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### ► **To cite this version:**

D.M.L. Diongue, G. Brunetti, C. Stumpp, Frederic Do, Olivier Roupsard, et al.. A probabilistic framework for assessing the hydrological impact of *Faidherbia albida* in an arid area of Senegal. *Journal of Hydrology*, 2023, 622, 129717 [16 p.]. 10.1016/j.jhydrol.2023.129717 . hal-04176592

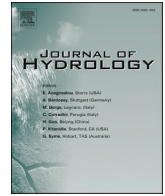
**HAL Id: hal-04176592**

**<https://hal.science/hal-04176592v1>**

Submitted on 16 Sep 2024

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## Research papers

## A probabilistic framework for assessing the hydrological impact of *Faidherbia albida* in an arid area of Senegal

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## ARTICLE INFO

**Keywords:**  
Arid areas  
HYDRUS  
Surrogate  
Calibration  
Phreatophyte

## ABSTRACT

The *Faidherbia* tree (*Faidherbia albida*) is frequently used as an intercrop in Sahelian agroforestry parklands due to its multi-purpose advantages and reverse phenology. However, its effect upon the water balance remains unclear, due to the challenges in directly measuring water fluxes in the underlying vadose zone. Mechanistic hydrological models can be inversely calibrated on transient observations and used to partition different hydrological components, but the computational burden of the analysis can become impractical if the model itself is computationally expensive. To overcome this limitation, and to provide novel insights into the hydrological role of *Faidherbia*, we combine a low-fidelity, one-dimensional hydrological model (HYDRUS-1D) with a kriging-based correction function to emulate the response of a high-fidelity, two-dimensional axisymmetric description of the system (HYDRUS-2D). Multiannual measurements of soil moisture and sap flow in a Senegal agroforestry parkland are used in conjunction with Bayesian inference to calibrate the resulting validated multifidelity surrogate, and to inversely estimate soil hydraulic and root water uptake parameters. Results show that the model can reproduce observations with good accuracy and limited uncertainty for both the calibration and the validation phases, and also confirm the phreatophytic behaviour of *Faidherbia* by indicating the existence of a moderately compensated root water uptake. Moreover, a local sensitivity analysis suggests that a fully compensated uptake could potentially reduce groundwater recharge by 13%. Interestingly, estimated soil hydraulic parameters hint at the possibility of root-induced changes in soil hydraulic properties that mimic preferential and/or macropore flow, resulting in sustained recharge fluxes ( $\approx 26\%$  of the annual precipitation). The analysis indicates that overall, *Faidherbia* could have a net positive effect upon the water balance in arid areas.

## 1. Introduction

Arid and semi-arid regions cover >40% of the Earth's land area (Koutroulis, 2019), and host about 3 billion people worldwide (Van der Esch et al., 2017). These regions are home to unique biodiversity and rich cultural heritages (Maestre et al., 2015), and provide essential ecosystem services (Bidak et al., 2015; N. Lu et al., 2018). However, the sustainable development of these areas may be seriously jeopardized by

ecological issues that accrue from scarcity of water resources (e.g., lack of surface water, and low amounts of precipitation) (Kuriqi et al., 2019). In Sub-Saharan Africa (SSA), arid regions are predicted to expand due to climate change (Feng & Fu, 2013). The resulting combination of high temperatures, extremely variable rainfall, low soil fertility, and recurrent but unpredictable droughts will threaten agriculture and food production. In addition, the rapid growth of megacities increases competition for water resources (Cherlet et al., 2018). Because the

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<https://doi.org/10.1016/j.jhydrol.2023.129717>

Received 2 January 2023; Received in revised form 3 May 2023; Accepted 20 May 2023

Available online 25 May 2023

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region lacks perennial surface water, groundwater is often the only source for meeting urban, industrial, and agricultural needs (Lapworth et al., 2017; MacDonald et al., 2012). Therefore, optimal use of groundwater is crucial for SSA's development—including the region's rural economies (FAO, 1999).

Optimizing that use requires an understanding of the hydrological impact of the region's agricultural practices. One such practice is agroforestry parklands, which are widespread because of their economic, social, and environmental benefits (Mbow et al., 2014). In the agroforestry parklands of Senegal, pearl millet and groundnut are often the major crops. However, the parklands' impact upon water balance is still unclear. Jackson et al. (2005) suggest that transpiration by the parklands' large, intercropped trees is detrimental to that balance, but other studies show that the trees' roots increase groundwater recharge by altering soil hydraulic properties (Bargués Tobella et al., 2014; Ilstedt et al., 2016). The intercropped tree species *Faidherbia albida* (Del.) A. Chev. (syn. *Acacia albida* Del.) is investigated extensively in the agricultural and ecological literature (Barnes & Fagg, 2003). Its uncommon reverse phenology (shedding all of its leaves at the beginning of the rainy season (Wickens, 1969)) benefits the major crops by providing a significant nitrogen input to the topsoil at the growing season. A further benefit for the major crops is that the leafless tree canopies intercept less light and rainfall (Rhoades, 1995).

