[
\frac{\sigma_b - \sigma_a}{\sigma_b}.
\]

3. Study area and datasets

a. Murrumbidgee River catchment

Investigation focused on a 200 000 km\(^2\) region of interest (ROI) located in southeast Australia. The study area surrounds the Murrumbidgee River catchment (~87 000 km\(^2\)) and was specifically chosen to illustrate the ranges in \( T_s \) and \( T_b \) across a diverse set of land uses, terrain, and climates in Australia. Across this ROI topography varies from the alpine areas of the Kosciusko National Park in the southeast to the low-lying plains of the Riverina in the west. Mean annual rainfall varies from nearly 1000 mm in the east to less than 200 mm in the west. Land use in the Murrumbidgee River catchment includes forestry, national park, dryland, irrigated cropping, and grazing. Data used in the investigation are described below and include the static datasets that define model inputs and the time-varying satellite observations and climate forcing data. A subset of these data is shown in Fig. 1.

b. Static input datasets

Both SEB and SEB–MRT models require the input of a number of spatially varying and, for the purposes of this study, temporally static parameters and variables. Inputs range from canopy micrometeorological parameters to soil physical and chemical properties and are available either directly as digital satellite images or as spatially distributed datasets from a variety of sources.

1) LAND COVER CLASSIFICATION

We used the 1-km\(^2\) land cover classification of the Australian Government Bureau of Rural Sciences that was prepared for the National Land and Water Resources audit (available online at http://adl.brs.gov.au/anrdll/php/). Land cover classes were grouped into four generalized categories: tall forests, shrublands, grasslands/crops, and water. Through the middle and northwest of the ROI is a mix of irrigated and rainfed cropping, horticulture, and grazing land uses, whereas in the mountain areas to the southeast, plantation forestry, conservation reserves, and grazing predominate.

2) DIGITAL ELEVATION MODEL (DEM)

Topographic information was obtained from the 9-s (~250-m resolution) DEM of the Australian Government Geoscience Australia (available online at http://www.ga.gov.au/nmd/products/digidat/dem_9s.htm). The elevation data for the ROI is displayed in Fig. 1a. The terrain ranges from the flat, semiarid shrub and grasslands in the northwest to the mountainous alpine terrain of the southeast.
3) VEGETATION PROPERTIES

The digital atlas of Australian vegetation cover of the Australian Survey and Land Information Group (1990) was used to provide vegetation cover classes consisting of growth form, canopy height (up to 30-m height), and species composition of the tallest vegetation stratum. These classes were converted to vegetation heights, zero plane displacement, roughness length, and average leaf width parameters based on generalized values for each vegetation cover class.

4) SOIL PROPERTIES

The Digital Atlas of Australian Soils soil texture classes were converted to porosity, clay and sand content, and field capacity using the interpretations of McKenzie and Hook (1992) and Rawls et al. (1993).

5) LEAF AREA INDEX (LAI)

Estimates of LAI for the study region were obtained using the numerical inversion of the broadband canopy radiative transfer model of Sellers (1985) and satellite-derived albedo images from the Moderate Resolution Imaging Spectroradiometer (MODIS) sensor. The visible (0.3–0.7 \( \mu \)m) and near-infrared (0.7–3.0 \( \mu \)m) albedos were obtained from the version 4 of the MODIS 16-day 0.05° global albedo product (MOD43C1; available online at http://www-modis.bu.edu/brdf/userguide/cmgalbedo.html), which are 16-day composites, normalized to local noon. The estimated LAI appears to be more realistic than that of the MODIS LAI product (MOD15A2; https://lpaac.usgs.gov/lpaac/products), which was shown to overestimate LAI in southeastern Australia (Hill et al. 2006). LAI varies from 0 to 1 in the northwest through to 6 in the mountain forests (Fig. 1b).

c. Satellite observations and climate driver data

1) CLIMATE DATA

Climate data used in the SEB, SEB–MRT, and water budget models were obtained from the archive of interpolated surfaces of Australian meteorological station observations (Jeffrey et al. 2001). These data are gridded for the whole continent at approximately 5-km resolution and date back to 1890. Specific data used by these models were the minimum and maximum daily temperatures, daily total shortwave radiation, 0900 [local time (LT)] vapor pressure, and daily total rainfall. The Murrumbidgee ROI has received well below average rainfalls for the years 2001–08, resulting in a dry soil profile and the lowest inflows by streams into the catchment in recorded history (Cai and Cowan 2008). The period 1 September–1 November 2005 was chosen for this study because it contained a series of rainfall events with which to test the observation operators through wetting and drying cycles.

2) LAND SURFACE TEMPERATURE

The most common way of estimating land surface temperature from satellite brightness temperature observations is via a split-window algorithm (SWA; Yu et al. 2008). LST retrievals via SWAs (e.g., Becker and Li 1990; Sobrino et al. 1994; Wan and Dozier 1996) exploit the differential absorption of radiation by atmospheric water.
vapor in spectral bands centered approximately on 11 and 12 μm, respectively. They are simple in form (representing linearizations of the thermal infrared radiative transfer equation) and are thus easy to implement operationally for large-scale estimation of LST.

SWA performance is essentially governed by the way in which the algorithm handles atmospheric water concentration, satellite view angle, and surface emissivity effects. Atmospheric water vapor may be estimated from brightness temperature data themselves (Sobrino et al. 1994), or it may be based on climatologies derived from other satellites or surface observations (Pinheiro et al. 2007). Adjustment for the increase in pathlength with off-nadir observations may be achieved explicitly by varying algorithm coefficients as a function of view angle (Wan and Dozier 1996) or by adding path correction terms to the SWA (Sun and Pinker 2005). The independent estimation of land surface emissivity can be achieved by relatively simple normalized difference vegetation index–based approaches (Sobrino and Raisouni 2000; Momani and Saradjian 2007) or by iterative, computational intensive approaches (Gillespie et al. 1998). The resultant accuracy of LST from these methods ranges from 0.4 to 1.75 K (Sobrino et al. 1994; Wan and Dozier 1996; Qin et al. 2001; Sória and Sobrino 2007; Wan 2008).

