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A sensitivity analysis of soil moisture retrieval from the Tau-Omega microwave emission model

Ian J Davenport (Member, IEEE), Jesus Fernández-Gálvez, R J Gurney

Abstract

The potential of the $\tau_\omega$ model for retrieving the volumetric moisture content of bare and vegetated soil from dual polarisation passive microwave data acquired at single and multiple angles is tested. Measurement error and several additional sources of uncertainty will affect the theoretical retrieval accuracy. These include uncertainty in the soil temperature, the vegetation structure and consequently its microwave single-scattering albedo, and uncertainty in soil microwave emissivity based on its roughness. To test the effects of these uncertainties for simple homogeneous scenes, we attempt to retrieve soil moisture from a number of simulated microwave brightness temperature datasets generated using the $\tau_\omega$ model. The uncertainties for each influence are estimated and applied to curves generated for typical scenarios, and an inverse model used to retrieve the soil moisture content, vegetation optical depth and soil temperature. The effect of each influence on the theoretical soil moisture retrieval limit is explored, the likelihood of each sensor configuration meeting user requirements is assessed, and the most effective means of improving moisture retrieval indicated.

Keywords: passive microwave, sensitivity analysis, soil moisture.

Front page footnote:

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I. INTRODUCTION

Satellite-based passive microwave radiometers operating at L-band are currently in development for deployment on three missions, Aquarius, SMOS (Soil Moisture and Ocean Salinity) and HYDROS (HYDROsphere State). SMOS and HYDROS are intended for use to measure soil moisture. Whilst HYDROS will acquire data at a fixed look-angle of 40º from nadir, SMOS will deploy a synthetic aperture system enabling it to acquire observations of individual sites over a range of angles up to about 50º from nadir. The use of these systems to measure soil moisture content would be of value in atmospheric, hydrological, and dynamic global vegetation and carbon dynamics models. Although objectives are different for each class of model, soil moisture plays an important role in each discipline.

In atmospheric models, the principle interest in soil water is its impact on evaporation and sensible/latent heat partitioning at scales that are appropriate for simulating the forcing of atmospheric processes. In hydrological applications the focus is generally on water balance components - infiltration, surface run-off, evaporation, deep percolation and changes in water content of the vadose zone. In dynamic global vegetation models the principal interest is in quantifying the distribution of vegetation with implications for the terrestrial component of the current global CO\textsubscript{2} budget. An analysis of end-user requirements [1] found that a volumetric water content accuracy of 0.04 m\textsuperscript{3} m\textsuperscript{-3} or 4% in absolute terms was realistic for atmospheric modelling applications, though this may prove inadequate for modelling soil profiles down to the root zone.

The soil surface usually has some coverage by vegetation. The emission of microwave radiation by soil, and the effect on the radiation of passing through vegetation can be described by the $\tau$-$\omega$ model [2,3]. This model predicts the microwave radiation observed above soil of a given composition and moisture content covered by a vegetation layer of a known microwave optical depth and single-scattering albedo. The model can be used to retrieve variables such as soil moisture, vegetation microwave optical depth, and soil temperature [4,5,6], but a number of assumptions underlie it. In this work we study the limits on the variables that can be retrieved from this model as a function of the instrument sensitivity, and the impact of uncertainty in some of the parameters the model relies upon. We assume throughout that the model is a valid representation of microwave emission, so the results are necessarily theoretical limits on accuracy rather than a practical error budget, and subject to increase because of the simplification that the model represents.

Firstly, we consider the consequences of instrumental noise and bias on variable retrieval from measured microwave brightness temperature data, by generating data using a forward model to produce brightness temperature values for known values of variables, adding noise or bias, and attempting to retrieve the same variables from the degraded data. Making measurements from the ground or alternative remote sensing sources can allow us to add information to assist the model in retrieving variables, so we consider the effect of giving the model information about the surface temperature and density of vegetation cover. We then test the impact of other influences on the model. One common assumption is that the microwave single-scattering albedo from vegetation can be ignored [7,8]. We examine the effect of setting this to zero, or using an erroneous value, and explore the best retrieval strategy to minimise error arising
from uncertainty in this parameter. Soil roughness, small-scale variations in the soil surface elevation of a few centimetres, can have a significant effect on the microwave emissivity of the soil. The difficulty in measuring surface roughness can consequently cause errors in interpretation of microwave data. We employ a simple model of the effect of soil roughness on emissivity [9] to examine its effect on variable retrievals.

Pardé et al. [10] examined retrieval accuracy of soil moisture from multiple-angle L-band measurements using a seven-variable iterative retrieval from actual microwave observations and soil moisture measurements, showing the sensitivity of soil moisture retrievals to (i) the initial estimates of variables required by an iterative retrieval approach, and (ii) the accuracy with which these variables are known. Uncertainty in the error present in the microwave measurements, estimated between 1 and 3 K, and its high level compared to the projected error of satellite systems made some of the effects difficult to distinguish. We have here attempted firstly to remove the effect of initial variable estimates by using a retrieval that does not depend on them, and secondly to extend our understanding of the relative effects of uncertainty in the different components of the $\tau$-$\omega$ model to a lower measurement error regime closer to that we expect a satellite system to achieve.
II. SENSITIVITY ANALYSIS TECHNIQUE

A. Model description

A simple radiative transfer formulation, the $\tau$-$\omega$ model [2,3] is used for describing the emission of microwave radiation from the soil surface. In the $\tau$-$\omega$ model, the brightness temperature, $T_B$, of a top layer (soil and vegetation) medium is the sum of three terms: the canopy attenuated soil emission, the direct vegetation emission and the vegetation emission reflected by the soil and attenuated by the canopy. There is also a fourth term which is the soil-reflected and two way canopy-attenuated down-welling sky brightness temperature, but this term may be considered negligible in the first instance. The brightness temperature can be expressed as:

$$T_B = \varepsilon_{\text{soil}} T_{\text{soil}} e^{-\tau} + (1 - \omega) T_{\text{veg}} (1 - e^{-\tau}) + (1 - \varepsilon_{\text{soil}}) (1 - \omega) T_{\text{soil}} (1 - e^{-\tau}) e^{-\tau}$$

where $\varepsilon_{\text{soil}}$ is the soil emissivity, $\omega$ is the single scattering albedo within the canopy, $\tau$ is the optical depth of the canopy, $\alpha$ is the look angle from nadir, $T_{\text{soil}}$ is the soil temperature and $T_{\text{veg}}$ is the vegetation temperature.

