Research Article

An Air-to-Soil Transition Model for Discrete Scattering-Emission Modelling at L-Band

Hong Zhao,¹ Yijian Zeng,¹ Jun Wen,² Xin Wang,³ Zuoliang Wang,³ Xianhong Meng,³ and Zhongbo Su^{1,4}

¹Department of Water Resources, Faculty of Geo-Information Science and Earth Observation (ITC), University of Twente, 7514 AE Enschede, Netherlands

²College of Atmospheric Sciences, Plateau Atmosphere and Environment Key Laboratory of Sichuan Province, Chengdu University of Information Technology, Chengdu 610225, China

³The Key Laboratory of Land Surface Process and Climate Change in Cold and Arid Regions, Northwest Institute of Eco-Environment and Resources, Chinese Academy of Sciences, Lanzhou 730000, China

⁴The Key Laboratory of Subsurface Hydrology and Ecological Effect in Arid Region of Ministry of Education, School of Water and Environment, Chang'an University, Xi'an 710054, China

Correspondence should be addressed to Zhongbo Su; z.su@utwente.nl

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Topsoil structures and inhomogeneous distribution of moisture in the soil volume will induce dielectric discontinuities from air to bulk soil, which in turn may induce multiple and volume scattering and affect the microwave surface emission. *In situ* ELBARA-III L-band radiometer observations of brightness temperature T_B^p ($p = H$ or V polarization) at the Maqu site on the Eastern Tibetan Plateau are exploited to understand the effect of surface roughness on coherent and incoherent emission processes. Assisted with *in situ* soil moisture (SM) and temperature profile measurements, this study develops an air-to-soil transition (ATS) model that incorporates the dielectric roughness (i.e., resulted from fine-scale topsoil structures and the soil volume) characterized by SM and geometric roughness effects, and demonstrates the necessity of the ATS model for modelling L-band T_B^p . The Wilheit (1978) coherent and Lv et al. (2014) incoherent models are compared for determining the dielectric constant of bulk soil in the ATS zone and for calculating soil effective temperature T_{eff} . The Tor Vergata discrete scattering model (TVG) integrated with the advanced integral equation model (AIEM) is used as the baseline model configuration for simulating L-band T_B^p . Whereafter, the ATS model is integrated with the foregoing model for assessing its performance. Results show the ATS-based models reduce the underestimation of T_B^p (≈ 20 –50 K) by the baseline simulations. Being dynamic in nature, the proposed dielectric roughness parameterization in the ATS model significantly improves the ability in interpreting T_B^p dynamics, which is important for improving SM retrieval at the global scale.

1. Introduction

Soil moisture (hereafter SM) is of significant importance for weather and climate predictions by controlling the partition of heat and water fluxes on the land-atmosphere interface [1–3]. Passive L-band microwave remote sensing has become the most promising technique for measuring near-surface SM by properly quantifying contributions from vegetation and the ground surface [4–6]. Independent L-band brightness temperature observations and radiative transfer models (e.g., the Community Microwave Emission Model [7]), if

integrated with land surface models in a data assimilation framework, can be used for estimating soil physical properties [8–12], which are crucially important for understanding SM dynamics [13, 14].

The efforts related to microwave remote sensing of the land surface may be traced back to the work of Peake [15], which demonstrates the complementary relationship between emission and scattering and shows such with data from Straiton [16]. This may be called the scattering-emission radiative transfer approach. The more recent works are those of Fung [17] and Chen [18] on an advanced integral

equation model (AIEM) for a rough bare soil surface, and Ferrazzoli [19, 20] on a discrete scattering model (Tor Vergata model) for a vegetated surface. These approaches consider a uniform soil moisture and soil temperature (SMST) profile and use a surface value of the dielectric constant with roughness parameters for the calculation of the surface reflectivity, by integrating the bistatic scattering coefficients over the half-space above the surface. The other line of work is that of Njoku and Kong [21] and Wilheit [22], which uses the stratified coherent radiative transfer approaches to calculate the microwave emission of a medium with the nonuniform temperature profile to account for the nonuniform SMST profile for natural soil (e.g., coherent model). That is to say, the SMST profile is used to determine the smooth surface reflectivity and soil effective temperature T_{eff} . Due to its simpler formulation, the Wilheit [22] model is widely used and followed by the simplified semiempirical models [5, 23–26] for applications in airborne and satellite microwave remote sensing. Generally, these models use the Fresnel equations to obtain the surface reflectivity with roughness corrections, and they have continued into the zeroth-order radiative transfer model used for the Soil Moisture and Ocean Salinity (SMOS) [4] and the Soil Moisture Active Passive (SMAP) [6] SM retrievals [27, 28]. On the other hand, these models do not retain the coherent character as in the Wilheit model, mainly due to the simplified T_{eff} parameterization scheme [23, 29]. To investigate the impact of T_{eff} on microwave radiometry, Lv [29] used an analytical formulation to physically explain various T_{eff} schemes, all of which having their roots in the scheme of Choudhury [23], and proposed the Lv's T_{eff} scheme (e.g., incoherent model). In this study, we will investigate how Wilheit [22] coherent and Lv [29] incoherent models affect T_{eff} and associated brightness temperature (T_B^p , with $p = \text{H or V polarization}$) simulations.

Another research focus of microwave radiometry is the surface roughness effect. The geometric roughness resulting from the variation of surface heights influences surface scattering and is modelled by the physically based AIEM. However, AIEM assumes isotropic roughness properties for a homogenous dielectric half-space and does not account for the dielectric effects due to heterogeneities in the soil characteristics (e.g., composition, moisture content, and bulk density). On the other hand, the fact is that lateral structures (e.g., the unfilled surface composed of organic matter and clods) significantly smaller than the observation wavelength (e.g., $\lambda_0 = 21$ cm, at L-band) influence the manner of wave propagation and induce the impedance mismatch of the rough surface between air and soil. The aforementioned heterogeneities produce dielectric roughness (namely, the large dielectric discontinuities at the soil surface and within the soil volume) and may in turn induce the volume and multiple scattering processes, which will affect the microwave surface emission. The model parameters used in the zeroth-order radiative transfer models may implicitly account for both the geometric and dielectric roughness effects. However, they are site-specific empirical ones, obtained by using the best-fit approaches based on limited field observations and model simulation results. An air-to-soil transition (hereafter ATS)

model [30]—an intermediate modelling approach between physical and semiempirical approaches—is suggested to describe the roughness effects from topsoil structures on the L-band radiation as an impedance matching between the dielectric constants of air and bulk soil. In the original ATS model [31, 32], the structured topsoil is taken as a transition layer with a geometric thickness h , considering that the volume fraction of soil materials increases with depth in the ATS zone. The h is related with s (the height standard deviation with Gaussian distribution, centered around lateral separation) by $s(h) = 0.2489h$ [30, 31]. As the geometric surface roughness (i.e., s) does not experience the pronounced change, h is a fixed peak-to-trough transition layer thickness induced by topographical effects and independent of soil moisture. However, regarding h to be constant is questionable due to the fact that the dielectric properties of the topsoil and the soil volume may be modulated by inhomogeneity related to moisture. This study will develop an enhanced ATS model with a new h parameterization to investigate a soil moisture-dependent dielectric roughness at the topsoil structures and the soil volume on the L-band radiation. The Maqu site (33.91°N, 102.16°E) on the eastern Tibetan Plateau meadows providing comprehensive field observations [33–36] will be taken as the study area to validate the model.

With the ATS dielectric layer obtained, an “equivalent” homogenous dielectric entity that acts as the ground scattering-emission medium can be assumed with a given dielectric constant and surface geometric roughness. The AIEM [18], which uses a more complete expression of the single scattering terms to keep the acceptable energy conservation for calculating bistatic scattering and emission, will be employed for simulating soil surface scattering. As the research object is a natural grassland, the Tor Vergata model simulating vegetation scattering is coupled with AIEM (TVG+AIEM) for the overall vegetation-soil scattering-emission modelling. The coupled model including the ATS model (TVG+AIEM+ATS) is further used to investigate the impacts on h estimations and T_B^p simulations by adapting Wilheit's or Lv's stratified model, or using SM at the single-layer depth of 2.5 cm (*in situ* measurements) given its topmost role in surface emission [22, 37]. Finally, the applicability and uncertainty of the enhanced ATS model on L-band radiometry modelling are discussed.

