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1 **Towards soil moisture profile estimation in the root zone using L- and P-band**
2 **radiometer observations: A coherent modelling approach**

3 Foad Brakhasi ^{a,*}, Jeffrey P. Walker^a, Nan Ye ^a, Xiaoling Wu^a, Xiaoji Shen^{a,b}, In-Young Yeo^c,
4 Nithyapriya Boopathi^d, Edward Kim^e, Yann Kerr^f, and Thomas Jackson^g

5
6 ^a Department of Civil Engineering, Monash University, Clayton, Australia

7 ^b Yangtze Institute for Conservation and Development, Hohai University, Nanjing, China

8 ^c School of Engineering, The University of Newcastle, Callaghan, Australia

9 ^d IITB-Monash Research Academy, Mumbai, India

10 ^e NASA Goddard Space Flight Center, Greenbelt, USA

11 ^f Centre d'Etudes Spatiales de la Biosphère, Toulouse, France

12 ^g USDA ARS Hydrology and Remote Sensing Laboratory (Retired), Beltsville, USA

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29 **Corresponding author.*

30 *E-mail addresses: foad.brakhasi@monash.edu, brakhasi.f@gmail.com.*

31 **ABSTRACT**

32 Precision irrigation management and crop water stress assessment rely on accurate estimation
33 of root zone soil moisture. However, only the top 5 cm soil moisture can be estimated using
34 the two current passive microwave satellite missions, Soil Moisture and Ocean Salinity
35 (SMOS) and Soil Moisture Active Passive (SMAP), which operate at L-band (wavelength of
36 ~21 cm). Since the contributing depth of the soil to brightness temperature increases with
37 observation wavelength, it is expected that a P-band (wavelength of ~40 cm) radiometer could
38 potentially provide soil moisture information from deeper layers of the soil profile. Moreover,
39 by combining both L- and P- bands, it is hypothesized that the soil moisture profile can be
40 estimated even beyond their individual observation depths. The aim of this study was to
41 demonstrate the potential of combined L-band and P-band radiometer observations to estimate
42 the soil moisture profile under flat bare soil using a stratified coherent forward model.
43 Brightness temperature observations at L-band and P-band from a tower based experimental
44 site across a dry (April 2019) and a wet (March 2020) period, covering different soil moisture
45 profile shapes, were used in this study. Results from an initial synthetic study showed that the
46 performance of a combined L-band and P-band approach was better than the performance of
47 using either band individually, with an average depth over which reliable soil moisture profile
48 information could be estimated (i.e. with a target root mean square error (RMSE) of less than
49 $0.04 \text{ m}^3/\text{m}^3$) being 20 cm for linear and 15 cm for second-order polynomial functions. Other
50 functions were also tested but found to have a poorer performance. Applying the method to
51 the tower-based brightness temperature achieved an average estimation depth of 28 cm (20
52 cm) and 5 cm (5 cm) during the dry and wet periods respectively when using a second-order
53 polynomial (linear) function. These findings highlight the opportunity of a satellite mission
54 with L-band and P-band observations to accurately estimate the soil moisture profile to as deep
55 as 30cm globally.

56 **Keywords:** Soil moisture profile estimation, Coherent model, Multi-frequency, L-band, P-
57 band, Passive microwave

58 **1. Introduction**

59 Soil moisture is a key state variable in the water, energy, and carbon cycles (Falloon et al.,
60 2011; Zhang et al., 2019). While soil moisture accounts for only a small fraction of the
61 freshwater globally (0.15%), it has an important impact on rainfall-runoff processes (Brocca et
62 al., 2012), regulates net ecosystem exchange (Chu et al., 2019), constrains food security (Sadri
63 et al., 2020), and influences land-atmosphere interactions (Yuan et al., 2020). However, many
64 studies have shown large variability in the spatial and temporal distribution of soil moisture,
65 especially in the top 20 cm of the soil (Shi et al., 2014), emphasizing the necessity of monitoring
66 these variations. Moisture in this region of the soil profile limits the plant's photosynthetic
67 activity and transpiration (Seneviratne et al., 2010; Reich et al., 2018). In addition, information
68 on the root zone soil moisture is used for irrigation scheduling (Liang et al., 2016),
69 understanding of plant stress and pesticide management (Malone et al., 2004; Jiang et al.,
70 2021). As compared to estimation of moisture in the shallow layer, root zone soil moisture
71 estimation is more challenging (Etminan et al., 2020). Accurate spatial and periodic mapping
72 of this vital variable through direct measurement is almost impossible due to its cost-intensive
73 and time-consuming measurement, higher spatio-temporal variability, and non-linear
74 relationship with surface soil moisture (Das and Mohanty, 2006; Sabater et al., 2007; Hu and
75 Si, 2014; Gao et al., 2019).

76 Microwave remote sensing techniques have been identified as the most promising approach for
77 global observation of near-surface soil moisture content (Karthikeyan et al., 2017).
78 Specifically, passive microwave remote sensing at L-band has been widely adopted with
79 current remote sensing satellites dedicated to the monitoring of soil moisture, including the
80 European Space Agency (ESA) Soil Moisture and Ocean Salinity (SMOS; Kerr et al., 2010)

81 and the National Aeronautics and Space Agency (NASA) Soil Moisture Active Passive
82 (SMAP; Entekhabi et al., 2014) missions. While L-band can observe a deeper layer of soil than
83 shorter wavelengths, its soil moisture measurement is limited to just a few centimeters of the
84 soil (Zheng et al., 2019; Shen et al., 2020, 2022a). Therefore, researchers have investigated
85 different techniques for estimating the root zone soil moisture from surface soil moisture
86 including multiple regression (Qiu et al., 2010; Mahmood et al., 2012), data assimilation
87 (Walker et al., 2001; Baldwin et al., 2017), and statistical/empirical methods such as machine
88 learning (Carranza et al., 2021; Karthikeyan and Mishra, 2021; Xia et al., 2022), principle of
89 maximum entropy (Mishra et al., 2018; Zhou et al., 2016), and exponential filters (Mishra et
90 al., 2020). The approach chosen is usually based on the application, level of complexities
91 involved and the amount of a priori information available. When it comes to applications on a
92 large scale, the number of inputs needed is of utmost importance, especially in areas where data
93 is scarce. As a result, approaches that require minimal inputs have gained attention in these
94 types of applications. Generally, all the models require establishing a relationship between
95 surface and root-zone soil moisture. However, the relationship between the two is often
96 nonlinear and becomes weaker with depth, making it challenging to capture using conventional
97 statistical techniques (Ford et al., 2014).

98 The multiple regression models are simple and relatively straightforward to interpret, but they
99 have limitations in handling complex non-linear relationships between input and output
100 variables. These models are also sensitive to outliers, which means that even a small number
101 of extreme values can significantly affect the results. Conversely, machine learning algorithms
102 are well-suited to handle non-linear relationships between inputs and outputs, making them
103 suitable for modeling complex soil moisture patterns. However, they require large amounts of
104 training data to produce accurate estimates, which can be difficult to obtain in some cases.
105 Additionally, some machine learning algorithms can be difficult to interpret, making it

106 challenging to understand the physical basis for their predictions and to identify areas for
107 improvement. There is also a risk of overfitting, where the algorithm becomes too specialized
108 to the training data and does not generalize well to new data. The principle of maximum entropy
109 method does not rely on prior information about the profile, but it requires the values of surface
110 soil moisture, the average moisture content, and the moisture content of the bottom-most layer,
111 which are difficult to obtain. The exponential filter only requires the time series of surface soil
112 moisture, which is easily available from microwave sensors, however sensitivity is reduced
113 during prolonged dry periods and in deeper layers where plant uptake is the main factor
114 affecting root-zone moisture movement due to the assumption of no transpiration and constant
115 hydraulic conductivity.

116 Current regional or global scale root zone soil moisture products such as Soil Moisture Ocean
117 Salinity (SMOS) level 4 RZSM data, Soil Moisture Active Passive (SMAP) level 4 RZSM
118 data, the Japanese 55-year Reanalysis (JRA-55), National Centers for Environmental
119 Prediction (NCEP) Reanalysis version 1 (NCEP R1) and 2 (NCEP R2), the Modern-Era
120 Retrospective analysis for Research and Applications, Version 2 (MERRA-2), the fifth
121 generation European Centre for Medium-Range Weather Forecasts (ECMWF) atmospheric
122 reanalysis (ERA-5), and the Global Land Data Assimilation System (GLDAS) are based on
123 assimilation of surface soil moisture into land surface models (LSMs) or global hydrological
124 models (GHMs) (Xu et al., 2021). The Ensemble Kalman Filter is a widely used assimilation
125 algorithm in land surface models, but its implementation is claimed to be inappropriate because
126 of non-linear relationships between observations and model states (Clark et al., 2008).

127 Compared with L-band (1.4 GHz; 5cm sensing depth), P-band (750 MHz) has been shown to
128 be more sensitive to soil moisture over deeper layers (~10 cm; Shen et al., 2020). As the L-
129 band and P-band emissions are derived from different depths in the soil (Shen et al., 2020),
130 there is the potential to derive insights into the depth variation of soil moisture by using the

131 two together. Some researchers have used P-band radar alone (Tabatabaenejad et al., 2013,
132 2015, 2016, 2017; Sadeghi et al., 2016; Chen et al., 2018; Etminan et al., 2020; Yueh et al.,
133 2020) or combined with L-band radar (Du et al., 2015; Chen et al., 2016, 2017; Azemati et al.,
134 2019; Yi et al., 2019) to estimate root zone soil moisture. While their results have shown the
135 concept to be promising, they have typically applied constraints, been limited to snapshot
136 retrieval, and been applied to radar rather than radiometer observations. Moreover, a
137 comprehensive investigation of the different mathematical functions that might be used to
138 represent the soil moisture profile is lacking. Importantly, compared with a radiometer, radar
139 is more sensitive to vegetation and surface roughness (Engman and Chauhan, 1995), and thus
140 it is possible that multi-frequency L- and P-band radiometer observations could provide more
141 accurate soil moisture profile estimation than that obtained from radar.

142 The aim of this research was to study the use of multi-frequency (L- and P-band) radiometry
143 to estimate the root zone profile for flat bare soil. The forward stratified coherent model of
144 Njoku and Kong (1977) was applied to calculate brightness temperature (TB) from soil
145 moisture and temperature profiles. While the coherent and incoherent models have the same
146 general trend, the former includes phase-interference oscillations (Ulaby and Long, 2014). The
147 main differences between them relate to the effects of interference, which is a function of
148 frequency and the steepness of soil moisture profile near the surface (Schmugge and
149 Choudhury, 1981). When data from regions of rapid sub-surface moisture variations (rapid
150 drying out or a region having a subsurface water table) are interpreted with depth, the
151 incoherent models become inaccurate, since coherent reflections are not accounted for. Also,
152 when there is considerable diurnal surface temperature variation, incoherent models become
153 inaccurate for longer wavelengths. Thus, the coherent models of Njoku and Kong (1977) and
154 Wilheit (1978) were introduced and formulated in terms of continuous and discrete varying
155 dielectric constant within the soil, respectively. Only a small difference was observed between

156 the Njoku and Wilheit models (Schmugge and Choudhury, 1981) and so in this research the
157 Njoku model was used.

158 The analysis has considered single or dual-frequency, single or dual-polarization, single or
159 multi-incidence angle, and snapshot or time series retrieval options. Several mathematical
160 functions have been investigated as representative functions of the soil moisture profile, namely
161 i) Linear (hereafter Li), ii) Exponential (Exp), iii) Second-order Polynomial (Pn2), iv)
162 simplified solution of the Richards' Equation (RE), v) Parametrized second-order polynomial
163 from the simplified solution of the Richards' Equation (PRE), vi) Third-order Polynomial
164 (Pn3), and vii) Piecewise Linear (PL).