In this work, we have used a vegetation classification–based approach to estimate surface emissivity and applied the SWA of Key et al. (1997) to the 11- and 12-μm channel brightness temperature data from the Advanced Very High Resolution Radiometer (AVHRR) onboard the National Oceanic and Atmospheric Administration-18 (NOAA-18) polar orbiting satellite. These data have an approximate overpass time for the study area of 1400 LT. All NOAA-18 AVHRR imagery for the period September–November 2005 were obtained from Commonwealth Scientific and Industrial Research Organisation (CSIRO) archives (King 2003). The SWA coefficients were derived for a range of atmospheric water content and view angle scenarios with the reported accuracy compared with in situ measured LST of <2 K.

Estimates of LST at 1-km resolution across the study area for the relatively cloud-free image on 2 October 2005 are presented in Fig. 1c. Evident in these data is the northwest–southeast gradient in $T_s$, with higher values associated with lower LAI in the northwest, whereas cooler $T_s$ occur at higher elevations in mountains and forests. The fine texture variation in $T_s$ shows some coincidence with LAI, but it is mediated by soil water availability via the effect of latent and sensible heat loss on canopy temperatures. Water bodies, snow, and small amounts of residual cloud are visible as a speckling of cooler $T_s$ across the region.

3) MICROWAVE BRIGHTNESS TEMPERATURES

The earth’s atmosphere is essentially transparent to microwave radiation in the frequency range 1–15 GHz. Therefore, unlike thermal brightness temperature observations, satellite-based microwave $T_b$ measurements may be considered direct observations of emissions from the land surface. The accuracy of microwave brightness temperature measurements is therefore a function of antenna characteristics and signal deconvolution strategies (Ashcroft and Wentz 2000). Reported instrument errors for $T_b$ from the Scanning Multichannel Microwave Radiometer (SMMR) onboard Nimbus are between 0.3 and 0.7 K (Njoku and Li 1999). Brown et al. (2008) claim that antenna error contributes 0.9 K to the overall radiometric accuracy of 1.68 K for the Microwave Imaging Radiometer with Aperture Synthesis (MIRAS) onboard the planned Soil Moisture and Ocean Salinity (SMOS) satellite (Barré et al. 2008). Similarly, the planned Soil Moisture Active Passive (SMAP) instrument has specification for a brightness temperature relative accuracy of 1.5 K (available online at http://smap.jpl.nasa.gov). Another factor affecting the microwave brightness temperature accuracy in unguarded frequency bands (e.g., those centered on 6.9 and 10 GHz) is radio frequency interference (RFI). It has been shown that RFI is likely to contaminate microwave signals in the more populous region of the globe (Njoku et al. 2005). In the Murrumbidgee catchment study area, the error introduced by RFI is likely to be negligible based on the global distribution determined by Njoku et al. (2005), therefore this error is ignored here.

In this work, we have used the microwave brightness temperature observations from the Advanced Microwave Scanning Radiometer for Earth Observing System (AMSR-E) aboard the Aqua satellite (Njoku et al. 2003) with an approximate overpass time for the ROI of 1330 h (local time). Specifically, we have used the gridded level-3 land surface product resampled to a global 25-km grid [AMSR-E Aqua daily L3 surface soil moisture, interpretive parameters, and quality control Equal-Area Scalable Earth Grids (EASE-Grids; AE_Land3), available online at http://nsidc.org/] for the period September–November 2005.

The microwave brightness temperature observation ($T_b$) from AMSR-E for October 2005 (Fig. 1d) shows a different spatial pattern to $T_s$ across the study area. The two regions where $T_b$ are highest (~280 K) occur in the north and southwest as a result of a dry soil surface layer. The spatial distribution of rainfall that occurred three and six days prior to the displayed image has moistened the soil immediately below the surface, leading to the visible band of cooler $T_b$ between 270 and 275 K running.
northwest–southeast across the ROI. Three areas of coolest \( T_b \) are marked A1–A3 in Fig. 1d and are discussed further in section 4.

4. Results

a. Modeled \( T_s \) and \( T_b \)

Observation operators \( H_t \) and \( H_m \) were used to compute modeled \( T_s \) and \( T_b \), respectively, across the study area for daily modeled soil moisture between 1 September 2005–1 November 2005 (see later discussion of temporal variation in proportional constraint) and for two extremes of soil moisture content (i.e., wilting point and field capacity) on 2 October 2005. The single model output provides a spatial estimate of the variability in upper and lower bounds of \( T_s \) and \( T_b \) across the ROI (Fig. 2) corresponding to wilting point and field capacity modeled temperatures, respectively. Comparison of Fig. 1c with Figs. 2a and 2d show that observed \( T_s \) from the AVHRR on this day are bounded by the upper and lower modeled \( T_s \) (Fig. 2), except for pixels contaminated by water, snow, or cloud. Thus, soil moistures for each pixel in Fig. 1c reside within the range of wilting point and field capacity for this region. It can also be seen that the range in modeled \( T_s \) (difference between top and bottom panels) is greatest in the lowest relief and lowest LAI parts of the landscape, whereas the least range in \( T_s \) occurred in the mountain forests of the southeast.