This paper is organized as follows. The *in situ* SMST profiles and the ELBARA-III observed T_B^p on Maqu site are described in the first part of Section 2. In the second part of Section 2, a brief description of the TVG model is introduced. The improved ATS model is described together with Wilheit [22] and Lv [29] models. The configurations of different simulation experiments are also explained. Results about the performance of the enhanced ATS model and seasonal T_B^p simulations are shown in Section 3, as well as how coherent and incoherent models and SM at 2.5 cm influence T_B^p simulations. The applicability and uncertainty of ATS models in T_B^p simulations are discussed in Section 4, as well as the impacts of geometric roughness on the performance of the ATS model. The potential advantage of the ATS model that can be used for improving satellite-based SM retrievals is

FIGURE 1: MODIS/Terra+Aqua Leaf Area Index (500 m resolution) original data with filtered data using the HANTS algorithm.

discussed in Section 4. Conclusions and outlooks are drawn in Section 5.

2. Materials and Methods

2.1. In Situ Measurements at Maqu Site. The Tibetan Plateau observatory for soil moisture and soil temperature (Tibet-Obs) was built and maintained since 2006 onwards [14, 33, 34, 38] to provide comprehensive observations for land surface modelling community and for validating SM retrievals from satellite microwave remote sensing and reanalysis SM datasets [35, 39–41]. In 2016, an *in situ* Dicke-type radiometer ELBARA-III at L-band (1.4 GHz) has been mounted at the Maqu site (33.91°N, 102.16°E) of the Tibet-Obs, providing T_B^p observations at different incidence angles (between 40° and 70° in steps of 5°) for investigating L-band microwave radiometry for eastern Tibetan alpine meadows [42–45]. Detailed descriptions of ELBARA-III radiometry setup can be found in [36], as well as a schematic overview (see Figure 1 in [36]).

In this study, a dense profile of SMST (at 2.5, 5, 10, 20, 35, 60, and 80 cm below the soil surface) collected from the SMST_LC pit near the ELBARA-III (see Figure 1 in [36]) in the first period between 08/08/2016 and 30/11/2016 is used. Detailed descriptions of SMST measurements can be found in [36]. The analyses of this study will focus on the *in situ* observed data and the T_B^p simulations in the late-monsoon (August to September) and post-monsoon (October to November) periods in 2016. To keep consistent with the SMAP incidence angle, the T_B^p data analysis is confined to the angle of 40°. Additionally, Leaf Area Index (LAI) is an important input parameter for vegetation modelling in the Tor Vergata model, determining the number of grass as discrete dielectric scatters. Time series of LAI extracted from MCD15A2H-MODIS/Terra+Aqua Leaf Area Index (500 m resolution) (<https://lpdaac.usgs.gov/products/mcd15a2hv006/>) is processed with the harmonic analysis of the time series (HANTS) algorithm [46] to remove the cloud contamination. The results in Figure 1 show a reliable interpreted LAI. Furthermore, meteorological observation data in the Maqu site [36] are used to support the analysis. The data mainly involve precipitation intensity, air temperature, and surface albedo with ground

surface temperature deriving from the *in situ* four components radiation measurement (i.e., up- and down-welling shortwave and longwave radiations).

2.2. Methods

2.2.1. Tor Vergata Discrete Scattering-Emission Model. The TVG [19, 20] assumes the soil as a homogeneous infinite half-space with a rough interface, and the overlying vegetation is represented as an ensemble of discrete dielectric scatters. The scattering modelled by TVG involves three components: vegetation volume scattering, soil surface scattering, and the component resulted from vegetation-surface interactions. The TVG model has been investigated over the Maqu area [42, 47–49]. As in [47], the grass leaves at the Maqu site are described by dielectric thin discs with a random distribution of orientation. The bistatic scattering and extinction (absorption plus scattering) cross sections of the dielectric discs are computed by applying the Rayleigh-Gans approximation at L-band [50] (① in Figure 2), in which Mätzler [51] model is used for calculating vegetation dielectric constant. Subsequently, the contributions from all discs (scatters) are integrated using the matrix doubling algorithm (② in Figure 2), thereby the scattering and transmission matrices are computed for the whole vegetation (③ in Figure 2). Vegetation parameters such as the disc radius, disc thickness, numbers of discs (i.e., the ratio of LAI to the area of the disc), and plant moisture content used in this study are calibrated ones from [47, 48], and they are found insensitive to the emissivity for L-band [49].

The soil surface scattering is computed by adopting AIEM, in which the soil dielectric constant and surface roughness parameters (i.e., the standard deviation of surface heights s , the correlation length of surface height L , and the assumed exponential autocorrelation function for natural surface) are needed as inputs. In the previous version of TVG adopted for the Maqu site, the grassland litter component is included [47]. The litter layer, however, is not implemented in this study. One reason is that the grassland on the Tibetan Plateau is grazed by sheep and yaks [33] and litter in most areas is decomposed (see two snapshots in supplementary materials). On the other hand, for nature land surface, there does exist a soft transition zone of the dielectric constant from air to bulk soil than in a case of an abrupt surface,

FIGURE 2: Flowchart illustrating the procedure for the forward T_B^p simulations by the coupled TVG and AIEM model including the ATS model. ①-⑩ represent the workflow. The square rectangle represents inputs and parameters, and the rounded rectangle in orange refers to models and algorithms. The outermost dash blue box encloses elements in the TVG+AIEM+ATS model. Inside three dash boxes in blue enclose elements in modelling scattering of vegetation, soil parts, and their combination, respectively. The black dashed box inside the upper blue dash box is with inputs used for computing scattering and transmission matrices. The black dashed box inside the lower blue dash box is with inputs used for calculating the dielectric constant, and the dashed arrow points to inputs used for ATS-based simulations (see Section 2.2.4). Detailed descriptions of the ATS model are seen in Section 2.2.2, as well as Wilheit coherent and Lv incoherent models in Section 2.2.3.

as for example at calm sea [30]. Therefore, our focus in this paper is to improve air-to-soil dielectric transition (ATS) modelling. Ignoring the litter part in the modelling system is for simplicity but also reduces numerous input parameters that may degrade the performance of the model.

In this study, the enhanced ATS model (see Section 2.2.2) will be used to obtain the effective dielectric constant (④ in Figure 2). Two components: incoherent bistatic scattering coefficients (computed by the AIEM, ⑤ in Figure 2) and coherent specular reflection coefficients (computed by the Fresnel equations corrected by roughness factor, ⑤ in Figure 2) are computed for the composite air-to-soil medium scattering. The same matrix doubling algorithm is then used to combine the calculated vegetation contribution with that of the air-soil medium (⑥ in Figure 2). Subsequently, the emissivity $e_p(\theta_i)$ on p polarization (i.e., H or V) at an incidence angle θ_i is obtained by applying energy conservation law with integrating the bistatic scattering coefficients over the half-space above the surface (⑦-⑧ in Figure 2). Due to the low vegetation emission at L-band, the physical temperature of vegetation is assumed the same as that of soil in this study. The soil effective temperature T_{eff} can be estimated using either Wilheit [22] coherent or Lv [29] incoherent models (see Section 2.2.3) (⑨ in Figure 2). Finally,

$T_B^p (= e_p(\theta_i) \cdot T_{\text{eff}})$ is computed using the emissivity $e_p(\theta_i)$ multiplied by T_{eff} (⑩ in Figure 2). Figure 2 shows the flow-chart of forward T_B^p simulations by the coupled TVG and AIEM model including the ATS model. Parameter values used for TVG+AIEM+ATS running are listed in Table 1.

2.2.2. The Air-to-Soil Transition (ATS) Model. Vegetated soil medium is composed of a substantial amount of loose dirt, plant debris, and crumbs scattered on the surface and a much denser soil entity lying beneath (Figure 3(a)). Driven by changing weather systems such as after dry and sunny conditions following rainfall events, wetted plant debris and large clods on the surface dry out more quickly than bulk soil beneath the surface. Affected by roots and air pockets present in the soil volume, it produces an inhomogeneous layer between soil structures near the surface and bulk soil at the bottom. All these effects may lead to a large spatial variability in SM at the soil surface and within the soil volume [30]. Consequently, it induces different (e.g., wet-dry layers) interfaces existing in the soft transition zone of the dielectric constant from air to bulk soil (ATS). The ATS zone may extend over the peak-to-trough geometric thickness for the natural smooth surface, especially when the soil surface is dry and

TABLE 1: Input parameters of the integrated ATS+AIEM+TVG model used in this study.