165 **2. Data**

166 As part of the P-band Radiometer Inferred Soil Moisture project (PRISM;
167 www.prism.monash.edu), a comprehensive tower-based experiment site was established at
168 Cora Lynn, Victoria, Australia from October 2017 to September 2021 to advance the state of
169 microwave remote sensing technology readiness (Fig. 1). The tower was instrumented with the
170 Polarimetric P-band Multi-beam Radiometer (PPMR) and the Polarimetric L-band Multi-beam
171 Radiometer (PLMR), operating at 0.742-0.752 GHz and 1.400-1.425 GHz, respectively. The
172 tower was located at the center of 4 quadrants, each with a size of 75 m \times 75 m, in order to
173 observe different land cover conditions but similar soil moisture status (Shen et al., 2020). The
174 PPMR has a phased array antenna with four beams having 30° beamwidth, distributed at angles
175 of $\pm 15^\circ$ and $\pm 45^\circ$ from the normal to the antenna plane, and the PLMR has six antenna beams
176 having 15° beamwidth distributed at angles $\pm 7.5^\circ$, $\pm 21^\circ$, and $\pm 38.5^\circ$ from the normal to the
177 antenna plane. These radiometers could not only be rotated in azimuth to look at the different
178 quadrants but tilted to change the look angles, which was done automatically according to a
179 predefined schedule. Footprints of PLMR and PPMR for two extreme incidence angles of 30°
180 and 60° are shown in Fig. 1. At the middle border of each quadrant ground stations (called

181 stations 126, 127, 128 and 136) were installed, equipped with hydra-probes that simultaneously
 182 measured the soil moisture and temperature from the soil surface to 60 cm depth at 5 cm
 183 intervals. Soil texture analysis was also conducted for different locations and depths, providing
 184 an average (standard deviation, depth 5cm, depth 20 cm, depth 50 cm) soil texture of 18.3% (\pm
 185 3.15%, 18%, 17%, 17%) clay, 13.7% (\pm 5.89%, 12%, 11%, 20%) sand, and 68% (\pm 5.12%,

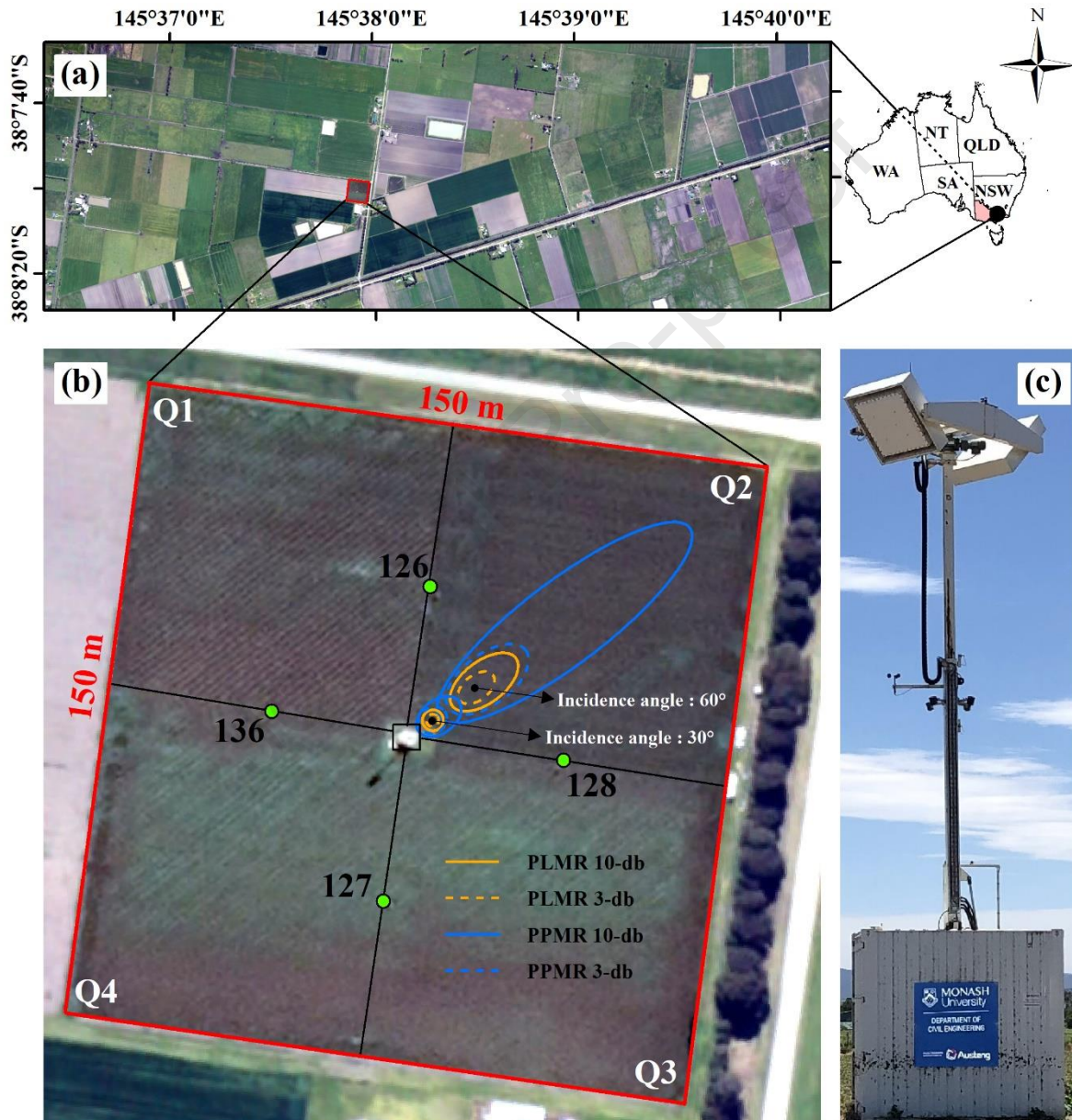


Fig. 1. Location map (a) of the experimental site (b) having a tower (c) at the center of a paddock at Cora Lynn, Victoria, Australia. The colored ovals represent the footprints of the microwave radiometers. The green dots represent the stations installed at the borders of the quadrants Q1 to Q4.

186 71%, 69%, 62%) silt, indicating a silty loam soil. The quadrants were maintained under
 187 different conditions in terms of vegetation type (corn, wheat, grass or bare) and surface
 188 roughness (smooth, furrow and bench furrow with parallel or perpendicular row orientation;
 189 (Shen et al., 2022b)). For simplicity, this research has focused on the flat bare soil condition.
 190 The performance of a multi-frequency optimization approach was investigated using
 191 experimental data of soil moisture and temperature profiles from the soil surface to 60 cm depth

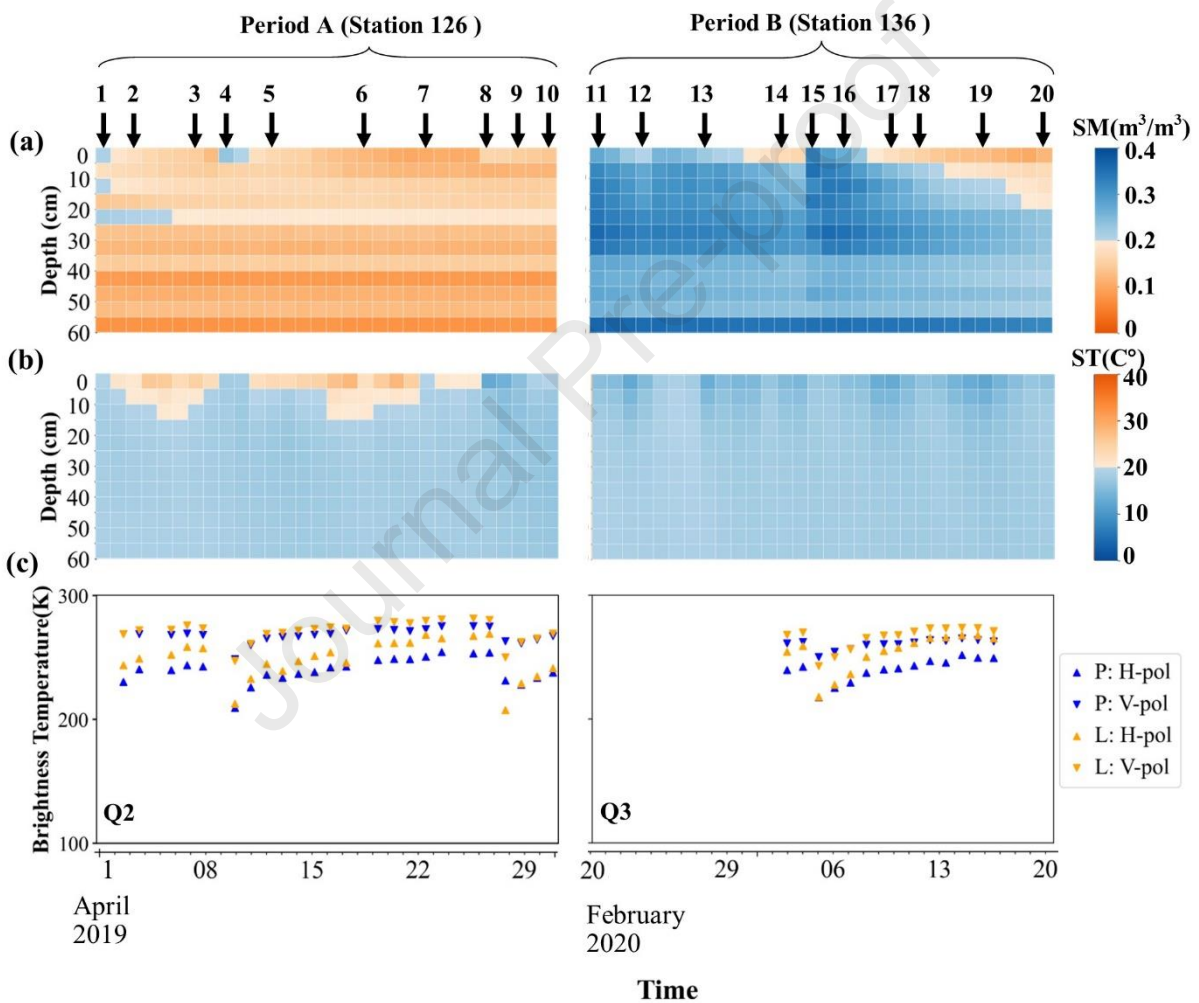


Fig. 2. Evolution time series of (a) soil moisture and (b) soil temperature as a function of depth were measured at Cora Lynn station number 126 (period A) and 136 (period B), and (c) brightness temperature from PPMR and PLMR at quadrant 2 over Period A (1st - 30th April 2019) and quadrant 3 over Period B (20th February to 20th March 2020). The twenty black arrows show the timing of the soil moisture and temperature profiles used for snapshot and time series retrieval in the synthetic study.

192 in 5 cm increments, covering soil moisture conditions ranging from 0.07 to 0.35 m³/m³. Data
 193 from stations 126 and 136 as shown in Fig. 2 (a and b), and tower-based TB as shown in Fig.
 194 2 (c), were used under flat and bare soil conditions for two periods, namely A (1st to 30th April,
 195 2019) and B (20th February to 20th March, 2020). Fig. 2 (a and b) shows the high variability
 196 of moisture and temperature in the near-surface layer relative to deeper layers in the profile. It
 197 is seen during Period A that variation of soil moisture in the deeper layers was much lower
 198 than Period B, with high variability of moisture in almost all of the soil layers. Despite rapid
 199 drying of the surface and shallow layers, the deeper layers of the soil were slow to respond (see
 200 soil moisture at deeper layers in Fig. 2 (a)). Compared to soil moisture, soil temperature has a

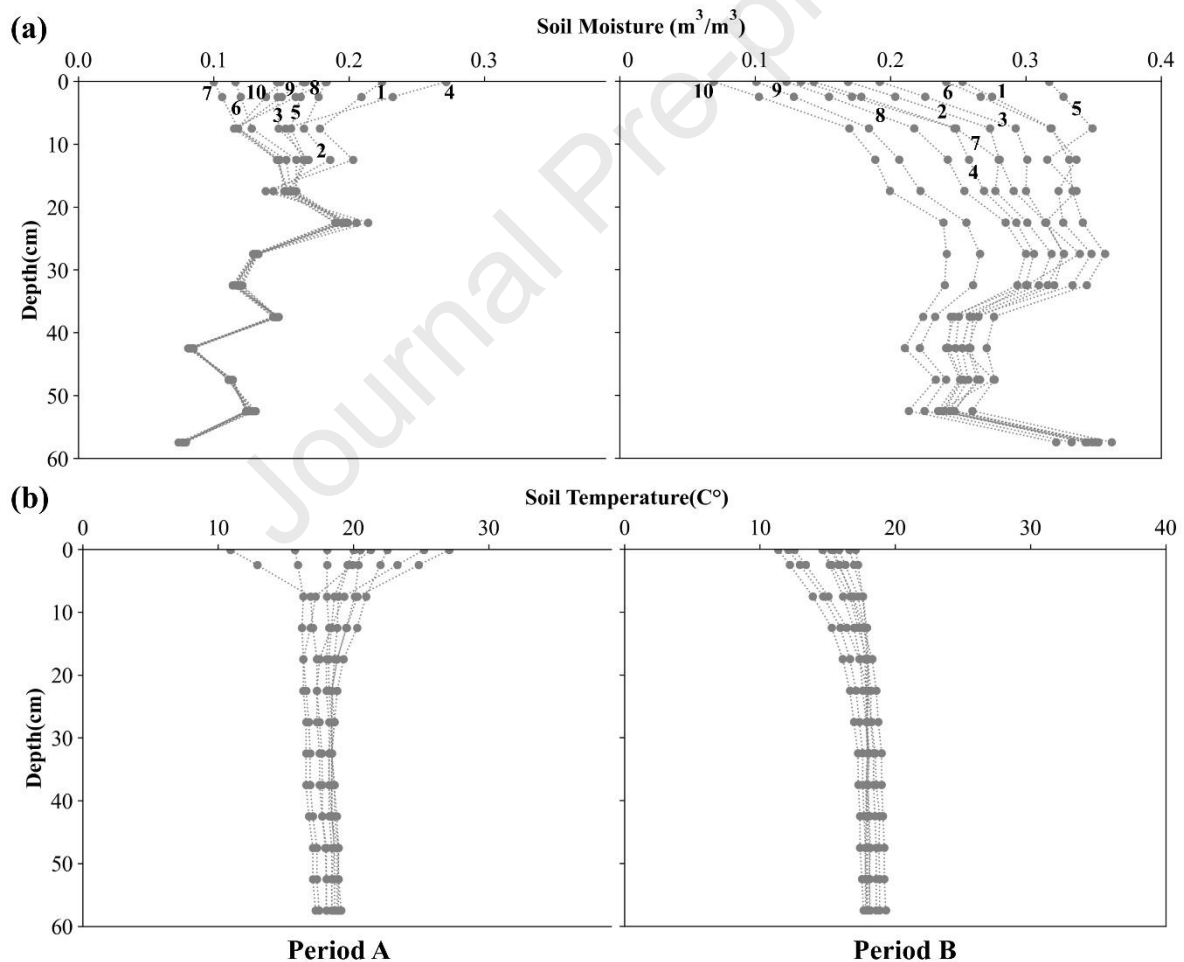


Fig. 3. Selected (a) soil moisture and (b) temperature profiles for this research. All of these soil moisture profiles were used in investigating different mathematical functions to represent the soil moisture and soil temperature profile.