Because of these benefits, much effort has been devoted to understanding the “Faidherbia effect” upon ecosystem services and crops (Louppe et al., 1996; Tschakert et al., 2004; Roupsard et al., 2020; Leroux et al., 2020; Faye et al., 2021; T. Lu et al., 2022; Dierks et al., 2022). To understand how *Faidherbia*'s sustains its peculiar reverse phenology in an arid region, Roupsard et al. (1999) studied the species' sap flows and water potentials, and the isotopic compositions of relevant water fractions. The results showed that *Faidherbia* obtains most of its water from the groundwater, thus enabling this species to grow during the dry season with little indication of drought stress. However, *Faidherbia*'s hydrological impact remains poorly understood despite all of this scientific effort. The main difficulty lies in measuring water fluxes in the vadose zone beneath the trees. These fluxes can be inferred from other measurements, but the results frequently fail to tie together all components of the hydrological balance coherently.

An additional challenge to understanding these fluxes is the multi-dimensional morphological complexity of the tree roots' spatial distribution. A comprehensive theoretical framework for reproducing that complexity is offered by mechanistic vadose-zone hydrological models such as HYDRUS or SWAP (van Dam et al., 2008; Šimůnek et al., 2016). These models can discriminate the different water-balance components, but to do so, the models must describe the system's hydrologic functioning satisfactorily. Satisfactory descriptions can be generally achieved by combining data from multiple transient observations (e.g., transpiration rates and volumetric water content) with specific numerical techniques (e.g., Bayesian inference and optimization strategies) to calibrate and validate the model, and therefore to assess its predictive uncertainty (Brunetti et al., 2019a; Vrugt et al., 2008; Wöhling and Vrugt, 2011). Once the model is calibrated, it can be used to *probabilistically* separate all hydrological components (e.g., recharge and evapotranspiration fluxes), and to discern the effects of physical factors such as roots and soil.

At present, this type of approach presents multiple general and case-specific challenges. One of these challenges is that the calibration procedure requires thousands of model executions in order to assess the models' uncertainties. The computational burden of that assessment can easily become prohibitive if the model itself is computationally expensive. Modelling of fluxes in the soil-tree domain is especially susceptible to this problem because the above-mentioned morphological complexity of root systems requires a numerical model that is at least 2D axisymmetric (i.e., that has cylindrical symmetry). (See, for example, Deb et al., 2013). Supercomputers or distributed computing clusters might be able to handle the job, but are not widely available. An appealing alternative

is to reduce the computational workload by using surrogate-based models in place of the complex original *high-fidelity* model (Razavi et al., 2012). When used for calibration purposes, surrogate modelling frequently aims to build an emulator that can calculate the objective function (or the likelihood) for different input parameters as if the function were being computed using the original *high-fidelity* model (e.g., a 2D axisymmetric one). Because the emulator can do the calculations in much less time, the calibration procedure is made feasible (Brunetti et al., 2017).

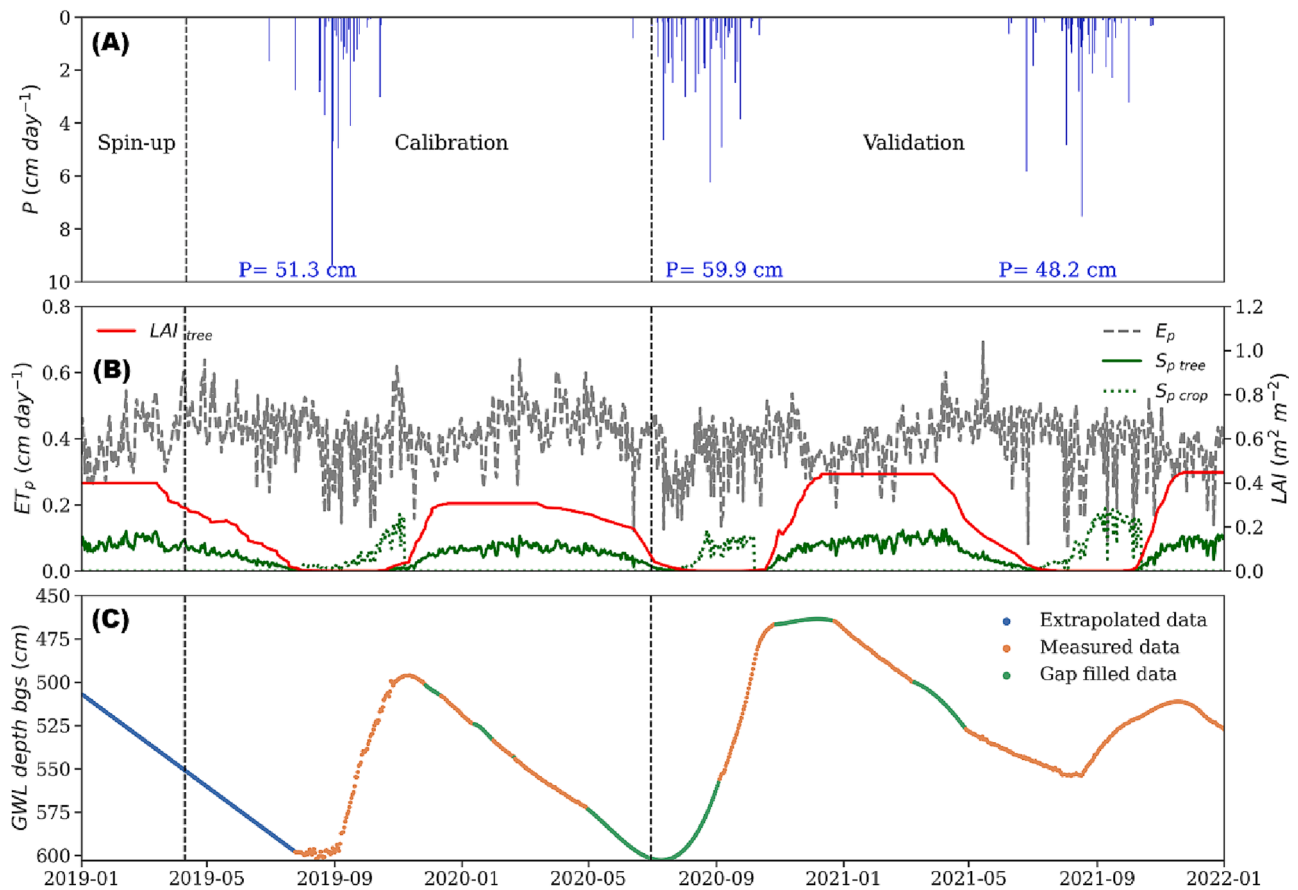
A diversity of water-related studies have used so-called “response-surface surrogates” successfully; including kriging, radial basis functions, and polynomial chaos expansion (Asher et al., 2015; Keating et al., 2010; Laloy et al., 2013; Razavi et al., 2012; Zeng et al., 2018; X. Zhang et al., 2009). However, when the dimensionality of the inverse problem is moderately high (e.g., >10), the necessary training of these surrogates requires an impractically high number of executions of the high-fidelity model in order to achieve a good coverage of the parameters space (O'Hagan, 2006). A possible remedy is to use *low-fidelity*, physically based surrogates, which are essentially cheaper-to-run approximations of the original complex models. For example, the surrogate model can be 1D instead of 2D (Razavi et al., 2012). When the surrogate uses the same theoretical framework and parameters as the high-fidelity model, the discrepancy between their respective response surfaces is expected to be limited. This discrepancy can be corrected by using an appropriate function that relates the responses of the low- and high-fidelity models. The so-called *multifidelity* approach develops the necessary correction function by using response-surface surrogates, which is generally easier to reconstruct because the low-fidelity response surface is supposedly a good approximation to the high-fidelity one. By thus reducing computational cost while mimicking the output of a high-fidelity forward model simulation, multifidelity surrogate analysis makes itself highly attractive for calibrating vadose zone hydrological models.