	Parameter name	Value	Reference
TVG: vegetation part	Leaf area index (LAI)	MCD15A2H, Figure 1 in the text	
	Plant moisture content (kg kg^{-1})	0.59	Wang et al., 2018 [48]
	Leaves: disc radius (cm)	1.4	Dente et al., 2014 [47]
	Leaves: disc thickness (cm)	0.02	Dente et al., 2014 [47]
	Leaves: disc angular distribution	Random	Dente et al., 2014 [47]
ATS+AIEM: soil part	Volumetric soil moisture and soil temperature	<i>In situ</i> measurements at 2.5, 5, 10, 20, 35, and 60 cm	Su et al., 2020 [36]
	Soil texture	<i>In situ</i> measurements	Zhao et al., 2018 [38]
	The standard deviation of surface heights (cm)	0.9	Dente et al., 2014 [47]
	Correlation length (cm)	9	Dente et al., 2014 [47]
	Autocorrelation function	Exponential	Dente et al., 2014 [47]
Sensor configuration	Incidence angle ($^\circ$)	40	
	Frequency	1.4 GHz	
	Polarization	H and V	

FIGURE 3: The sketch of the air-to-soil transition (ATS) model (a) and the dielectric depth profile in the ATS zone (b). $V_h(z^*)$ refers to the cumulative probability of density of $S_h(z^*)$, and $1 - V_h(z^*)$ corresponds to the total air volume fraction of the ATS zone. h is the total dielectric roughness thickness (unit: cm) of a soil area with the order λ_0 by λ_0 ($\lambda_0 = 21$ cm at L-band). h_{ss} (unit: cm) refers to the dielectric roughness thickness at the topsoil structures. h_{sv} (unit: cm) is the dielectric roughness thickness in the soil volume. $z = 0$ is the average surface geometric height with standard deviation s (unit: cm). The ECH2O 5TM probes (Decagon Devices, Inc., USA) are located at different depths (e.g., 2.5 and 10 cm). (b) describes the h under wet and dry soil conditions with s of 0.9 cm, in which ϵ'_{soil} is the real part of the dielectric constant of bulk soil, $\epsilon_{soil} = 17.3 + i2.2$ for $SM = 0.31 \text{ m}^3/\text{m}^3$, and $\epsilon_{soil} = 5.1 + i0.4$ for $SM = 0.1 \text{ m}^3/\text{m}^3$.

electromagnetic waves from deep layers can transmit towards the surface.

Assuming L less than the wavelength λ_0 in free space, a concept of dielectric roughness (h , L) is proposed for the

ATS zone, in which h is a dielectric roughness thickness characterizing the depth of interfaces, not only resulting from topsoil structures (h_{ss}) affected by both irregularities (i.e., geometric roughness) of the soil surface and inhomogeneous

distribution of moisture but also due to inhomogeneity within soil volume (h_{SV}) that is related to soil porosity and moisture. The dielectric roughness thickness h for the ATS zone is assumed as a sum of h_{SS} and h_{SV} (see Figure 3(a)).

$$h = h_{SS} + h_{SV}. \quad (1)$$

Due to the difficulty to have detailed volumetric information on inhomogeneous mediums (e.g., loose dirt, plant debris, and bulk soil mixed with roots) along the ATS zone, the Fermi-Dirac distribution function [52] is used in this study to construct the dielectric depth profile, given an exponential dependence of the roughness thickness on SM [31, 53]. Subsequently, an “equivalent” homogenous dielectric ATS zone with a given dielectric constant is produced as a consequence of the impedance match over the ATS zone, which is used for calculating scattering of the ATS medium by AIEM (see Section 2.2.1).

In this study, h is taken as the SM-dependent roughness parameter. Modulated by SM, h varies and the probability density function $S_h(z^*)$ for dielectric roughness height is assumed to have an exponential distribution with a rate parameter α , considering the exponential attenuation with regard to water content and (physical) height on surface emission [30, 31, 54]. $S_h(z^*)$ is formulated by Equation (2):

$$S_h(z^*) = \alpha \exp(-\alpha z^*), \quad z^* \geq 0. \quad (2)$$

As h is also affected by geometric roughness, the depth dependence of the volume fraction of soil materials that backbone variations of the dielectric profile is consequently related to the dielectric height distribution and can be described as the cumulative distribution of $S_h(z^*)$. Specifically, the integral of $S_h(z^*)$ over depth $z^* - V_h(z^*)$ represents the volume fraction of soil materials and $1 - V_h(z^*)$ for the air volume fraction (Equation (3)):

$$1 - V_h(z^*) = \exp(-\alpha z^*), \quad z^* \geq 0. \quad (3)$$

At the soil surface, h_{SS} is backbone by topographic effects and is related to $2s$ as the surface geometric height (see Figure 3(a)). h_{SS} in this study is also assumed depending on both incidence angle and polarization reported by previous investigations by [25, 55, 56]. If assuming that the air volume fraction is one at an arbitrary position on the top of the surface structures where $z^* = 0$ (z^* is away from the average surface geometric height $z = 0$ for nadir observation), since more soil particles occupy the hollows of topsoil structures on the lateral scale with increasing depth ($z^* > 0$), the air volume fraction in the topsoil structures decreases (see Figure 3(a)). The decreased air volume is filled by the increased volume of soil materials, and the resultant effect of moisture on h_{SS} can be described by logarithmic SM (Equation (4)). While h_{SS} decreases when the soil surface is wet, the surface may become “saturated” when it is sufficiently wet, namely, the soil moisture reaches field capacity

(FC), at which $z^* = 0$ moves to $z^* = z = -s$ and makes h_{SS} close to $2s$. h_{SS} is then given as follows:

$$h_{SS} = \begin{cases} 2 \cdot s \cdot (-\ln(SM)) \cdot \cos^{Np}(\theta_i), & SM < FC, \\ 2 \cdot s, & SM \geq FC, \end{cases} \quad (4)$$

where θ_i is the incidence angle. Np is a polarization modulation parameter, and Np is set at 0 for H polarization and -1 for V polarization. SM is volumetric soil moisture.

With z^* deepening in the ATS zone, when the topsoil structures on the whole lateral scale tend to be fully filled with soil materials (see Figure 3(a)), the soil texture (i.e., porosity) and SM profile become the dominant factors whose effects can be represented by h_{SV} , which is the depth where the air volume fraction of the ATS zone equals to a maximum volume of pore space in the soil (porosity) (Equation (5)).

$$h_{SV} = \frac{-\ln(\text{porosity})}{\alpha}. \quad (5)$$

Affected only by moisture in the soil volume (this is where SM is measured), the parameter of the distribution α can be estimated by the power attenuation coefficient as in [23, 57], which is determined by λ_0 and the complex dielectric constant of bulk soil in the ATS zone as follows:

$$\alpha = \frac{2\pi}{\lambda_0} * \frac{\epsilon_{\text{soil}}''}{\sqrt{\epsilon_{\text{soil}}'}}, \quad (6)$$

where $\epsilon_{\text{soil}} = \epsilon_{\text{soil}}' + i\epsilon_{\text{soil}}''$, ϵ_{soil}' is real part, and ϵ_{soil}'' imaginary part of the soil dielectric constant of the ATS zone. In this study, soil porosity is set of 0.62 according to laboratory measurements [38], and FC is valued of $0.35 \text{ m}^3/\text{m}^3$ for silt loam soil. The sketch of the improved ATS model is shown in Figure 3(a).

The Fermi-Dirac distribution function [52] shown in Equation (7) is used to describe the dielectric depth profile $\epsilon(z^*)$ for the ATS zone. The steepness parameter k_{AS} in Equation (8) is related to s and SM effects.

$$\epsilon(z^*) = \epsilon_{\text{air}} + \frac{1}{1 + \exp(-(z^* - h_{SV})/k_{AS})} (\epsilon_{\text{soil}} - \epsilon_{\text{air}}), \quad (7)$$

$$k_{AS} = \exp(-\alpha z^*) \cdot s. \quad (8)$$

Figure 3(b) shows two estimated h and the correspondingly derived $\epsilon(z^*)$ under wet and dry soil conditions. The same temperature can be assumed of all layers in the ATS zone due to small influences from temperature change on the dielectric constant of (organic) soils [58]. As such, a coherent radiative transfer model can be used to compute the overall coherent reflectivity for the ATS zone from $\epsilon(z^*)$, which is based on a matrix formulation of the boundary conditions at dielectric discontinuities derived from Maxwell's equations [59]. The coherent model is performed for a total depth of h with the thickness of each layer set to 1 mm, which is less than one-tenth of the wavelength

λ_0 . This coherent model predicts a trend of reflectivity as a function of layer thickness but is characterized by enhanced oscillations due to coherent interactions among multiple reflected waves, and this process can be smoothed by natural variations of layer thickness around its average value and an averaging procedure [60]. Considering the impacts of both surface geometric roughness and SM at the bottom of the ATS zone, the average dielectric surface ($z_{\text{avg}}^* = h/2$ along z^* , see Figure 3(a)) is assumed varying downward with a depth measured by s multiplied by logarithmic SM (Equations (9)–(10)).

$$z_{\text{avg}}^* = h/2, \quad (9)$$

$$z_{\text{lb}}^* = \frac{h}{2} - \ln(\text{SM}) \cdot s. \quad (10)$$

Consequently, reflectivities obtained at this layer thickness ($z_{\text{avg}}^* \leq z^* \leq z_{\text{lb}}^*$) are averaged, and the effective dielectric constant of an equivalent homogenous dielectric ATS zone (used for calculating the scattering by AIEM) is computed by minimizing an objective function between the obtained reflectivities and those computed for the ATS zone using Fresnel equations [60].