The soil emissivity is calculated from the Fresnel equations, incorporating the dielectric constant of the soil which is derived from the Wang and Schmugge [11] model, assuming a soil texture of SAND=60%, CLAY=20%, incorporating the wilting point of soil [12] assuming a bulk density of 1.3 g.cm$^{-3}$, and component relative dielectric constants of 3.2, 1 and 5.5 for bound water, air and soil particles respectively. The dielectric constant of water was derived by modified version of the Debye equation for the relative dielectric constant [13], the high frequency dielectric constant [14], the static dielectric constant of water as described by Klein and Swift [15] and the relaxation time of pure water [16]. We use the earlier and more widely-published versions of the Fresnel equations relating reflectivity to dielectric constant and look angle [17] rather than the apparently erroneous expressions appearing in some literature [18,19] which yield the square roots of the values for reflectivity.

B. Retrieval accuracy assessment methodology

The forward model described above was used to generate a family of brightness temperature curves describing a range of soil and vegetation conditions. In all cases, the soil and vegetation temperatures are assumed to be the same, represented by the surface temperature, $T_s$, set at 293 K. Six test scenarios were devised by using all the combinations of soil moisture content $\theta = 0.1$ and 0.4 m$^3$m$^{-3}$, and microwave optical depth $\tau = 0.0$, 0.2 and 0.6. Both the horizontally (H) and vertically (V) polarised brightness temperatures were generated in the forward model at the look angles 0, 10, 20, 30, 40 and 50° from nadir, creating twelve brightness temperature values, representing what a perfect multiple-look-angle microwave radiometer instrument would measure if the $\tau$-$\omega$ model is an accurate representation of reality. These brightness temperatures are then perturbed in a range of ways to simulate possible observing errors, and the inversion is applied to find the values of soil moisture, vegetation optical depth and surface temperature which produce a curve that fits most accurately.
C. Model Inversion technique

The sensitivity of soil moisture retrieval to initial variable estimates is evident in Pardé et al. [10], so for this work we devised a retrieval system independent of initial estimates, which only relies on knowing the plausible range of each variable. The retrieval technique inverts the $\tau-\omega$ model by finding the set of three input variables soil moisture content $\theta$, vegetation optical depth $\tau$ and surface temperature $T_s$ which generate a brightness temperature curve which best matches the ‘observed’ input curve. The brightness temperature curves for comparison are calculated for all combinations of values of $T_s$ between 263 and 313 K with a step of 0.1 K, all values of $\tau$ between 0.0 and 1.0 with a step of 0.01, and all values of $\theta$ between 0.0 and 0.5 m$^3$m$^{-3}$ with a step of 0.01 m$^3$m$^{-3}$. Since the value of soil bulk density used for the model is 1.3 g·cm$^{-3}$, 0.5 m$^3$m$^{-3}$ is the maximum possible value of soil moisture content. The 50 K temperature range is used to denote a situation where no independent observations are available to infer the surface temperature. To simulate the case where surface temperature is known from an external source with an accuracy of 2 K, the model retrieval is constrained to retrieve $T_s$ within 2 K of the known input value. The set of variables which best fit the observed data best are judged by minimizing the sum of the squares of the difference between the input ‘observation’ and the simulated curves.

Once an initial best fit to the input curve is obtained, a second stage refines the retrieved $\theta$, $\tau$ and $T_s$ estimates by repeating the procedure using smaller steps in the variable space around the best fit $\theta$, $\tau$, $T_s$ values. In this stage the best fit $T_s$ is estimated to within 0.01 K, $\theta$ to within 0.001 m$^3$m$^{-3}$, and $\tau$ to within 0.0001. If the single-scattering albedo $\omega$ and soil roughness are also retrieved, as in later sections, their values are accurate to 0.001. The best model fit is determined by minimising the sum of the squared differences between the input points on the brightness temperature curves and the modelled points. The horizontally and vertically polarised data are fitted simultaneously. To simulate retrievals from a multiple-angle dual-polarization data set such as a synthetic aperture system such as SMOS might provide, brightness temperatures at six angles and two polarisations are fitted. To simulate single look-angle data such as HYDROS might provide, only the H and V brightness temperatures at 40º look-angle were fitted. Since retrieving three variables from the two observations leads to a range of possible exact solutions depending on the variable constraints, when retrieving fits from single-angle data, we present the statistics from retrievals assuming nine $T_s$ values covering the $T_s$ constraint range. For example, if we know that the surface temperature is between 291 and 295 K, then we retrieve the best fits for soil moisture and vegetation optical depth for the assumptions $T_s=291, 291.5, 292, 292.5, 293, 293.5, 294, 294.5$ and 295 K. Mean and RMS errors and other statistical measures are then calculated over these assumptions.
D. Model Inversion validation

