1 Integrating process-related information into an ANN for root-

2 zone soil moisture prediction

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11 Abstract. Quantification of root-zone soil moisture (RZSM) is crucial for agricultural applications and soil sciences. 12 RZSM impacts processes such as vegetation transpiration and water percolation. Surface soil moisture (SSM) can be 13 assessed through active and passive microwave remote sensing methods, but no current sensor enables direct RZSM 14 retrieval. Spatial maps of RZSM can be retrieved via proxy observations (vegetation stress, water storage change, and 15 surface soil moisture) or via land surface model predictions. In this study, we investigated the combination of surface 16 soil moisture information with process-related inferred features involving artificial neural networks (ANNs). We 17 considered the infiltration process through the soil water index (SWI) computed with a recursive exponential filter and 18 the evaporation process through the evaporation efficiency computed based on a MODIS remote sensing dataset and 19 simplified analytical model, while vegetation growth was not modeled and only inferred through normalized difference 20 vegetation index (NDVI) time series. Several ANN models with different sets of features were developed. Training was 21 conducted considering in situ stations distributed several areas worldwide characterized by different soil and climate 22 patterns of the International Soil Moisture Network (ISMN), and testing was applied to stations of the same data 23 hosting facility. The results indicate that the integration of process-related features into ANN models increased the 24 overall performance over the reference model level in which only SSM features were considered. In arid and semi-arid 25 areas, for instance, performance enhancement was observed when the evaporation efficiency was integrated into the 26 ANN models. To assess the robustness of the approach, the trained models were applied on observation sites in Tunisia, 27 Italy and South-India that are not part of ISMN. The results reveal that joint use of surface soil moisture, evaporation 28 efficiency, NDVI and recursive exponential filter represented the best alternative for more accurate predictions in the 29 case of Tunisia, where the mean correlation of the predicted RZSM based on SSM only sharply increased from 0.443 to 30 0.801 when process-related features were integrated into the ANN models in addition to SSM. However, process-31 related features have no to little added value in temperate to tropical conditions.

32 Keywords: root-zone soil moisture, artificial neural networks, evaporation efficiency, exponential filter.

33 1 Introduction

34 Soil moisture is a major land parameter integrated into several agricultural, hydrological and meteorological 35 applications (Koster et al., 2004; Anguela et al., 2008) This essential climate variable (ECV) consists of two 36 components, namely, surface soil moisture (SSM) (0-5 cm) and root-zone soil moisture (RZSM). RZSM corresponds 37 to the soil moisture in the region in which the main vegetation rooting network is developing. Its definition varies 38 depending on vegetation type and pedoclimatic conditions. The importance of RZSM is mainly highlighted in 39 agricultural applications through vegetation stress and water needs and in carbon and nitrogen cycles, as RZSM 40 influences biogeochemical activities in soil (Martínez-Espinosa et al., 2021). RZSM is nonlinearly related to SSM 41 through different hydrological processes, such as diffusion processes. RZSM may be extracted by evaporation at the 42 surface, through root extraction or by capillary rises (Calvet et Noilhan, 2000). SSM quantification is achieved through 43 three main sources: in situ measurements, model estimates and remote sensing-based products. Microwave remote 44 sensing technologies involving sensors such as the Soil Moisture and Ocean Salinity (SMOS) (Kerr et al., 2010), Soil 45 Moisture Active Passive (SMAP) (Entekhabi et al., 2010) Advanced Microwave Scanning Radiometer (AMSR) (Owe 46 et al., 2008) and Advanced Scatterometer (ASCAT) (Wagner et al., 2013) have been employed to retrieve SSM at 47 coarse resolutions. Current satellite sensors can only provide surface soil moisture information because of the shallow 48 penetration depth of spaceborne data (on the order of a few centimeters) (Wagner et al., 2007). Fine-spatial resolution 49 synthetic aperture radar (SAR) data can also be applied in synergy with optical data to retrieve soil moisture (Zribi et 50 al., 2011; Hajj et al., 2014; Dorigo et al., 2011), but again for surface soil moisture. The International Soil Moisture 51 Network (ISMN) is an exhaustive data hosting facility focused on soil moisture data and associated ancillary 52 information. The ISMN provides in situ soil moisture measurements collected from operational soil moisture networks 53 worldwide (Dorigo et al., 2011). Various models can be adopted to estimate RZSM, such as land surface models 54 (Surfex (Masson et al., 2013), ISBA (Noilhan et al., 1996), CLM (Oleson et al., 2010), JULES (Best et al., 2011), etc.) 55 or dedicated crop models such as Aquacrop (Raes et al., 2009) or SAFYE (Battude et al., 2017). While these models 56 provide the advantage of physical process-based estimates, these estimates depend on the availability and accuracy of 57 ancillary information. Model predictions are often enhanced by the implementation of data assimilation techniques, 58 such as the land data assimilation system (LDAS) (Sabater et al., 2007; Entekhabi et al., 2020).

59 Data-driven methods such as artificial neural networks (ANNs) have also been commonly applied in hydrology as 60 detailed for instance by the ASCE Task Committee on Application of Artificial Neural Networks in Hydrology (2020) 61 and in (Tanty el al., 2015). One of their advantages is that these models do not require an explicit model structure to 62 accurately represent the involved hydrological processes but instead construct a relationship between the given inputs 63 and the process of interest. Therefore, ANNs are regarded as dynamic input-output mapping models heavily relying on 64 the provided training data relevant to target values (Pan et al., 2017). Moreover, ANNs only require a one-time 65 calibration to provide soil moisture estimations once instrument data are loaded and thus generate relatively low 66 computational costs (Kolassa et al., 2018). These advantages explain the approach to estimate RZSM based on surface 67 information with ANNs in various methodologies (Pan et al., 2017; Grillakis et al., 2021; Souissi et al., 2020). In this 68 paper, we do not address ANN applications as a model twin where the ANN model is trained on the target for 69 mimicking purposes and subsequently generates predictions while requiring a short computation time or fewer input 70 simplifications. Here, we are instead interested in the adoption of ANNs as independent models trained on in situ 71 observations. Within this context, Pan et al. (2017) successfully applied an ANN as a model for shallow 20-cm root 72 zone soil moisture prediction with a global correlation coefficient of 0.7. Grillakis et al. (2021) proposed employing an 73 ANN as a means to calibrate and regionalize the time constant of a recursive exponential filter, which was thereafter 74 applied at the regional scale. A combined implementation of Bayesian probabilistic approach and an ANN to infer

75 RZSM at different depths from optical UAV acquisitions via local training was also applied (Hassan-Esfahani et al., 76 2017). Multitemporal averaged features to predict RZSM based on only SSM and investigated the transferability of a 77 trained ANN across different climatic conditions globally were proposed in (Souissi et al., 2020). Temporal information 78 can be considered in ANNs through recurrent neural networks (RNNs), long short-term memory (LSTM) architectures 79 (Liu et al., 2021), 1D convolutional neural networks (CNNs), or multitemporal averaging. In (Souissi et al., 2020), 80 median, maximum, and minimum correlation values of 0.77, 0.96, and 0.65 were respectively reported across training, 81 validation and test datasets. The use of climatic variables such as precipitation and surface temperature and intrinsic 82 surface properties such as soil texture and land cover has also been considered in ANNs (Liu et al., 2021). The choice 83 of variables depends not only on the data availability but also on the objectives. Finally, ANN-based approaches pertain 84 to the more general term of machine learning approaches, and within this framework, the random forest approach has 85 been applied to root zone soil moisture prediction (Carranza et al., 2021). The aforementioned studies have investigated 86 the application of multiple information sources to predict root zone soil moisture. The input features are commonly 87 curated for quality, and correlation analysis is conducted to determine the useful inputs, while physical processes are 88 not considered. In this paper, we introduce process-related features based on simplified analytical models representing 89 the major processes contributing to root zone soil moisture dynamics. In this work, RZSM refers to a point observation 90 of water content in a depth ranging between 30 and 55cm. We investigate the impact of the application of different 91 process-related variables on the precision of RZSM predictions as well as the robustness of our approach. (1) We start 92 from a previously developed ANN model (Souissi et al., 2020), and we extend the feature list to include NDVI time 93 series, surface soil temperature and process-related variables, namely, the soil water index given by a recursive 94 exponential filter and remote sensing-based evaporation efficiency. (2) The robustness of the approach is assessed 95 through additional tests involving stations not included in the ISMN database in Tunisia, Italy, and South-India. (3) 96 Climatic analysis is conducted to infer the most indicative process-related features for each climate pattern.