Few studies to date have calibrated vadose zone hydrological models via this approach (Man et al., 2018, 2021; Zheng et al., 2019). Therefore, the present study uses it to efficiently calibrate and validate a high-fidelity, two-dimensional axisymmetric HYDRUS model of the vadose zone underlying a *Faidherbia* tree in an agroforestry parkland in Senegal. The data used in the validation are from multiannual comprehensive measurements of sap flows, and of volumetric water contents at different depths. The validated multifidelity surrogate merges HYDRUS-1D and a kriging-based correction function to emulate the response of HYDRUS-2D. The surrogate is coupled with a Monte Carlo Markov Chain (MCMC) algorithm to inversely estimate soil hydraulic and root water uptake parameters, and to assess the model's predictive uncertainty. Parameters that were estimated via the surrogate are then transferred into the high-fidelity HYDRUS-2D model for validation purposes. Then, the validated HYDRUS-2D model is used to discriminate the different water fluxes; explain their interrelations; and assess their effects upon the hydrological balance. The realistic application of a multifidelity surrogate-based approach to calibrate a hydrological model of the vadose zone is a novel contribution in this field. The results can be valuable for a better understanding of water balances in agroforestry parklands in arid areas.

## 2. Materials and methods

### 2.1. Case study description and data analysis

The study area is part of the “Faidherbia-Flux” (FLUXNET/SN-Nkr) collaborative platform (<https://lped.info/wikiObsSN/?Faidherbia-Flux>), located in the agroforestry parkland of Sob village (135 km from Dakar) within the Senegal Groundnut basin (Roupsard et al., 2020). Soils are predominantly sandy, of a type known locally as “Dior soil” (loamy sand or Arenosols according to the USDA and FAO). The tree-based cropping system is dominated by *Faidherbia albida*, planted at a density of 13 trees ha<sup>-1</sup>. Canopy cover is 9.6% in the main, 1-ha



**Fig. 1.** Boundary conditions used for the following quantities during the three phases of modelling: (A) rainfall ( $P$ ); (B) potential soil evaporation ( $E_p$ ); potential crop transpiration ( $S_{p\ crop}$ ); potential tree transpiration ( $S_{p\ tree}$ ); tree leaf area index ( $LAI_{tree}$ ); (C) groundwater level (GWL); and depth below the ground surface (bgs). The three phases and their respective time intervals are: spin-up (from 01 to 01-2019 to 10-04-2019), calibration (from 11 to 04-2019 to 30-06-2020), and validation (from 01 to 07-2020 to 31-12-2021).

instrumented plot. The annual crop rotation includes rainfed millet and groundnut. Climate is of Soudano-Sahelian type, with a four-month rainy season from late June to early October, and a long dry period for the rest of the year. The average temperature is 29.8 °C; reference evapotranspiration ( $ET_0$ ) is 1500 mm  $y^{-1}$ ; and long-term average rainfall is around 600 mm  $y^{-1}$ . The top unconfined aquifer is a Continental Terminal (CT) formation (Oligo-Miocene to Pliocene), with a shallow brackish water 4.5–6.0 m below the ground surface. This aquifer overlies an impervious Eocene marl-limestone bedrock at a depth of around 40 m.