Modeled \( T_b \) (Figs. 2b and 2e) shows a similar southwest–northeast banding as \( T_s \) across the ROI. Aggregation of the 1-km grid cells to 25 km (Figs. 2c and 2f) allowed for direct comparison with observed \( T_b \) (Fig. 1d). Once again, the observed \( T_b \) is bounded by the upper and lower modeled \( T_b \) (Figs. 2c and 2f), except for areas marked A1–A3 in Fig. 1d. These areas have lower \( T_b \) than estimated by the model even at field capacity, suggesting that either standing water is present on the soil surface at the time of image acquisition or that open water in dams or lakes is “contaminating” observed \( T_b \). Although major dams and lakes are associated with these areas (A1 is centered on Hume Dam, A2 is on the hydroelectric water supply dams of Lakes Eucumbene and Jindabyne, and A3 is on the natural intermittently filled Lake George), there is also temporal variation in \( T_b \) for these areas between September and November 2005 (data not presented). This indicates that intermittent standing water is a key factor that is likely to influence microwave emissions from these areas.

The range in \( T_b \) is greatest in the northwest where a large fraction of bare soil is visible to the sensor. The range in \( T_b \) is least for the high relief, tall forests (marked A2 in Fig. 1d) as a result of the presence of the high biomass, strong relief, and high vegetation moisture contents, which act to scatter passive microwave emissions from the soil. In addition, as explained earlier, the differences in the pixel pattern of modeled and observed \( T_b \) in area A2 is due to dams of the Snowy Mountains Hydroelectric Scheme’s remaining snowpack at the highest elevations and surface water, which interferes with the soil passive microwave signal.
The range of modeled $T_s$ in Figs. 2a and 2d is plotted as a function of LAI for the three vegetation types in Figs. 3a and 3c. The highest surface temperatures for soils at wilting point (Fig. 3a) are associated with an increasing fraction of bare soil (LAI < 2). At field capacity (Fig. 3c), higher rates of evapotranspiration from soil and vegetation suppressed the range in modeled $T_s$ across all LAI, with the most pronounced effects when LAI was less than 2.

Similar analyses were conducted on modeled micro-wave brightness temperature (Fig. 4). The range of modeled $T_b$ in Figs. 2b and 2c is plotted as a function of LAI in Figs. 4a and 4c. These data show an increase in $T_b$ with decreasing LAI in dry soils. This increase in $T_b$ (Fig. 4a) is due to both a decrease in the surface dielectric constant under dry conditions at lower biomass densities and a higher soil source temperature with increased radiation incident on the soil surface. For soils at field capacity (Fig. 4c), modeled $T_b$ was up to 5 K lower than at wilting point for pixels where LAI was <2. At these LAI, the microwave emissions from the soil surface dominated the $T_b$ signal over vegetation moisture. At higher LAI, the soil signal was progressively attenuated by biomass microwave emissions, and the difference between $T_b$ at wilting point and field capacity approached zero.

b. Model sensitivity

Sensitivity of modeled $T_s$ to perturbations in the two extremes of soil moisture status ($\delta T_s / \delta \theta$) were computed and displayed as functions of LAI in Figs. 3b and 3d. The sensitivity is greater (more negative) under dry soils (Fig. 3b) than at field capacity (Fig. 3d), particularly when LAI was >2. However, sensitivities differed
between the three vegetation classes. Relatively low sensitivities were observed for shrublands at all LAI and for all vegetation classes when LAI approached zero. Maximal sensitivity was observed for forests and grasslands/crops at high LAI (Fig. 3b). The sensitivity was suppressed in forest and grassland/crops when soils were at field capacity (Fig. 3d). Differences in sensitivities among vegetation types are due to physiological differences in maximum stomatal conductance to water vapor ($g_{\text{max}}$) between these classes ($g_{\text{max}}$ forest, 10 mm s$^{-1}$; grassland/crop, 20 mm s$^{-1}$; shrub = 5 mm s$^{-1}$) based on Jones 1992 and Bell and Williams 1997. The banding of points evident within a vegetation class (e.g., Fig. 3b) arose from soils of different soil moisture holding capacities ($\theta_{\text{min}} - \theta_{\text{max}}$). Higher sensitivity was observed for soils having lower water holding capacity.

Modeled brightness temperature sensitivity ($\frac{\delta T_b}{\delta \theta_s}$) under dry soils is highest (most negative for LAI < 2.5 (Fig. 4b), but it rapidly diminishes to zero at LAI > 3 as a result of vegetation microwave emissions obscuring the soil signal. For soils at field capacity, the sensitivity remains strong even at relatively high LAI (i.e., between −5 and −10 up to an LAI ≈ 4) with differences in sensitivity evident among vegetation classes (e.g., shrublands are more sensitive than grassland/crops).

c. Analysis error

The relationship between model sensitivity to perturbation in soil moisture ($\frac{\delta T}{\delta \theta}$) and analysis, observation, and background variances ($\sigma_a$, $\sigma_o$, and $\sigma_b$) are illustrated for the scalar case [Eq. (3)] in Fig. 5 for “accurate” and “uncertain” modeled soil moistures. Note that this analysis assumes that the model bias in soil moisture (propagated through the observation operators to bias in modeled $T_a$ or $T_b$) and observation bias has been already eliminated. In each case, the rate at
which the analysis error ($\sigma_a$) approached the background error ($\sigma_b$) varied depending on the sensitivity term $\delta T/\delta \theta$: the lower the sensitivity (less negative), the more rapidly $\sigma_a$ approached $\sigma_b$ and the poorer the constraint provided by an observation. The rate at which these curves approached the limit $\sigma_b$ also depended on $\sigma_b$ itself. In Table 1, we considered the proportional constraint [Eq. (4)] as a measure of efficacy of the observations to constrain modeled soil moisture in the assimilation for three cases of observation error, two background errors ($\sigma_b = 0.025 \text{ m}^3 \text{ m}^{-3}$ (accurate case) and $0.05 \text{ m}^3 \text{ m}^{-3}$ (uncertain case)].