Retrieval sensitivity was tested by generating 500 test curves with random input values evenly distributed across the ranges $T_s$ between 263 and 313 K, $\tau$ between 0.0 and 0.6, and $\theta$ between 0.1 and 0.4 m$^3$ m$^{-3}$. These values were used to generate the forward curves, and the inversion described above was used to attempt to retrieve them. For the six-angle data, $\theta$ was retrieved with an RMS error of 0.0005 m$^3$ m$^{-3}$, $\tau$ was retrieved with an RMSE of 0.001, and $T_s$ with an RMSE of 0.05 K. For the single-angle data, attempting to retrieve three variables ($\theta$, $\tau$, $T_s$) using only two measurements means that there are a number of valid solutions, and $\theta$ retrieval accuracy depends on constraint of the other variables. To quantify this, runs were carried out with different constraints on $T_s$. The RMS errors, the 90th and 99th percentile errors, and the worst case errors for $\theta$ retrieval are shown in Figure 1. The worst cases always corresponded to the highest soil moisture, highest vegetation optical depth scenarios. In this graph, a 1 K constraint means that the temperature is known to within 1 K, so the retrieval is constrained to a total temperature range of 2 K. A 0 K constraint therefore means that the temperature is known to within 0 K, i.e. exactly known, so that at 0 K the error shown is that for a two-variable retrieval. The error distributions for the soil moisture retrieval were generally gaussian and symmetrical in shape. For example, in the 2 K $T_s$ constraint case, the RMS error was 0.013 m$^3$ m$^{-3}$, the worst case, which was high soil moisture and high vegetation optical depth, gave an error of 0.042 m$^3$ m$^{-3}$, 90% of the errors were below 0.020 m$^3$ m$^{-3}$, and 99% were below 0.032 m$^3$ m$^{-3}$. Thus, if the surface temperature is known only to within 2 K, then in the worst case the soil moisture retrieval error already exceeds the 0.04 m$^3$ m$^{-3}$ user requirement, before measurement error and other uncertainty effects considered in later sections are accounted for.

Figure 1. RMS soil moisture retrieval error for a single-angle dual polarization system with surface temperature constraint.
III. THE EFFECT OF INSTRUMENT BIAS AND NOISE

A. Motive

An uncertainty or error is associated with any given measurement, and in this case the measurement made by a microwave radiometer is the brightness temperature. The projected measurement error for the HYDROS instrument for example is currently estimated as 0.64 K [20]. Bias and system noise-induced random error in the measured brightness temperature values will perturb the retrieved values of soil moisture, vegetation optical depth and soil temperature.

B. Method

We calculated horizontally and vertically polarised brightness temperature curves as described in Section II. A number of degraded curves were then generated by adding biases between 0.2 K and 5.0 K, both positive and negative, and normally-distributed noise with a standard deviation (σ) between 0.05 and 2.00 K. The inverse model then attempted to retrieve the input variables soil moisture content \( \theta \), vegetation optical depth \( \tau \), and surface temperature \( T_s \). The inversion also attempted to retrieve these variables from just the 40º H and V brightness temperatures, to simulate a single-angle system. Ignorance of the surface temperature is simulated by allowing the inversion to retrieve the surface temperature, \( T_s \), within a 50 K range between 263 K and 313 K. This range represents an effectively unconstrained retrieval, as if no external temperature information is available, as we will always know the surface temperature better than this, from climatology or other independent observations. To simulate the effect of independent \( T_s \) knowledge, retrievals were attempted whilst constraining \( T_s \) to within 2 K of the input value.
Figure 2. RMS error in $\theta$ retrieval for systematic bias on the brightness temperature curves.
Figure 3. The effect of random brightness temperature noise on retrieving $\theta$, (a) RMS errors over the six $\theta, \tau$ scenarios, (b) RMS errors just for the worst scenario $\theta=0.4, \tau=0.6$. 
Figure 4. As Figure 3, showing the retrieval error for vegetation optical depth, \( \tau \).

Figure 5. As Figure 3, showing the six-angle RMS retrieval error for surface temperature, \( T_s \), for the case where the surface temperature in the model is only limited to the 50 K range 263-313 K.
C. Results

The soil moisture retrieval accuracy for each system with bias is shown in Figure 2. Notably the six-angle system performs worse at high bias when the surface temperature is constrained to within 2 K, since the bias renders this temperature constraint inaccurate. Allowed the wider 50 K temperature range, the soil moisture retrieval is better at biases over 2 K. The retrieval accuracy over all $\theta$, $\tau$ scenarios with noise for soil moisture, vegetation optical depth and surface temperature are shown in Figures 3, 4 and 5 respectively. The worst $\theta$, $\tau$ scenario in each case is the high soil moisture, high vegetation optical depth case ($\theta$=0.4, $\tau$=0.6), and the soil moisture retrieval errors for this scenario alone are presented in Figure 3(b).

1) Soil moisture retrieval

Constraining the retrieved surface temperature for the single-angle system to within 2 K of the input yields a soil moisture content retrieval RMSE of 0.020 m$^3$m$^{-3}$ for $\sigma = 0.50$ K noise. This compares to 0.012 m$^3$m$^{-3}$ for the six-angle retrieval without any temperature constraint. The best results are unsurprisingly obtained with a multiple-angle system with surface temperature constrained to within 2 K, where the RMSE is 0.010 m$^3$m$^{-3}$. For higher noise levels, the multiple-angle temperature-constrained system performs significantly better than both the multi-angle temperature ignorant and single-angle temperature-constrained systems. In work using a seven-variable retrieval from actual multiple-angle observations, though with an uncertain measurement error estimated as within the range 1-3K, Pardé et al. [10] obtain a soil moisture retrieval RMS error around 0.06 m$^3$m$^{-3}$.

The lower limit on the temperature-constrained single-angle system discussed in Section II.D and Figure 1 can be seen in Figures 2 and 3, as both plots approach RMS errors of 0.013 m$^3$m$^{-3}$ with the lowest bias and noise respectively. A tighter constraint on the surface temperature would result in a lower asymptotic error as indicated in Figure 1.

2) Vegetation optical depth retrieval

Figure 4 shows the retrieval errors for the vegetation optical depth, $\tau$, for the same set of runs. Again, the six-angle system performs noticeably better than the single-angle system, and constraining the surface temperature further improves the retrieval. More surprising is the high degree of accuracy in the retrieval of this variable. For the six-angle retrieval cases, keeping the system noise below $\sigma = 0.5$ K allows optical depth to be retrieved with an RMSE below 0.011, and for the single-angle system with 2 K $T_s$ constraint below 0.023. This high retrieval accuracy means that in order to improve the model retrieval of soil moisture, supplementary vegetation information must exceed these levels, and we will examine this more closely in Section IV.