97 2 Materials and Methods

98 The proposed methodology entails the construction of several ANN models with both direct (SSM, surface temperature, 99 and NDVI) and intermediate sets of features (soil water index and evaporation efficiency) computed based on 100 simplified analytical models. An overview of the processing configuration is shown in Figure 1. Standard scaling is 101 applied to each dataset separately so that the different inputs fall into the same range of values, then the ANN outputs 102 are descaled to make the comparison with actual values of RZSM possible.

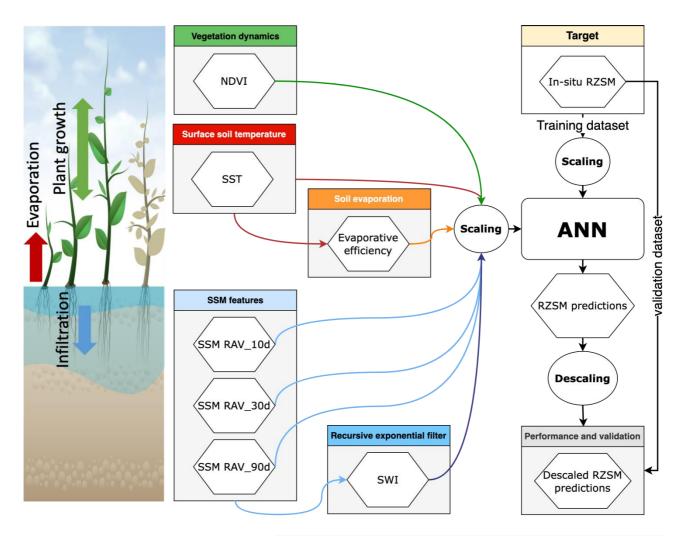


Figure 1. Overview of the processing configuration showing the components of the model: the tested models are variations of thisANN with a different combination of inputs (see Table 1). The scaling and descaling are applied to each dataset separately.

106 This approach results in a combination of ANN models (Table 1). Each model has one or more process-related

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107 features in addition to three SSM features which correspond to backward rolling averages of in-situ SSM computed

108 over 10,30 and 90 days. All the ANN model hyperparameters remain the same except the number of input features.

109 **Table 1.** ANN model configurations with the respective input variables ; *: rolling averages of SSM over 10 days; **: rolling

110 averages of SSM over 30 days; ***: rolling averages of SSM over 90 days; ****: number of parameters of the ANN model.

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Model	SSM_10d_RAV*	SSM_30d_RAV**	SSM_90d_RAV***	SST	NDVI	SWI	EVAP	Nb****
Features								
ANN_SSM	Х	Х	Х					101
ANN_SSM_TEMP	Х	Х	Х	Х				121
ANNI SSM NIDVI	Х	Х	Х		Х			121
ANN_SSM_NDVI	Λ	Α	Α		Λ			121
ANN_SSM_EXP-	Х	Х	Х			Х		121
FILT-T5								
AND COM EVAD	Х	Х	Х				X	121
ANN_SSM_EVAP-	Λ	Λ	Λ				Λ	121

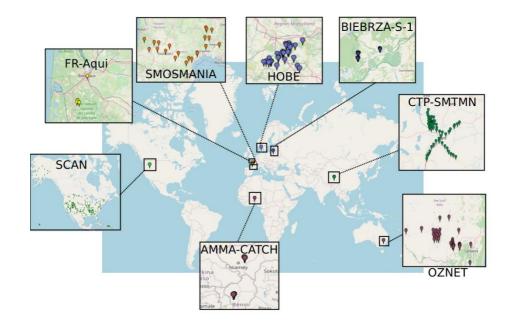
EFF-B60							
ANN_SSM_NDVI_E	Х	Х	Х	Х	Х	Х	161
VAP-EFF-B60_EXP-							
FILT-T5							

The model with the simplest starting point is ANN_SSM based on (Souissi et al., 2020). The most complex model includes the full set of inputs. Intercomparison of the model performance provides information on the added value of each input. All input features are scaled, and training is performed on each of these features based on scaled in situ RZSM data retrieved from the ISMN. The RZSM model predictions are validated against an independent set of observations.

# 117 2.1 Datasets

# 118 2.1.1 ISMN soil moisture data

119 The first training and test operations were conducted on eight ISMN networks previously considered in (Souissi et al., 120 2020). Figure 2 shows the distribution of the considered soil moisture networks with different soil textures and climatic 121 parameters (cf. appendix B). For each station, the RZSM observation point is located between 30 and 55cm (Table 2). 122 For each soil moisture hourly acquisition, ISMN provides quality flags. Quality flags can be marked as 'C' (exceeding 123 plausible geophysical range),' D' (questionable/dubious), 'M' (missing), or 'G' (good) (Dorigo et al., 2011). Category 124 'D' has subset flags namely 'D01' for which in situ soil temperature  $< 0^{\circ}$ C, 'D02' that flags points at which in situ air temperature  $< 0^{\circ}$ C as well as 'D03' that also flags areas where GLDAS soil temperature  $< 0^{\circ}$ C. In our study, only soil 125 126 moisture data which quality flag is marked 'G' were retained.



127

Figure 2. International Soil Moisture Network (ISMN) network distribution (adapted from the ISMN web data portal
 (https://www.geo.tuwien.ac.at/insitu/data_viewer/); scale: 1 cm=1000 km).

130 **Table 2.** Overview of the considered ISMN and external networks.

Network	Country	Number of Selected	Selected RZSM Depth	SM
Network	Country	Stations (cm)		Sensors
AMMA-CATCH	Benin, Niger	5 (3 in Benin and 2 in Niger)	40	CS616
BIEBRZA-S-1	Poland	3	50	GS-3
CTP-SMTMN	China	54	40	EC-TM/5TM
HOBE	Denmark	29	55	Decagon-5TE
FR-Aqui	France	5	30, 34, 50	ThetaProbe ML2X
OZNET	Australia	19	30	Hydra Probe-CS616
SCAN	USA	209	50	Hydraprobe-Sdi-12/Ana
SMOSMANIA	France	22	30	ThetaProbe ML2X

# 132 2.1.2 External soil moisture data

133 The external networks only considered to assess the transferability and robustness of the approach were employed for 134 validation. The trained models are run for predictions only over these sites. They have been selected to cover semi-arid, 135 moderate and tropical semi-arid climates.

<u>Tunisian site</u>: The Merguellil site is located in central Tunisia (9°54 E; 35°35 N). This site is characterized by a semiarid climate with highly variable rainfall patterns (average equal to 300mm/year), very dry summer seasons, and wet winters. The Merguellil site represents an agricultural region where croplands, namely, olive groves and cereal fields, prevail (Zribi et al., 2021). At this study site, a network of continuous thetaprobe stations installed at bare soil locations provided moisture measurements at depths of 5 and 40 cm. All measurements were calibrated against gravimetric estimations. Data were obtained from the Système d'Information Environmental (SIE) web application catalog.

- <u>Italian site</u>: The Landriano site is located in northern Italy (Pavia province, Lombardia region). This station is located in a maize field, which was monitored in 2006 and from 2010 to 2011 (Masseroni et al., 2014). The average rainfall in Pavia province is of 650–700 mm, the climate is classified as 'Cfa' (cf. appendix A) and the field is irrigated by the border method with an average irrigation amount of approximately 100 to 200 mm per application with one to two applications per season due to the presence of a shallow groundwater table. Soil moisture measurements were performed with time domain reflectometer (TDR) soil moisture sensors. Five TDR soil moisture sensors were installed along a profile at depths of 5, 20, 35, 50, and 70 cm.
- 150Indian site: The Berambadi watershed is located in Gundalpet taluk, Chamarajanagara district, in the southern151part of Karnataka state in India and covers an area of approximately 84 km². The average rainfall is equal to152800 mm/year and the climate is classified as Aw (cf. appendix A). Hydrological variables have been intensively153monitored since 2009 in the Berambadi watershed by the Environmental Research Observatory ORE BVET154and AMBHAS Observatory. The soil moisture levels at the surface (5 cm) and root zone (50 cm) are monitored

with a HydraProbe sensor at different agricultural sites across the watershed, and in the current study, 4 stations were chosen.