The effective roughness parameters obtained from model calibration are recommended to be used in the physically based surface backscatter model [61, 62]. In this study, s is taken as 0.9 cm and L as 9.0 cm in Maqu case [47]. These two calibrated values consider the high correlation between s and roughness slope (s/L) [61, 63]. SM of the lower boundary of the ATS zone used for calculating h_{SS} (see Equation (4)), ϵ_{soil} and associated h_{SV} (see Equations (5)–(6)) for L-band is difficult to obtain, but can be regarded as the representative SM. The measured SM at 2.5 cm is considered as the representative SM, because the reflectivity of a stratified dielectric is primarily determined by changes in the real part of the refractive index over a depth of about 1/10 and 1/7 wavelengths (~ 2.5 cm for L-band) [22]. It is to note that representative SM is also obtained by considering the impact of SMST profile on soil microwave emissions through either Wilheit [22] or Lv [29] stratified models (see Section 2.2.3). The Mironov dielectric model [58] is used to calculate ϵ_{soil} throughout the whole study period, and the soil texture (i.e., clay fraction and bulk density) information is based on laboratory measurements [38].

2.2.3. Wilheit Coherent Model and Lv Incoherent Model. In this study, we regard the Wilheit [22] model as coherent because the electromagnetic wave considered in the model is formulated with amplitude and phase, and the electromagnetic energy flow through the plane is given by the Poynting vector with retaining coherent character. In reality, when a rapid drying out of the surface occurs, there are dry and wet layers with the depth. Reflections from the air-soil interface and the dry-wet soil interface may interfere, resulting in the wave from deep layers adding to the surface energy density constructively (in phase) or destructively (out of phase), or in between (i.e., adding of two waves). By contrast, Lv [29] model is taken as incoherent, because the model derivation is

based on radiation intensity (i.e., with only amplitude considerations but without phase) [23]. T_{eff} and associated T_B^p simulations by these two models are expected to provide physical insights on interactions of microwaves with soil medium. From an application perspective, it can help determine whether coherent and incoherent effects are needed to be considered for modelling emission for natural surface, whose status changes with meteorological and hydrological conditions.

(1) Wilheit Coherent Model. In Wilheit [22] model, soils are treated as a layered plane dielectric medium. The basic assumption is that there is a reflection for the incident radiation on the air-soil interface and the thermal equilibrium in each following layer (i.e., beneath the interface) of this stratified medium. That is to say, only the absorption and transmission of electromagnetic waves are considered in each layer. The fraction of absorption (f_i^p) can be calculated by solving Maxwell's equations with the aid of boundary conditions at the interfaces for a coherent electromagnetic wave propagating through the layered soil [22]. If T_i is the temperature of the i th layer, under thermodynamic equilibrium, the layer radiates energy equal to the product of the fractional absorption f_i^p and the temperature T_i . In terms of the conservation of energy, the reflectivity of the smooth air-soil interface R_s^p is described by Equation (11):

$$R_s^p = 1 - \sum_{i=1}^N f_i^p, \quad (11)$$

where N represents the total number of discrete soil layers. As such, the representative SM (SM_Wil) used for determining h is the one resulting in a minimum root mean square error difference between the obtained reflectivities and those computed for a set of SM through the Fresnel equations [60]. Wilheit [22] also defined the thermal sampling depth δ_T as the average depth, at which the upwelling thermal radiation from the soil originates. δ_T is a function of integrals over the imaginary part of the refraction index but calculated using an approximation (Equation (12)).

$$\delta_T = \frac{\sum x_i f_i}{\sum f_i}, \quad (12)$$

where x_i is the depth of the i th layer and f_i^p ($p = H, V$ polarization) is the weighting function (e.g., the fraction of absorption) for that layer as previously defined. The average soil temperature over the δ_T is regarded as the soil effective temperature T_{eff} and calculated by Equation (13).

$$T_{\text{eff}} = \frac{\sum f_i T_i}{\sum f_i}. \quad (13)$$

(2) Lv Incoherent Model. The soil effective temperature is defined as the net intensity at the soil surface, which is a

TABLE 2: Configuration of simulation experiments.

Experiments	AIEM	ATS	$T_{\text{eff\_Lv}}$	$T_{\text{eff\_Wil}}$	Emissivity
(1) Base-Wil	+			+	SM_Wil, computed based on <i>in situ</i> SMST at 2.5, 5, 10, 20, 35, and 60 cm
(2) Base-Lv	+		+		<i>In situ</i> SM at 2.5 cm
(3) ATS-Wil	+	+		+	SM_Wil, computed based on <i>in situ</i> SMST at 2.5, 5, 10, 20, 35, and 60 cm
(4) ATS-Lv	+	+	+		SM_Lv, computed based on <i>in situ</i> SMST at 2.5, 5, 10, 20, 35, and 60 cm
(5) ATS-Lv2.5	+	+	+		<i>In situ</i> SM at 2.5 cm

superposition of intensities emitted at various depths [23]. The formula is as follows:

$$T_{\text{eff}} = \int_0^{\infty} \alpha(z) T_s(z) \exp \left[-\int_0^z a(z') dz' \right] dz, \quad (14)$$

where $T_s(z)$ is the soil temperature at depth z . $\alpha(z)$ is the attenuation coefficient related to the complex soil dielectric constant $\epsilon = \epsilon' + i\epsilon''$ at depth z . For low-loss dielectric and nonmagnetic soil medium, $\alpha(z)$ can be expressed as [23, 64]

$$\alpha(z) = \frac{2\pi}{\lambda_0} \cdot \frac{\epsilon''(z)}{\sqrt{\epsilon'(z)}}. \quad (15)$$

Assuming uniform SM and texture in each layer, a discrete formulation of (14) is derived by Lv [29].

$$T_{\text{eff}} = T_{s,1} (1 - e^{-\alpha_1 \Delta z_1}) + \sum_{i=2}^{N-1} T_{s,i} (1 - e^{-\alpha_i \Delta z_i}) \prod_{j=1}^{i-1} e^{-\alpha_j \Delta z_j} + T_{s,N} \prod_{j=1}^{N-1} e^{-\alpha_j \Delta z_j}, \quad (16)$$

where 1, i , and j represent the soil layers. N shares the same meaning as in Equation (11). T_s is soil temperature. α is the attenuation coefficient given in Equation (15), and Δz is soil thickness. $1 - e^{-\alpha_i \Delta z_i}$ is defined as the weight function for the i th layer [65]. By assuming uniform dielectric properties of soils throughout the emitting layer and a linear soil temperature gradient along the soil optical depth, the soil temperature at one time of the soil optical depth is proved equivalent to T_{eff} . The depth corresponding to one soil optical thickness is defined as the penetration depth of soil effective temperature δ_{PD} [57] as follows:

$$\begin{cases} \int_0^{\delta_{\text{PD}}} \Delta z_i \alpha(z) dz = 1, \\ \delta_{\text{PD}} = \frac{\lambda_0 \sqrt{\epsilon'}}{2\pi \epsilon''}, \end{cases} \quad (17)$$

where Δz , α , and ϵ share the same meanings as in Equations (15), (16). The *in situ* SM at 2.5 cm is used for calculating δ_{PD} in this case. Measured SM at depths above

δ_{PD} are integrated using the weight function (in Equation (16)) for obtaining the representative SM (SM_Lv, Equation (18)) that considers the impacts of profile SMST. The δ_{PD} (Lv's model) and δ_T (Wilheit's model) are referred to as sampling depths of soil effective temperature in the following analysis.

$$\begin{aligned} \text{SM}_{\text{Lv}} = & \text{SM}_1 (1 - e^{-\alpha_1 \Delta z_1}) + \sum_{i=2}^{\delta_{\text{PD}}-1} \text{SM}_i (1 - e^{-\alpha_i \Delta z_i}) \prod_{j=1}^{i-1} e^{-\alpha_j \Delta z_j} \\ & + \text{SM}_{\delta_{\text{PD}}} \prod_{k=1}^{N-1} e^{-\alpha_k \Delta z_k}, \end{aligned} \quad (18)$$

where SM_i refers to SM at i layer. The other symbols in Equation (18) share the same meanings as in Equation (16).