3) Surface temperature retrieval

Figure 5 shows the retrieval errors for the surface temperature from the six-angle data for the cases where $T_s$ is allowed a range of 50 K. $T_s$ is retrieved reasonably accurately at low noise levels, with an RMSE of 1.6 K for $\sigma=0.5$ K noise.
D. Conclusions

1. A six-angle system has a sensitivity to brightness temperature bias in retrieving soil moisture content which is nearly linear with bias up to about 5 K, giving a RMSE of 0.015 m$^3$m$^{-3}$ for a 5 K bias error if the soil temperature is unknown, though constraining the surface temperature and having a bias which pushes the observations outside this constraint increases this error.

2. The single-angle system is subject to a limiting accuracy in soil moisture content retrieval based on the extent of surface temperature constraint. If the temperature is known to within 2 K it is about 0.013 m$^3$m$^{-3}$, and the error then rises uniformly with bias up to 0.062 m$^3$m$^{-3}$ at 5 K.

3. With brightness temperature noise of 0.50 K, a single-angle sensor with 2 K surface temperature constraint has an RMSE error in soil moisture content retrieval of 0.020 m$^3$m$^{-3}$. A six-angle system with no temperature constraint has an RMSE of 0.012 m$^3$m$^{-3}$, and constraining the surface temperature to within 2 K allows the six-angle sensor to retrieve soil moisture content with an RMSE of 0.10 m$^3$m$^{-3}$.

4. The high accuracy of retrieval of vegetation optical depth is a useful result for vegetation study, however it also means that the potential to improve soil moisture content retrieval by supplying extra information about the vegetation is limited, and we study this further in Section IV. It should be noted that this result may not hold for a heterogeneous canopy.

5. The six-angle system can estimate the surface temperature to within 3 K for system noise below 1 K.

6. Comparison between the single- and multiple-angle systems should bear in mind that the single observation measurement error for a single-angle system will likely be lower than for a multiple-angle system, if only due to the simpler instrument design.
IV. THE EFFECTS OF ASSIMILATING INDEPENDENT MEASUREMENTS OF VEGETATION OPTICAL DEPTH AND SURFACE TEMPERATURE

A. Motive

Estimates can be made of the vegetation optical depth and soil surface temperature from either land-based or remotely-sensed data, often with temperature data assimilated into a weather forecasting model. Do these measurements improve the ability to retrieve soil moisture from the brightness temperature curves?

B. Method

We test the impact of four possible levels of independent information on the vegetation microwave optical depth; unknown, known to within 0.10, known to within 0.01 and known exactly. Four levels of independent surface temperature information were simulated by forcing it to exactly the input value, constraining it to within 2 K and 5 K of the input value, and constraining it to the 50 K range between 263 K and 313 K, to represent ignorance of the surface temperature. Inversions from the brightness temperature curves with systematic noise added to the individual points were carried out as in Section III.
Figure 6. Six-angle dual-polarisation soil moisture content (θ) retrieval error with brightness temperature noise level when the retrieval algorithm is given constraints on surface temperature ($T_s$) and vegetation optical depth ($\tau$). The $\tau$ unknown and $\tau$ known to within 0.1 results are indistinguishable in (a).
Figure 7. Single-angle dual-polarisation soil moisture content ($\theta$) retrieval error with brightness temperature noise level, when the retrieval algorithm is given constraints on surface temperature ($T_s$) and vegetation optical depth ($\tau$).
Figure 8. Soil moisture retrieval RMSE obtained by constraining surface temperature at different noise levels using (a) the single-angle system, (b) the six-angle system.
C. Results

1) Six-angle sensor

The effects of constraining surface temperature and vegetation optical depth for a six-angle system are shown in Figure 6 and 8(b). The performance improvement given by independent surface temperature and vegetation optical depth information is dependent on the noise level of the instrument. At a likely noise level of $\sigma = 0.50$ K, and with no knowledge of the surface conditions, the soil moisture content may be retrieved to better than $0.012 \text{ m}^3/\text{m}^3$ RMSE. Given an optimistic view of possible supplementary information, if a temperature estimate can be made to within 2 K, and vegetation optical depth to within 0.01, this would only improve the estimate to $0.009 \text{ m}^3/\text{m}^3$ RMSE. The improvement in retrieval ability is more marked for higher noise levels, halving the RMSE at 2 K noise. As suggested in Section III, there is confirmation here that the model retrieves vegetation optical depth so well that adding independent vegetation information is redundant, unless it is accurate to within about 0.01 of the actual value. Pardé et al. [10] similarly see only a marginal impact of constraining vegetation optical depth, between 0.07 and 0.06 $\text{m}^3/\text{m}^3$ for $\tau$ constraint with a standard deviation of 2.00 and 0.01 respectively, at their estimated measurement error level of 1-3 K. They also find that tightening temperature constraint at this higher instrument measurement error level reduces the soil moisture retrieval RMS error from around 0.09 $\text{m}^3/\text{m}^3$ for a constraint of standard deviation 10K to about 0.06 $\text{m}^3/\text{m}^3$ for 1 K, comparable to the improvement shown in Figure 8(b).

2) Single-angle sensor

The effects of constraining surface temperature and vegetation optical depth for a single-angle system are shown in Figure 7 and 8(a). Constraining the surface temperature exactly, effectively removing it as a variable in Figure 7(a), and adding an independent 0.01 accurate measurement of the vegetation optical depth has much the same effect as with the six-angle system, approximately halving the soil moisture content retrieval error. However, we can see in Figure 7(b) that if there is temperature uncertainty, the improvement in soil moisture retrieval is small compared to the limiting error imposed by this uncertainty, as indicated in Figure 1. It is worth noting that in cases where the optical depth is tightly constrained, the surface temperature range is similarly constrained at low instrumental noise levels, and if we allow the retrieval to fit the surface temperature, then for noise levels of 0.25 K and below, the soil moisture retrieval RMSE can be improved slightly for 5 K $T_s$ constraint. In the best case this brings the “$\tau$ known exactly” curve down to an RMSE of $0.021 \text{ m}^3/\text{m}^3$ at the lowest noise level, the “$\tau$ known to within 0.01” curve down to $0.025 \text{ m}^3/\text{m}^3$, and the “$\tau$ known to within 0.1” curve down to $0.034 \text{ m}^3/\text{m}^3$. 