The data that the authors used to design this research work and to validate the resulting model were collected during an intensive, three-year field experiment (from 2019 to 2021). Meteorological data were provided by an automatic station (CR1000, Campbell Sci.) equipped with classical automatic sensors that made measurements every 30 sec, and averaged them to every 30 min. Measured parameters included rainfall events (TE25MM); air temperature and relative humidity at 2 m above the ground (CS215); and wind speed at 4.5 m above ground level (Wind Master sonic anemometer (Gill Instruments, Lymington, UK). Wind speeds at 2 m were then estimated.  $ET_0$  was computed according to the FAO-56 Penman-Monteith equation (Allen, 1998).

To estimate the amount of water used by *Faidherbia* trees, we neglected water storage, and assumed that the water use was equal to the transpiration, which was estimated from sap flows. These flows had been measured during 2019–2021 via the single-probe, transient-thermal-dissipation method (Do et al., 2011), with a cyclical heating of 600 sec every 30 min. The total sap flow [ $LT^{-1}$ ] was calculated for each tree, and averaged between trees to yield a mean flow for an average tree of

the stand. The 2019–2021 experiments also monitored the Leaf Area Indices (LAIs) of 15 *Faidherbia* trees, including the four whose sap flows were being measured. The LAIs were measured every 10 days, using a LAI2200 device (Li-Cor, USA) to measure transmittances.

During 2019–2021, volumetric soil-water contents were measured in shaded areas (under tree canopies) at depths of 20, 40, 60, 80, 120, 140, 160, 180, 280, and 380 cm. These data were recorded using automated time-domain reflectometers (TDR, type CS655 Campbell), which were installed horizontally in a well that was dug close to the tree. The TDRs installed at a depth  $-180 < z \leq 0$  cm were locally calibrated with data on gravimetric water contents and bulk densities. The calibration procedure is explained in details in the [Supplementary Material](#). In contrast, TDR sensors installed at a depth  $z < -180$  cm used the factory calibration curve, which leads to an accuracy of  $\pm 3\%$ . Levels of the groundwater table were continuously recorded from August of 2019 by using pressure sensors (Rugged TROLL 100, coupled with Baro-TROLL 100 for barometric compensation, In-Situ, USA). The sensors were emplaced in a piezometer close to the locations of the above-mentioned TDRs. Missing data were gap-filled via cubic interpolation. A linear interpolation was used to extrapolate data back to January 2019, based upon dry-season recession curves.

Soil profiles were sampled at different depth intervals to analyse for dry bulk density and soil texture (percentages of sand, silt, and clay). Textural analyses were performed at the Institute of Soil Physics and Rural Water Management, University of Natural Resources and Life Sciences, Vienna. The sand fractions were determined by sieving; silt and clay fractions were determined via sedimentation. The analyses revealed that in the 0–100 cm depth interval, the texture was loamy

sand, with an average bulk density of  $1.7 \text{ g cm}^{-3}$ . The clay percentage was uniform at about 2.2%, but the sand percentage decreased from 85.4% at the soil surface to 77.8% at 60 cm. In contrast, the soil from 100 down to 500 cm had a sandy-loam texture. Contents of clay (2.9–5.5%) and silt (29.3–34.7%) were higher than in the 0–100 cm layer, but the sand content was lower (67.8–59.8%).

Densities of tree root lengths were characterized underneath tree canopies and far from them, per. For this purpose, those authors excavated 1-m-square sampling pits to a depth of 1.5 m. Results showed that about 62% of *Faidherbia*'s fine roots were distributed within the deep soil layer (100–150 cm), versus 35% in the 30–100-layer depth, and only 3% in the upper layer (0–30 cm). Interestingly, root densities in the 50–100 cm depth interval were significantly higher outside of the canopy. Although no root-density data for depths > 150 cm were investigated via excavation, field observations that were made during installation of TDRs indicate that *Faidherbia* roots extend far into the deep layer and the capillary fringe. This agrees with what reported in Roupsard et al. (1999).

Because we would use the above-described data set (i.e., from all of the 2019–2021 observations) to perform a multifidelity surrogate analysis, we partitioned that data into three chronological groups (one for each phase of the modelling): spin-up (from 01 to 01-2019 to 10–04-2019); calibration (11–04-2019 to 30–06-2020); and validation (01–07-2020 to 31–12-2021) (Fig. 1).