201 strong day to day variation and cooling of the near-surface layer relative to deeper layers for
202 Period A compared with Period B (Fig. 2 (c)).

203 In an initial synthetic study, the twenty soil moisture and soil temperature profiles in Fig. 3,
204 selected from the two periods in Fig. 2 to cover the different profile shapes identified in Fig. 4,
205 were used to predict TB values for developing the soil moisture profile estimation process. The
206 selected data were used for answering questions including: i) if single or multi-frequency
207 provide better results; ; ii) if single or multi-incidence angles yield better results; iii) if single
208 (H or V) or dual (H and V) polarization provide a more robust solution; iv) which mathematical
209 function(s) provides the best results; v) whether a snapshot or time series approach performs
210 best; and vi) the impact of soil temperature profile approximation on the soil moisture profile
211 estimation accuracy?

212 **3. Methodology**

213 Quantification of soil moisture using passive microwave remote sensing relies on a model,
214 which in its simplest form can be a regression model, or in its most complex form a physical
215 model. Microwave emission models are physical models that take the form of either a coherent
216 or an incoherent model for soil moisture estimation. In this research, the coherent stratified
217 model of Njoku and Kong (1977) was employed.

218 *3.1 Forward model background*

219 A vertically inhomogeneous half-space model (Njoku and Kong, 1977), hereafter referred to
220 as the Njoku model, was used as the forward model to simulate TB at the sensor level. The
221 theory behind such an approach uses electromagnetic fluctuations and electromagnetic wave
222 propagation as formulated by Stogryn (1970), which established a relationship between emitted
223 energy and the properties of the medium (surface roughness, soil moisture, and physical

224 temperature). Mathematically, TB at H (Eq.1) and V (Eq.2) polarization from the Njoku model
 225 is written as:

$$TB_H = \frac{k}{\cos\theta} \int_{-\infty}^0 dz T(z) \epsilon_r''(z) |\psi(z)|^2 \quad (1)$$

$$TB_V = \frac{1}{k \cos\theta} \int_{-\infty}^0 dz T(z) \epsilon_r''(z) \cdot \left\{ \left| \frac{1}{\epsilon_r(z)} \frac{d\phi(z)}{dz} \right|^2 + \left| \frac{k_x \phi(z)}{\epsilon_r(z)} \right|^2 \right\} \quad (2)$$

226 where $K = \frac{2\pi}{\lambda}$ is the free space wave number, $k_x = k \sin\theta$, θ is the angle of observation,
 227 $\epsilon_r(z) = \epsilon_r'(z) + i\epsilon_r''(z)$ is the complex dielectric constant profile, and $T(z)$ is the soil
 228 temperature profile. The functions $\psi(z)$ and $\phi(z)$ are solutions of the following two second-
 229 order differential equations (Eq.3 and Eq.4):

$$\left\{ \frac{d\psi(z)}{dz} + ik \cos\theta [2 - \psi(z)] \right\}_{z=0} = 0 \quad (3)$$

$$\left\{ \frac{d\phi(z)}{dz} + i\epsilon_r(z) k \cos\theta [2 - \phi(z)] \right\}_{z=0} = 0. \quad (4)$$

230 These wave propagation equations are solved in conjunction with the boundary condition for a
 231 smooth surface. From the perspective that at lower frequencies more information about soil
 232 moisture comes from the deeper layers of the soil, Tsang et al. (1975) reformulated Eq.1 and
 233 Eq.2 for a large number of horizontal layers. This was then incorporated by Njoku and Kong
 234 (1977) and referred to as a stratified medium approach for smooth and bare soil according to
 235 Eq.5 (for H polarization) and Eq.6 (for V polarization):

$$TB_H = \frac{k}{\cos\theta} \sum_{l=1}^N \frac{\epsilon_l'' T_l}{\epsilon_0} \left(\frac{|A_l \exp(-ik_{lz} d_l)|^2}{2k_{lz}''} \{1 - \exp[2k_{lz}''(d_{l-1} - d_l)]\} \right. \quad (5)$$

$$- \frac{|B_l \exp(-ik_{lz} d_l)|^2}{2k_{lz}''} \{1 - \exp[-2k_{lz}''(d_{l-1} - d_l)]\}$$

$$- \left(\frac{[A_l \exp(-ik_{lz} d_l)][B_l \exp(-ik_{lz} d_l)]^*}{2ik_{lz}' } \right) \{1$$

$$- \exp[-i2k_{lz}'(d_{l-1} - d_l)]\}$$

$$+ \left(\frac{[A_l \exp(-ik_{lz} d_l)]^* [B_l \exp(-ik_{lz} d_l)]}{2ik_{lz}' } \right) \{1$$

$$- \exp[-i2k_{lz}'(d_{l-1} - d_l)]\} + \frac{k}{\cos\theta} \frac{\epsilon_t'' T_t}{\epsilon_0} \frac{|T_h|^2 \exp(-2k_{tz}'' d_n)}{2k_{tz}''}$$

$$TB_V = \frac{k}{\cos\theta} \sum_{l=1}^N \frac{\epsilon_l'' T_l}{\epsilon_0 |k_l|^2} (|k_{lz}|^2 \quad (6)$$

$$+ k_x^2) \left[\frac{|C_l \exp(-ik_{lz} d_l)|^2}{2k_{lz}''} \{1 - \exp[-2k_{lz}''(d_l - d_{l-1})]\} \right.$$

$$- \frac{|D_l \exp(ik_{lz} d_l)|^2}{2k_{lz}''} \{1 - \exp[2k_{lz}''(d_l - d_{l-1})]\}$$

$$+ \frac{|k_{lz}|^2 - k_x^2}{|k_{lz}|^2 + k_x^2} \left(\frac{[C_l \exp(-ik_{lz} d_l)][D_l \exp(-ik_{lz} d_l)]^*}{2ik_{lz}' } \{1$$

$$- \exp[-i2k_{lz}'(d_l - d_{l-1})]\}$$

$$- \frac{[C_l \exp(-ik_{lz} d_l)]^* [D_l \exp(ik_{lz} d_l)]}{2ik_{lz}' } \{1$$

$$- \exp[-i2k_{lz}'(d_l - d_{l-1})]\} \right]$$

$$+ \frac{k}{\cos\theta} \frac{\epsilon_t'' (|k_{tz}|^2 + k_x^2) T_t}{\epsilon_0 |k_t|^2} |T_v|^2 \frac{\exp(-2k_{tz}'' d_n)}{2k_{tz}''},$$

236 where θ is the incidence angle, index l is the ID of the layer, $k = \frac{2\pi}{\lambda} = \omega \sqrt{\mu_0 \epsilon_0}$ is the

237 wavenumber in free space (λ is the wavelength, ω is the frequency in radian/sec, μ_0 is the

238 permeability of free space, ϵ_0 is the permittivity of free space), $\epsilon_l = \epsilon_l' + i\epsilon_l''$ is the complex
 239 permittivity of the l^{th} layer, $\frac{\epsilon_l}{\epsilon_0}$ is the dielectric constant of l^{th} layer, T_l is the temperature in the
 240 l^{th} layer, $k_l = \omega\sqrt{\mu_0\epsilon_l}$ is the wavenumber in the l^{th} layer, $k_{lz} = k_{lz}' + ik_{lz}'' =$
 241 $k\sqrt{\epsilon_l/\epsilon_0 - \sin^2\theta}$, d_l is the depth below the surface, and n is the total number of horizontal
 242 layers. The quantities A_l, B_l, C_l, D_l, T_h and T_v are wave amplitudes that are related to each
 243 other by propagation matrices. The impact of surface roughness was considered based on a
 244 semi-empirical approach (referred here to as the HQN model) which was proposed by (Wang
 245 and Choudhury, 1981) and developed by (Wigneron et al., 2001) through Eq.7.

$$r_{GP}(\theta) = \left[(1 - q_P(\theta))r_{GP}^*(\theta) + q_P(\theta)r_{GQ}^*(\theta) \right] \exp(-h_P(\theta)\cos^{n_P}(\theta)), \quad (7)$$

246 where q_P (with $P = H$ and $Q=V$ or $P = V$ and $Q=H$) is a polarization mixing factor, h_P is a
 247 surface roughness parameter, and n_P is the angular dependence of the surface roughness. The
 248 parameter h_P was calculated using (Wigneron et al., 2001) by Eq.8:

$$h_P = 1.3972 * \left(\frac{rms}{lc} \right)^{0.5879}, \quad (8)$$

249 where rms and lc are the RMS height and correlation length measured at the field for the two
 250 study periods. The parameter q_P was set to 0 for both L- and P- bands. The parameter n_P was
 251 calibrated using Eq.7 and the Njoku model from another period of data, yielding values of -
 252 0.50 (1.80) and -0.333 (0.415) at H (V) polarizations for L-band and P-band respectively. The
 253 parameter r_{GP}^* is the specular reflectivity calculated from the Fresnel equations for H (Eq.9)
 254 and V (Eq.10) polarizations such that:

$$r_{GH}^* = \left| \frac{\cos(\theta) - \sqrt{\epsilon_r - \sin^2(\theta)}}{\cos(\theta) + \sqrt{\epsilon_r - \sin^2(\theta)}} \right|^2 \quad (9)$$

$$r_{GV}^* = \left| \frac{\epsilon_r \cdot \cos(\theta) - \sqrt{\epsilon_r - \sin^2(\theta)}}{\epsilon_r \cdot \cos(\theta) + \sqrt{\epsilon_r - \sin^2(\theta)}} \right|^2, \quad (10)$$

255 where $\varepsilon_r = \varepsilon_r' - i \cdot \varepsilon_r''$ is the relative soil dielectric constant which includes real (') and
 256 imaginary (") parts, and θ is the incidence angle. Using the coherent model, the emissivity is
 257 calculated in each layer, so by adjusting the calculated surface layer emissivity for roughness
 258 before multiplying by the physical temperature, the roughness can be included in the overall
 259 TB estimate by summing the TB contributions from each layer. Using the stratified coherent
 260 model to calculate the TB, with inputs of soil moisture and temperature, requires selecting an
 261 appropriate soil dielectric model, profile depth and a number of horizontal layers (profile depth
 262 divided by layer thickness). Here the multi-relaxation generalized refractive mixing dielectric
 263 model (Mironov et al., 2013, 2014) was used, as it considers the interfacial (Maxwell-Wagner)
 264 relaxation of water in the soil, which is significant at P band (Zhang et al., 2020). Schmugge
 265 and Choudhury (1981) recommended there be a total of 100 layers in 1 m profile depth (layer
 266 thickness varies from 0.003 cm at the surface to 1 cm at a depth of 9 cm and 5 cm at a depth of
 267 40 cm) for 1.4 GHz frequency and higher. However, based on a sensitivity analysis using a
 268 combination of synthesized soil moisture and temperature profiles at various incidence angles
 269 using L- and P-band and H/V polarization, the profile depth and the number of horizontal layers
 270 did not exceed 0.9 m and 56 (when the layer thickness was 0.016). However, for preventing
 271 error from the numerical configuration of the model, they were set to 1 m and 0.01 m
 272 respectively, with 100 layers.