D. Conclusions

1) Six-angle sensor

1. Better defining the vegetation optical depth is of marginal utility in improving soil moisture retrieval. In no case does the assimilation of even the most accurate vegetation optical depth information into the model as much as halve the vegetation-ignorant retrieved soil moisture error, and around $\sigma = 0.5$ K the improvement is negligible.

2. Figure 8 (b) gives an indication of the value of additional independent temperature information, seemingly of greater value, as we might expect from the temperature retrieval curve in Figure 5. The soil moisture retrieval error is reduced to 50%-80% of its temperature-ignorant level by constraining the surface temperature to within 2 K.

2) Single-angle sensor

1. Where surface temperature is constrained to 2 K or better, the effect of adding vegetation optical depth information is negligible, unless it is accurate to within 0.01.

2. Where the surface temperature is less constrained, if it is known to 5 K or worse, accurate vegetation optical depth information can be of use. Figure 7 shows that vegetation optical depth needs to be measured more accurately than to within 0.10 to be of use, and Figure 4 indicates that to improve on the model estimation of $\tau$, and therefore improve the model accuracy, $\tau$ needs to be independently estimated to 0.02 or better to offer any value.
V. THE EFFECT OF ERRORS IN VEGETATION SINGLE-SCATTERING ALBEDO

A. Motive

The microwave single-scattering albedo of vegetation $\omega$ is a function of plant geometry, and so varies according to plant species. There are limited experimental data on this parameter, but for selected crops it varies from 0.04 for grasses and mixed farming areas, to 0.08 for mixed farming and woodland areas to 0.12 for trees [2,3,8], and for natural vegetation in semi-arid regions the value is typically around 0.05 [21]. However, it is often assumed zero to simplify the model [7,8]. In observations encompassing areas tens of kilometres in diameter, vegetation types with a range of albedo will frequently be evident. It is therefore important to know how sensitive retrievals will be to uncertainty and generalisation in albedo. In the work we describe here, we assume that a whole pixel has the same value of single-scattering albedo.

B. Method

Ideal brightness temperature curves were created using a range of values of $\omega$ between 0.00 and 0.12 at 0.001 steps, for each of the six $\theta,\tau$ scenarios described in Section II. Multiple-angle and single-angle retrievals were performed for the assumptions $\omega = 0.00, 0.06$ and 0.10. Soil temperature was constrained to within 2 K of the forward model input value of 293 K.

C. Results

The errors in retrieving volumetric soil moisture using each of the retrieval assumptions for $\omega$ are shown in Figures 9 and 10, and summaries of mean errors and worst cases are in Table 1. The $\theta,\tau$ scenario giving rise to the worst overall $\theta$ error is not always the same for all input values of $\omega$, so the worst case lines in Figures 9 and 10 are derived for each input value of $\omega$. Using the single-angle retrieval, and assuming $\omega = 0.0$ and 0.1, as in Figures 9(a) and (c), the worst scenario is consistently $\theta = 0.4, \tau = 0.6$; in all other cases the worst scenario is either this or $\theta = 0.1, \tau = 0.6$ depending on the input value of $\omega$. As expected, the worst case scenarios were always those with the highest vegetation optical depth. In Figure 10, the flat regions of soil moisture error of 0.10 m$^3$m$^{-3}$ indicate where constraining the soil moisture to the physically-plausible range between 0.0 and 0.5 m$^3$m$^{-3}$ has suppressed an unrealistic higher error.

<table>
<thead>
<tr>
<th>Assumed $\omega$</th>
<th>Retrieval errors for soil moisture content over six $\theta,\tau$ scenarios (m$^3$m$^{-3}$)</th>
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<tr>
<td></td>
<td>Multiple-angle system</td>
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<tr>
<td></td>
<td>Mean error</td>
</tr>
<tr>
<td>0.00</td>
<td>0.010</td>
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<tr>
<td>0.06</td>
<td>0.010</td>
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<td>0.10</td>
<td>0.020</td>
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Table 1. Errors in retrieval of soil moisture content, for sites with the single-scattering albedo $\omega$ between 0.00 and 0.12, with the retrieval algorithm making assumptions for the value of $\omega$, over the six $\theta,\tau$ scenarios.
D. Conclusions

The single-angle system clearly needs information on the vegetation single-scattering albedo. It is likely that some additional information could be acquired, in the form of a multispectral acquisition and classification, or other land cover information, to determine the target vegetation type and consequently an estimate of the single-scattering albedo could be made for any region studied by a single-angle microwave radiometer. Whilst this approach would reduce the worst effects of albedo errors, Figure 9(b), the plot with lowest soil overall moisture retrieval errors by assuming $\omega = 0.06$, shows that even an error of 0.01 in albedo estimation yields an mean error of 0.019 m$^3$ m$^{-3}$, and 0.010 m$^3$ m$^{-3}$ for the worst $\theta, \tau$ scenario, which is in this case the soil moisture 0.10 m$^3$ m$^{-3}$, vegetation optical depth 0.60 scenario. If such albedo-induced errors in soil moisture retrieval are to be avoided, albedo must be estimated with an accuracy better than 0.01.

The six-angle system shows a lower sensitivity to variation in single-scattering albedo, and given the increased information in the shape that multiple-angle retrieval can acquire, there may be adequate information in the multiple angle data to retrieve single-scattering albedo from the data simultaneously with soil moisture. In Figure 11 we show the results of an analysis where six-angle input brightness temperature curves are generated with a range of $\omega$ between 0.00 and 0.12, and we attempt to retrieve it in addition to the usual three variables, essentially a four variable ($\theta, \tau, T_s, \omega$) retrieval. Compared to the three variable retrieval, it performs only slightly worse at low noise levels, certainly better than assuming a fixed value of $\omega$. Pardé et al. [10] similarly show that using a retrieval which also fits $\omega$, does not cause soil moisture retrieval error to vary significantly from their mean of 0.06 m$^3$ m$^{-3}$. 
Figure 9. Mean and maximum magnitude of retrieval error of soil moisture content from single-angle data generated with a range of single-scattering albedo $\omega$ values, where surface temperature is known to within 2 K. Retrievals assume (a) $\omega = 0.00$, (b) $\omega = 0.06$, (c) $\omega = 0.10$. 
Figure 10. Mean and maximum magnitude of retrieval error of soil moisture content from six-angle data devised with a range of single-scattering albedo $\omega$ values, where surface temperature is known to within 2 K. Retrievals assume (a) $\omega = 0.00$, (b) $\omega = 0.06$, (c) $\omega = 0.10$. 
Figure 11. Soil moisture retrieval error from a four variable retrieval of $\theta, \tau, T_s, \omega$ from six angle data with a range of input $\omega$, where surface temperature is known to within 2 K. The retrieval curve from the three-variable retrieval where $\omega$ is known in Figure 3(a) is also shown (dashed) for comparison.
VI. THE EFFECT OF SOIL ROUGHNESS