## 2.2. Modelling theory

### 2.2.1. Water flow

The variably saturated water flow in a 2D axisymmetric domain is described by the following Richards equation:

$$\frac{\partial \theta(h)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[ rK(h) \frac{\partial h}{\partial r} \right] + \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - S_a(h) \quad (1)$$

where  $\theta$  is the volumetric water content [ $\text{L}^3\text{L}^{-3}$ ];  $h$  is the pressure head [L];  $t$  is time [T],  $r$  is the radial space coordinate [L];  $z$  is the vertical coordinate [L];  $K$  is the unsaturated hydraulic conductivity [ $\text{LT}^{-1}$ ]; and  $S_a(h)$  is a sink term [ $\text{L}^3\text{L}^{-3}\text{T}^{-1}$ ], defined as a volume of water removed from a unit volume of soil per unit of time, due to plant water uptake. By setting  $r = 0$ , eq. (1) reduces to the one-dimensional Richards equation. Soil hydraulic properties are parameterized via the unimodal van Genuchten-Mualem (Mualem, 1976; van Genuchten, 1980) (VGM) model, as follows:

$$\theta = \begin{cases} \frac{\theta_s - \theta_r}{(1 + (\alpha|h|)^n)^m} + \theta_r & \text{if } h \leq 0 \\ \theta_s & \text{if } h > 0 \end{cases} \quad (2)$$

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (3)$$

$$K = \begin{cases} K_s \Theta^L \left[ 1 - (1 - \Theta^{\frac{1}{m}})^2 \right]^2 & \text{if } h \leq 0 \\ K_s & \text{if } h > 0 \end{cases} \quad (4)$$

$$m = 1 - \frac{1}{n} \quad (5)$$

where  $\theta_r$  [ $\text{L}^3\text{L}^{-3}$ ] is the residual soil water content;  $\theta_s$  [ $\text{L}^3\text{L}^{-3}$ ] is the saturated soil water content,  $K_s$  [ $\text{LT}^{-1}$ ] is the saturated hydraulic conductivity;  $\alpha$  [ $\text{L}^{-1}$ ] and  $n$  [-] are empirical shape parameters;  $L$  indicates the tortuosity [-], which is frequently assumed equal to 0.5 (Mualem, 1976); and  $\Theta$  is the effective saturation [-].

Compensated Root Water Uptake and Soil Water Evaporation.

The reference evapotranspiration demand is partitioned into potential transpiration ( $S_p$ ) and potential soil water evaporation ( $E_p$ ) using the measured LAI (Brunetti et al., 2019b; Ritchie, 1972; Sutanto et al., 2012). The following equation converts  $S_p$  to actual transpiration,  $S_a$ :

$$\frac{S_a(h)}{S_p} = \frac{1}{S_p} \int_{\mathcal{R}} S_a(h, x, y, z) dx dy dz = \int_{\mathcal{R}} a(h, x, y, z) b(x, y, z) dx dy dz = \omega \quad (6)$$

where  $S_a(h, x, y, z)$  is actual root water uptake [ $\text{L}^3\text{L}^{-3}\text{T}^{-1}$ ];  $a(h, x, y, z)$  is a dimensionless water-stress response function;  $b(x, y, z)$  is a dimensionless root-density distribution function; and  $\omega$  is a dimensionless water-stress index. Eq. (6) describes root water uptake for a general three-dimensional problem, but can be easily particularized for 1D vertical and 2D axisymmetric domains. Because this study models the hydrological effects of two vegetation species (i.e., *Faidherbia* and groundnut-millet), their effects are distinguished in the model by first specifying the root density and the potential transpiration rate for each vegetation (using the time series of LAI), and by then using eq. (6) to calculate their respective actual root water uptakes. Their sum of the two uptakes constitutes the actual sink term in eq. (1).

Based upon results from isotope methods, Roupsard et al. (1999) suggested that *Faidherbia* behaves mostly as a phreatophyte, but alternatively uses all root compartments along the vadose-zone profile. To account for this effect, the two models incorporate a dimensionless root adaptability factor,  $\omega_c$  (which modulates the index  $\omega$  that is presented in eq. (6)).  $\omega_c$  is a threshold value above which any reduction in root water uptake that occurs in stressed parts of the root zone is fully compensated by an increased uptake from unstressed parts. The range of values for  $\omega_c$  is  $0 \leq \omega_c \leq 1$ . Root water uptake is not compensated when  $\omega_c = 1$ , but is fully compensated when  $\omega_c = 0$ . For a detailed explanation, please see Šimunek and Hopmans (2009).

The root water stress response ( $a$ , in eq. (6)) depends upon the soil pressure head  $h$ . To model this stress, we used Skaggs et al.'s (2006b) smooth, s-shaped function:

$$a(h) = \frac{1}{1 + \left( \frac{h}{h_{50}} \right)^p} \quad (7)$$

where  $h_{50}$  is the pressure head value at which the root water uptake is reduced by 50% [L], and  $p$  is a dimensionless empirical shape parameter. The  $a$  value ranges from 0 to 1. Because actual root water uptake depends upon root density, the models include a spatially explicit root-density function ( $b(x, y, z)$  in eq. (6)). This function modulates the uptake at each mesh node in the soil-domain models, and is based on the formulation proposed by Vrugt et al. (2001). Both models neglect the effect of salinity upon root water uptake, because no comprehensive measurements from the area of study are available to characterize solute distribution in the soil domain.

Potential soil water evaporation ( $E_p$ ) is converted to actual evaporation ( $E_a$ ) as long as the surface is sufficiently moist and the pressure head at the soil surface doesn't exceed the minimum allowed pressure head  $h_{crit}$  [L]. This value ( $h_{crit}$ ) is estimated from the relative humidity and air temperature. However, to avoid numerical-convergence issues when solving the Richards equation, the models restrict values of  $h_{crit}$  such that the corresponding soil water contents are at least 0.005 higher than the residual water content  $\theta_r$  [ $\text{L}^3\text{L}^{-3}$ ].