# 157 **2.1.3 Surface soil temperature**

In addition to in situ soil moisture, the ISMN optionally includes meteorological and soil variables that are available over specific time periods. Values of the situ surface soil temperature among these variables can be employed as a useful indicator of the soil moisture data quality. The soil temperature was provided in Celsius, and the plausible values range from -60 to 60 °C. Regarding soil moisture data, surface soil temperature data were also provided with quality flags (Dorigo et al., 2011). However, the drawback is that this variable is not available in all networks, which is the case with the AMMA-CATCH network.

## 164 **2.1.4 Normalized difference vegetation index**

165 We considered the remote sensing-based normalized difference vegetation index (NDVI) to infer vegetation dynamics. 166 We extracted this index from the Moderate Resolution Imaging Spectroradiometer (MODIS) Vegetation Indices 167 product (MOD13Q1 version 6). MODIS Vegetation Indices (MOD13Q1) version 6 data are generated at 16-day 168 intervals and a 250-m spatial resolution as a Level 3 product. This product provides two primary vegetation layers. The 169 first vegetation layer is the NDVI, which is referred to as the continuity index of the existing National Oceanic and 170 Atmospheric Administration-Advanced Very High Resolution Radiometer (NOAA-AVHRR)-derived NDVI. The 171 algorithm chooses the best available pixel value from all the acquisitions over the 16-day period. The criteria 172 considered are low cloud coverage, low view angle, and highest NDVI value (Huete et al., 1999). To obtain daily 173 NDVI values, we conducted linear interpolation of the 16-day product.

# 174 **2.1.5 Potential evapotranspiration**

175 Similarly, we assessed the impact of considering a remote sensing-based evaporation efficiency, which is initially 176 defined as the ratio of actual to potential soil evaporation, on RZSM prediction. The computation details of this variable 177 will be detailed later (cf. Section 2.2.2). We employed the remote sensing-based potential evapotranspiration (PET) to 178 compute the evaporation efficiency. We extracted the PET from the MOD16A2 Evapotranspiration/Latent Heat Flux 179 version 6 product, which is an 8-day composite dataset produced at a 500-m pixel resolution. The algorithm used for 180 MOD16 data product collection is based on the logic of the Penman–Monteith equation, which employs inputs of daily meteorological reanalysis data along with MODIS remote sensing data products such as vegetation property dynamics, 181 182 albedo, and land cover. The MOD16A2 product provides layers for the composite evapotranspiration (ET), latent heat 183 flux (LE), potential ET (PET) and potential LE (PLE). The pixel values for the PET layer include the sum of all eight 184 days within the composite period (Running et al., 2017). To obtain daily PET values, we performed a linear 185 interpolation over the 8-day product and then we divided by eight the interpolated value.

### 186 **2.2 Methods**

# 187 **2.2.1 Recursive exponential filter**

188 Two ANN models presented in Table 1 contained extra knowledge on infiltration process information based on the 189 outputs of the recursive exponential filter (Stroud, 1999) as a feature. The recursive exponential filter was first introduced by Wagner et al. (1999) to estimate the soil water index (SWI) from surface soil moisture. SWI is computedas follows:

 $SWI_{t_n} = SWI_{t_{n-1}} + K_n(ms(t_n) - SWI_{t_{n-1}})$ (1)

194 where:

195 SWIt_n is the soil water index at time  $t_n$ , 196  $ms(t_n)$  is the scaled surface soil moisture at time  $t_n$  (scaled between maximum and minimum 197 values), 198  $K_n$  is the gain at time  $t_n$ , which occurs in [0,1] and is given by:  $K_n = \frac{K_{n-1}}{\frac{K_{n-1} + e^{-\frac{(t_n - t_{n-1})}{T}}}{(t_n - t_n)}}$  (2) and 199 200 T is a time constant and is the only required tuning parameter to compute the recursive 201 exponential filter. 202 For the initialisation of the filter, gain  $K_1 = 1$  and  $SWI_{(t1)}^* = ms(t_1)$ 203 Regarding T values, we considered an empirical list ([1,3,5,7,10,13,15,20,40,60]), which was partly inspired by (Paulik 204 et al., 2014) ( $T \in [1,5,10,15,20,40,60,100]$ ). Given the list of T values, recursive exponential filter outputs were 205 computed for all of the stations (346 stations) given each T value. Based on the correlation values between the in situ 206 RZSM values and the recursive exponential filter-based RZSM pre-estimates, we established the optimal time variable 207 T, hereafter referred to as T_{best}, for each station.

### 208 2.2.2 Evaporative efficiency

An ANN model with evaporation efficiency input was also developed. This variable, which is defined as the ratio of the actual to potential soil evaporation, was first introduced in (Noilhan, J. and Planton, 1989; Jacquemin et al., 1990; Lee et al., 1992) and thereafter readapted in (Merlin et al., 2010) to include the soil thickness. In our work, we use a modified evaporation efficiency formulation, based on the third model developed in (Merlin et al., 2010), which can be expressed as follows (cf. appendix C):

- 214
- 215

$$\beta = \left[\frac{1}{2} - \frac{1}{2}\cos(\pi\theta/\theta_{max})\right]^{P*} \qquad (3)$$

4

216 where:  $-\beta$  is evaporation efficiency

217 -  $\theta$  is the water content in the soil layer of thickness L.

218 -  $\theta_{max}$  is the maximum soil moisture at each station.

219 - P* is a parameter computed as follows:

$$P^* = \frac{PET}{2B} (4)$$

P*, a proxy of parameter P (cf. appendix C), represents an equilibrium state controlled by retention forces in
the soil, which increase with the thickness L of considered soil and by evaporative demands at the soil surface.
-PET is the potential evapotranspiration (PET) extracted from the MODIS 500-m 8-day product (MOD16A2).

- 224 The soil evaporation efficiency computed by model 3, developed in (Merlin et al., 2010), decreases when PET
- 225 increases. Retention force and evaporative demand make the term P increase (replaced by P*), as if an increase of
- 226 potential evaporation LE_p (here replaced by PET) at the soil surface would make the retention force in the soil greater.
- 227 Merlin et al. (2010) tested this approach at two sites in southwestern France using in situ measurements of actual
- evaporation, potential evaporation, and soil moisture at five different depths collected in summer. Model 3 was able to
- 229 represent the soil evaporation process with a similar accuracy as the classical resistance-based approach for various soil
- 230 thicknesses up to 100 cm. Merlin et al. (2010) affirm the parameterization of P as function of  $LE_p$  (here PET) indicates
- 231 that  $\beta$  cannot be considered as a function of soil moisture alone since it also depends on potential evaporation.
- 232 Moreover, the effect of potential evaporation on  $\beta$  appears to be equivalent to that of soil thickness on  $\beta$ . This
- equivalence is physically interpreted as an increase of retention forces in the soil in reaction to an increase in potentialevaporation.

### 235 **2.2.3** Artificial neural network implementation

236 The multilayer perceptron (MLP), which is a multilayer feed-forward ANN, is one of the most widely applied ANNs, 237 mainly in the field of water resources (Abrahart and See, 2007) The multilayer perceptron contains one or more hidden 238 layers between its input and output layers. Neurons are organized in layers such that the neurons of the same layer are 239 not interconnected and that any connections are directed from lower to upper layers (Ramchoun et al., 2016). Each 240 neuron returns an output based on the weighted sum of all inputs and according to a nonlinear function referred to as 241 the transfer or activation function (Oyebode and Stretch, 2019). The input layer, consisting of SSM values and/or other 242 processrelated variables, is connected to the hidden layer(s), which comprises hidden neurons. The final ANN-derived 243 estimates of the ANN are given by an activation function associated with the final layer denoted as the output layer, 244 based on the sum of the weighted outputs of the hidden neurons.