273 *3.2 Mathematical representation of soil moisture and temperature profile*

274 Several mathematical functions including Li (Eq.11), Exp (Eq.12), Pn2 (Eq.13), Pn3 (Eq.14),
 275 PL (Eq.15), RE (Eq.16) and PRE (Eq.21) were selected from literature (Reutov and Shutko,
 276 1986; Tabatabaenejad et al., 2015; Cuenca et al., 2016). Mathematically these functions are:

$$SM(z) = az + c \quad (11)$$

$$SM(z) = c + b(\exp(-az) - 1)/(\exp(-az_1) - 1) \quad (12)$$

$$SM(z) = az^2 + bz + c \quad (13)$$

$$SM(z) = az^3 + bz^2 + dz + c \quad (14)$$

$$SM(z) = c + az + b(z - z_1)x, \quad (15)$$

277 where z is depth (positive downward) and a , b , c and d are coefficients of the related function.
 278 Table 1 shows the boundaries of each parameter. The parameters a in Eq.11 and Eq.15
 279 represent the profile slope of soil moisture content, while in Eq.12 and Eq.13 along with d in
 280 Eq.14 control the shape of the profile. Parameter b in Eq.12 is the change of moisture from the
 281 surface to the depth z_1 (0.6 m in this study), while in Eq.15 its value along with the a parameter
 282 is the slope of the second piece of the piecewise linear function. The parameter c in Eq.11 to
 283 Eq.15 represents the surface soil moisture content. Parameter z_1 in Eq.12 is the depth after
 284 which the soil moisture can be considered constant, while Eq.15 contains two linear segments
 285 that join at the depth z_1 . Moreover, the binary vector x in Eq.15 is mathematically written as:
 286 if ($z \leq z_1, 0, 1$). Notably, each of these functions has different computational requirements and
 287 degrees of complexity for fitting the shape variables. For example, the linear function has only
 288 two shape variables, while the exponential and second-order polynomial functions have three

Table 1. The boundaries of parameters used in the mathematical functions. SP (Shape Parameter; unitless), SSM (Surface Soil Moisture; % in Equations 12, m³/m³ in the rest), and ΔSM (the change of moisture in the profile from surface to the bottom of the profile (here 60 cm); %). The numbers in the brackets show the boundary [lower, upper] of each parameter.

Equation	a	b	c	d
11	Slope [-0.83, 0.83]	-	SSM [0, 0.5]	-
12	SP [-50, 50]	ΔSM [-35, 35]	SSM [0, 50]	-
13	SP [-1, 1]	SP [-1, 1]	SSM [0, 0.5]	-
14	SP [-1, 1]	SP [-1, 1]	SSM [0, 0.5]	SP [-1, 1]
15	Slope [-1, 1]	Slope [-1, 1]	SSM [0, 0.5]	-

289 shape variables, and the third-order polynomial and piecewise linear each have four shape
 290 variables. The simplified solution to Richards' equation Eq.16 has five parameters, two of
 291 which are empirical parameters (h_{cM} and P) related to effective capillary drive and soil pore
 292 size distribution respectively, given for different soils in Table 1 (51.64 and 10.84 respectively
 293 for the silty loam soil used here) of Sadeghi et al. (2016), while the rest (a , b , and c) are
 294 parameters controlling the shape of the profile and do not have any physical meaning.
 295 Consequently, these were parametrized according to the value of soil moisture at the top (θ_1),
 296 middle (θ_2), and bottom (θ_3) of the investigated depth (z_1 , z_2 and z_3) as follows (Sadeghi et
 297 al., 2016):

$$SM(z) = (az + b \exp\left(\frac{z}{h_{cM}}\right) + c)^{\frac{1}{P}} \quad (16)$$

$$a = \frac{\theta_3^P - \theta_1^P - A(\theta_2^P - \theta_1^P)}{z_3 - z_1 - A(z_2 - z_1)} \quad (17)$$

$$b = \frac{\theta_2^P - \theta_1^P - a(z_2 - z_1)}{\exp\left(\frac{z_2}{h_{cM}}\right) - \exp\left(\frac{z_1}{h_{cM}}\right)} \quad (18)$$

$$c = \theta_1^P - az_1 - b \exp\left(\frac{z_1}{h_{cM}}\right) \quad (19)$$

$$A = \frac{\exp\left(\frac{z_3}{h_{cM}}\right) - \exp\left(\frac{z_1}{h_{cM}}\right)}{\exp\left(\frac{z_2}{h_{cM}}\right) - \exp\left(\frac{z_1}{h_{cM}}\right)}. \quad (20)$$

298 Assuming $P = 1$ and/or h_{cM} is larger than the investigation domain ($\frac{z}{h_{cM}} < 1$) leads to a
 299 second-order polynomial approximation (Eq.21):

$$SM(z) = az + b \exp\left(\frac{z}{h_{cM}}\right) + c. \quad (21)$$

300 It is worth noting that the unknown parameters of Eq.16 and Eq.21 include the soil moisture
 301 value at the surface, middle, and bottom of the soil profile (0, 30 and 60 cm in the application
 302 here). When $P > 1$, and $\theta_1 < \theta_2 < \theta_3$ or $\theta_1 > \theta_2 < \theta_3$, the calculated soil moisture profile using

303 Eq.16 is undefined for a part of the profile. To solve this problem, P is considered as 1 so that
304 the second-order polynomial in Eq.21 can be used.

305 Data throughout the period December 2017 to December 2019, having different wetting and/or
306 drying regimes, was used to identify typical profile shapes and analyze the seven mathematical
307 functions identified from literature for approximating soil profile conditions. This step was
308 undertaken to aid in estimating the root zone soil moisture profile, as estimating a few shape
309 parameters is a simpler task than estimating directly the soil moisture at multiple depths in the
310 soil. The profile types (or shapes) are distinguished by changes in their moisture gradient, and
311 their dynamic response to precipitation, evapotranspiration, soil properties etc. Type 1 in Fig.
312 4 (a) is a soil moisture profile that has little variation with depth (gradient or slope which can
313 be decreasing, stable, or increasing). Type 2 in Fig. 4 (b) is a dry case with higher soil moisture
314 at depth due to exfiltration. Type 3 in Fig. 4 (c) occurs when rain has wetted the soil near the
315 surface and this has moved down through the soil column as plug flow, resulting in a sharp
316 gradient neat the bottom of the profile. It could also happen if there are large differences in the
317 soil texture such that the shallow layer can hold the moisture while the bottom of the profile
318 does not. Type 4 in Fig. 4 (d) is where infiltration has occurred (due to rainfall) on the profile
319 of Type 1, such that the profile takes a concave shape. Type 5 in Fig. 4 (e) is the most complex,
320 taking on a S shape likely due to alternate wetting and drying cycles, resulting in substantial
321 moisture variation throughout the profile. Samples of observed soil moisture profiles along
322 with a typical soil temperature profile and their comparison with the fitted functions are
323 illustrated in Fig. 4.

324 From the analysis it was concluded that depending on the time of the year, site, and its soil
325 texture and infiltration dynamics, a mathematical function with a higher number of parameters
326 will typically represent the soil moisture profile more accurately. The average RMSE (from
327 surface to 60 cm depth) between soil moisture profiles from the fitted function and observed

328 soil moisture profiles were 0.026 (PL), 0.028 (Pn3), 0.03 (Pn2 and PRE), 0.032 (Exp), 0.034
 329 (RE), and 0.035 (Li) (the unite is m^3/m^3). However, the greater number of parameters also

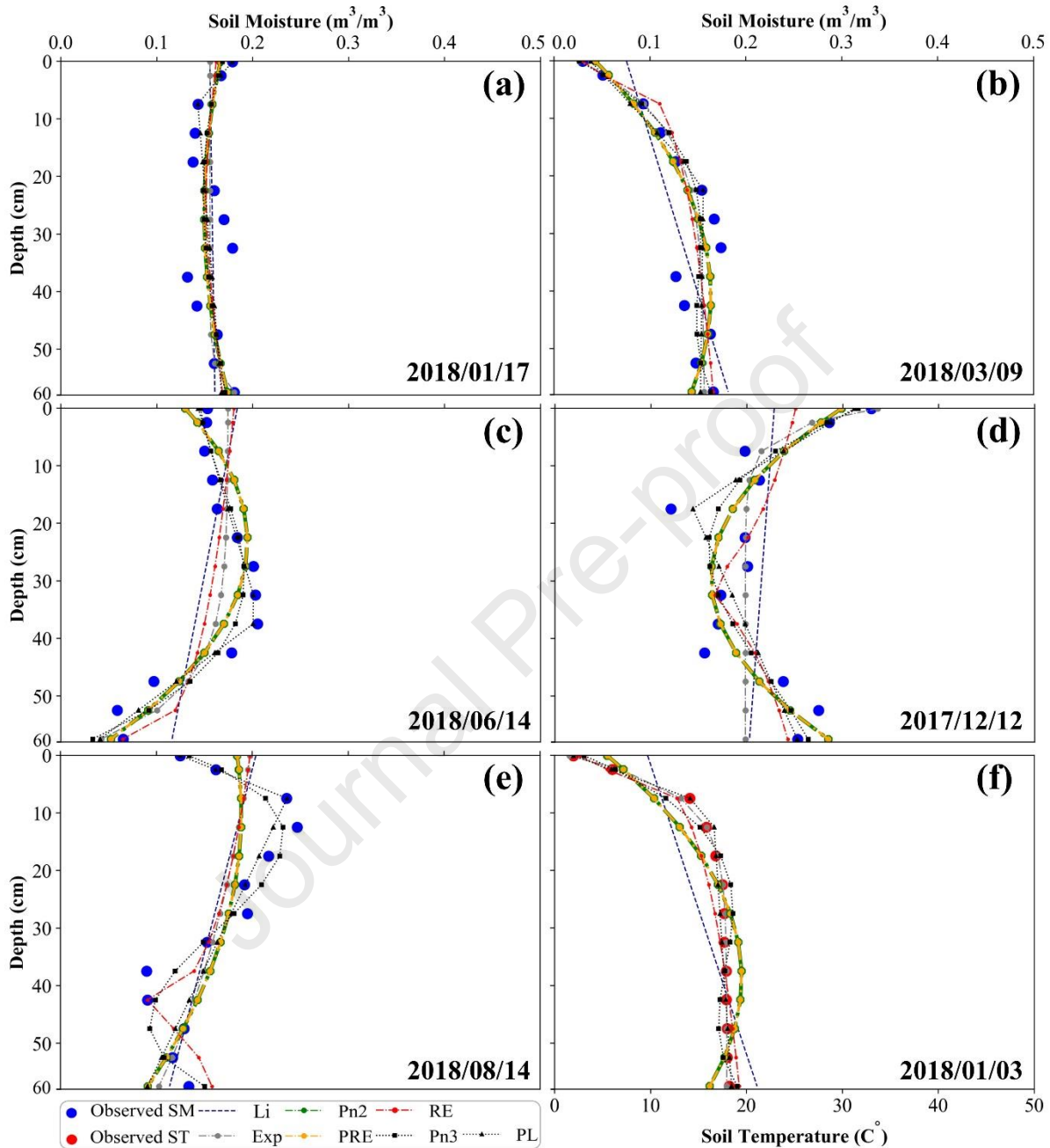


Fig. 4. Examples of (a) to (e) soil moisture and (f) soil temperature profile shapes encountered in Cora Lynn over the period December 2017 to December 2019 along with fitted mathematical functions (Li: Linear, Exp: Exponential, Pn2: second-order Polynomial, PRE: Parametrized second-order polynomial from simplified solution of Richard Equation, RE: simplified solution of Richards' Equation, Pn3: third order Polynomial, and PL: Piecewise Linear). Note: Both Pn2 and PRE functions resulted in exactly the same values, meaning that the curves were overlapped.

330 brings greater challenges to identify them. In this research, Eq.11 to Eq.16 and Eq.21 were
 331 considered as the mathematical representation of soil moisture profiles.

332 3.3 Inversion scheme

333 Radiative transfer equations used for forward models like the Njoku model need the
 334 distribution of soil moisture and temperature throughout the profile to simulate TB at the sensor
 335 level. Moreover, the output from the forward model should be able to closely mimic the TB
 336 that would be recorded by the sensor. Critically, validity of the forward model is a prerequisite
 337 for success of the inverse problem. For the synthesis study, it was assumed that the forward
 338 model met this criterion, while for the field application, roughness parameters were first
 339 calibrated to an independent period of data. In order to estimate the soil moisture profile, each
 340 of the above assumed mathematical functions was applied to calculate soil moisture as a
 341 function of depth. Accordingly, the parameters of the associated mathematical function were
 342 derived from matching predicted and observed TB using the cost function in Eq.22 through the
 343 coherent model in Eq.5 and Eq.6 by the process explained in Fig. 6. Accordingly, using the
 344 Njoku model the TB expected from an L-band and P-band radiometer were simulated
 345 separately and constrained using Eq.22.

$$L(\bar{x}) = \frac{1}{N} \left[\sum_{p=h,v} |TB_{f,p}(\bar{x}) - TB_{f,p}|^2 \right], \quad (22)$$

346 where (\bar{x}) represents the parameters of interest, $TB_{f,p}$ and $TB_{f,p}(\bar{x})$ are the calculated and
 347 observed TB, N is the number of observations, p and f represent the polarization (H or V) and
 348 frequency, respectively.