## 2.3. Model calibration and uncertainty assessment

### 2.3.1. Inverse estimation of soil hydraulic and root water uptake parameters

The Richards equation and the root water uptake equations [i.e., eq. (1) and (6)] include several parameters that must be defined. In the present study, we fixed the values of some of these parameters, and calibrated the others based upon the volumetric water content and sap flow observations from 2019 to 2021. Specifically, the residual water content,  $\theta_r$ , is set to 0 for all soil horizons because the soil is mainly sandy (Brunetti et al., 2020). The tortuosity factor,  $L$ , is set to the common value of 0.5 (van Genuchten, 1980). For groundnut-millet, the root water uptake parameters  $h_{50}$  and  $p$  are set equal to  $-800$  cm and 3, respectively. These values provide a good approximation to the

**Table 1**

Calibrated model parameters and their prior bounds; calculated means; 3%, and 97% High-Density Intervals (HDIs); and the ESS of the parameters' posterior distributions from the Bayesian analysis.

Parameter <sup>†</sup>	Parameter description	Parameter bounds	Posterior distribution		Effective Sample Size
			HDI 3%	Mean	
Soil layer (1): $0 \leq z \leq -100$ cm					
$\theta_{s1}$ [ $\text{cm}^3\text{cm}^{-3}$ ]	Saturated water content	(0.2, 0.5)	0.35	0.45	780
$\alpha_1$ [ $\text{cm}^{-1}$ ]	VGM shape parameter	(0.001, 0.3)	0.01	0.013	459
$n_1$ [-]	VGM shape parameter	(1.1, 5)	2.2	2.5	621
$K_{s1}$ [ $\text{cm day}^{-1}$ ]	Saturated hydraulic conductivity	(100, 10,000)	200	750	543
Soil layer (2): $-100 < z \leq -200$ cm					
$\theta_{s2}$ [ $\text{cm}^3\text{cm}^{-3}$ ]	Saturated water content	(0.2, 0.5)	0.21	0.24	578
$\alpha_2$ [ $\text{cm}^{-1}$ ]	VGM shape parameter	(0.001, 0.3)	0.01	0.014	710
$n_2$ [-]	VGM shape parameter	(1.1, 5)	1.8	2.05	756
$K_{s2}$ [ $\text{cm day}^{-1}$ ]	Saturated hydraulic conductivity	(100, 10,000)	700	1,500	480
Soil layer (3): $-200 < z \leq -600$ cm					
$\theta_{s3}$ [ $\text{cm}^3\text{cm}^{-3}$ ]	Saturated water content	(0.2, 0.5)	0.24	0.31	865
$\alpha_3$ [ $\text{cm}^{-1}$ ]	VGM shape parameter	(0.001, 0.3)	0.04	0.065	761
$n_3$ [-]	VGM shape parameter	(1.1, 5)	1.35	1.43	672
$K_{s3}$ [ $\text{cm day}^{-1}$ ]	Saturated hydraulic conductivity	(100, 10,000)	500	1,300	501
Roots					
$h_{50}$ (cm)	S-shaped function's parameter	(-50, -800)	-140.1	-71.8	497
$p$ (-)	S-shaped function's exponent	(1.01, 4)	1.1	1.3	598
$\omega_c$ (-)	Roots adaptability factor	(0, 1)	0.31	0.39	731

<sup>†</sup>The subscripts 1, 2, and 3 indicate the first, second, and third soil horizons, respectively.

piecewise linear Feddes function used by Diongue et al. (2022b) to describe the actual root water uptake of groundnut-millet. By using these assumptions, only 15 model parameters needed to be calibrated, including the saturated water content,  $\theta_s$ , the VGM shape parameters,  $\alpha$  and  $n$ , the saturated hydraulic conductivity,  $K_s$ , for three soil horizons; the root adaptability factor,  $\omega_c$ ; and root water uptake parameters,  $h_{50}$  and  $p$ .

### 2.3.2. Bayesian inference

The Bayesian inference is used to inversely estimate soil hydraulic and root water uptake parameters and to therefore assess their uncertainty. The definition of a parameters' prior distribution and a likelihood function are required to infer the parameters posterior distribution. The prior distribution is set to be bounded uniform for all parameters. Upper and lower bounds (Table 1) are chosen based on the prior information available regarding the soil textural composition, followed by a comprehensive literature review.

Selection of the likelihood functions took into consideration the types of observations that are included in the Bayesian framework, and the characteristics of each observation's measurement errors. To a large degree, those observations consisted of soil-moisture measurements. Because the final, calibrated model is intended to reproduce the deterministic part of each observed signal, the error model for each measurement should approximate the properties of the measurement's remaining stochastic part. That part depends upon the measurement device. The TDR CS655 that was used to measure soil moisture during the 2019–2021 field study determines the velocity of electromagnetic pulses as they traverse a wave-guide that is inserted into the soil. The pulses are independent of each other, thereby excluding the possibility of autocorrelation in the measurements' errors. Moreover, the procedure that was used for calibrating the TDR CS655 in the upper soil layers led to Gaussian homoscedastic residuals (Caldwell et al., 2018) with  $\sigma = 0.015$  (Supplementary Material).