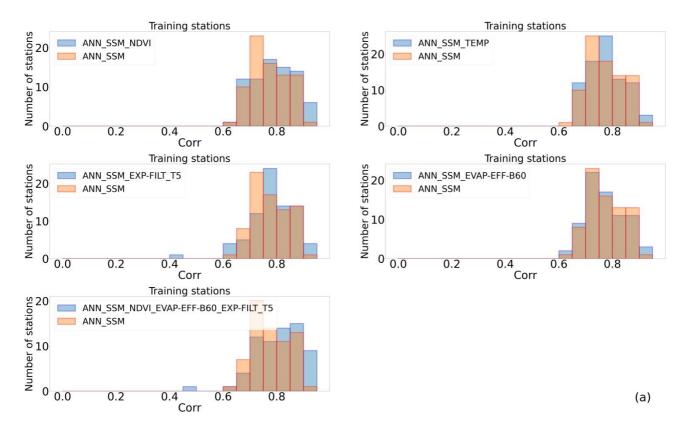
- 245 We started with the ANN model developed in (Souissi et al., 2020), whose architecture consists of one hidden layer 3 246 of 20 hidden neurons, a tangent sigmoid function as the activation function of the hidden layer, a quadratic cost 247 function as the loss function and the stochastic gradient descent (SGD) technique as the optimization algorithm. 248 This model was developed to estimate RZSM based on only in situ SSM information. SSM was not applied as a 249 feature of hourly values but was employed in the form of three features, namely, SSM rolling averages over 10, 30 250 and 90 days. Additional ANN models were developed to study, through each model, the impact of the application 251 of the NDVI, SWI, evaporation efficiency and the surface soil temperature as features. A model combining surface 252 soil moisture, NDVI, evaporation efficiency and recursive exponential filter was further considered. These ANN 253 models were trained and validated on the 122 ISMN stations considered of good quality after a data filtering step 254 as detailed in (Souissi et al., 2020). Training of the above ANN models was conducted considering 70% of these 255 122 stations. Thirty percent was reserved for validation, and testing was conducted at the rest of stations. So in 256 summary, 122 stations were considered for the training/validation of the ANN models and 224 stations, if all input 257 data are available, were used for testing. In a second step, tests were conducted on data external to the ISMN 258 database namely on sites of Tunisia, Italy and India. The trained models over ISMN are used only in prediction 259 mode over these sites. The data for SSM in addition to the other features are used as inputs and RZSM is predicted 260 in outputs.**Results**
- 261 **3.1 Exponential filter characteristic time length**

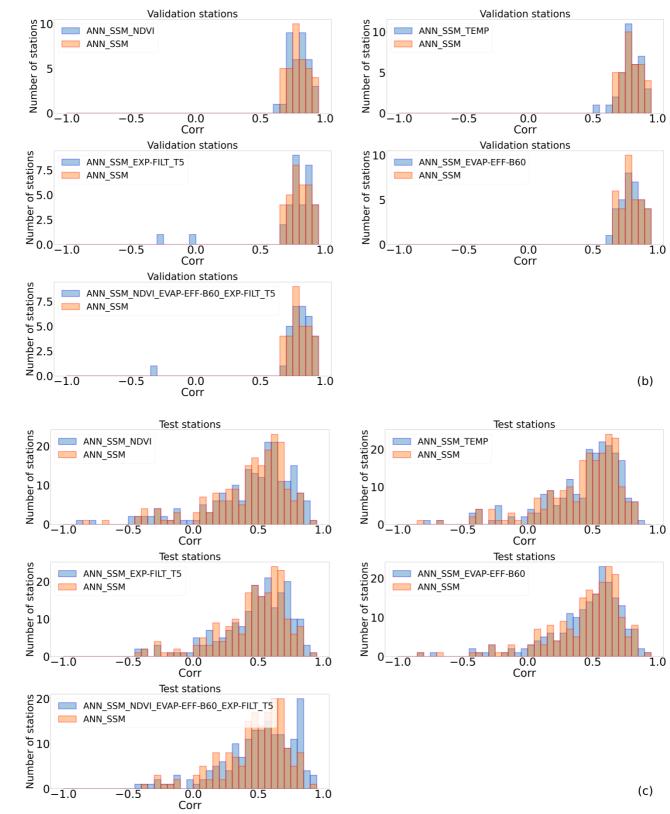
- 262 A large proportion of the stations attained an optimal time constant (T_{best}) value equal to 60 days which suggests an
- abnormally long infiltration time. These stations belong to the SCAN network and exhibit an RZSM acquisition depth
- of 50 cm, in contrast other networks such as SMOSMANIA, for instance, where RZSM is retrieved at 30 cm. The high
- values correspond to correlation with seasonal dynamics rather than infiltration processes. This depth could explain the
- anomalously long infiltration time. This is consistent with (Paulik et al., 2014) in which the average T value with the
- 267 highest correlation (T_{best}) increased with increasing depth of the in situ observations.
- For comparison purposes, Paulik et al. (2014) found that 23.98% of the stations achieved  $T_{best}$ =5 days, while 21.58% of the stations achieved  $T_{best} \ge 60$  days (60 or 100 days).
- Albergel et al. (2008) considered an average  $T_{best}$  value of 6 days for the SMOSMANIA network. This value represented the average  $T_{best}$  value for all stations belonging to the SMOSMANIA network. In our case, the average  $T_{best}$  value for all stations of the SMOSMANIA network reached 9 days. In this study, an average  $T_{best}$  value could be established for each station or each network. However, this is not relevant to our work because we aim to evaluate maps of remote sensing data in next steps, and thus, we did not compute  $T_{best}$  at each location. We fixed the value of T to 5 days as a median infiltration time.

#### 276 **3.2 Intercomparison of the ANN models**

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The distribution histograms for training, validation and test stations (Fig. 3) show that the integration of the considered process-related features improved the prediction accuracy in certain cases compared to the reference. Time series of good and less good quality of fit were provided in appendix E for training, validation and test stations using reference model ANN_SSM and the most complex ANN model.





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Figure 3. Correlation histograms of all tested ANN models compared to ANN_SSM (a) on training stations (b) on validation stations
 (c) on test stations (cf. appendix D for RMSE histograms)

In terms of the NDVI, 65.82%, 45.71% and 55.22% stations attained better correlation values with ANN_SSM_NDVI
 than those obtained with ANN_SSM for the training, validation and test stations, respectively. RMSE decreased for

- 44.3%, 40.0% and 40.3% of the stations with ANN_SSM_NDVI compared to model ANN_SSM for training,
  validation and test stations, respectively (Table 3).
- 290 In regard to the ANN_SSM_TEMP model that integrates the soil surface temperature, 49.4%, 55.56% and 59.35% of
- the training, validation and test stations exhibited higher correlation values than those obtained with the ANN_SSM
- 292 model, respectively. RMSE decreased with ANN_SSM_TEMP compared to model ANN_SSM for 25.3%, 38.89% and
- 293 42.99% of the training, validation and test stations, respectively.
- In addition, model ANN_SSM_EXP-FILT-T5 that integrates the simplified infiltration based features yielded slightly
  better correlations, and 64.56%, 60.61% and 63.68% 62.62% of the training, validation and test stations attained better
  correlations than those obtained with model ANN_SSM, respectively. Besides, RMSE decreased for 36.71 %, 42.42 %
  and 50.25% of the training, validation and test stations with ANN_SSM_EXP-FILT-T5 compared to model
  ANN_SSM, respectively.
- 299 Regarding the evaporation efficiency, we considered different values of fitting parameter B (Eq. 4) such that B 300 remained within the [50,60] interval. This parameter can be fitted using different variables, such as the wind speed or 301 relative humidity. Comparisons based on the correlation values provided by the different models for each B value 302 indicated that the performance was insensitive to the B value. Thus, we fixed the B value to 60 W m-2. Comparison of 303 models ANN_SSM and ANN_SSM_EVAP-EFF-B60 revealed that 54.55%, 52.94% and 52.33% of the training, 304 validation and test stations attained higher correlation values with the latter model, respectively. RMSE was reduced for 305 28.57%, 41.18% and 48.19% of the training, validation and test stations with ANN SSM EVAP-EFF-B60 compared 306 to model ANN_SSM, respectively.
- 307 Finally, we investigated the impact of the joint application of the NDVI, recursive exponential filter (T= 5 days)
- 308 and evaporation efficiency (B=60 W m⁻²) in the ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5 model. The
- 309 surface soil temperature was not included, as its effect is included in the evaporation process. At 84.06%, 61.29% and
- 310 62.07% of the training, validation and test stations, the correlation value obtained with this model was higher than that
- 311 obtained with the ANN_SSM model, respectively. In addition, RMSE was minimized for 62.32%, 54.84% and 54.02%
- 312 of the training, validation and test stations with ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5 compared to
- 313 model ANN_SSM, respectively.
- Considering model ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5, only one training station had a decrease in correlation by more than 0.1 namely station 'Lind#1' (network 'SCAN') compared to reference model ANN_SSM. All inputs were not available at the same dates which implied a significant reduction in data points (cf. appendix F). The decrease in correlation and increase in RMSE didn't exceed 0.1 and 0.01 m³/m³, respectively, for the rest of stations of lower performance metrics with the most complex ANN.
- 319 Similarly for validation stations, only one station had a decrease in correlation above 0.1, namely station 'PineNut'
- 320 (network 'SCAN'), with model ANN SSM NDVI_EVAP-EFF-B60_EXP-FILT-T5. This decrease can be also
- 321 explained because of data shortage (cf. appendix F). The decrease in correlation and increase in RMSE didn't exceed
- 322 0.1 and 0.01 m³/m³, respectively, for the rest of stations of lower performance metrics with the most complex ANN.
- Regarding test stations, correlation decrease by more than 0.1 and RMSE increase by more than 0.01 m³/m³with model ANN SSM NDVI EVAP-EFF-B60 EXP-FILT-T5 compared to model ANN SSM was detected for only 2 stations.