A. Motive

Soil roughness is rarely known accurately unless a ground survey has been carried out, however it has an effect on soil emissivity. What is the effect of assuming that soil roughness is negligible, or of having inadequate information?

B. Method

To test the effect of soil roughness on the retrieval of soil moisture, the soil reflectivity $R$ was modified using the expression for the effect of rough soil proposed by Choudhury et al. [9]:

$$ R = R_0 e^{-h \cos^2 \alpha} $$

(2)

where $R_0$ is the reflectivity of flat soil, $\alpha$ is the look angle, $h$ is the roughness factor given by

$$ h = 4\sigma_s^2 \left( \frac{2\pi}{\lambda} \right)^2 $$

(3)

where $\sigma_s$ is the standard deviation of the soil surface elevation and $\lambda$ is the microwave wavelength. Values for $h$ range from 0.0 for flat to 0.3 at maximum, and the average is given as 0.1 [9]. For a 21 cm radiometer, the maximum 0.3 indicates a surface with $\sigma_s = 9$ mm, which is slightly lower than some recently cultivated sites. We found [22] that a field recently harrowed with a rotary cultivator gave a surface with a peak-trough range of 3 cm, and a standard deviation of 9.8 mm over a 1 m distance, and a recently-ploughed site with a peak-trough range of about 5 cm had an elevation standard deviation of 15.7 mm over 1 m. However, since these sites were cultivated only a few days before measurement, and we would expect them to flatten quickly with weather conditions, the maximum of 0.3 was considered appropriate for this study.

Brightness temperature curves were generated using the six $\theta, \tau$ scenarios described in Section II, and $h$ between 0.0 and 0.3. These were then inverted using the assumptions $h = 0.0$ and $h = 0.1$. Inversions assumed knowledge of the soil temperature to within 2 K, and were attempted with the multiple-angle and single-angle dual polarisation data.
Figure 12. The range of soil moisture content retrieval error from a single-angle sensor caused by error in the assumption of soil roughness $h$, whilst constraining surface temperature to within 2 K of the input value. The lines represent minimum, mean and maximum errors over the $\theta, \tau$ scenarios. The retrievals assume (a) $h=0.0$, (b) $h=0.1$. 
Figure 13. The range of soil moisture content retrieval error from a multiple-angle sensor caused by error in the assumption of soil roughness $h$, whilst constraining surface temperature to within 2 K of the input value. The lines represent minimum, mean and maximum errors over the $\theta, \tau$ scenarios. The retrievals assume (a) $h=0.0$, (b) $h=0.1$. 
C. Results

<table>
<thead>
<tr>
<th>Assumed $h$</th>
<th>Retrieval errors for soil moisture content over all $\theta,\tau,h$ scenarios (m$^3$m$^{-3}$)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Multiple-angle system</td>
<td>Single-angle system</td>
</tr>
<tr>
<td></td>
<td>Mean error</td>
<td>Maximum error</td>
</tr>
<tr>
<td>0.00</td>
<td>0.054</td>
<td>0.137</td>
</tr>
<tr>
<td>0.10</td>
<td>0.039</td>
<td>0.111</td>
</tr>
</tbody>
</table>

Table 2. Errors in retrieval of soil moisture content, for sites with the roughness $h$ between 0.00 and 0.30, with the retrieval algorithm making assumptions for the value of $h$, over the six $\theta,\tau$ scenarios

Figures 12 and 13 show the retrieval error caused by an erroneous assumption of the value of roughness, and Table 2 shows the mean and maximum errors over the range of input $h$. Notably the retrievals from the multiple-angle data are affected far more than from the single-angle data. These errors are far higher than the error induced by system noise, and so will dominate the overall error budget, if these wrong assumptions are made. This somewhat counter-intuitive result, that the multiple angle sensor data leads to a less accurate retrieval than the single-angle approach when the wrong roughness is selected, is explained by the look-angle dependence of the roughness correction. Whilst a model fitting to the two single angle observations at H and V polarisations can do so whilst only accounting for the displacement caused by the roughness error, fitting the six point H and V curves through the data with the wrong roughness assumption makes the best fit alter the retrieved temperature and soil moisture content to match the shape. Significant errors in retrieved soil moisture result from this. Whilst this result indicates that a multiple-angle sensor is less able to cope with the angle-dependent effects of an error in assumed roughness, the substantial alteration in the curve shape caused by soil roughness also means that a multi-angle sensor will be able to retrieve roughness independently. Figure 14 shows the soil moisture retrieval curve for a set of scenarios having a range of soil roughnesses between 0.0 and 0.3, with a surface temperature known to within 2 K. Extracting roughness as a fourth variable adds around 0.01 m$^3$m$^{-3}$ error compared to the three-variable retrieval of Figure 3. Pardé at al. [10] also show that the soil moisture retrieval error induced by retrieving soil roughness increases by about 0.01 m$^3$m$^{-3}$, or slightly more depending on the initial $h$ estimate in the iterative retrieval.
Figure 14. RMS error in soil moisture retrieval from six-angle data, with input soil roughness $h$ between 0.00 and 0.30, and the retrieval fitting $\theta, \tau, T_s, h$. The surface temperature is assumed known to within 2 K. The $\theta, \tau, T_s$ retrieval curve from Figure 3 is also shown (dashed) for comparison.