<table>
<thead>
<tr>
<th>$\sigma_b$ (m$^3$ m$^{-3}$)</th>
<th>$\delta T/\delta \theta$ (K (m$^3$ m$^{-3}$)$^{-1}$)</th>
<th>$\sigma_a$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.025</td>
<td>$-2.5$</td>
<td>3.0</td>
</tr>
<tr>
<td></td>
<td>$-1.0$</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td>$-0.5$</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>$-0.25$</td>
<td>1.9</td>
</tr>
<tr>
<td></td>
<td>$-0.05$</td>
<td>10.6</td>
</tr>
<tr>
<td></td>
<td>$-0.025$</td>
<td>29.3</td>
</tr>
<tr>
<td></td>
<td>$-0.01$</td>
<td>10.6</td>
</tr>
<tr>
<td></td>
<td>$-0.005$</td>
<td>55.3</td>
</tr>
<tr>
<td></td>
<td>$-0.0025$</td>
<td>29.3</td>
</tr>
<tr>
<td></td>
<td>$-0.001$</td>
<td>55.3</td>
</tr>
<tr>
<td></td>
<td>$-0.0005$</td>
<td>29.3</td>
</tr>
</tbody>
</table>

At low sensitivities ($\delta T/\delta \theta = -2.5$), an observation of error $= 1.25$ K provided virtually no constraint on the analysis state. In this case, the proportional constraint [Eq. (4)] was <1%. However, when sensitivities were greater ($\delta T/\delta \theta = -10$), a reduction in error of up to 7% was observed with an observation error of 1.25 K. With an increase in the observation accuracy to 0.5 K, the relative constraint increased to >10% for the accurate case but up to ~30% for the uncertain case. At higher sensitivities, such as those observed for microwave $T_b$ (Figs. 4b and 4d), the proportional constraint provided by $\sigma_o = 1.25$ K is substantial (29%) when the background soil moisture was “uncertain” and increased considerably to ~63% for observation errors of 0.5 K. Further improvements in the observation error to within the noise of the instrument ($\sigma_o = 0.25$ K) yielded significant improvements in the reduction of analysis error (Table 1) but observations of this accuracy from satellite are unlikely in the foreseeable future.

Temporal variation in the proportional constraint [Eq. (4)] provided by $T_s$ and $T_b$ observations is shown in Figs. 6a, 6b, 7a, and 7b for two contrasting vegetation types: semiarid woodlands and tall forests. In semiarid open woodlands and under moist conditions following rainfall, the reduction in background error in $\theta_{s1}$ afforded by $T_b$ observations can be up to 50% or 30% for uncertain and accurate cases, respectively (Fig. 6a). However, this constraint reduces rapidly to zero as soils dry. In contrast, $T_s$ observations provide virtually no reduction in background error in $\overline{\theta}$ for open woodlands (Fig. 6b). For tall forests, the reduction in background error in $\theta_{s1}$ from the assimilation of $T_b$ observations (Fig. 7a) was an order of magnitude less than for semiarid woodlands (Fig. 7a) but with the same decrease in proportional constraint as the soil surface dried (Fig. 7a). The reduction in background error provided by $T_s$ observations was up to 8% for the uncertain case (Fig. 7b); however, in this case the constraint on $\overline{\theta}$ increased as the soil profile dried rather than decreased as for $T_b$. For a cropping/pasture site in the central Murrumbidgee catchment, the proportional constraint provided by $T_s$ and $T_b$ observations was midway between these extremes, with each observation type contributing up to a maximum of 10% and 20%, respectively (data not presented).

The bottom panels of Figs. 6c and 7c provide preliminary information on model-observation bias. In the semiarid woodland, modeled $T_s$ consistently underestimated observations by an average of 4.0 K and modeled $T_b$ consistently overestimated observations, particularly when rainfall was frequent and/or heavy, by an average of 9.6 K (Fig. 6c). For tall forests (Fig. 7c), these model-observation biases $T_s$ and $T_b$ were reduced to an average of 1.6 and 1.8 K, respectively, but with the
same sign. This result indicates a better performance by the water balance model in tall forests rather than in semiarid woodlands but with potentially similar sources of bias.

5. Discussion

The efficacy of an observation type as a constraint on hydrological and hydrometeorological models is a function of the sensitivity of modeled observation to perturbation in the model state, the observation error, and the background error, and is expressed as the difference (relative or absolute) between the analysis and background errors. This study has shown that both thermal and microwave satellite observations can provide effective observational constraint on the modeled profile and surface soil moisture contents but only under certain conditions. Furthermore, the characteristics at which the observational constraint is maximal for \( T_s \) and \( T_b \) observations are complimentary—a fact that can be exploited to improve the estimation of soil moisture by satellite observations. Under a weak constraint, the water balance model will operate through time without any feedback from observations. However, under conditions where thermal and microwave observations together or separately provide a strong constraint, the model is benefited by a sequential adjustment that takes into consideration the orthogonal information contained in each observation type.