- 325 Both stations, namely station 'S-Coleambally' and 'Widgiewa' which belong to network 'OZNET', significantly lose in
- 326 data volume when process-related variables are integrated in ANN and more precisely because of NDVI data
- 327 availability (cf. appendix F). For the rest of test stations, correlation decreased and RMSE increased simultaneously by
- 328 less than 0.1 and 0.01 m³/m³, respectively, whith model ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5.
- 329 Table 3. Proportion of the stations which performance enhances using the ANN models enriched with process-related features
- 330 compared to model ANN_SSM (*: % of stations at which the correlation improves over the model ANN_SSM level; **: % of stations
- at which RMSE improves over the model ANN_SSM level)

Model	Training stations		Validation stations		Test stations	
	% of stations	% of stations	% of stations	% of stations	% of stations	% of stations
	$(\operatorname{corr}\uparrow)^*$	$(\text{RMSE}\downarrow)^{**}$	$(\operatorname{corr}\uparrow)^*$	$(\text{RMSE }\downarrow)^{**}$	$(\operatorname{corr}\uparrow)^*$	$(\text{RMSE}\downarrow)^{**}$
ANN_SSM_NDVI	65.82	44.3	45.71	40.0	55.22	40.3
ANN_SSM_TEMP	49.4	25.3	55.56	38.89	59.35	42.99
ANN_SSM_EXP-FILT-T5	64.56	36.71	60.61	42.42	63.68	50.25
ANN_SSM_EVAP-EFF-B60	54.55	28.57	52.94	41.18	52.33	48.19
ANN_SSM_NDVI_EVAP- EFF-B60_EXP-FILT-T5	84.06	62.32	61.29	54.84	62.07	54.02

333	Table 4. Proportion of the stations which	correlation decreases using the ANN model	ls enriched with process-related features

334 compared to model ANN_SSM ( $\Delta_{corr}$ =corr_{ANN_SSM} - corr_{ANN_SSM_X}, X denotes a or a combination of process-related variables)

Model	Training stations		Validation stations		Test stations		
	% of stations	% of stations	% of stations	% of stations	% of stations	% of	
	corr $\downarrow$ and	corr $\downarrow$ and	corr $\downarrow$ and	corr $\downarrow$ and	corr $\downarrow$ and	stations	
	$0.05 < \Delta_{corr} < 0.1^*$	$\Delta_{corr} > 0.1^*$	$0.05 < \Delta_{corr} < 0.1^*$	$\Delta_{corr} > 0.1^*$	$0.05 < \Delta_{corr} < 0.1$	corr $\downarrow$ and	
					*	$\Delta_{corr} > 0.1^*$	
ANN_SSM_NDVI	3.8	0	2.86	0	9.95	5.97	
ANN_SSM_TEMP	0	1.2	0	2.78	4.67	3.27	
ANN_SSM_EXP-FILT-T5	6.33	1.27	3.03	9.09	6.97	3.48	
ANN_SSM_EVAP-EFF-B60	10.39	1.3	0	2.94	6.74	5.7	
ANN_SSM_NDVI_EVAP- EFF-B60_EXP-FILT-T5	4.35	1.45	6.45	3.23	9.2	6.9	
_							

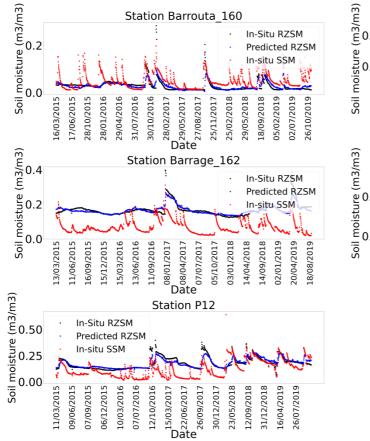
336 Always in terms of the general performance of model ANN SSM NDVI EVAP-EFF-B60 EXP-FILT-T5, about 337 75% of the stations have an RMSE less than  $0.05 \text{ m}^3/\text{m}^3$  and around half of the stations have an RMSE less than 0.04338  $m^3/m^3$ . This accuracy is consistent, for instance, with the target value in SMAP (Entekhabi et al., 2010) and SMOS (Kerr et al., 2010) missions which is equal to 0.04 m³/m³ and also to the average sensor accuracy adopted by Dorigo et 339 340 al. (2013) which is equal to 0.05 m³/m³. Overall, the most complex model ANN_SSM_NDVI_EVAP-EFF-B60_EXP-341 FILT-T5 can successfully characterize the soil moisture dynamics in the root zone since half of the stations have a 342 correlation value greater than 0.7. Pan et al. (2017) developed different ANN models to estimate RZSM at depth of 343 20cm and 50cm over the continental United States using surface information. They found that half of the stations have 344 RMSE less than 0.06 m³/m³ and more than 70% of stations have correlation above 0.7 when predicting RZSM at 20cm. 345 However, the developed ANN was less effective in RZSM prediction at 50cm which is also in accordance with 346 (Kornelsen and Coulibaly, 2014). In our study, the densest soil moisture network is 'SCAN', located in the USA. Soil 347 moisture was predicted at a depth of 50cm over this network. Around half of the stations have a correlation value of 348 above 0.6 and RMSE less than 0.04 m³/m³ after the integration of process-related inputs. Pan et al., (2017) suggests that 349 the use of only time-dependent variables may not be sufficient for the ANN models to accurately predict RZSM and 350 suggests adding soil texture data.

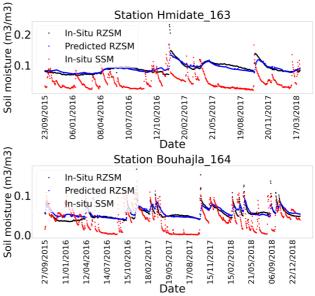
351

# 352 **3.3 Robustness of the approach**

353 To further assess the robustness of our approach, which involves RZSM prediction using the different ANN models 354 with different features, we predicted RZSM at 40 cm at sites not previously considered in previous parts of the study. 355 The selected stations are located in: the Kairouan Plain, a semiarid region in central Tunisia, Landriano site located in 356 the North of Italy, and the Berambadi watershed located in Gundalpet taluk, South-India. In the case of the Kairouan 357 Tunisia, model ANN_SSM yielded moderate- to low-precision predictions, as highlighted by the performance metrics 358 listed in Table 5. The time series (cf. appendix G) show that the RZSM predictions followed the SSM seasonality, 359 which was reflected by the false peaks generated in the RZSM predictions whenever a sharp increase or decrease 360 occurred in the SSM values. This observation was also found in (Souissi et al., 2020). Actually, the Kairouan Plain is 361 characterized by a semiarid environment where rainfall events infrequently occur and the level of evaporation is high. 362 The reference model ANN_SSM shows its limitations to accurately predict RZSM in areas with no alternate wet and 363 dry cycles.

364 However, the consideration of additional features, namely, the NDVI, evaporation efficiency and SWI in the ANN 365 models resulted in a good agreement between the in situ and predicted RZSM values (Fig. 4). The correlation values 366 were improved by 60.04%, 169.5%, 112.02%, 80.23% and 53.7% at stations Barrouta-160, Hmidate 163, 367 Barrage_162, Bouhajla_164 and P12, respectively, with the ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5 model 368 over ANN SSM model values. Similarly, RMSE values were reduced (Table 5). As shown in figure 4, the most 369 complex ANN model is able to capture the variations of RZSM. This finding highlights the added value of our hybrid 370 approach based on an association of a machine learning method with process-related variables. Instead of injecting 371 uncertain information in physical models, such as soil properties, we used a nonparametric method related to physical 372 processes without using forcing data that may be subject to errors and potentially lead to inaccurate tracking of the 373 long-term evolution of soil moisture.