349 Given the complex analytical form of this physics-based emission model, an iterative
 350 optimization scheme was used to minimize the cost function and estimate the desired soil
 351 moisture profile parameters of interest. Different optimization algorithms were analysed,
 352 including simulated annealing (SA), genetic algorithm (GA), particle swarm optimization

353 (PSO) and their combinations, to estimate soil moisture profiles under two nominal conditions
 354 (a dry case and a wet case). According to the results (not shown here), PSO alone consistently
 355 produced the best results and so was selected for optimization of the soil moisture profile shape
 356 parameters in this study. PSO is a stochastic evolutionary computation technique that relies on
 357 the social behavior of swarms of fish, bees, and other animals. Each solution in PSO can be
 358 considered as a particle, except that they share their information and interact locally with each
 359 other and with the community. These interactions lead to a global behavior which is less likely
 360 to get stuck in a local minimum. A schematic of the algorithm search for the global minima is
 361 shown in Fig. 5. By randomly initializing parameters, any particle (blue circle in Fig. 5 (a)) in
 362 the search space has an initial position whose value is the cost function. The next position of
 363 the particles is determined by Eq.23:

$$x^i[t + 1] = x^i[t] + v^i[t + 1] \quad (23)$$

$$v^i[t + 1] = wv^i[t] + c_1r_1(x^{i,best}[t] - x^i[t]) + c_2r_2(x^{g,best}[t] - x^i[t]), \quad (24)$$

364 where $x^i[t]$ is the current position of the particle, $v^i[t + 1]$ (Eq.24) is the speed for the next
 365 position which is a function of movement in the direction of the previous position $wv^i[t]$, the
 366 best experience of the particle $x^{i,best}[t] - x^i[t]$ and movement in the direction of the best

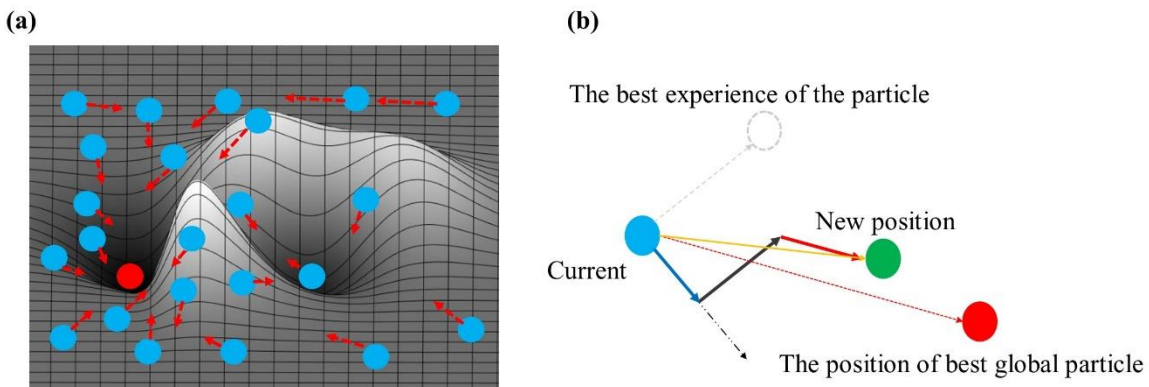


Fig. 5. (a) Schematic view of the particle swarm intelligence and (b) movement of a particle based on the theory of the PSO algorithm.

367 particle $x^{gbest}[t] - x^i[t]$, w is inertial weight between 0.6 and 0.9, slowing the particle and
368 helping it to converge around x^{gbest} , c_1 and c_2 (between 1.2 and 1.5) are acceleration constants
369 and r_1 and r_2 are random numbers between 0 and 1. A sample of the movement for one particle
370 is shown in Fig. 5 (b).

371 Different strategies were considered to retrieve the soil moisture profile shape parameters (as
372 shown in Fig. 6), including using the a) L-band observations alone, b) P-band observations
373 alone, c) L- and P-band observations jointly (namely LP method), and d) retrieving the surface
374 soil moisture parameter in each of the functions using the L-band observation and the rest of
375 the shape parameters using the P-band observation (namely L_P method). In the L_P method,
376 the soil moisture profile was first estimated using the L-band alone (method (a)). Because L-
377 band is more sensitive to surface soil moisture, just the parameter related to the surface soil
378 moisture in each of the used mathematical functions (parameter c in Eq.11 to Eq.15 and
379 parameter θ_1 related to Eq.16 and Eq.21) was accepted and fed into the next step, which then
380 retrieves the remaining parameters using P-band. It should be noted here that the estimated
381 surface soil moisture using the coherent stratified model from L-band is the soil moisture at the
382 air-soil interface and not the average soil moisture from surface to 5 cm depth. In order to
383 compare the result of the different strategies, the number of iteration (100) and the parameters
384 of the PSO algorithm (w , c_1 and c_2) along with the convergence criteria (< 0.01 K) for
385 minimizing the cost function were considered equal. A flowchart of soil moisture profile
386 estimation using the coherent stratified model is shown in Fig. 6.

387 In soil moisture profile estimation using each of the strategies, first a mathematical function
388 was considered and then the corresponding parameters of the function were generated
389 randomly and dependently. In applying all of the seven mathematical functions, first, surface
390 soil moisture as a parameter of the function was generated and then the rest of the parameters
391 were generated in a way that the change of soil moisture from the surface to the investigated

403 constant (< 0.01 K), then the algorithm interrupts the optimization process by changing the
404 parameters w , c_1 and c_2 , and randomly generating a new population. The algorithm saves the
405 last cost function and the corresponding parameters in a separate matrix and starts generating
406 parameters from the beginning. If it doesn't get stuck in the local minimum, it generates the
407 parameters so that it will converge the cost function. Finally, the matrix containing the smallest
408 cost function of each ten successive iteration were sorted based on its cost values and the
409 corresponding parameters of the smallest selected as the final output. The soil moisture profile
410 was then calculated from the retrieved parameters using the corresponding mathematical
411 function and the RMSE between estimated and observed soil moisture profile calculated.
412 Moreover, the practical depth for estimating the soil moisture profile from the relevant
413 mathematical function with a satisfactory level of accuracy (RMSE less than $0.04 \text{ m}^3/\text{m}^3$) was
414 approximated.

415 Experimental data of various soil moisture and temperature profile shapes (Fig. 2) collected
416 from ground Stations 126 and 136 in Cora Lynn under flat bare soil were used as input to the
417 coherent model to demonstrate the potential for profile estimation. Retrieved shape parameters
418 for the soil moisture profile were evaluated by comparing the derived profile against the
419 original profile used to produce the observed TB, with and without TB error imposed. A
420 uniform distribution of noise (low noise: $-1 \sim +1$ K, and high noise: $-4 \sim +4$ K) was imposed
421 on the TB observations, and each soil moisture profile estimated 10 times (realization) using
422 different realizations of noise. The analysis considered single and dual-frequency, single and
423 dual-polarization, and single and multi-incidence angle, snapshot and time series. Additionally,
424 the soil temperature profile was considered as known, or assessed for approximation using a
425 simple method.

426 In approximating the soil temperature profile, first a time series of the 6 AM profiles was
427 extracted from discrete measurements and interpolated to a continuous profile. The 12 soil

428 temperature measurements of each profile were related to depths of 2.5 (0-5 cm) to 57.5 (55-
429 60 cm) in 5 cm increments. The gradient between 2.5 and 7.5 cm was used to estimate the soil
430 temperature at the surface. The soil temperature below 57.5 cm up to 100 cm was considered
431 constant and equal to the soil temperature at depth of 57.5 cm. Second, a general profile was
432 calculated based on the whole set of 6 AM soil temperature profiles. Then surface soil
433 temperature (measured or estimated from a land surface model) for that day could be added to
434 the general profile shape and the soil temperature profile of that day approximated. The reason
435 behind using the general profile shape lies in the fact that 6 AM soil temperature profiles
436 through the year have a similar profile shape, but with an offset.

437 **4. Results and discussion**

438 In this section, the result from the soil moisture profile estimation methods as described in
439 section 3.3 are first presented and discussed. The performance of the best method from the
440 synthetic study is then evaluated using experimental data.

441 *4.1 Soil moisture profile estimation*

442 To explore the potential of the proposed soil moisture profile estimation models explained in
443 the methodology section, the 20 soil moisture profiles shown in Fig. 3 were estimated
444 individually using the four methods with dual H and V polarization, incidence angle of 40° ,
445 and the seven mathematical functions used to represent the soil moisture profile. The average
446 final value of the cost function in the case of low (0.58 K) and high (0.96 K) noise scenarios
447 using the LP method demonstrated the robustness of the inversion scheme. The depth for
448 reliable estimation and error (RMSE) was calculated for each soil moisture profile at different
449 depths over the top 60 cm profile, containing in situ soil moisture measurements at 12 depths.
450 The result (Fig. 7 for high noise scenario and Fig-Sm. 1 in supplementary material for low
451 noise scenario) showed that as the depth increased, the RMSE typically increased because of
452 the reduced contribution of the soil dielectric profile to the total emission from the soil.

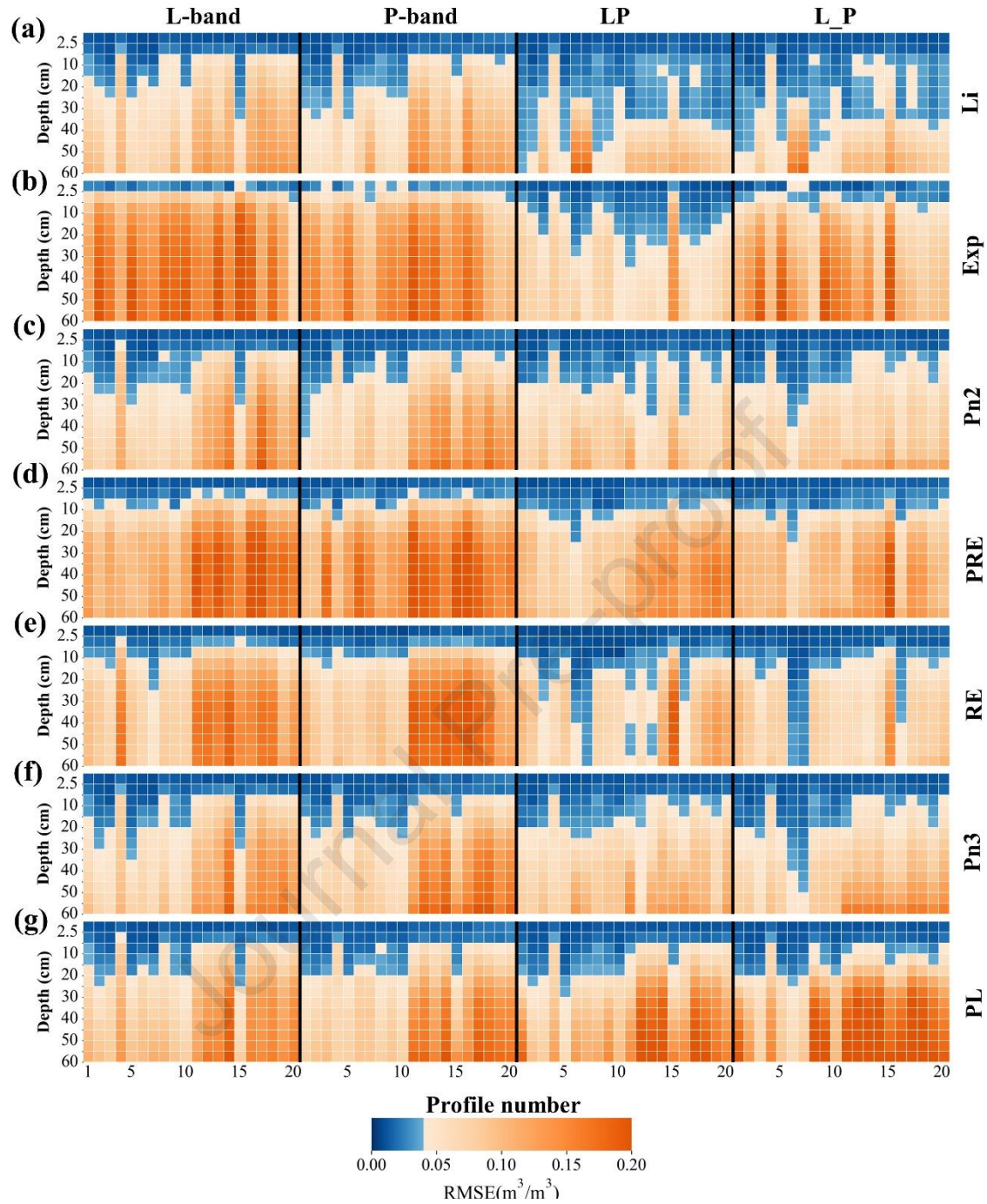


Fig. 7. Heatmap of RMSEs (average of ten perturbations under high noise scenario) between retrieved and observed soil moisture profile using L-band only (first column), P-band only (second column), LP band jointly (third column), and L_P method (last column). Each row shows results for a mathematical function representing the soil moisture profile including (a) linear, (b) exponential, (c) second-order polynomial, (d) derived second order polynomial from simplified solution of Richard equation, (e) simplified solution of Richard equation, (f) third-order polynomial, and (g) piecewise linear. Note: the blue color represents the RMSE below the target RMSE (0.04 m³/m³).