2.2.4. Configuration of Simulation Experiments. To assess the importance of the ATS model in seasonal T_B^p simulations, five experiments involving Wilheit coherent model and Lv incoherent model for the soil part are carried out. The first two experiments are called “Baseline,” only using the AIEM +TVG without the ATS model integrated. The baseline experiments are configured with both Wilheit's and Lv's models, which can reflect the impacts of effective soil temperature and effective soil moisture, respectively, on T_B^p simulations. Considering the emission is sensitive to SM at top layers [42], the *in situ* measured SM at 2.5 cm is used to calculate the dielectric constant of bulk soil for the second experiment, which is equivalent to the concept of representative SM based on Wilheit's model. Furthermore, a total soil depth of 60 cm is used for these two stratified models, since the *in situ* measured SM at 60 cm is almost constant during the study periods.

The third and fourth experiments integrate the ATS model with the combination of Wilheit's and Lv's models separately (named “ATS-Wil” and “ATS-Lv”) to reflect the effects of the dielectric roughness on T_B^p simulations. Specifically, the SM_Wil and SM_Lv are used, respectively, to determine the dielectric constant of bulk soil and the T_{eff} (i.e., $T_{\text{eff\_Wil}}$ and $T_{\text{eff\_Lv}}$) (see Figure 2). Furthermore, the fifth experiment is considered with the combination of Lv's model and the 2.5 cm SM for calculating the dielectric constant of bulk soil, evaluating the effectiveness of Lv's weighted SM approach (see Figure 2). Table 2 summarizes the configurations of simulation experiments.

With the Wilheit [22] model, properties such as the layer thickness d and the interpolation method to estimate the

FIGURE 4: Comparisons of estimated dielectric roughness thickness (h) from the third (ATS-Wil), fourth (ATS-Lv), and fifth (ATS-Lv2.5) experiments, supported by comparisons of SM during the late-monsoon period. SM_Wil is the representative SM derived from Wilheit coherent model using the Fresnel equations (e.g., via minimizing the objective function of reflectivity difference). SM_Lv represents the weighted SM derived from Lv incoherent model and SM_2.5 cm refers to *in situ* measured SM at 2.5 cm.

SMST in each layer from a limited number of observations are noted affecting model simulations. Similar to [66], the linear interpolation is used in this study. Considering the high sensitivity of coherent models to optical thickness, a preliminary test was carried out to investigate the sensitivity of the Wilheit model to the soil layer thickness d . The results confirm the use of 1 mm for d in Wilheit model simulations, which is consistent with that in [66].

3. Results

3.1. The Late-Monsoon Period

3.1.1. The Dielectric Roughness Thickness (h) and the Sampling Depths of Soil Effective Temperature (δ_{PD} and δ_T). As a constant difference of the dielectric roughness thickness (h) between H and V polarizations is assumed (see Equations (1), (4)-(5)), only the estimated h for H polarization is analyzed. Figure 4 shows comparisons of h from the third (h_{Wil}), fourth (h_{Lv}), and fifth ($h_{Lv\_SM2.5\text{ cm}}$) experiments (bottom panel), together with the representative SM derived from Wilheit's (SM_Wil) and Lv's (SM_Lv) models and the *in situ* SM at 2.5 cm (SM_2.5 cm) (upper panel). SM_Wil is found changing coincidentally with SM_2.5 cm, and this might be due to the sampling depth of SM determined by Wilheit model being the order of about one-tenth

wavelength (approximately 2.5 cm at L-band). SM_Wil is also seen slightly higher than SM_2.5 cm when soils go through the transition of dry-wet-dry during the midmonsoon period. Comparatively, a slight variation of SM_Lv is seen in this period, and this is the consequence of Lv incoherent model with an assumed uniform SM distribution in the profile. Correspondingly, h_{Lv} cannot increase as much as h_{Wil} and $h_{Lv\_SM2.5\text{ cm}}$ do when soils become drier. The Wilheit model can simulate h with obvious variations when soils experience dry and wet conditions, due to its capability of considering the effect of SM profile in calculating the dielectric constant of bulk soil. Compared to $h_{Lv\_SM2.5\text{ cm}}$, h_{Wil} is slightly lower in the soil drying process (Figure 4). Wet soils at deep layers considered in the Wilheit model lead to the smooth increase of the h when the soil surface becomes drier. h is estimated exceeding over 10 cm in dry conditions (e.g., $SM \approx 0.1\text{ m}^3/\text{m}^3$) (Figure 4). When SM increases and is greater than $0.3\text{ m}^3/\text{m}^3$, h estimated from all schemes decrease (Figure 4).

Figure 5 shows that the sensing depths of effective temperature derived from Lv model (δ_{PD}) and Wilheit model (δ_T) have the same variations and approach each other during the whole late-monsoon period. Due to considerations of the coherent effect in the Wilheit model, constructive interference might exist for reflections from the air-soil interface and the dry-wet soil interfaces (drying front), and δ_T is found

FIGURE 5: Comparisons of the sampling depths of soil effective temperature estimated by Wilheit coherent model and Lv incoherent model (δ_T and δ_{PD}), and also the T_{eff} ($T_{\text{eff-Wil}}$ and $T_{\text{eff-Lv}}$) during the late-monsoon period. $ST_{2.5 \text{ cm}}$ refers to *in situ* soil temperature measured at 2.5 cm.

higher ($\sim 2.3 \text{ cm}$) than δ_{PD} (Figure 5). $T_{\text{eff-Wil}}$ is close to $T_{\text{eff-Lv}}$, but both have a phase lag reflecting the propagation of periodic temperature waves from the deep soil, compared to the *in situ* soil temperature at 2.5 cm ($ST_{2.5 \text{ cm}}$). T_{eff} as a resultant of the superposition of the foregoing waves at various depths within the soil does not show as much variation as $ST_{2.5 \text{ cm}}$, because the latter experiences rapid diurnal variations due to direct solar radiation, and this kind of variation becomes damped with increasing soil depth. As such, $ST_{2.5 \text{ cm}}$ is higher than $T_{\text{eff-Wil}}$ and $T_{\text{eff-Lv}}$ at midday but lower at midnight. $T_{\text{eff-Wil}}$ is slightly larger ($\sim 0.2 \text{ K}$) than $T_{\text{eff-Lv}}$ especially at midday and midnight (Figure 5), whereas their differences reduce when soils are wet following rainfall events (see sharp jumps of $SM_{2.5 \text{ cm}}$ in Figure 4). Figure 5 shows a negligible difference ($\sim 0.2 \text{ K}$) between $T_{\text{eff-Wil}}$ and $T_{\text{eff-Lv}}$, while the varied thermal sampling depth ($\sim 2.3 \text{ cm}$) of soil temperature is noted important for determining the optimal mounting depth for observations as claimed by [65].

3.1.2. The T_B^p Simulation. Figure 6 shows that the two baseline simulations underestimate T_B^H in the whole late-monsoon period, signifying that considering only impacts of effective soil temperature and effective soil moisture cannot close the discrepancy between simulations and observations. However, the underestimation of T_B^H ($\approx 30\text{--}50 \text{ K}$) is obviously compensated by integrating the ATS

model. T_B^H simulated by the ATS-based models are close to ELBARA-III observations in magnitude before late August, in which the ATS-Wil and ATS-Lv2.5 simulations match to observation while the ATS-Lv model presents underestimations. T_B^H simulated by the ATS-based models continue to be consistent with observations in September when the soil surface is wet. This indicates the necessity of the ATS model for surface emission modelling for H polarization during the late-monsoon period.

For V polarization, Figure 6 shows that the two baseline models simulate T_B^V well in August but underestimate T_B^V ($\approx 20 \text{ K}$) in September when the soil surface is wet. By integrating the dielectric roughness in the ATS model, the underestimation is reduced, similarly as for H polarization. The ATS-based models show slight underestimations compared to ELBARA-III observations before late August but are closer to observations than baseline simulations. The ATS-Wil model performs better than the ATS-Lv model for T_B^V modelling in this period. While all ATS-based models have the same performances and capture T_B^V well during the end-monsoon period (September), despite discrepancies occurring after big rainfall events (e.g., on 25/08/2016). The ATS model is seen improving the modelling of surface emission also for V polarization during the late-monsoon period.