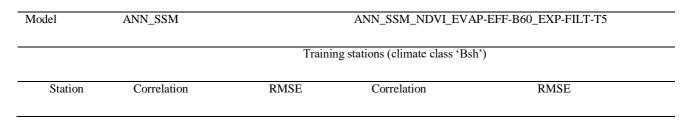


374 375

Figure 4. In situ SSM, in situ RZSM, and predicted RZSM series at the stations in the Kairouan Plain (Tunisia) with model 376 ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5 (cf. appendix G for larger figure format).

377 A second comparison can be conducted between the quality of fit of these independent datasets and training datasets. 378 Actually, the climate class of the Tunisian stations is 'Bsh' (cf. appendix A). At the training stage, no station falls into 379 the climate class 'Bsh' (cf. appendix A). However, some training stations fall under a similar climate class which is 380 'Bsk' (cf. appendix B). Table 5 presents correlation and RMSE values for these training stations and Tunisian sites with 381 both models ANN SSM and ANN SSM NDVI EVAP-EFF-B60 EXP-FILT-T5. For all training stations, 382 performance metrics are slightly enhanced with the most complex ANN model compared to reference model 383 ANN_SSM, except for stations GrouseCreek, Harmsway and Lind#1 which performance decreases. Overall, the range 384 of correlation values is similar for training and external validation stations with model ANN_SSM_NDVI_EVAP-EFF-385 B60_EXP-FILT-T5 and RMSE is well reduced for Tunisian stations compared to training stations. Given the results on 386 unseen datasets, namely on Tunisia, the performance of the most complex ANN model is good as it is able to generalize 387 the patterns present in the training dataset.

388 Table 5. Performance metrics of models ANN SSM and ANN SSM NDVI EVAP-EFF-B60 EXP-FILT-T5 at training stations of 389 climate "Bsk" and Tunisian stations of climate "Bsh".



Banandra	0.701	0.05	0.764	0.046
(OZNET)				
DRY-LAKE	0.674	0.031	0.692	0.03
(OZNET)				
CPER (SCAN)	0.691	0.032	0.695	0.032
EPHRAIM	0.758	0.051	0.791	0.046
(SCAN)				
GrouseGreek	0.818	0.033	0.802	0.035
(SCAN)				
HarmsWay	0.705	0.034	0.622	0.038
(SCAN)				
Lind#1	0.605	0.055	0.483	0.022
(SCAN)				
		Ext	ternal test stations (Tunisia)	
Station	Correlation	RMSE	Correlation	RMSE
Barrouta_160	0.463	0.021	0.714	0.016
Hmidate_163	0.318	0.019	0.834	0.011
Barrage_162	0.416	0.035	0.864	0.019
Bouhajla_164	0.435	0.016	0.733	0.01

391 At the South-Indian stations, the ANN_SSM model yielded a good agreement even without the integration of process-392 related features (Table 6). The NDVI added little to nonsignificant improvement at station Bheemanbidu. The same 393 observation was made at the Italian site. The application of multiple features performed the best under arid conditions, 394 e.g., in Tunisia. In the tropical and temperate climate regions, this was not the case. The presence of clouds in the 395 MODIS NDVI and potential evapotranspiration products could explain this observation at sites of South-India and 396 North-Italy. In South-India, for instance, the maximum variability in soil moisture occurred during the monsoon season, 397 which is characterized by a large amount of clouds. Moreover, the coarse resolution of MODIS NDVI product makes it 398 sometimes not adapted to the considered site. (Chen et al., 2016) investigated the impact of sample impurity and 399 landscape heterogeneity on crop classification using coarse spatial resolution MODIS imagery. They showed that the 400 sample impurity such as mixed crop types in a specific sample, compositional landscape heterogeneity that is the 401 richness and evenness of land cover types in a landscape, and configurational heterogeneity that is the complexity of 402 spatial structure of land cover types in a specific landscape are sources of uncertainty affecting crop area mapping when 403 using coarse spatial resolution imagery. High resolution NDVI from sensors like Sentinel-2 could have been used in 404 this exercise to mitigate the spatial resolution issue, however, MODIS data were privileged in order to provide NDVI 405 and PET from the same sensor.

406 Table 6. Performance metrics of models ANN_SSM, ANN_SSM_NDVI and ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5 at

407

the sites in South-India and Northern Italy.

ANN_SSM ANN_SSM_1		ANN_SSM_NDVI	M_NDVI ANN_SSM_NDVI_EV		
				EFF_B60_EXP-FILT-T5	
		INDIA			
Correlation	RMSE	Correlation	RMSE	Correlation	RMSE
0.813	0.04	0.78	0.042	0.744	0.044
0.76	0.046	0.784	0.044	0.763	0.046
0.825	0.038	0.787	0.04	0.743	0.044
0.713	0.024	0.713	0.024	0.633	0.025
		Italy			
Correlation	RMSE	Correlation	RMSE	Correlation	RMSE
0.861	0.038	0.827	0.041	0.841	0.038
	Correlation 0.813 0.76 0.825 0.713 Correlation	Correlation         RMSE           0.813         0.04           0.76         0.046           0.825         0.038           0.713         0.024           Correlation         RMSE	INDIA           Correlation         RMSE         Correlation           0.813         0.04         0.78           0.76         0.046         0.784           0.825         0.038         0.787           0.713         0.024         0.713           Italy         Correlation         RMSE	INDIA         Correlation       RMSE       Correlation       RMSE         0.813       0.04       0.78       0.042         0.76       0.046       0.784       0.044         0.825       0.038       0.787       0.04         0.713       0.024       0.713       0.024         Italy       Correlation       RMSE	EFF_B60_EXP-FI         INDIA       INDIA         Correlation       RMSE       Correlation         0.813       0.04       0.78       0.042       0.744         0.76       0.046       0.784       0.044       0.763         0.825       0.038       0.787       0.04       0.743         0.713       0.024       0.713       0.024       0.633         Italy       Italy       Correlation       RMSE       Correlation

408

### 409 **4 Discussion**

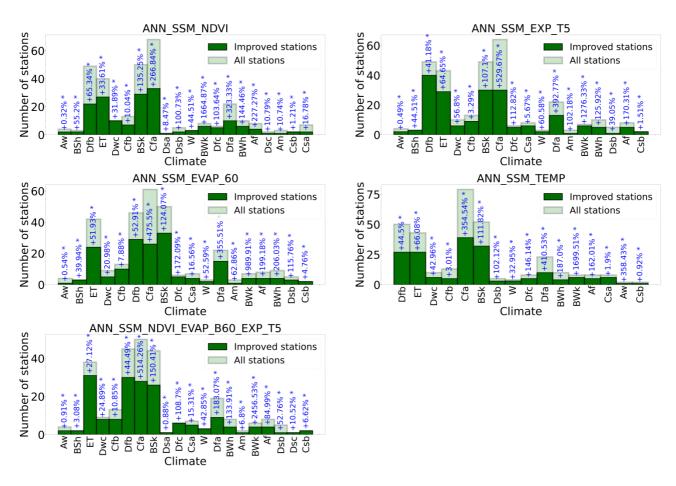
410 Climate analysis of the results yielded by the different models indicated that among all models, the climate class with 411 the highest mean correlation change rate (Fig. 5) was class BWk (cf. appendix A), which regroups desert areas where 412 the link between SSM and RZSM is weak due to high evaporative rates. Class Dfa (cf. appendix A), which includes 413 areas experiencing harsh and cold winters, also yielded a high mean correlation change rate (>100%). Similarly, at 414 stations of this climate type, the link between the surface and root zone is poor. In regard to class Cfa (cf. appendix A), 415 in which more than 80% of the total stations belongs to SCAN network, the high mean correlation change rate could be 416 explained by the surface-subsurface decoupling phenomena detected within this network, as previously reported in 417 (Souissi et al., 2020). The model with the largest number of stations with improved predictions over the ANN_SSM 418 model predictions was ANN SSM NDVI EVAP-EFF-B60 EXP-FILT-T5. Actually, the coupled use of process-419 related features in the ANN models exerted a greater impact on the prediction accuracy than that exerted by the one-at-420 a-time application of these features. In model ANN SSM NDVI EVAP-EFF-B60 EXP-FILT-T5, the three process-421 based features jointly employed seemed to counterbalance the weight of these three SSM features. In this model, the 422 process-related features were equally represented versus the SSM information depicted by these three features. The 423 redundancy of the considered SSM information could explain the limited impact of the one-at-a-time addition of 424 process-related features the joint addition of the three process-related features.