The fact that the observed \( T_b \) and \( T_s \) (Figs. 1c and 1d) fall within the endpoints of modeled \( T_b \) and \( T_s \) (Fig. 2) confirms that the observation operators \( H' \) and \( H'' \) are functioning realistically in this study, given available climate, soils, and vegetation data. The exception is where errors were introduced by standing water, snow, and cloud, as these conditions are not represented by the observation operators (these would be masked out in an operational assimilation scheme). The analysis of model sensitivities to perturbation in states showed that the sensitivity of \( T_s \) to profile moisture content was minimal in circumstances where low maximal stomatal conductance is an inherent plant trait (e.g., in shrublands), large fractions of soil surface were visible to the sensor (i.e., low LAI), soil water holding capacity was large (i.e., large \( \theta_{\text{max}} - \theta_{\text{min}} \)), and/or profile soil moisture content was near saturation (Fig. 3). Conversely, the sensitivity of \( T_b \) to surface layer soil moisture was minimal under conditions of high LAI, dense woody biomass, and low soil moisture content (Fig. 4). Maximal sensitivity for \( T_s \) occurred under drying soil—where vegetation stomata were strongly responsive to available water, such as in sands and sandy-loam soils, which have a smaller water holding capacity than clay soils—and at high LAI (Fig. 3). These results highlight the importance of
accurate information on soil and vegetation physical properties because $\delta T_s / \delta \theta_s$ is dependent on both the range in soil moisture between wilting point and field capacity and canopy cover. Under conditions of maximal sensitivity, maximum information on soil moisture content from an observation is mapped to state variables by the assimilation. In the ROI, this occurred primarily throughout the moderate-to-high relief and in well-developed canopies of the forest, cropping regions, and pastures (LAI > 2) in a band that extended from the northeast to south and southeast in Fig. 1. Little information on profile soil moisture content was provided by $T_s$ observations under sparse canopies in the flat terrain of the western part of this ROI (Fig. 3).

The conditions under which $T_s$ and $T_b$ provide strong constraints on $\theta_s$ and $\theta_u$ are approximately the converse for each observation type (Figs. 6 and 7). This means that the prospect for significant improvements in model performance by employing both observation types at the same time within a data assimilation scheme is considerable. This is because when conditions vary such that one observation type is ineffective at constraining model soil moisture, the other observation type can potentially act as a strong constraint on model dynamics. This dynamic variation in the proportional constraint is evidenced in Figs. 6a, 6b, 7a, and 7b where an initially wet profile undergoes drying to near-wilting point, with more rapid drying of the surface layers than deeper in the profile. In a wet soil and full canopy with stomata fully open, observations of $T_s$ provide little constraint on profile moisture content (Fig. 7b), whereas microwave observations of $T_b$ provide a stronger constraint on surface layer moisture (Fig. 7a). With the drying of the upper soil layers, observations of $T_b$ cease to constrain modeled surface moisture content, whereas observations of $T_s$ provide an increasingly strong constraint on profile moisture content. For a semiarid location, the majority of the observational constraint through time was provided by microwave observations of surface soil moisture, particularly under wet soils (Fig. 6a) with little constraint on $\theta_s$ provided by observations of $T_s$. This dynamic variation in the strength of observational constraints from multiple satellite sensors can be exploited in regional-scale hydrological and hydrometeorological data assimilations using “multiple constraints” approaches (e.g., Barrett 2002; Barrett et al. 2005; Raupach et al. 2005; McCabe et al. 2008; Renzullo et al. 2008) that also take into account the varying frequency of observations (Figs. 6c and 7c) to provide the most accurate estimation of soil moisture initial conditions possible. This will lead to subsequent benefits for the prediction of latent and sensible heat fluxes to the atmosphere, runoff, streamflow, and soil water availability.

The magnitude of observation errors is critical in determining the efficacy of satellite data as constraints on models. Increasing measurement error, bias, and infrequent data reduce the effectiveness of observations as constraints (Figs. 5–7; Table 1). Currently, the range in accuracy for observed $T_s$ from SWAs is 0.4–1.75 K (see section 2c), and the present study has shown that for $\sigma_a > 1.5$ K, these errors are too large for satellite thermal observations to be an effective constraint on modeled soil moisture content, especially when the background error is small (e.g., $\sigma_b = 0.025$ m$^3$ m$^{-2}$ in Fig. 5). For an
uncertain background (0.05 m$^3$ m$^{-3}$), these observations provide a marginal improvement in the analysis errors but only under conditions when the sensitivity ($\delta T_s/\delta u_z$) is maximal. It would appear, therefore, that the prospects for individual thermal observations imparting constraint on profile soil moisture estimation will only improve if observation error can be reduced to $\sim$1 K. Despite the apparent limitation this may impose, the serial nature of satellite observations, their spatial and temporal correlations, and the “memory” of soil moisture stores contained in the model equations act to stabilize model dynamics in a time series when observations have large errors or are absent. Further work is needed to determine how to best exploit multiple thermal observations acquired at key times of the day (Kustas and Norman 1999; Anderson et al. 2007; Crow et al. 2008) and to incorporate vegetation greenness (Gillies and Carlson 1995; Carlson 2007) to further improve estimates of root-zone soil moisture.

In the case of microwave $T_b$, the requirement for close tolerances on observation errors is to some degree obviated by the strong sensitivity (Fig. 4), and any improvement in the accuracy of these observations would be expected to further increase the strong constraint on modeled $\theta_{1z}$ (Fig. 5). These results concur with estimated error reduction using ensemble Kalman filter methods by Reichle et al. (2002). They found a reduction in root-mean-square error for surface soil moisture of up to $\sim$80% using passive microwave when compared against values obtained without assimilation. However, these improvements can only be achieved where the potential bias from an incorrect specification of canopy optical depth, soil temperature, surface roughness, and surface emissivity is removed—and these biases can be substantial (Draper et al. 2009; Wagner et al. 2007). Assuming that these biases can be eliminated through the accurate and independent estimation of LAI and optical depth, the use of a coupled SEB–MRT model to provide soil and vegetation temperatures, and through accurate information on soil physical properties, the prospects for improved prediction of surface soil moisture from data assimilation constrained by passive microwave observations is good. The exceptions to this are the conditions under which the sensitivity of $T_s$ is low or where the observation operator performs badly, such as in mountainous terrain, high biomass forests, or where standing water or snow is present.