3.2. The Post-Monsoon Period. Due to the page limit, similar analyses for the post-monsoon period are presented in the

FIGURE 6: Comparisons of simulated T_B^p by different models to the ELBARA-III observed T_B^p during the late-monsoon period. p refers to H or V polarization mode. Base-Lv and Base-Wil refer to experiments using AIEM+TVG in combination with Wilheit's and Lv's models separately. ATS-Lv and ATS-Wil represent experiments using ATS+AIEM+TVG in combination with Wilheit's and Lv's models separately. ATS-Lv2.5 denotes experiments using ATS+AIEM+TVG in combination with Lv's model and soil moisture at 2.5 cm for calculating the dielectric constant of bulk soil.

supplementary materials. Results show that (1) the estimated h within 4–6 cm is corresponding to surface SM changes within $0.24\text{--}0.32\text{ m}^3/\text{m}^3$ (Figure S1). The SM_Wil and SM_Lv and associated h_{Lv} and h_{Wil} (Figure S1) are consistent with SM_2.5 cm and $h_{\text{Lv\_SM2.5 cm}}$ correspondingly during the post-monsoon period before the soil freezing-dominated period, where the surface soil temperature is below 0°C (e.g., from 26/11/2016 to 30/11/2016, see Figure S2). While during the surface freeze-thaw transition period, in which the surface soil temperature changes along the freezing level 0°C (e.g., from 12/11/2016 to 25/11/2016, Figure S2), the SM_Wil and SM_Lv and associated h_{Lv} , h_{Wil} and $h_{\text{Lv\_SM2.5 cm}}$ (Figure S1) show less diurnal variations than those of SM_2.5 cm. (2) Estimated δ_T is higher ($\sim 1.6\text{ cm}$) than δ_{PD} most of the time during the post-monsoon period (Figure S3), and values of $T_{\text{eff\_Wil}}$ and $T_{\text{eff\_Lv}}$ are almost the same. (3) Two baseline simulations underestimate T_B^p ($\approx 20\text{--}50\text{ K}$) in the post-monsoon period (Figure S4), while T_B^p simulated by the ATS-based models are much closer to observations. It is to note that when the weather system changes and soils start to experience freeze-thaw processes, T_B^p simulated by the ATS-based models deviate from observations.

4. Discussion

4.1. Applicability and Uncertainty of the ATS Model. The enhanced ATS model in this study stems from the original ATS model [31, 32, 54], considering the effect of roughness

components within the observation λ_0 and finding the impedance match for the ATS zone [30]. The enhanced ATS model with the new parameterizations of dielectric roughness effects maintains physical considerations and helps improving T_B^p simulations.

The dielectric roughness thickness h is a key parameter in the ATS model, which is parameterized comprising two components. One is dielectric roughness within the soil volume (h_{SV}); the other is dielectric roughness induced by SM from the soil surface and geometric roughness effects (h_{SS}). Figure 7 shows during the study period, with SM decreasing (see SM from 0.2 to $0.1\text{ m}^3/\text{m}^3$ in Figure 4), the contribution from the soil volume to the dielectric roughness thickness (h_{SV}/h) increases (Figure 7), while that from the surface (h_{SS}/h) decreases, and it is vice versa when SM increases (see SM from 0.15 to $0.3\text{ m}^3/\text{m}^3$ in Figure 4). This is reasonable because as the soil dries out, emissions originate from the deep layers and the spatial heterogeneity of the dielectric constant within the soil volume becomes much larger and enhances dielectric roughness effects, and it is the other way around when soils are wet. This phenomenon is also reported by [31, 53, 55, 67], in which the site-specific empirical soil roughness parameter H_R [25, 68] is obtained for zeroth-order radiative transfer models.

With SM decreasing, the scattering medium (e.g., loose dirt, plant debris, and crumbs) at the soil surface becomes drier and more transparent for electromagnetic wave transmission, thus, the contribution to the dielectric roughness from the soil surface (h_{SS}/h) decreases as shown in Figure 7.

FIGURE 7: Comparisons of the ratio of h_{SV} and h_{SS} to h from the third (ATS-Wil), fourth (ATS-Lv), and fifth (ATS-Lv2.5) experiments for the late-monsoon period.

Conversely, with SM increasing, the scattering medium including senescent vegetation (see decreased LAI in Figure 1) lying on soils becomes wet and may trigger litter effects and leads to roughness (h_{SS}/h) increasing (see Figure 7). This is in line with findings from [69, 70], in which higher values of the calibrated H_R are used to account for surface effects related to litter over the grassland. Moreover, given the parameterization of h_{SS} related to both geometric roughness and SM, the scaled h_{SS} (namely, h_{SS}/h) can be comparable to H_R , which implicitly accounts for both the geometric and dielectric roughness effects. The h_{SS}/h is found ranging from 0.31 to 0.42 (see Figure 7), and these values are close to the $H_R (= 1.3972 \cdot (s/L)^{0.5879})$ from [53] and $H_R (= (0.9437 \cdot s / (0.8865 \cdot s + 2.29143))^6)$ from [71], with the same s and L used in this study. In another study over grass in the Goulburn River catchment, Australia [72], H_R is approximated of 0.4.

Correspondingly, for associated T_B^p modelling during the late-monsoon period, two baseline simulations have high Pearson correlation coefficients ($R \geq 0.87$) while consistently underestimated the observation. T_B^p simulated by the ATS-based model only considering h_{SS} are higher than those from two baseline simulations but still underestimated the observed T_B^p (see Section 3 in the supplementary materials). However, the ATS-based models by considering the impacts of both h_{SS} and h_{SV} greatly compensate underestimations by the foregoing simulations, with more simulation results closely aligned to 1:1 line as shown in Figures 8(a) and 8(b) and Figure S9 (in the supplementary materials). The simulated T_B^p have similarly high R (≥ 0.85) but much lower root mean square errors (RMSEs ≤ 9.2 K for T_B^H and 8.0 K

for T_B^V) than baseline simulations (RMSEs over 37 K for T_B^H and 12 K for T_B^V). The ATS-Wil and ATS-Lv2.5 models perform better than the ATS-Lv model in this period as more clustered points aligned along 1:1 line are seen in Figures 8(a) and 8(b) and better matches to observations shown in Figure 6. This underlines the importance of obtaining the realistic SM that can reflect the moisture status of the ATS zone and implies that the coherent effects can be considered during the late-monsoon season. With changing weather systems in the post-monsoon periods, the ATS-based models maintain the performance with lower RMSEs (≤ 12.5 K for T_B^H and 10.9 K for T_B^V) than baseline simulations (RMSEs over 39 K for T_B^H and 18 K for T_B^V), in which the ATS-Lv2.5 and ATS-Lv models with lower RMSEs perform better than the ATS-Wil model (Figure S5). This may indicate that the coherent effects occurring in the late-monsoon period may be disrupted due to freeze-thaw processes during this period.

The ATS-based models underestimate T_B^p for soils undergoing surface freeze-thaw processes, and simulated T_B^p have weak diurnal variations (see Figure S4). The estimated dielectric roughness derived from the ATS-based models in this period (see Figure S6) is also found having slight variations for the ATS-based models, which the stable δ_T and δ_{PD} and associated T_{eff_Wil} and T_{eff_Lv} (see Figure S1 and Figure S3) may partially account for. As air temperature and ground surface temperature impose the topmost roles in affecting the soil surface freeze-thaw process, the appropriate temperature information is necessary to refine the h estimation for soils during the freeze-thaw transition period. On the other hand, the

FIGURE 8: Simulated $T_B^p(\text{K})$ from the Base-Lv, Base-Wil, ATS-LV, ATS-Wil, and ATS-Lv2.5 experiments against the ELBARA-III $T_B^p(\text{K})$ at Maqu site. (a, b) T_B^H and T_B^V , respectively, for the late-monsoon period (from 08/08/2016 to 30/09/2016). R refers to the Pearson correlation coefficient, and RMSE is the root mean square error and calculated by $\sqrt{(1/n)(T_B^p\text{-m} - T_B^p\text{-o})^2}$ (where n is the number of observations). Base-Lv and Base-Wil refer to experiments using AIEM+TVG in combination with Wilheit's and Lv's models separately. ATS-Lv and ATS-Wil represent experiments using ATS+AIEM+TVG in combination with Wilheit's and Lv's models separately. ATS-Lv2.5 denotes experiment using ATS+AIEM+TVG in combination with Lv's model and soil moisture at 2.5 cm for calculating the dielectric constant of bulk soil.

freeze-thaw processes exaggerate the inhomogeneity in the soil media (e.g., composed of ice in pores mixed with preexisting crack, or melted liquid water mixed with ice, organic matter, and soil solid). The formed ice affects the dielectric constant of bulk soil during the nighttime and early morning, and the melted surface (soil) water does that during the daytime. Without the soil ice content and surface (soil) water information considered in the ATS model parameterizations, the ATS model cannot capture such mixtures and accurately model h and associated T_B^p . If we can further take into account surface (soil) liquid water and ice content for the h estimation, the performance of the ATS model for L-band radiometry of the freeze-thawed soil is expected to be improved. It is to note that soil ice content cannot be measured directly *in situ* but can be retrieved indirectly via assimilating proximal sensing signals [73]. The inclusion of soil ice content, surface liquid water fraction, and ground surface temperature into the ATS model will be explored in further studies. A similar improvement can be expected to implement for T_B^p modelling with rainfall events, such as by ATS model considering surface water effects when the accumulated intensities of rainfall become greater than soil infiltration

capacity of the surface, and the formed surface water may block the soil emission from the deep layers.