454 1 to 10 in Fig. 7 and Fig-Sm. 1) as compared to Period B (profile numbers 11 to 20 in Fig. 7
 455 and Fig-Sm. 1) due to the higher penetration depth of L- and P-band wavelengths in drier
 456 profiles (Rao et al., 1988). Taking all the mathematical functions and the twenty soil moisture
 457 profiles into account, it was found that the LP method outperformed other methods (Fig. 8).
 458 The two different levels of noise in the synthetic study aimed to represent the impact of
 459 calibration and model uncertainty. The average estimation depth of the methods under low
 460 (high) noise scenarios were 5 (4) cm at L-band, 6 (5) cm at P-band, 13 (12) cm with LP method,
 461 and 11 (10) cm for L_P method. Thus, it is clear that the performance of the two wavelengths
 462 together is better than the performance of a single wavelength. Since the sensitivity to factors
 463 which affect soil emission is frequency dependent (e.g. penetration depth is increased in the
 464 soil at longer wavelengths), obtaining higher accuracy and getting information from deeper
 465 layers are expected to be achieved by combining the two L-band and P-band frequencies. More
 466 specifically, there are many profile options that could lead to the same P-band TB prediction.
 467 However, adding an additional frequency at L-band constrains these options and thus leads to

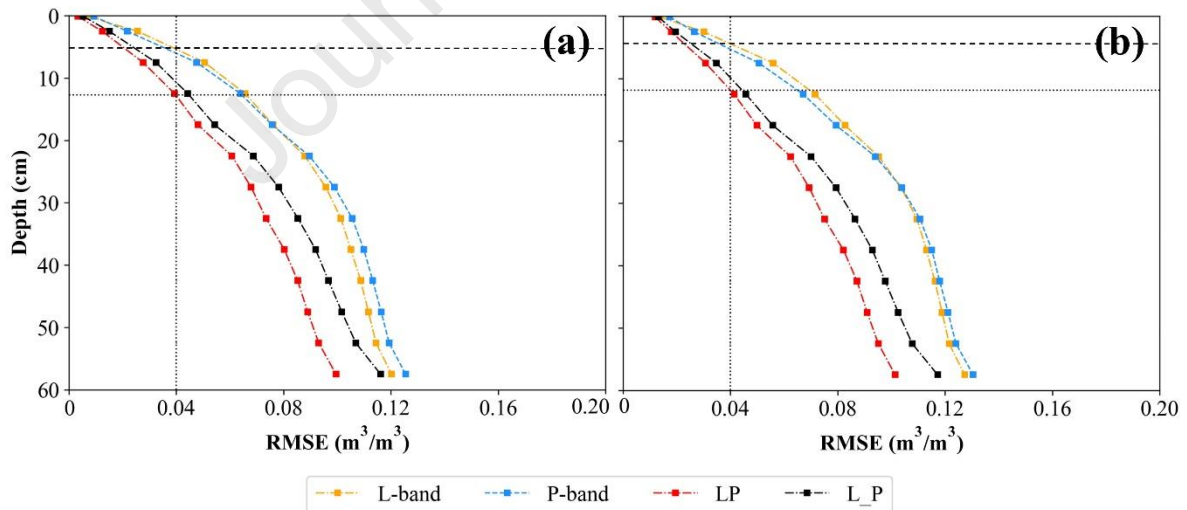


Fig. 8. Comparison of the methods for (a) low noise and (b) high noise scenario. Note: the RMSE axis is the average RMSE of 10 realizations and 7 mathematical functions. The vertical and horizontal dotted lines show the target RMSE (0.04 m³/m³) and the associated maximum estimation depth respectively. The dashed horizontal line shows worst case scenarios of estimation depth.

468 a more accurate extrapolation. The L_P method was the next best performing method followed
 469 by the P-band and finally L-band only models. Regardless of the applied noise scenario or the
 470 period, the RMSE of the L-band model predicted shallower surface soil moisture than the P-
 471 band model (Fig. 8). This is because the P-band signal carries information about the soil
 472 moisture from much deeper layers of the soil. The performance of the individual mathematical
 473 functions representing the soil moisture profile was investigated. For this reason, the estimation
 474 depth of the methods was calculated as shown in Fig. 9. The linear function with only two
 475 parameters (Eq.11) could estimate the soil moisture up to a depth of 31 cm (mean of low and
 476 high noise scenarios) at LP and 30 cm at L_P method, outperforming all other functions.
 477 Additionally, the average estimation depth of the Pn2 function (17 cm) was comparable with
 478 Pn3 (17.5 cm) using each of the LP or L_P methods. The RE function recommended by Sadeghi
 479 et al. (2016) led to an estimation depth of 12 cm at both LP and L_P methods. The PL function
 480 using LP (L_P) method was the next best function with estimation depth 9 (12) cm. Although
 481 applying the Exp function resulted in an estimation depth of 12 cm using the LP method, the
 482 lowest estimation depth was achieved using this function with 1 cm at L-band alone, 2 cm at
 483 P-band alone and 4 cm for L_P method. Also, using the PRE function an average estimation
 484 depth of 4 cm (10 cm) was achieved using L-band or P-band (LP or L_P) methods. The reason

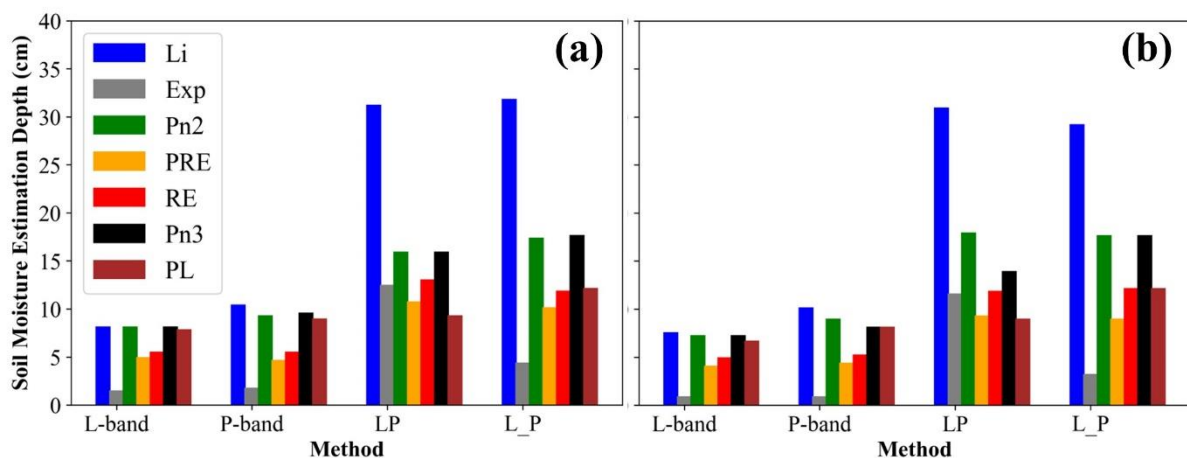


Fig. 9. The estimation depth of methods according to assumed moisture profile functions based on target RMSE 0.04 m³/m³ under (a) low and (b) high noise scenarios.

485 of achieving lower estimation depth using the Exp function could be linked to the fact that a
486 small change in the shape parameters (a and b in Eq.12) of this function leads to a huge change
487 in the profile shape. Additionally, function PRE could capture the shape of the profiles that are
488 dominant in Period B (Fig. 3). Except Exp, PRE, and RE functions, the depth of estimation of
489 the other functions were similar using L-band or P-band methods and were 8 cm and 9 cm
490 respectively. The results obtained using the employed functions were similar at least for depths
491 less than 10 cm (Fig. 7 and Fig. 10). Therefore, if the intention is to estimate the soil moisture
492 not deeper than 10 cm, any of these functions can be expected to give a similar result. The
493 linearity of soil moisture variation at the lower depth could be a possible reason for achieving
494 such similar results, thus enabling most of these functions to capture the shape of the profile at
495 the lower depths. However, as the depth increased, the RMSE between the estimated and
496 observed soil moisture profile increased (Fig. 7 and Fig. 10). This synthetic study clearly shows
497 the effectiveness of the LP method in estimating the soil moisture profile with the best
498 mathematical functions of Li followed by Pn2 function. Therefore, the LP method was selected
499 as the most robust method and thus the main focus of the further analysis of this research.

500 *4.2 Time series estimation of soil moisture profile*

501 The optimization algorithm (PSO) used in this study is population-based and so the particles
502 share information together while searching the global minimum. In the snapshot retrieval, one
503 global minimum is found by 50 particles during every iteration. For example, considering a
504 second-order polynomial for retrieving parameters a , b , and c , the 50 particles search for
505 finding one global minimum. By increasing the number of observations (known) in a fixed
506 time-window, more parameters can be retrieved. If a 30 day estimation period of soil moisture
507 profiles is considered using the second-order polynomial function instead of retrieving one set
508 of a , b , and c , 30 sets of parameters are retrieved. However, in a drying down period, these 30
509 parameters of a , b , and c change gradually and so can build a density of global minima in the

510 search space. As a result, finding 30 global minima (built by 30 days \times 3 parameters) by 50
511 particles is much easier than finding one global minimum. Accordingly, PSO is expected to
512 give a better result with the time series approach, because it is able to incorporate the prior
513 knowledge of the previous time step to get the value for the next time step as it understands the
514 relationship between these parameters through time. As a result, the motivation of using time
515 series retrieval is proposed.

516 The temporal behaviour of soil moisture is usually characterized by a relatively slow dry-down
517 process following an abrupt increase from precipitation or irrigation. Therefore, dry down
518 periods of soil moisture in Period A and B were considered to compare the time series and
519 snapshot retrieval methods. The purpose of selecting the dry-down periods was for partially
520 removing the uncertainties in calibration and forward modeling in the multi-temporal soil
521 moisture profile estimation. The Period A is characterized by simple soil profile shapes and
522 relatively lower soil moisture with average $0.13 \text{ m}^3/\text{m}^3$ (minimum $0.07 \text{ m}^3/\text{m}^3$ and maximum
523 $0.23 \text{ m}^3/\text{m}^3$) while Period B has more complex profile shapes with an average of $0.27 \text{ m}^3/\text{m}^3$
524 (minimum $0.13 \text{ m}^3/\text{m}^3$ and maximum $0.35 \text{ m}^3/\text{m}^3$). Fig. 10 shows the comparison between the
525 snapshot and time series estimation for the two periods using the LP method. It is concluded
526 that except the Li function, the time series outperformed the snapshot estimation under low
527 (high) noise scenario by 0.01 (0.01) m^3/m^3 for RE, 0.01 (0.02) m^3/m^3 for PRE, 0.02 (0.02)
528 m^3/m^3 for PL, 0.008 (0.01) m^3/m^3 for Exp, 0.004 (0.008) m^3/m^3 for Pn3, and 0.006 (0.002)
529 m^3/m^3 for Pn2 functions. Function Li showed an exception in which RMSE increased by 0.006
530 (0.003) under low (high) noise scenarios when using the time series approach.