For these reasons, we assumed that the error residuals are uncorrelated and normally distributed, with constant variance,  $\sigma^2$ . Those assumptions lead to the following form for the log-likelihood function  $\ell(\mathbf{u})$ :

$$\ell(\mathbf{u}) = -\frac{k}{2} \ln(2\pi) - \frac{k}{2} \ln(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^k \left( y_i(\mathbf{u}) - \tilde{y}_i \right)^2 \quad (8)$$

where  $k$  is the number of observations,  $y_i(\mathbf{u})$  and  $\tilde{y}_i(\mathbf{u})$  are the  $i$ th

model realization and its corresponding measured value, respectively. It is worth noting that although other forms of the likelihood function [e.g., first-order autoregressive (Wöhling & Vrugt, 2011)] might improve the quality of the model's fitting, they could also compromise the objectivity of subsequent assessments of the model's adequacy. For that reason, we opted to use a traditional, measurement-motivated Gaussian likelihood function, followed by model predictive checks for both the calibration and validation period to discuss the model adequacy.

Because the calibration procedure includes sap flows, and locally and factory calibrated TDR measurements, the final log-likelihood function  $L(\mathbf{u})$  is the aggregated sum of single log-likelihoods for each  $j$ th measurements sets:

$$L(\mathbf{u}) = \sum_{j=1}^3 \ell_j(\mathbf{u}) \quad (9)$$

$\sigma$  are assumed equal to 0.01 cm/day for the sap flow, 0.015 and 0.03 (-) for the locally (i.e.,  $-180 < z \leq 0$  cm) and factory (i.e.,  $z < -180$  cm) calibrated volumetric water contents, respectively.

Having selected the prior distribution and likelihood function for each of the 15 parameters, we then used a hybrid Monte Carlo Markov Chain (MCMC) ensemble sampler to estimate the parameters' posterior distributions. The algorithm combines the differential evolution snooker move developed by Ter Braak and Vrugt (2008) with the affine-invariant stretch move proposed by Goodman and Weare (2010). To improve the algorithm convergence, chains were initialized by random sampling from a multivariate normal distribution that is centred upon the global optimum,  $x_{opt}$ . This optimum was identified via the Gradient-based Comprehensive Learning Particle Swarm Optimization (G-CLPSO) that Brunetti et al. (2022) developed for the HYDRUS model. The main diagnostic for monitoring the convergence of the MCMC sampler was the Integrated Autocorrelation Time (IAT), which is the number of steps (ensemble moves) required for the chain to produce independent samples from the true parameter's posterior distribution. After convergence, the Python package ArViz (Kumar et al., 2016) is used to calculate further diagnostic metrics, such as the High-Density Intervals (HDIs) and the effective sample size. Further details about MCMC sampling and convergence assessment are reported in the Supplementary Material.

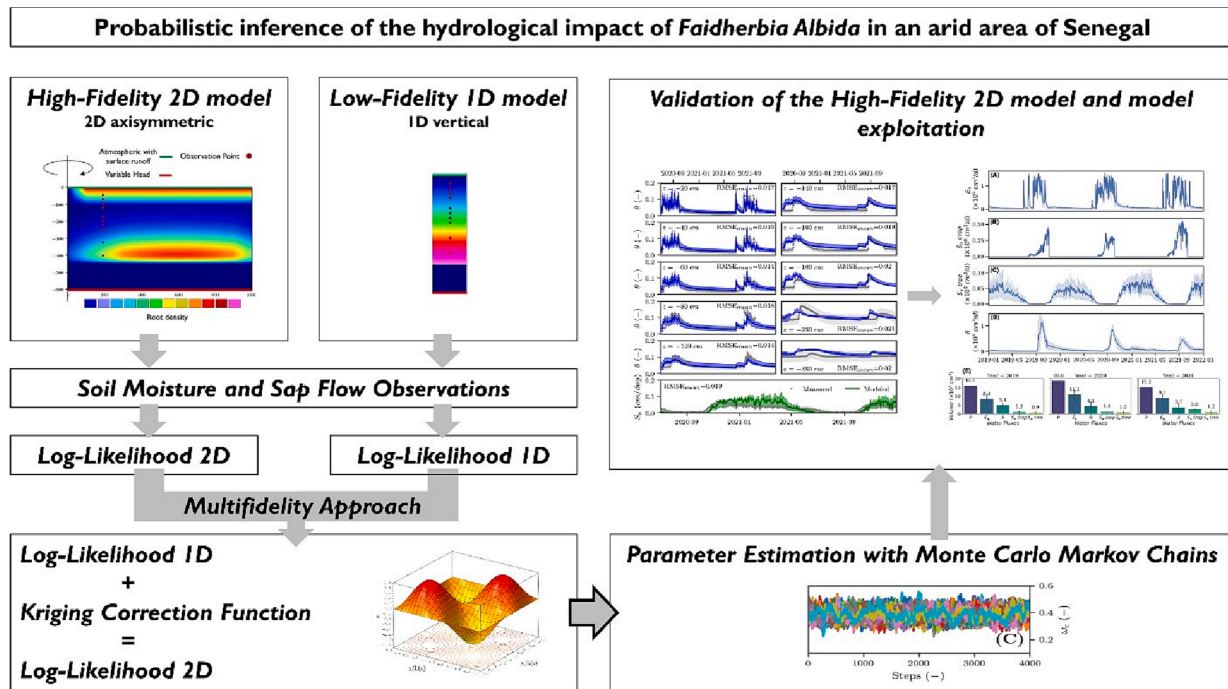


Fig. 2. A schematic of the modelling approach. The framework combines a low-fidelity *cheap-to-run* 1D model with a kriging-based correction function to approximate the log-likelihood function computed using a high-fidelity 2D axisymmetric model. The approximated log-likelihood is then used in conjunction with a Monte Carlo Markov Chain algorithm to inversely estimate soil hydraulic and root water uptake parameters, and quantify their uncertainty. Estimated parameters are then used in the high-fidelity 2D model for validation purposes and model exploitation.