Comparison of modeled observations with satellite data (Figs. 6c and 7c) showed the consistent underestimation of $T_s$ and overestimation of $T_b$ by the water budget but with less bias evident for the tall forest site (Fig. 7c) than for open woodland (Fig. 6c). The identification of biases through the application of multiple constraints data assimilation is one of the major benefits of these methods. The sharp reduction in $T_s$ following rainfall relative to the model (Fig. 6c) is strongly suggestive of surface saturation and possibly pooling of water in run-on parts of the landscape. Consistent underestimation of $T_s$ is indicative of a modeled profile that is too wet relative to observations, which may indicate the possible underestimation of drainage or evapotranspiration terms of the model. Further work is required to elucidate the nature of these biases, to determine whether they arise from observations or from the model, to determine their spatial and temporal variations, and to develop correction functions for use in an operational data assimilation scheme.

6. Conclusions

The tangent linear model (TLM) for two observation operators were used to examine the sensitivities of thermal and microwave satellite observations to variations in profile and surface layer soil moisture. The TLM for $T_s$ showed the strongest sensitivity when soils were relatively dry, in grassland/crop and forest vegetation classes, at low soil water holding capacity, and when canopy leaf area index (LAI) exceeded 2.5. Low sensitivity of $T_b$ was observed where soils were at field capacity (across all vegetation types), in shrublands (as a result of low maximum stomatal conductance), and in sparse canopies where bare soils prevailed. The TLM for $T_b$ showed sensitivities 1–10 times greater than for $T_s$. Maximal sensitivities of $T_b$ to surface soil moisture content occurred when LAI was $<1.5$ in dry soils but up to an LAI of $\sim$4 when soils were at field capacity.

Satellite observations of thermal and microwave emissions of the land surface can provide strong constraints on root-zone soil moisture under specific conditions. Where potential sources of bias are eliminated and the observation errors reduced to $\sim$1 K, these observations offer good prospects for improved profile soil moisture prediction—particularly when combined in a “multiple constraints” data assimilation context. The multiple constraints methods have additional benefits of using orthogonal information in observations to increase the observational constraint on model dynamics and in identifying the presence of bias in the model and/or observations.

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**APPENDIX**

**Observation Model Operators and TLM Approximations**

Observation model operators and their respective TLM representation are given here. The observation operator for land surface temperature $H^T$ was developed from the equations of Friedl (1995, 2002) using the Jarvis (1976) formulation for canopy resistance to water vapor and the stomatal resistance scaling functions of Cox et al. (1998). The observation operator for microwave brightness temperature $H^m$ was based on the microwave radiative transfer theory presented in Wang and Schmugge (1980), Mo et al. (1982), Dobson et al. (1985), Njoku et al. (2003), and Owe et al. (2001).

(For more details, including model assumptions and limitations, refer to the references above.) Here only the pertinent components of each model for calculating temperature ($T_s$ or $T_b$) and the TLM are presented. Model variables and parameters are defined in Table A1.

### a. Land surface temperature

The SEB model used in this work comprised six nonlinear equations that describe the portioning of moisture and heat fluxes between the vegetation and soil surface layers and the overlying atmosphere (Friedl 2002). Key TLM equations are denoted by a $\delta$ symbol preceding each variable. Active variable in case of LST is $\delta_z$. A simple $N$-loop construct was considered the most efficient method of numerically solving the equations for