531 The effect of combining observations from different incidence angles, including 10, 20, and
532 40° , on the soil moisture profile estimation accuracy as compared to having observations at a
533 single incidence was assessed using the L-band, the P-band, and the LP method. It was found
534 that using one incidence angle at 40° with the LP method outperformed using multi-incidence

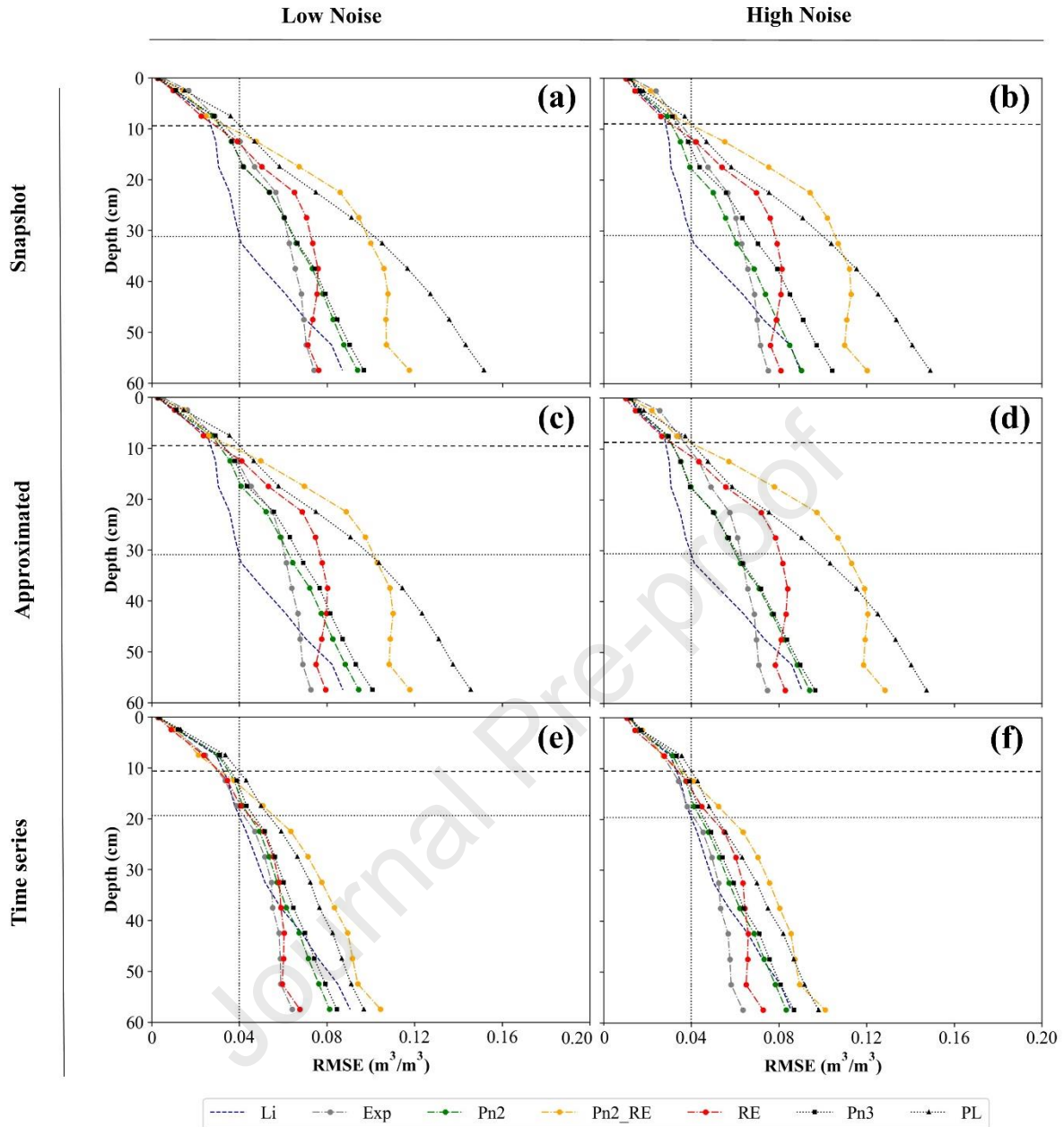


Fig. 10. Snapshot retrieval of soil moisture profiles using the combined L- and P-band method (H and V polarization and single 40° incidence angle) for (a and b) known and (c and d) approximated soil temperature profile using snapshot retrieval, and time series retrieval (e and f) with known soil temperature profile under low and high noise scenarios. The dashed and dotted horizontal lines show best and worst case scenarios of estimation depth.

535 angles at L-band or P-band alone (Fig-SM. 2). Taking all the mathematical functions into
 536 account, the result of the LP method using a combination of different incidence angles,
 537 including 40° , 20° and 40° , and 10° , 20° and 40° demonstrated (Fig-SM. 3) that two incidence

538 angles resulted in a $0.003 \text{ m}^3/\text{m}^3$ decrease in RMSE under low and high noise scenarios, while
539 remaining unchanged when three incidence angles were employed.

540 Investigation of single and dual-polarization retrieval from the LP method confirmed
541 expectations (Fig-SM. 4) that using H and V together resulted in better performance than when
542 using either polarization individually.

543 *4.3 Impact of approximation of soil temperature profile on the estimation accuracy*

544 The soil temperature profile is one of the important inputs of the microwave coherent model in
545 simulating TB, but obtaining this variable is challenging and has thus been a limitation for
546 large-scale applications. Therefore, an approximation method as explained in the methodology
547 section was considered and differences quantified between the approximated profiles from
548 actual temperature profiles and their impact on the simulated TB and soil moisture estimation.
549 It was found (not shown here) that approximation of the soil temperature profile leads to an
550 average RMSE between actual soil temperature profiles at 6 AM and approximated soil
551 temperature of around 3 K.

552 The impact of the soil temperature profile approximation on the TB estimation for soil moisture
553 profile estimation was investigated. Accordingly, TB was simulated for both L-band and P-
554 band using the coherent model from actual and approximated soil temperature profiles.
555 Considering the thermal sensing depth at L-band and P-band, it is obvious that if approximated
556 soil temperature profiles were calculated from the surface soil temperature, the RMSE of the
557 simulated and observed TB would be higher at P-band (4 K) as compared with L-band (3 K).
558 The reason is that thermal sensing depth at P-band is much deeper than for L-band, and P-band
559 is more sensitive to the temperature of the deeper layers. In the above analysis, a dry soil
560 moisture profile was considered. However, when a wet soil moisture profile was considered, a
561 much lower RMSE of TB was achieved when using the approximated soil temperature profile.
562 The reason is that when soil moisture is high, the penetration depth and the variation of soil

563 temperature near the surface decrease so that surface temperature is more realistic for
564 approximating the soil temperature profile.

565 It should be noted that, to investigate the impact of approximated soil temperature profiles on
566 soil moisture profile estimation, the twenty soil moisture profiles (Fig. 3) were estimated
567 individually using the LP method under low and high noise scenarios (Fig. 10 (c and d)). In the
568 low noise scenario, except Exp (decrease in RMSE by $0.001 \text{ m}^3/\text{m}^3$), Pn2 (decrease in RMSE
569 by $0.0005 \text{ m}^3/\text{m}^3$), and PL (decrease in RMSE by $0.001 \text{ m}^3/\text{m}^3$) function, and in the high noise
570 scenario except Pn3 (decrease in RMSE by $0.005 \text{ m}^3/\text{m}^3$) and PL (decrease in RMSE by 0.0001
571 m^3/m^3) functions, the retrievals from other functions were a little worse by average 0.002
572 m^3/m^3 . Therefore, the approximation method of soil temperature profile can be considered as
573 an appropriate substitution of having known soil moisture profile information when estimating
574 the soil moisture profile using coherent models.

575 *4.4 Estimating soil moisture profile using real experiment data*

576 In the synthetic study it was found that the LP method outperformed other methods, and that
577 using the time series approach gave better performance compared with snapshot retrieval.
578 Additionally, it was concluded that the two incidence angles 10° and 40° at both H and V
579 polarization led to the lowest RMSE. It was also shown that Li and Pn2 functions resulted in a
580 lower RMSE compared with the other options. Thus, using this configuration, the coincident
581 brightness temperature observations at L-band and P-band for the Period A and B profiles
582 shown in Fig. 2 were used for testing with real data. In the real study using real data, because
583 of the configuration of the tower, the brightness temperature observations were only available
584 at incidence angles of 45° (for Period A) and 40° (for Period B) for both L-band and P-band.
585 Therefore, the soil moisture was estimated using a single incidence angle. To assess the
586 performance of the proposed inversion scheme, the L-band and P-band observations (Fig. 2
587 (c); 26 days in Period A and 14 days in Period B) were first used along with simultaneous

588 measurements of soil moisture and temperature profiles (Fig. 2 (a and b)) for the two periods
 589 from the PRISM project. The numerical setup of the coherent model was considered the same
 590 as for the synthetic study with the same profile depth and number of layers. The brightness
 591 temperature was simulated using the coherent forward model and evaluated against
 592 observations at L-band and P-band for both periods. As explained in the methodology section,
 593 the roughness parameters h_p , q_p , and n_p in Eq.7, and soil temperature profile were considered
 594 as known.

595 Fig. 11 shows the predicted brightness temperature versus the respective L-band and P-band
 596 observations over the two Periods A and B. The V (4.4 K) and H (4.6 K) polarization achieved
 597 the best performance for L-band and P-band respectively, followed by V (6.9 K) and H (8.6 K)
 598 polarization at the P-band and L-band. The H polarization is more sensitive to roughness and
 599 so this could be the possible reason for higher RMSE at L-band compared with the V
 600 polarization. Following rainfall when the surface was drying out, the anomalous error in H
 601 polarization at L-band led to higher observed TB. However, the model used the average soil

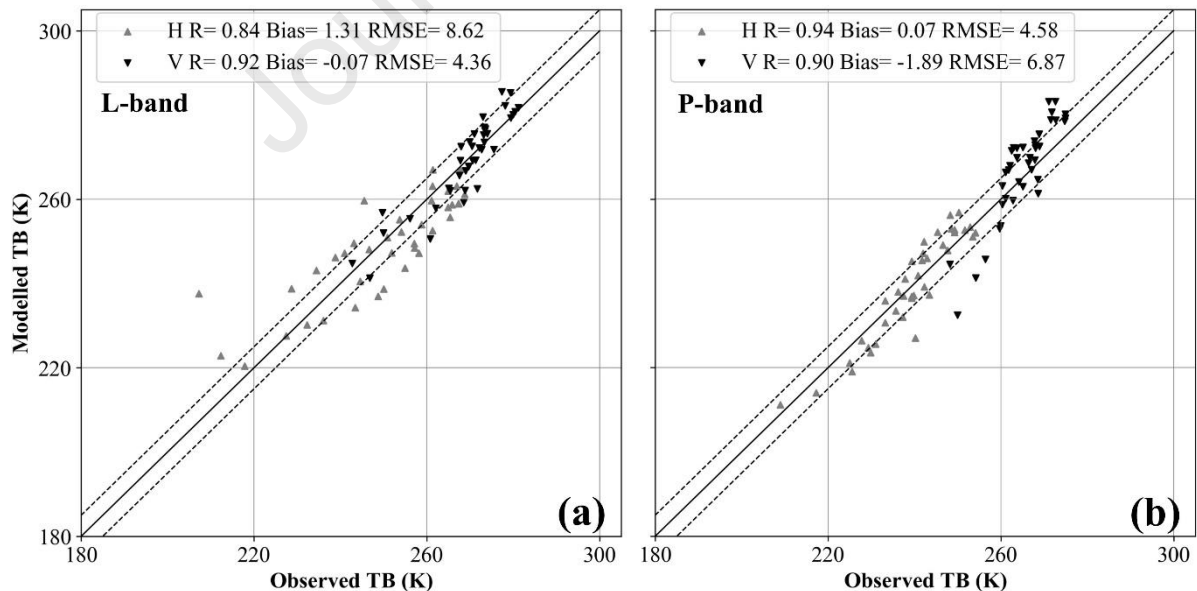


Fig. 11. Comparison of calculated brightness temperature from the coherent model and tower observations at (a) L-band and (b) P-band over bare soil. The dash lines denote ± 5 K offset. R refers to the Pearson correlation coefficient.

602 moisture below the surface (measured by ground stations), which was wetter than the surface
603 (due to infiltration), resulting in a relatively lower modelled TB. The source of anomalous error
604 in P-band and V polarization is unknown, with the model overestimating the TB. None of
605 these errors were removed from the calculations. Notably, there is a tendency for the Njoku
606 model to underestimate (overestimate) at low (high) soil moisture (especially at L-band)
607 (Njoku and O'Neill, 1982). Reasons for differences include: i) during a dry period, the soil
608 moisture at the skin is lower and drier than the deeper profile while during the wet period
609 (especially during rainfall), the surface tends to be saturated and it is wetter than deeper
610 profiles; ii) wind and rain showers modify the surface and the differences between surface
611 roughness characteristics change; iii) the skin soil moisture was constructed by having the slope
612 of soil moisture variation estimated using the sensor values at 2.5 and 7.5 cm which might not
613 be realistic.