425 In addition, Karthikeyan and Mishra (2021) demonstrated that at root depths beyond 20 cm, the importance of SSM

426 was notably lower than that at the 20-cm depth, signifying decorrelation between surface and deeper SM values, which

427 is in accordance with the findings in (Souissi et al., 2020), and it was further revealed that vegetation exhibits a higher

- 428 importance than that of meteorological predictors LST and precipitation. Kornelsen and Coulibaly (2014) indicated
- that evapotranspiration is the most important meteorological input for the prediction of soil moisture in the root zone
- 430 with the MLP, which reflects the importance of the water vapor flux in soil moisture state determination.



### 432

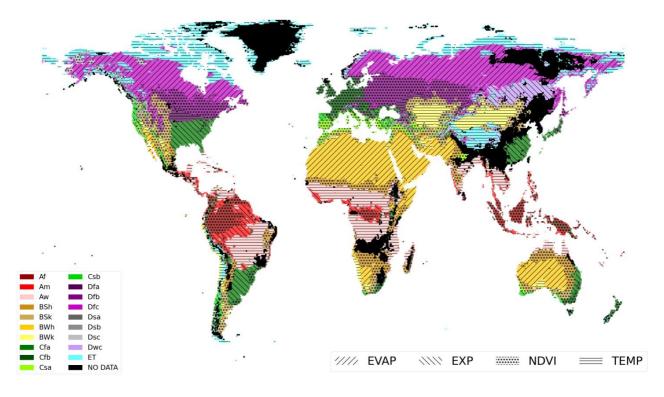
*Mean correlation change rate per climate class

Figure 5. Climate classification of the stations performing better with models (a) ANN_SSM_NDVI (b) ANN_SSM_EXP-T5 (c)
ANN_SSM_EVAP-60 (d) ANN_SSM_TEMP and (e) ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5 compared to model
ANN_SSM (Dark green corresponds to stations which correlation improved with complexified models, light green corresponds to
total stations, rate in blue correspond to mean correlation change rate per climate class).

$$437 \quad * corr_change_rate = mean(\frac{corr_{ANN}_{SSM}_{X} - corr_{ANN}_{SSM}}{corr_{ANN}_{SSM}} * 100) (5)$$

438 where X denotes a process-related variable (X  $\in$  ['NDVI', 'EXP-FILT-T5', 'EVAP-EFF-B60', 'TEMP']

The world map illustrated in Fig. 6, shows the best-performing ANN models based on the mean correlation change rate (Eq. 5). We assumed that the results in a given area of a specific climate class could be extended to other areas of the same climate class even if we did not consider the data for these areas. The climate classes without at least one station ware marked in black and labeled with 'NO DATA'



444 Figure 6. World map of best-performing ANN models per climate class based on the mean correlation change rate; colors
445 correspond to climate classes (cf. appendix A), hatches correspond to the most contributive input to the predictions namely: EVAP
446 (evaporation efficiency), EXP (exponential filter SWI), NDVI, TEMP (surface soil temperature).

In arid areas such as the eastern and western sides of the USA with high evaporation rates, ANN_SSM_EVAP-EFF-60 was the best performing model. Similarly, in bare areas of Africa, the Middle East and Australia where the Bwh climate class prevailed (arid desert hot climate; cf. appendix A), the evaporation efficiency was the best informative variable.

In the internal part of continental Europe and near the Mediterranean Basin, the NDVI was the most relevant indicator for RZSM estimation, where agricultural fields dominated. Similarly, the Great Plains region in the USA was deeply affected by the NDVI, as this region is a cultivated area. The same result could be obtained for regions belonging to climate class Bsh (arid steppe hot; cf. appendix A) and mainly covered by grassland and shrubland areas according to ESA CCI land cover maps.

In Nordic areas characterized by the ET climate class, the soil temperature was the most important root zone soil moisture indicator mainly because of the freeze-thaw events encountered in these regions. In tropical savannah wet areas (class Aw; cf. appendix A), the ANN_SSM_TEMP model was the best-performing model.

This classification definitely suffered limitations mainly provoked by the generalization of the climatic analysis results to areas not considered in this study. For instance, in regions of climate class Dfc (cold dry without a dry season, cold summer climate; cf. appendix A), we expect the temperature to serve as the most relevant indicator instead of the evaporation efficiency.

### 462 **5** Conclusion

443

In this study, we developed several ANN models to estimate RZSM based either on solely in situ SSM information
 or on a group of process-related features, in addition to SSM, namely, the soil water index computed with a recursive

465 exponential filter, evaporation efficiency, NDVI and surface soil temperature. Different regions across the globe with 466 distinct land cover and climate patterns were considered. The main conclusion of this study was that the consideration 467 of more features in addition to SSM information could enhance the accuracy of RZSM predictions mainly in regions where the link between SSM and RZSM is weak. 468

469 In arid areas with high evaporation rates, the most informative feature was the evaporation efficiency. In regions with 470 agricultural fields, the NDVI was, for example, the most relevant indicator to predict RZSM. Overall, the best 471 performing model included the surface soil moisture, NDVI, SWI and evaporation efficiency as features. The 472 robustness of the approach was further assessed through additional tests considering external sites in central Tunisia,

- 473 India and Italy. Similarly, the process-related features exerted a positive impact on the prediction accuracy when
- 474 combined with surface soil moisture in the case of Tunisia. The mean correlation across the five Tunisian stations
- 475 sharply increased from 0.44 when only SSM was considered to 0.8 when all process-related features were combined

476 with SSM. In India and Italy, the correlations were already high with the reference model ANN SSM. The change in

- 477 correlation after the addition of process-related features, namely NDVI, is about -0.04 which is nonsignificant, and is
- 478 potentially because of the cloudy conditions in India and noisy MODIS products. Also the crop heterogeneity and
- 479 sample impurity makes MODIS NDVI products not adapted to all sites.

480 As a research perspective, datasets can be separated in clusters corresponding to major climate classes and/or soil types.

481 More analysis can be conducted in this direction to eventually make connections between the different inputs and

482 climate/soil configurations.

483 Future work will examine the ability of the developed model to estimate RZSM across larger areas based on remote 484 sensing global soil moisture products. The use of remote sensing derived soil moisture products may yield lower 485 correlations with the reference model ANN_SSM which potentially implies further improvement when process-related 486 features are added.

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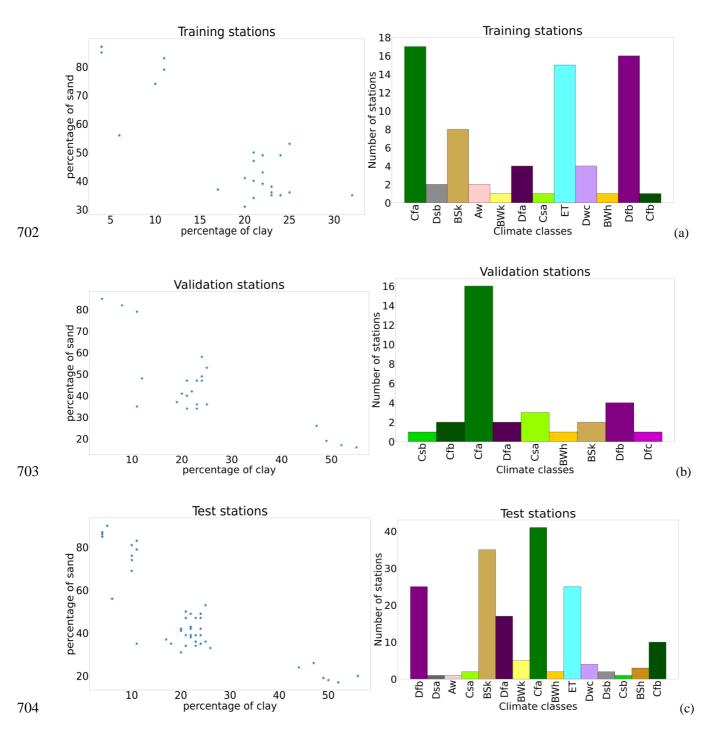
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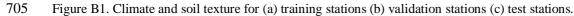
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664	Climate classes (Köppen classification):
665	Af: Tropical Rainforest
666	Am: Tropical Monsoon
667	As: Tropical Savanna Dry
668	Aw: Tropical Savanna Wet
669	• BWk: Arid Desert Cold
670	• BWh: Arid Desert Hot
671	• BWn: Arid Desert with Frequent Fog
672	BSk: Arid Steppe Cold
673	• BSh: Arid Steppe Hot
674	• BSn: Arid Steppe with Frequent Fog
675	Csa: Temperate Dry Hot Summer
676	Csb: Temperate Dry Warm Summer
677	Csc: Temperate Dry Cold Summer
678	Cwa: Temperate Dry Winter, Hot Summer
679	Cwb: Temperate Dry Winter, Warm Summer
680	Cwc: Temperate Dry Winter, Cold Summer
681	• Cfa: Temperate without a Dry Season, Hot Summer
682	• Cfb: Temperate without a Dry Season, Warm Summer
683	Cfc: Temperate without a Dry Season, Cold Summer
684	• Dsa: Cold Dry Summer, Hot Summer
685	Dsb: Cold Dry Summer, Warm Summer
686	Dsc: Cold Dry Summer, Cold Summer
687	• Dsd: Cold Dry Summer, Very Cold Winter
688	Dwa: Cold Dry Winter, Hot Summer
689	Dwb: Cold Dry Winter, Warm Summer
690	Dwc: Cold Dry Winter, Cold Summer
691	Dwd: Cold Dry Winter, Very Cold Winter
692	• Dfa: Cold Dry without a Dry Season, Hot Summer
693	• Dfb: Cold Dry without a Dry Season, Warm Summer
694	• Dfc: Cold Dry without a Dry Season, Cold Summer
695	• Dfd: Cold Dry without a Dry Season, Very Cold Winter
696	• ET: Polar Tundra
697	• EF: Polar Eternal Winter
698	• W: Water