D. Conclusions

1. If the soil roughness is unknown, for a single-angle sensor the optimal assumption that the roughness is 0.1 gives rise to a mean error of 0.014 m$^3$ m$^{-3}$ in the soil moisture retrieval over a range of roughness conditions, with a worst scenario error of 0.067 m$^3$ m$^{-3}$ (Table 2).
2. Because of the look-angle-dependent effect of soil roughness, assuming an erroneous value of soil roughness has a more marked effect with a multiple-angle sensor, giving rise to a mean error of 0.039 m$^3$ m$^{-3}$ if roughness is assumed to be 0.1, or 0.054 m$^3$ m$^{-3}$ if it is assumed to be 0.0, over the same range of scenarios (Figure 12(b)).
3. Because of the angle-dependent influence of soil roughness on the brightness temperature curve, the multiple-angle retrieval can retrieve soil roughness with a cost to soil moisture retrieval accuracy of about 0.01 m$^3$ m$^{-3}$, so it should be unnecessary to assume an erroneous value of roughness for a homogeneous pixel.
4. The strong influence of soil roughness on the shape of the brightness temperature curve may, however, have an effect for heterogeneous pixels, since a single roughness value will rarely be valid for more than a few square kilometres.
VII. THE COMBINED EFFECT OF
SINGLE-SCATTERING ALBEDO AND SOIL ROUGHNESS

A. Motive

Earlier sections tested the ability of analyses to retrieve soil roughness $h$ and the microwave single-scattering albedo, $\omega$, independently from multiple-angle sensor data; can simultaneous uncertainty in both these parameters be accommodated by the single- and multiple-angle sensors, and at what cost to the soil moisture retrieval error?

B. Method

For each of the six $\theta, \tau$ scenarios and for each noise level, 100 brightness temperature curves were generated, with values of $\omega$ generated randomly in a flat distribution with values between 0.00 and 0.12, and $h$ generated randomly in a flat distribution between 0.00 and 0.30. Each curve was subjected to the usual levels of noise, and retrievals attempted as described in earlier sections, with the surface temperature constrained to within 2 K of the input value. The multiple-angle system attempts to account for the variability by retrieving the roughness and single-scattering albedo from the data, whereas the retrieval from the single-angle data uses the best approximations determined in Sections V and VI, $\omega = 0.06$ and $h = 0.1$.

C. Results

The RMS errors in the retrieval of soil moisture for the single-angle and six-angle systems are shown in Figure 15 and 16, along with the retrieval curves for the cases where $h$ and $\omega$ are constant, and where they are independently allowed to vary. Whilst the compounded consequences of retrieving both variables creates an increased uncertainty in the soil moisture retrieval from the six-angle sensor, this is at an acceptable level for low noise values, with an RMSE of 0.028 m$^3$m$^{-3}$ for a system noise $\sigma = 0.50$ K.

For the single-angle sensor, compounding the errors serves to emphasise the dominance in the error budget of the uncertainty in the single-scattering albedo $\omega$, and given this variation in $\omega$, the soil moisture RMS error is between 0.07 and 0.08 m$^3$m$^{-3}$ at all noise levels. The RMS retrieval error for the worst scenario $\theta$=0.4 m$^3$m$^{-3}$, $\tau$=0.6, is not shown, but is constant across all noise levels at about 0.18 m$^3$m$^{-3}$.

D. Conclusions

Broad uncertainty in both the single-scattering albedo and surface roughness can be accommodated by a multiple-angle system. However, for the single-angle system, constraint of the single-scattering albedo is clearly essential to bring soil moisture retrieval error to a similar level.
Figure 15. The effects of unknown soil roughness $h$ and vegetation single-scattering albedo $\omega$ on the retrieval of soil moisture content from multiple-angle observations, showing the cases (i) where $\omega$ and $h$ are constant and known, (ii) where only $\omega$ varies and is fitted by the retrieval, (iii) where only $h$ varies and is fitted by the retrieval, and (iv) where both $\omega$ and $h$ vary and are fitted.
Figure 16. The effects of unknown soil roughness $h$ and vegetation single-scattering albedo $\omega$ on the retrieval of soil moisture content from single-angle observations, showing the cases (i) where $\omega$ and $h$ are constant and known, (ii) where only $\omega$ varies and the optimal assumption of $\omega = 0.06$ is used by the retrieval, (iii) where only $h$ varies and the optimal assumption of $h = 0.1$ is used, and (iv) where both $\omega$ and $h$ vary and are assumed as above.
VIII. CONCLUSIONS

A. Important factors

The effects of the following independent sources of error in the retrieval of near-surface soil moisture from microwave emission were investigated.

1) Surface temperature information

For a multiple-angle sensor, information on the surface temperature serves to improve the estimation of the soil moisture. Going from giving the retrieval a broad 50 K estimation range to a 2 K constraint approximately halves the six-angle system soil moisture retrieval error (Figure 3). The single-angle system is dependent on temperature information to provide a soil moisture estimation, a 2 K uncertainty in surface temperature alone yielding an RMS error in moisture retrieval of 0.13 m$^3$m$^{-3}$, rising to 0.042 m$^3$m$^{-3}$ for wet soil and deep vegetation. (Figure 1).

2) Brightness temperature measurement bias

The additional error yielded by a bias in brightness temperature measurement is relatively minor and largely linear, though the presence of bias needs to be accounted for in setting the surface temperature constraints. A 5 K bias would yield a 0.015 m$^3$m$^{-3}$ RMS soil moisture error for the six-angle system even if the surface temperature is known to only 50 K. The single-angle system constrained to 2 K yields a 0.062 m$^3$m$^{-3}$ RMS error for a 5 K bias.

3) Brightness temperature measurement noise

Normally-distributed noise with a standard deviation of 0.5 K causes RMS errors in soil moisture retrieval of 0.010 m$^3$m$^{-3}$ for the six-angle system with 2 K surface temperature constraint, 0.012 m$^3$m$^{-3}$ for the same system with the temperature only known within a 50 K range, and 0.020 m$^3$m$^{-3}$ for the single-angle system with 2 K surface temperature constraint. The worst case scenarios are usually where soil moisture and vegetation cover are high, and give rise to RMS errors of 0.017 m$^3$m$^{-3}$ for the six-angle and 0.039 m$^3$m$^{-3}$ for the single-angle cases at 0.5 K instrument noise (Figure 3).