614 In the synthetic study, it was found that applying the LP method using a linear and a second-
615 order polynomial within a time series retrieval resulted in the lowest RMSE. As a comparison
616 to the synthetic study, the soil moisture profiles were estimated for Periods A (26 days) and B
617 (14 days) using the LP model using the seven mathematical functions with both the time series
618 and snapshot approaches. The result in Fig. 12 shows that using snapshot (time series
619 approaches) the soil moisture profiles were estimated with lower RMSE in Period A (average
620 11 cm (21cm) estimation depth) as compared with Period B (average 4 cm (5cm) estimation
621 depth). The reason is that during the dry period when all layers had low moisture, the L-band
622 and P-band had a deeper observation depth. During the dry period (Period A), the time series
623 approaches outperformed the snapshot retrieval with an increasing estimation depth of 20 cm
624 for Exp, 15 cm for PL, 10 cm for Pn2 and Pn3, 5 cm for PRE and RE, and 3 cm for Li, resulting
625 in average increase of 10 cm. During the wet period (Period B), the time series approach still
626 resulted in an average increase of 1 cm, with 4cm, 4cm, and 3cm increase in estimation depth

627 of Exp, RE, and PRE respectively, unchanging for Pn3 and PL, and 1 cm decrease for Pn2 and
 628 Li functions. The time series approach using the LP method was found to be the most robust
 629 with a minimum estimation depth of 8 cm using the PRE function and maximum estimation

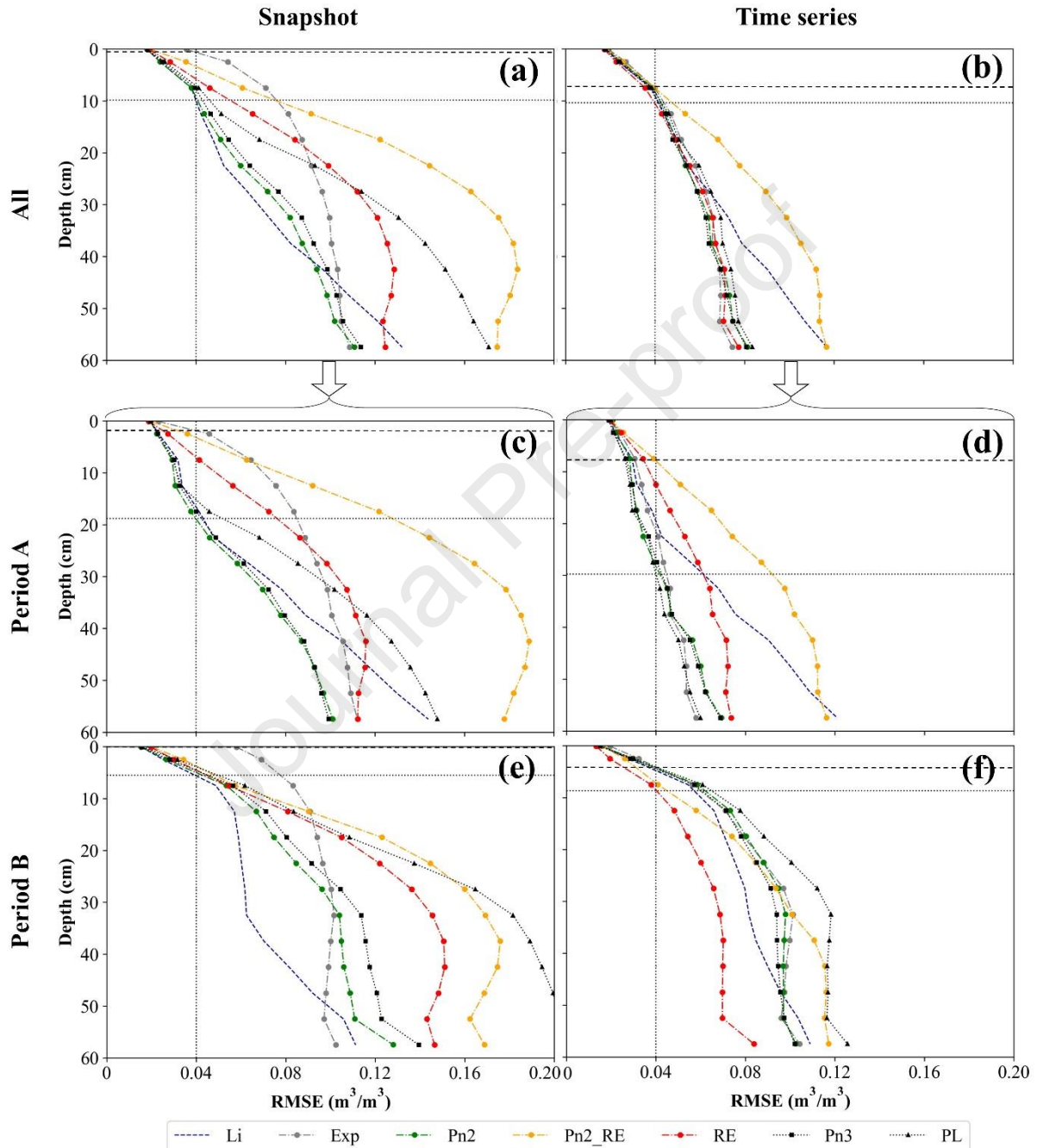


Fig. 12. The average RMSE calculated between in-situ and retrieved soil moisture profiles using LP method for (a) snapshot and (b) time series approaches decomposed to Period A (c and d) and Period B (e and f). The dashed and dotted horizontal lines show best and worst case scenarios of estimation depth.

630 depth of 28 cm using Pn2 and Pn3 functions over period A. Additionally, the result of the time
631 series approach for Period B had the minimum estimation depth of 5 cm using L, Exp, Pn2,
632 Pn3, and PL, and maximum estimation depth of 8 cm using the PRE and RE functions. Besides,
633 the time series approach is faster (0.5 second faster in retrieving each profile) and more precise
634 (standard deviation 0.015 (0.016) m^3/m^3 at the surface; 0.05 (0.06) m^3/m^3 at depth of 60 cm for
635 time series (snapshot) with lowest values for the Pn2 function) than the snapshot retrieval
636 approach. Moreover, the Exp, PRE and PL functions were found to be more sensitive to noise
637 in the observed brightness temperature compared to the other functions, resulting in the
638 snapshot retrieval approach having a higher RMSE when using these functions. In contrast, the
639 RE function is not sensitive to noise, however under some conditions (as explained in the
640 methodology) it has to be replaced with the PRE function resulting in a higher RMSE. The
641 time series retrieval can mitigate noise as explained in section 4.2 and so resulted in a much
642 lower RMSE as compared with the snapshot retrieval.

643 From this analysis it is concluded that the Pn2 function is the best function for estimating soil
644 moisture. Additionally, if the intention is estimating soil moisture below 20 cm, the Li function
645 with only two parameters can be considered as the best representation of soil moisture profile
646 especially during a wet season (Period B). The reason for a lower RMSE in the linear function
647 is the linearity of soil moisture in the shallow layer so that it is captured by this function. The
648 better performance of the PRE function during Period B is because during this period soil
649 moisture profiles had a large gradient at the shallow layers (up to 20 cm) and also showed some
650 changes of soil moisture value in the deeper layers, meaning that this function can capture their
651 shapes more easily. Some samples of estimated and observed soil moisture profiles for both
652 periods are shown in Fig. 13.

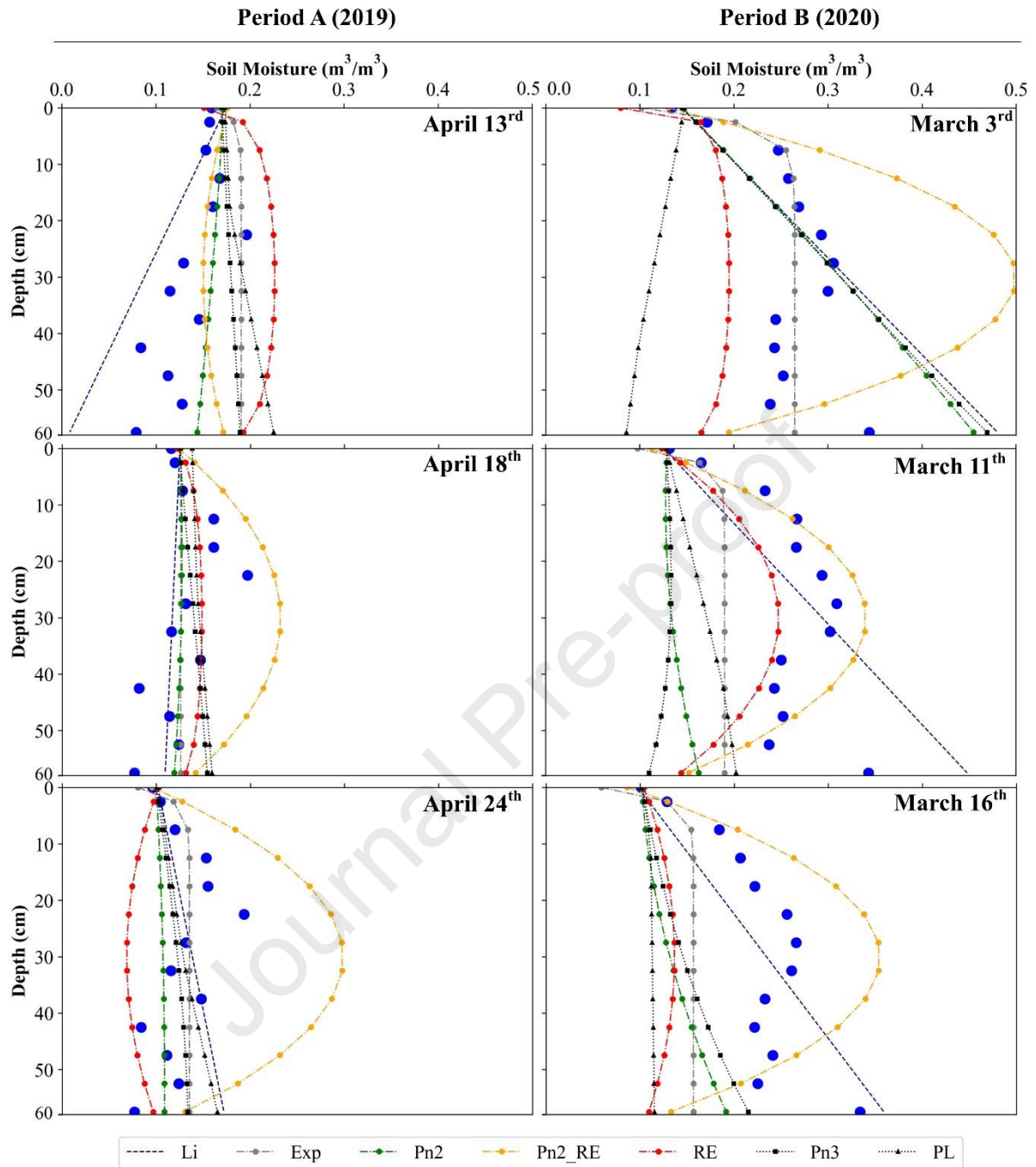


Fig. 13. Samples of estimated soil moisture profile using the LP method for the two periods A (left column) and B (right column) periods utilizing the time series approaches.

653 5. Conclusions

654 A soil moisture profile estimation strategy has been developed using L- and P-band radiometer
 655 observations together with a stratified coherent model and the PSO optimization algorithm.

656 Under low and high noise synthetic scenarios with RMSE lower than $0.04 \text{ m}^3/\text{m}^3$, the combined
657 use of L- and P-band dual polarization data outperformed both the L- or P-band method alone,
658 with an average estimation depth of 20 cm for the Li function and 15 cm for the Pn2 function
659 under both a wet and dry period with complex profiles, providing the more robust time series
660 approach was employed. Multi-incidence angle retrieval using 10° and 40° improved the
661 average RMSE by $0.002 \text{ m}^3/\text{m}^3$ and $0.005 \text{ m}^3/\text{m}^3$ under low and high noise scenarios
662 respectively as compared with single angle retrieval at 40° , while adding a third incidence angle
663 of 20° made no further improvement. Moreover, when approximating the soil temperature
664 profile with a simple method that uses a trend of the profile together with a surface soil
665 temperature measurement, there is little impact on the result. In a real-world experiment, the
666 combined L-band and P-band method using the time series retrieval approach and a second-
667 order polynomial representing the soil moisture profile outperformed the other methods tested,
668 with an RMSE less than $0.04 \text{ m}^3/\text{m}^3$ for depths up to 28 cm for a dry period but only to 5 cm
669 for a wet period. The success of this work demonstrates the potential of this approach, which
670 now requires further research to determine the most suitable mathematical functions for soil
671 moisture profile estimation in different regions around the world. Additionally, this study
672 demonstrates the potential of combining L-band and P-band radiometry for estimating soil
673 moisture in the root zone, proving the merit of this concept for the next generation radiometer
674 satellite mission.

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Highlights:

- 1- Combined L&P-band radiometry outperformed using either band alone.**
- 2- Second -order polynomial found best for soil moisture profile retrieval.**
- 3- Soil moisture profile retrieval via time series outperformed snapshot retrieval.**

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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