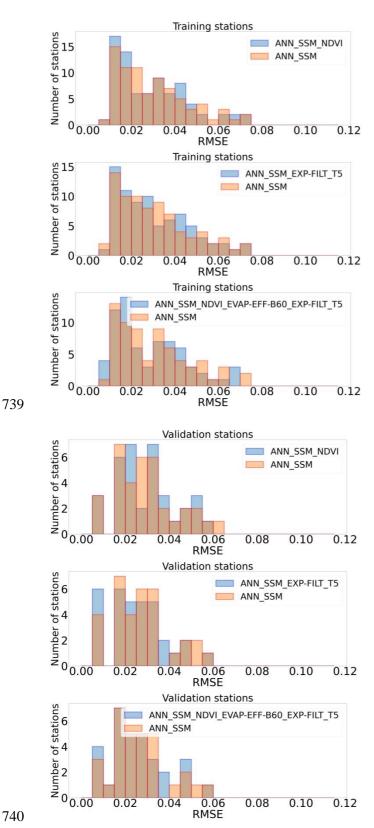
# **APPENDIX B**

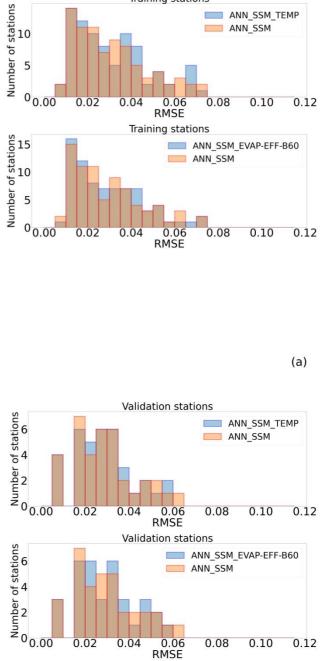




709	
710	APPENDIX C
711	Evaporation efficiency (section 2.2.2):
712 713	The standard equations to compute evaporation efficiency ( $\beta_3$ ) in (Merlin et al., 2010) are as follows:
714	$\beta_3 = \left[\frac{1}{2} - \frac{1}{2}\cos(\pi\theta_L/\theta_{max})\right]^p \qquad for \ \theta_L \le \theta_{max} \ (C3)$
715	$\beta_3 = 1 \text{ for } \theta_L > \theta_{max}$
716	where: $-\theta_L$ is the water content in the soil layer of thickness L.
717	- P is a parameter computed as follows:
718	$P = \left(\frac{1}{2} + A_3 \frac{L - L_1}{L_1}\right) \frac{L E_p}{B_3} (C4)$
719	- $\theta_{max}$ is the soil moisture at saturation.
720	$-LE_p$ is the potential evaporation.
721	- $L_1$ is the thinnest represented soil layer, and $A_3$ (unitless) and $B_3$ (W/m ² ) are the two best-fit parameters a
722	priori depending on the soil texture and structure, respectively.
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**APPENDIX D** 





Training stations

ANN_SSM_TEMP

ANN_SSM

(b)

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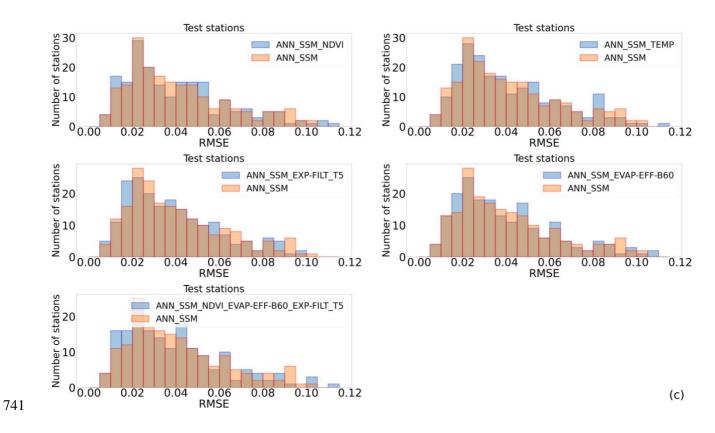
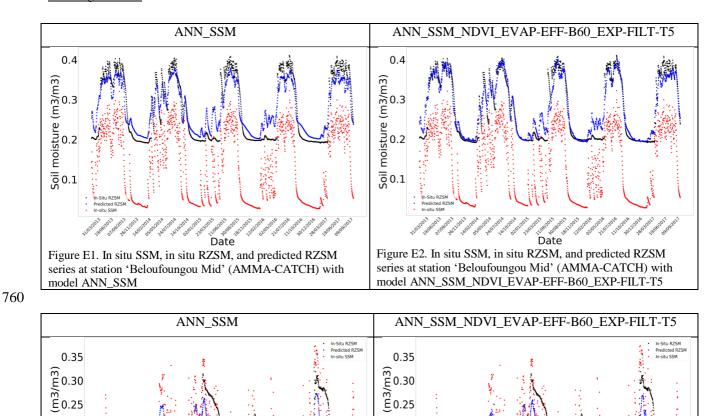


Figure D1. RMSE histograms of all tested ANN models compared to ANN_SSM (a) on training stations (b) on validation stations(c) on test stations.

#### 759 Training stations:



moisture 0.20

0.15

Date

Figure E4. In situ SSM, in situ RZSM, and predicted RZSM

series at station 'HarmsWay' (SCAN) with model ANN_SSM_NDVI_EVAP-EFF-B60_EXP-FILT-T5

.10 g 0.05

761

moisture

0.20 0.15

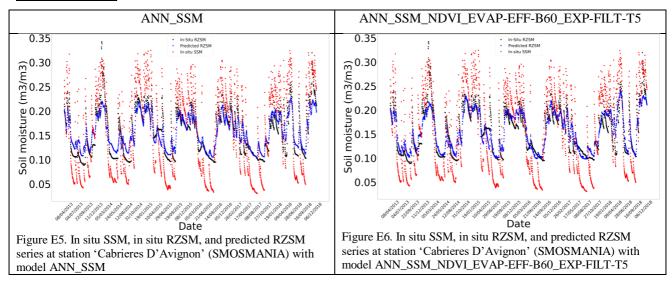
0.10

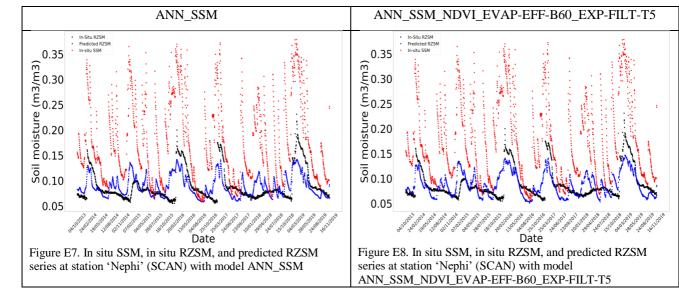
0.05

#### 762 Validation stations

Date

Figure E3. In situ SSM, in situ RZSM, and predicted RZSM series at station 'HarmsWay' (SCAN) with model ANN_SSM





# 765 ISMN test stations