4) Vegetation cover information

a) At brightness temperature noise level below a standard deviation of 0.50 K, adding vegetation optical depth information does not significantly improve the retrieval accuracy for soil moisture content, except for the single-angle system where very accurate information can compensate for lack of temperature information.

b) At all brightness temperature noise levels up to at least 2 K, both systems provide enough information to extract vegetation optical depth to better than 0.10 of its absolute value, so adding this level of information does not improve the soil moisture content accuracy over having no independent vegetation information.
c) Knowing the vegetation optical depth to within 0.01 of its absolute value does not improve the soil moisture content retrieval error at even the 2 K noise level to better than half of the vegetation-ignorant level.

5) Single-scattering albedo

General assumptions of microwave single-scattering albedo give rise to errors in soil moisture content retrieval up to 0.079 m$^3$m$^{-3}$ for a multiple-angle system using the optimal estimate of albedo=0.0, and up to 0.250 m$^3$m$^{-3}$ for a single-angle system using the optimal estimate of albedo=0.06. These can be reduced to acceptable levels by retrieving the albedo from six-angle data, but for the single-angle system, unless the albedo can be independently determined to better than 0.01 for the target site, albedo uncertainty will cause soil moisture retrieval mean errors of over 0.045 m$^3$m$^{-3}$ in cases of dense vegetation cover.

6) Soil roughness

a) Soil roughness has a strong angle-dependent effect on the brightness temperature. If unknown, the best assumption for a single-angle sensor is that the roughness is 0.1, and this gives rise to an mean error in the soil moisture content retrieval of 0.014 m$^3$m$^{-3}$ over a range of roughness conditions, with the worst scenario of a high roughness giving rise to an RMS error of 0.067 m$^3$m$^{-3}$.

b) The effect of a soil roughness error on the brightness temperature curve shape means that this approach works less well with a six-angle system, however given an unknown roughness, the retrieval is able to estimate soil roughness from the observations, yielding a soil moisture retrieval error about 0.01 m$^3$m$^{-3}$ higher than retrieving from a known roughness, if the surface temperature is known to within 2 K.

B. Overall conclusions – what independent information is necessary?

An absolute error of 0.04 m$^3$m$^{-3}$ (4%) is often cited as a target for the accuracy of retrieval of soil moisture content [1,20]. Of the observations that might be made to improve retrievals, surface temperature has clear value, particularly for a single-angle system, as indicated in Figure 1. Whilst it might be thought that the measurement of the vegetation optical depth would be a powerful tool in accounting for its effect and observing the soil beneath, retrievals from the $\tau - \omega$ model are surprisingly accurate in the estimation of the vegetation optical depth with the result that independent measurements would have to be implausibly accurate to be of use. However, the accurate estimation of the vegetation single-scattering albedo is an important factor. Whilst a multiple-angle sensor can retrieve this from observations, a heterogeneous area may have a range of vegetation types, and the use of an area average may well cause substantial error. For a single-angle sensor, with insufficient observations to be able to retrieve albedo, even the optimal general assumption of albedo=0.06 gives rise to an error of 0.040 m$^3$m$^{-3}$ in soil moisture retrieval over a range of vegetation/soil conditions, and 0.25 m$^3$m$^{-3}$ for the worst case. Clearly it is necessary to independently measure or estimate the albedo to use a single-angle sensor, to a better accuracy than 0.01 to keep the soil moisture RMS error below worst scenario error below the target of 0.04 m$^3$m$^{-3}$.
Soil roughness is a very difficult parameter to measure on the spatial scale and to the precision required for a satellite instrument (though not impossible [22]), so it must either be assumed, or retrieved from the measurements. For the multiple-angle system the angle-dependent effect of surface roughness makes it possible to retrieve it with only a minor degradation in soil moisture retrieval of about $0.01 \text{ m}^3\text{m}^{-3}$. The single-angle system requires an assumption of surface roughness, and assuming an optimal value of 0.1 gives a tolerable RMS soil moisture retrieval error of $0.014 \text{ m}^3\text{m}^{-3}$ over a range of vegetation and soil moisture conditions, though for the roughest surface it yields an soil moisture retrieval error of $0.067 \text{ m}^3\text{m}^{-3}$, which exceeds the target accuracy. It is difficult to see how this might be improved.

It can be seen from Figure 15 that if the brightness temperature measurement noise can be kept below a standard deviation of 0.5 K, without independent information on vegetation cover and soil roughness a multiple-angle system can retrieve soil moisture with an RMS error of $0.028 \text{ m}^3\text{m}^{-3}$, rising to $0.048 \text{ m}^3\text{m}^{-3}$ for the worst scenario where soil moisture is $0.4 \text{ m}^3\text{m}^{-3}$ and vegetation optical depth is 0.6.

A single-angle system is less able to cope with the problem of single-scattering albedo uncertainty. As indicated in Figure 16, retrieval using the best assumption yields RMSE errors in soil moisture between 0.07 and 0.08 $\text{ m}^3\text{m}^{-3}$ over a range of vegetation and soil roughness and moisture conditions. The most probable means of reducing this error is with an independent estimate of the single-scattering albedo.

Use of space-borne passive microwave radiometers will therefore require the simultaneous assimilation of this information, particularly to retrieve the surface temperature. Further work is required to examine the effects of the uncertainty in knowledge of the relationship between soil moisture and the soil dielectric constant which underpins the $\tau-\omega$ model, the temperature gradient between the canopy and the soil and within the canopy, sub-pixel heterogeneity [23], and how to retrieve profile moisture successfully from a time series of surface observations. This work also assumes that the $\tau-\omega$ model captures all the variability of the relationship, and this needs further testing. In particular, the parameterization of vegetation single-scattering albedo as a simple isotropic scalar increasingly seems an oversimplification.

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