Nevertheless, correspondences between T_B^p estimated by the ATS-based models and the observations indicate that the ATS model is necessary for L-band T_B^p modelling. The h parameterized in this study acting as a dynamic parameter can describe well the dielectric roughness at the soil surface and within the soil volume, which is significant for interpreting the observed T_B^p dynamics. The h_{ss} in this study is also related to the incidence angle and polarization. The N_p , the same as in the empirical roughness parameterization [25] is found with N_H of 0 and N_V of -1 for the best T_B^p simulations at Maqu site. This result supports the demonstration that different N values should be used for horizontal and vertical polarizations [55, 71, 74]. The applicability of N_p in other climate regimes needs to be further confirmed, but this is beyond the scope of this study.

4.2. The Impacts of Geometric Roughness on the Performance of the ATS Model. Geometric surface roughness parameters (s , L) have great impacts on surface scattering. s is considered in the dielectric roughness h parameterization and

TABLE 3: Comparisons of simulated T_B^p by different models with different s (0.75, 0.9, 1.2, 1.5, 2.5 cm) settings with constant L (9 cm) to ELBARA-III observations. Base-Lv and Base-Wil represent experiments using AIEM+TVG in combination with Wilheit's and Lv's models separately. ATS-Lv and ATS-Wil denote experiments using ATS+AIEM+TVG in combination with Wilheit's and Lv's models separately.

Polarization	Period Experiments s (cm)	Late-monsoon				Post-monsoon			
		Base-Wil R	Base-Wil RMSE (K)	ATS-Wil R	ATS-Wil RMSE (K)	Base-Lv R	Base-Lv RMSE (K)	ATS-Lv R	ATS-Lv RMSE (K)
H	0.75	0.9	40.1	0.85	23.0	0.37	41.4	0.13	28.8
	0.9	0.9	38.4	0.88	9.2	0.37	39.4	0.21	12.2
	1.2	0.9	34.0	0.89	20.8	0.37	34.5	0.37	20.6
	1.5	0.9	29.0	0.86	27.3	0.37	28.9	0.41	22.0
	2.5	0.9	11.3	0.89	9.8	0.38	12.1	0.36	11.6
V	0.75	0.88	12.8	0.84	14.8	0.55	18.3	0	12.3
	0.9	0.88	12.5	0.86	7.7	0.55	18.1	0.16	10.3
	1.2	0.88	11.7	0.73	17.6	0.54	17.1	0.48	13.9
	1.5	0.88	10.6	0.87	14.1	0.53	15.7	0.56	20.5
	2.5	0.87	7.5	0.87	7.4	0.48	10.2	0.45	9.6

affects the depth that determines variations of the effective dielectric constant of the air-to-soil medium (see Section 2.2.2). Considering the difficulty in determining the “true” values of s and L for natural grassland and their importance in calculating backscattering coefficients in AIEM [61], the effective geometric roughness parameters (s , L) obtained from satellite measurements in Maqu area [47] are used in this study as described in Section 2.2.2. To investigate the impacts of varying geometric roughness on the performance of baseline and ATS-based model T_B^p simulations, the sensitivity analyses by using a varying s in the range of (0.75, 0.9, 1.2, 1.5, 2.5 cm) with constant L of 9 cm (considering its lower impacts than s) are carried out. s of 0.9 cm is regarded for a smooth natural surface and s of 2.5 cm for a rough one for L-band in this case. The results shown in Section 3 and the aforementioned discussions have confirmed that both ATS-Wil and ATS-Lv2.5 models outperform in T_B^p simulations in the late-monsoon period and both ATS-Lv and ATS-Lv2.5 models do so in the post-monsoon periods except for the freeze-thaw transition period. Figures reflecting the impacts of geometric roughness are thus only displayed based on the ATS-Wil and ATS-Lv models together with the corresponding baseline models, and discussions are focused on the whole study period except for the freeze-thaw transition period. The error metrics involving R and RMSEs are listed in Table 3 to quantitatively describe the performances of models using varying s .

Simulated T_B^p (especially T_B^H) by the baseline models (Figure 9(a), Figure S7A) is very sensitive to s variations and simulations with large s (e.g., 2.5 cm) are closer to observations compared to those with small s during the late-monsoon and post-monsoon periods. Please also see reduced RMSEs with larger s in Table 3. However, most simulations cannot capture diurnal variations of T_B^p compared to observations. With the ATS model integrated, variations of T_B^p (especially T_B^H) can be captured, and the impacts of s variations on T_B^H during the late-monsoon period are reduced (i.e., see a narrow range of variations of

T_B^H with different s settings in Figure 9(b, 1)), although this is less apparent for T_B^V (Figure 9(b, 2), Figure S7B-2). T_B^p simulations with small s (e.g., 0.75 cm) present overestimations (Figure 9(b, 1)), which is opposite from those based on the Base-Wil model. T_B^p simulations with s of 2.5 cm are found consistent with those using s of 0.9 cm (similar large R and small RMSEs in Table 3) and match observations except during the soil freeze-thaw transition period (Figures S7A, B). However, the calculated microwave polarization difference index ($MPDI = (T_B^V - T_B^H) / (T_B^V + T_B^H)$) with s of 2.5 cm does not show the observed diurnal variations, while it does with s of 0.9 cm (Figure 9(c), Figure S7C). This indicates that the positive effects imposed by large geometric surface roughness (e.g., $s = 2.5$ cm) on surface emission may become dominant and balance the negative effects of SM in the ATS model. By contrast, the ATS model with s of 0.9 cm can continuously capture dynamic variations of dielectric roughness, not only at the soil surface related to the distribution of water and geometric roughness but also with the soil volume. Based on these analyses, the surface geometric roughness parameters ($s = 0.9$ cm and $L = 9$ cm) used in the ATS model are proved sufficient in this study. Surface geometric roughness may have slight changes due to the soil freeze-thaw processes such as frozen soil water causing volume expansion and melted surface water might smooth the surface, but this is beyond the scope of this study.

4.3. *The Impacts of Fixed h_{ss}/h Analog to H_R Used in SMAP and SMOS-CMEM Systems on T_B^p Simulations.* SMAP and SMOS brightness temperature forward modelling use the fixed soil roughness parameter H_R [25, 68] for SM retrievals at the global scale. Given the similarity between h_{ss}/h derived from the ATS model and H_R (see Section 4.1), this section attempts to investigate the impacts of fixed roughness parameters analogous to those used in SMAP and SMOS retrievals on T_B^p modelling. In the SMAP SM retrieval algorithms, the parameter H_R is assumed to be linearly related

FIGURE 9: Comparisons of simulated T_B^p by different models with different s (0.75, 0.9, 1.2, 1.5, and 2.5 cm) settings with constant L (9 cm) to ELBARA-III observations. (a, b) By the Base-Wil and ATS-Wil models, respectively, for the late-monsoon period. (c) The calculated MPDI ($= (T_B^V - T_B^H)/(T_B^V + T_B^H)$) with s of 0.9 cm and 2.5 cm for the late-monsoon period. Base-Lv and Base-Wil represent experiments using AIEM +TVG in combination with Wilheit's and Lv's models separately. ATS-Lv and ATS-Wil denote experiments using ATS+AIEM+TVG in combination with Wilheit's and Lv's models separately.

to s by $H_R = 0.1 \text{ cm}^{-1} \cdot s$ with s of 1.56 cm for grassland [75]. The default SMAP H_R of 0.156 is reported too low for T_B^p modelling on the Tibetan Plateau in comparisons to the recommended Wigneron soil roughness model [71] ($H_R = (0.9437 \cdot s / (0.8865 \cdot s + 2.29143))^6$) with the same s ($= 1.56$ cm) adopted [45]. For SMOS T_B^p long-term monitoring at ECMWF (European Centre for Medium-Range Weather Forecasts), the simple Wigneron soil roughness model [53] ($H_R = 1.3972 \cdot (s/L)^{0.5879}$) with s of 2.2 cm and L of 6 cm is used in the CMEM (Community Microwave Emission Modelling Platform) [76]. The Choudhury soil roughness model [68] ($H_R = (2ks)^2$) used in the SMOS SM

retrievals [27] has $H_R = 1.73$ if s of 2.2 cm is used as in CMEM, and this parameterization is found inferior compared to the simple Wigneron [53] soil roughness model [76]. It is to note this H_R ($= 1.73$) is different from the scaled h_{SS} (i.e., h_{SS}/h), which has a maximum value of one in this study. An alternative SMOS soil moisture product (SMOS-IC) [77] uses globally mapped H_R values decoupled from the optimized combined vegetation and roughness parameter TR ($= \tau_{\text{nad}} + (2/H_R)$, where τ_{nad} is vegetation optical depth at nadir [78]), by assuming a linear relationship between TR and LAI obtained from MODIS. As such, uncertainties of the obtained H_R are more related to vegetation properties than the surface roughness which is the primary

FIGURE 10: Simulated T_B^p by the ATS-Wil model using fixed roughness parameters compared to ELBARA-III observations for the late-monsoon period. SMOS-CMEM is with $h_{ss}/h = 0.77$ and SMAP with $h_{ss}/h = 0.58$.