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_1$, $c_2$, $c_4$</td>
<td>Constants used to scale water vapor pressure function; 0.611, 17.22, and 35.86</td>
<td>kPa, $-$, K</td>
</tr>
<tr>
<td>$c_3$</td>
<td>Offset used in water vapor pressure and microwave emissivity functions; 273.15</td>
<td>K</td>
</tr>
<tr>
<td>$c_5$, $c_6$, $c_7$, $c_8$</td>
<td>Coefficient used to calculate dielectric constant of water; 88.045, $-0.4147, 6.295 \times 10^{-4}$, and $1.075 \times 10^{-5}$</td>
<td>—</td>
</tr>
<tr>
<td>$e_{w0}$, $e_{w0}^0$, $e_{ss}$</td>
<td>Atmospheric vapor pressure of the mixed layer ($a$) and height of exchange within canopy ($0$); saturated water vapor pressure at leaf temperature ($v$); and vapor pressure of air in soil spaces between 0 and 2.5-cm depth ($ss$)</td>
<td>kPa</td>
</tr>
<tr>
<td>$e_r$</td>
<td>Rough surface emissivity</td>
<td>—</td>
</tr>
<tr>
<td>$f_{ss}$</td>
<td>Fraction of soil surface visible to thermal sensor</td>
<td>—</td>
</tr>
<tr>
<td>$h$</td>
<td>Soil surface roughness</td>
<td>—</td>
</tr>
<tr>
<td>$p_2$, $p_3$, $p_4$</td>
<td>Stomatal resistance model parameters (Cox et al. 1998)</td>
<td>W m$^{-2}$, kPa$^{-1}$, —</td>
</tr>
<tr>
<td>$r_m$, $r_s$, $r_w$, $r_s$, $r_ws$</td>
<td>Surface aerodynamic resistance to water vapor and heat exchange ($a$); resistance to heat exchange by foliage ($b$) and soil surface soil surface ($w$); and resistance to the exchange of water vapor by canopy ($c$) and soil surface ($ss$)</td>
<td>s m$^{-1}$</td>
</tr>
<tr>
<td>$A_u$</td>
<td>View zenith angle of microwave sensor</td>
<td>rad</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Specific heat of air at constant pressure</td>
<td>J kg$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$G$</td>
<td>Soil heat flux</td>
<td>W m$^{-2}$</td>
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<tr>
<td>$G_{max}$, $G_{min}$</td>
<td>Canopy maximum and minimum conductance to water vapor</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$I_{sw}$</td>
<td>Incident shortwave radiation</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$R$</td>
<td>Smooth soil reflectivity to horizontally polarized microwave radiation</td>
<td>—</td>
</tr>
<tr>
<td>$R_{n_i}$, $R_{n_s}$</td>
<td>Component of net radiation reaching vegetation canopy ($v$) and soil surface ($s$)</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$S_h$, $S_v$, $S_{th}$</td>
<td>Scaling function of stomatal conductance for incoming shortwave radiation ($l$), VPD ($v$), and average profile soil moisture content ($\theta$)</td>
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</tr>
<tr>
<td>$S_{a_{10}}$, $S_{a_{20}}$, $S_{a_{30}}$</td>
<td>Scaling function of stomatal conductance for soil moisture from 0 to 2.5-cm depth</td>
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</tr>
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<td>$T_{0_i}$, $T_{v_i}$, $T_{ss}$</td>
<td>Temperature of air at height of heat and water vapor exchange within the canopy ($0$), temperature of canopy foliage ($v$), and soil surface ($ss$)</td>
<td>K</td>
</tr>
<tr>
<td>VPD</td>
<td>Vapor pressure deficit</td>
<td>kPa</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Linear scaling function of soil water availability</td>
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<td>$\alpha_1$, $\alpha_2$, $\alpha_3$, $\alpha_4$, $\alpha_5$, $\alpha_6$</td>
<td>Microwave dielectric constant of soil, water, and air mixture; dielectric constant of air ($a$), ice ($i$), rock ($r$), and water ($w$); and water absorbed by clay ($c$) in the soil</td>
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</tr>
<tr>
<td>$\gamma$</td>
<td>Psychometric constant</td>
<td>kPa K$^{-1}$</td>
</tr>
<tr>
<td>$\gamma_{WS}$</td>
<td>Constant used in Wang and Schmugge (1980) model</td>
<td>—</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of air</td>
<td>kg m$^{-3}$</td>
</tr>
<tr>
<td>$\theta_{max}$, $\theta_{min}$</td>
<td>Volumetric soil moisture at field capacity (max) and wilting point (min)</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$\theta_{w1}$</td>
<td>Surface layer volumetric soil moisture content (0–2.5-cm depth)</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$\theta_{f}$</td>
<td>“Transition” soil moisture content where soil moisture saturates pore spaces</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$\theta_{ss}$</td>
<td>Profile average volumetric soil moisture content</td>
<td>m$^3$ m$^{-3}$</td>
</tr>
<tr>
<td>$\omega_0$, $\Gamma$</td>
<td>Single scattering albedo and vegetation transmissivity of microwave radiation</td>
<td>—, —</td>
</tr>
</tbody>
</table>
the temperatures and water vapor pressure values and computing the TLM. The method was found to rapidly converge to solution (e.g., temperature estimates converged to within 0.5 K within \( N = 5 \) iterations). Computation begins with the initialization \( T_v = T_0 = T_{ss} = T_a, e_v^0 = e_0 = e_{ss} = e_a, \) and \( \delta T_v = \delta T_0 = \delta T_{ss} = 0, \) and the algorithm proceeds as follows:

Algorithm Begin [\[
\begin{align*}
\beta &= \frac{\bar{\theta} - \theta_{\min}}{\theta_{\max} - \theta_{\min}} \\
\delta \beta &= \frac{1}{\theta_{\max} - \theta_{\min}} \delta \bar{\theta} \\
S_{\theta} &= \frac{1 - \exp(-p_4 \beta)}{1 - \exp(-p_4)} \\
S_v &= 1 - p_3 \text{VPD} \\
S_i &= \frac{I_{sw}}{1000} + \frac{p_2}{I_{sw} + p_2} \\
\delta S_{\theta} &= p_4 e^{-p_4 \beta} \left( 1 - e^{-p_4 \beta} \right) - \delta \beta \\
r_{ss} &= 5000 \exp(-15 \theta_{1i}) \\
\end{align*}
\]

\[
\delta e_0 = \left( \frac{e_v r_v + e_a (r_v + r_w)}{r_v + r_a(r_{ss} + r_w) + r_a(r_v + r_{ss} + r_v + r_w)} \right) \left( \frac{(r_a + r_{ss} + r_w)(e_{ss} r_a (r_v + r_w) + [e_v^0 r_a + e_a (r_v + r_w)](r_{ss} + r_w))}{[(r_v + r_a)(r_{ss} + r_w) + r_a(r_v + r_{ss} + r_v + r_w)]^2} \right) \delta T_v \\
+ \left( r_a r_v + r_{ss} \right) \left( r_v + r_a(r_{ss} + r_w) + r_a(r_v + r_{ss} + r_v + r_w) \right) \delta e_v \\
\]

\[
T_v = T_0 + \left( \frac{e_v^0 - e_v^0}{r_v} \right) + r_b \frac{R_{n}}{C_p} \\
\delta T_v = \delta T_0 + \left( \frac{r_b}{\gamma(r_v + r_w)} \right) \delta e_0 - \left( \frac{r_b}{\gamma(r_v + r_w)} \right) \delta e_v \\
T_{ss} = \frac{r_w}{C_p} \left[ -G + R_{n} + pC_p(e_v^0 - e_v^0) + \frac{C_p T_0}{r_w} \right] \\
\delta T_{ss} = \delta T_0 + \left( \frac{r_w}{\gamma(r_{ss} + r_w)} \right) \delta e_0 - \left( \frac{r_w}{\gamma(r_{ss} + r_w)} \right) \delta e_v \\
T_0 = \frac{r_b r_v T_a + r_a r_b T_{ss} + r_a r_w T_v}{r_b r_w + r_a(r_v + r_w)} \\
\delta T_0 = \left( \frac{r_a r_b}{r_b r_w + r_a(r_v + r_w)} \right) \delta T_{ss} + \left( \frac{r_a r_w}{r_b r_w + r_a(r_v + r_w)} \right) \delta T_v \\
\text{End Do}
\]
b. Microwave brightness temperature

The coupled SEB–MRT model used in this work uses the soil and vegetation temperatures computed in the SEB model earlier. Key TLM equations are denoted by a δ symbol preceding each variable. Active variable in case of microwave brightness temperature is $\theta_{s1}$. Again, a simple N-loop construct was considered the most efficient method of numerically solving the equations for the temperatures and water vapor pressure values and computing the TLM.

Algorithm Begin

$$T_s = f_{ss} T_{ss} + (1 - f_{ss}) T_v$$
$$\delta T_s = f_{ss} \delta T_{ss} + (1 - f_{ss}) \delta T_v$$
$$r_{ss} = 5000 \exp(-15 \theta_{s1})$$
$$\delta r_s = -75000 \exp(-15 \theta_{s1}) \delta \theta_{s1}$$

Do 1 \ldots N

$$e^a = c_1 \exp\left[\frac{c_2(T_v - c_3)}{T_v - c_4}\right]$$
$$\delta e^a = c_1 \exp\left[\frac{c_2(T_v - c_3)}{T_v - c_4}\right] \left[\frac{c_2(T_v - c_3)}{(T_v - c_4)}\right] \delta T_v$$
$$e_{ss} = c_1 \exp\left[\frac{c_2(T_{ss} - c_3)}{T_{ss} - c_4}\right] S_{\theta_{s1}}$$
$$\delta e_{ss} = c_1 \exp\left[\frac{c_2(T_{ss} - c_3)}{T_{ss} - c_4}\right] \left[\frac{c_2(T_{ss} - c_3)}{(T_{ss} - c_4)}\right] S_{\theta_{s1}} \delta T_{ss}$$
$$+ c_1 \exp\left[\frac{c_2(T_{ss} - c_3)}{T_{ss} - c_4}\right] \delta S_{\theta_{s1}}$$
$$e_0 = \left[\frac{e_{ss} r_a (r_b + r_v) + [e^a r_a + e_a (r_b + r_v) \delta \theta_{s1}] (r_{ss} + r_w)}{(r_b + r_v)(r_{ss} + r_w) + r_a (r_b + r_{ss} + r_v + r_w)}\right]$$

$$T_v = T_0 + \left(\frac{e_0 - e^a}{r_v} + \frac{r_v R_{n_v}}{(r_b + r_v)}\right) \frac{r_b T_0}{\rho C_p}$$
$$\delta T_v = \delta T_0 + \left[\frac{r_b}{\gamma(r_b + r_v)}\right] \delta e_0 - \left[\frac{r_b}{\gamma(r_b + r_v)}\right] \delta e^a_v$$
$$T_{ss} = \frac{r_w}{\rho C_p} \left[-G + R_n + \frac{\rho C_p (e_0 - e_{ss})}{\gamma(r_{ss} + r_w)} + \frac{C_p T_0}{r_w}\right]$$
$$\delta T_{ss} = \delta T_0 + \left[\frac{r_w}{\gamma(r_{ss} + r_w)}\right] \delta e_0 - \left[\frac{r_w}{\gamma(r_{ss} + r_w)}\right] \delta e_{ss}$$
$$- \left[\frac{(e_0 - e_{ss}) r_w}{\gamma(r_{ss} + r_w)^2}\right] \delta r_{ss}$$
$$T_0 = \frac{r_b r_a r_v T_a + r_a r_b T_{ss} + r_a r_v T_v}{r_b r_a r_v + r_a (r_b + r_v)}$$

End Do

$$e_w = c_5 + c_6 (T_{ss} - c_3) + c_7 (T_{ss} - c_3)^2 + c_8 (T_{ss} - c_3)^3$$
$$\delta e_w = [c_5 + c_6 (T_{ss} - c_3) + c_7 (T_{ss} - c_3)^2] \delta T_{ss}$$
$$e_x = e_i + \left(e_w - e_i\right) \frac{\theta_{s1}}{\theta_i} \gamma_{WS}$$
$$\delta e_x = \frac{\theta_{s1}}{\theta_i} \gamma_{WS} \delta e_w + \left(e_w - e_i\right) \frac{\theta_{s1}}{\theta_i} \gamma_{WS} \delta \theta_{s1}$$
$$e = \theta_{s1} e_x + (P - \theta_{s1}) e_a + (1 + P) e_r$$
\[ \delta e = (e_s - e_v) \delta \theta_s + \theta_s \delta e_v \]

\[ R = \left[ \frac{\cos(A_n) - \sqrt{e - \sin^2(A_n)}}{\cos(A_n) + \sqrt{e - \sin^2(A_n)}} \right] ^2 \]

\[ \delta R = \frac{2\cos(A_n) \left[ \sqrt{e - \sin^2(A_n)} - \cos(A_n) \right]}{\sqrt{e - \sin^2(A_n) \left[ \sqrt{e - \sin^2(A_n)} + \cos(A_n) \right] ^3} \delta e \]

\[ e_r = 1 - R \exp[-h \cos^2(A_n)] \]

\[ \delta e_r = -\exp[-h \cos^2(A_n)] \delta R \]

\[ T_b = T_{ss} e_v \Gamma + (1 - \omega) T_v (1 - \Gamma) \]

\[ + (1 - e_v)(1 - \omega) T_v (1 - \Gamma) \]

\[ \delta T_b = (\Gamma e_r T_{ss} + (\Gamma T_{ss} - (1 - \Gamma) \Gamma T_v (1 - \omega) \delta e_r \]

\[ + (1 - \Gamma)(1 - \omega) + (1 - \Gamma)(1 - \omega)(1 - e_v)) \delta T_v \]

\}\ Algorithm End.

REFERENCES