TABLE 4: Comparisons of simulated T_B^p by the ATS-based models using fixed roughness parameters compared to ELBARA-III observations. SMOS-CMEM is with $h_{ss}/h = 0.77$ and SMAP with $h_{ss}/h = 0.58$. The ATS-Wil model is for the late-monsoon period and the ATS-Lv model for the post-monsoon period.

Polarization	Period Experiments	Late-monsoon		Post-monsoon	
		R	RMSE (K)	R	RMSE (K)
H	SMOS-CMEM	0.89	10.7	0.40	11.5
	SMAP	0.89	28.7	0.29	26.9
V	SMOS-CMEM	0.87	7.6	0.47	9.2
	SMAP	0.87	9.7	0.51	13.3

interest of this paper. On the other hand, the obtained H_R is directly applied for SMOS-IC retrieval, and there is no quantified relationship between H_R and geometric roughness parameters (s , L). Given the large impact of s on ATS+AIEM+TVG modelling (see Section 4.2), SMOS-IC H_R is not a good choice used for comparisons in this study. To facilitate the comparison, h_{ss}/h is set as constant to match $H_R = 0.77$ (used in SMOS-CMEM) and $H_R = 0.58$ (suggested in SMAP over the Tibetan Plateau), respectively, during the study period. The same s and L adopted in SMOS-CMEM and SMAP are used for ATS-based model simulations. The N_p parameter is set the same as in this study (i.e., 0 for H polarization and -1 for V polarization).

T_B^H simulated by the ATS-based models with the SMAP setting (i.e., $h_{ss}/h = 0.58$) are found lower than observations during the late-monsoon (Figure 10, RMSE of 28.7 K in Table 4) and post-monsoon periods (Figure S8, RMSE of 26.9 K in Table 4). By contrast, moderate underestimations are seen for T_B^V simulations (Figure 10, Figure S8) with

RSME of 9.7 K and 13.3 K (Table 4) for the late-monsoon and post-monsoon periods, respectively. This may explain why only T_B^V is used in SMAP soil moisture retrieval algorithms [79], which might be due to its less sensitivity to changes of surface roughness (see a narrower dynamic range of T_B^V simulations than T_B^H in Figure 9, and T_B^p (50°) simulation results in Section 4 of the supplementary materials). The similar finding is also reported by [80]. T_B^p simulated by the ATS-based models with the SMOS-CMEM setting (i.e., $h_{ss}/h = 0.77$) are found close to observations during the late-monsoon and post-monsoon periods (RMSEs ≤ 13.3 K in Table 4) but do not have observed strong diurnal variations (Figure 10, Figure S8). Furthermore, the fixed roughness parameter cannot capture temporal variations in roughness characteristics related to changing surface conditions driven by the weather system, especially during the soil freeze-thaw transition period. In contrast, the proposed ATS model in this study (see Section 4.1) has the potential to reflect the dynamics of dielectric

roughness related to surface conditions, which is important for improving SM retrievals at the global scale.

In summary, the enhanced ATS model coupled with the AIEM+TVG model is validated for the use for natural grassland. The proposed ATS model, as a physically based one, is expected to be applied once all parameters are available for the area of interest (e.g., bare soil, cropland, and forest). Parameters such as wavelength and polarization are from sensor configuration. The roughness parameters (i.e., s , L , and Np) are very difficult to estimate but effective ones can be obtained by calibration using satellite backscatter and brightness temperature observations and soil moisture measurements as introduced by [47, 61]. When *in situ* measurements are not available, the most consistent input of profile SMST can be estimated by using land surface models (LSMs), such as Community Land Model (CLM) [81] and Noah LSM [82], while the simulation results shall be validated to assure the accuracy. Soil texture information can be obtained from global and regional soil maps, for instance, SoilGrids1km [83] suggested for the Tibetan Plateau [38]. It is to note that AIEM used in this study only involves single scattering terms [80]. Once the multiple scattering term is incorporated, the ATS model shall be coupled with the updated version to make the calculation of scattering more realistic.

Last but not least, we would like to highlight the potential uses of the ATS model for microwave multifrequency (i.e., commonly used 1-10 GHz) applications, because it considers the wavenumber factor when parameterizing the dielectric roughness h_{SV} induced by inhomogeneity in the soil volume (see Equations (5, 6)) and leads to h scaling with wavelength. On the other hand, the developed ATS model can be applied to the active microwave case. As radar backscatter depends not only on soil moisture dynamics but also on the surface roughness, and better quantification of the latter can contribute to substantial improvements of soil moisture retrieval [61, 84, 85]. When the surface roughness issue is better tackled with our proposed method, better understanding of the vegetation scattering-emission can be focused, as that will contribute further to soil moisture retrieval of vegetated regions.

5. Conclusions

In this study, the Tor Vergata discrete scattering model (TVG) coupled with the advanced integral equation model (AIEM) is used as a basis to investigate the effect of surface roughness on coherent and incoherent emission processes. The developed air-to-soil transition (ATS) model with a proposed dielectric roughness parameterization is integrated with the TVG+AIEM model to investigate seasonal T_B^p signals as observed by ELBARA-III radiometer on an eastern Tibetan alpine meadow. The Wilheit [22] coherent and Lv [29] incoherent models are compared in quantifying the dielectric constant of bulk soil in the ATS zone together with *in situ* SM at 2.5 cm and in calculating soil effective temperature T_{eff} (T_{eff_Wil} and T_{eff_Lv}). The penetration depths representing the sensing depth of T_{eff} derived from the coherent (δ_T) and incoherent (δ_{PD}) models are also compared.

The reduced discrepancy (≈ 20 –50 K) between the modelled and observed T_B^p demonstrates that the ATS model is a necessity in seasonal L-band T_B^p simulations. The dielectric roughness thickness h parameterized in the ATS model can describe well the surface roughness resulted from fine-scale topsoil structures characterized by SM and geometric roughness effects and from the soil volume that is due to the heterogeneous distribution of SM. The proposed dielectric roughness can replace the fixed roughness parameter H_R and capture dynamics of surface roughness related to hydrometeorological conditions. The consideration of dynamic dielectric roughness is important for improving SM retrievals at the global scale, for which the fixed H_R is used in current state-of-the-art processing. Furthermore, the soil porosity and logarithmic SM considered in the h parameterization enhances the physical link between microwave emission models and land surface models, which might improve retrievals of soil physical properties and contribute to developing soil monitoring system utilizing space-based earth observation data with *in situ* data and modelling, especially for remote areas such as the third pole region.

The ATS model combined with Wilheit's coherent model (ATS-Wil) can be applied for T_B^p simulations for soils that are in the quasi-equilibrium condition, such as thawed soils with vegetation cover during the late-monsoon season and the beginning of the post-monsoon period. The ATS model combined with Lv incoherent model (ATS-Lv) is applicable for T_B^p simulations for soils undergoing complex physical processes driven by rapidly changing weather systems, such as the freeze-thaw processes after heavy rainfall events during the post-monsoon season. The ATS model using the *in situ* SM at 2.5 cm (ATS-Lv2.5) can be applied during the whole study period except during the soil freeze-thaw transition period. The discrepancy between modelled and observed T_B^p during the soil freeze-thaw transition period suggests a potential enhancement of the ATS model by considering the effects of ground surface temperature, surface water fraction, and liquid water-ice mixtures in calculating h .

Conflicts of Interest

The authors declare no competing interests.

Authors' Contributions

H.Z. proposed the method and wrote the paper. Z.S. and Y.Z. conceptualized the method and revised the paper. J.W., X.W., Z.W., and X.M. provided and investigated data.

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Supplementary Materials

1. Result analyses for the post-monsoon period, including Figures S1-S4. 2. Figures S5-S8 for the post-monsoon period to support Discussions in the text. 3. Comparisons of T_B^p simulations by considering the impacts of only h_{SS} and $h_{SS} + h_{SV}$, including Figures S9-S10 and Table S1. 4. T_B^p simulations for incidence angles of 50° and 60°, including Figures S11-S12. 5. Two snapshots of Maqu region in Figure S13. (*Supplementary Materials*)

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