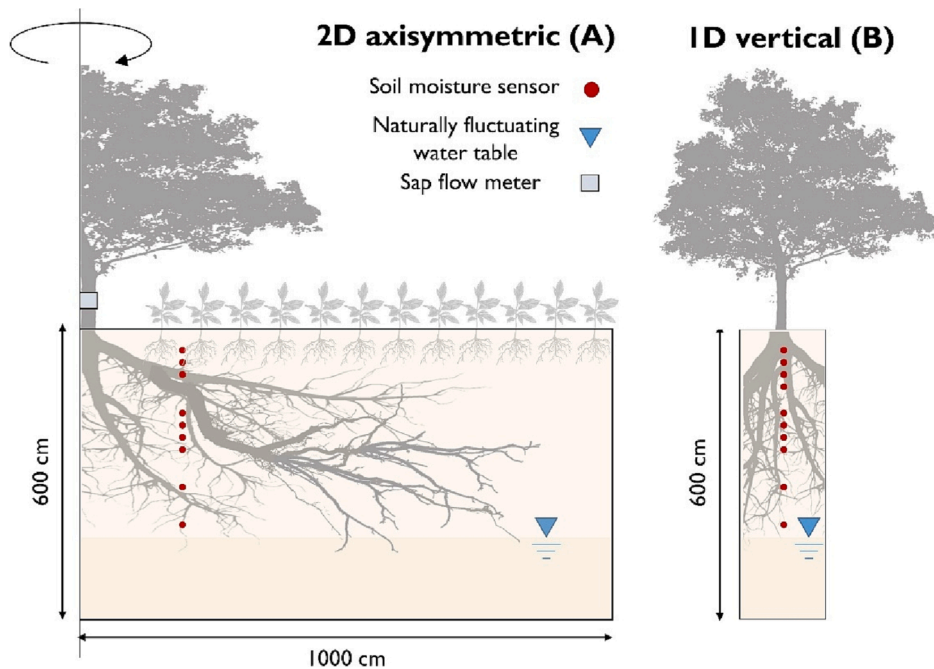


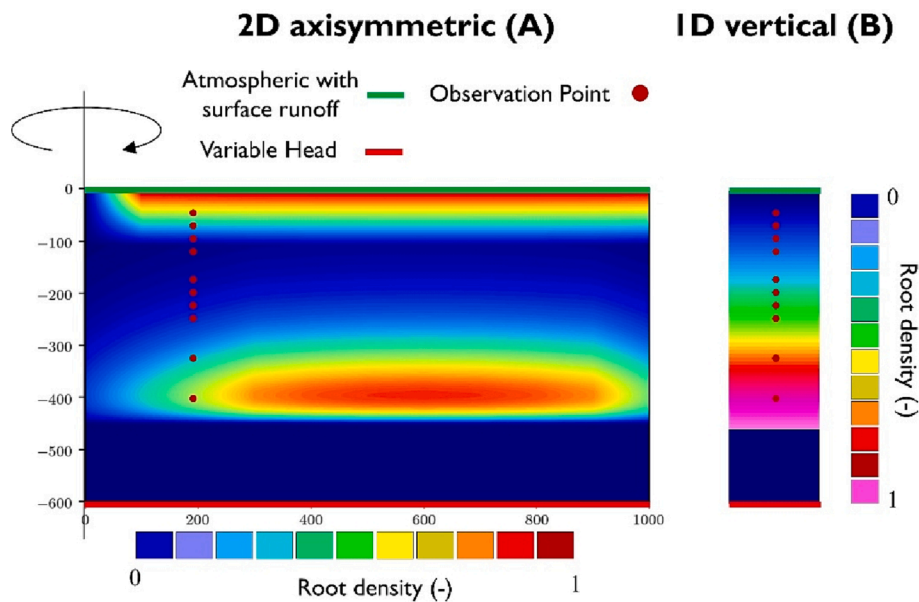
Fig. 3. Schematic of the high-fidelity axisymmetric 2D model (A) and low-fidelity 1D vertical model (B), showing also the approximate position of the naturally fluctuating water table, the position of soil moisture sensors and sap-flow meter, and the approximate distribution of roots for crops and the tree. The tree's root distribution extends beyond the dripline area; its density increases with depth until the capillary fringe.

2.4. Multifidelity surrogate analysis

2.4.1. The multifidelity approach

A schematic of the multifidelity modelling approach is shown in Fig. 2. As noted above, this study sought to produce both a high-fidelity model and a *cheap-to-run* low-fidelity model. Because our purpose was to

elucidate the hydrological role of an intercropped *Faidherbia* tree in the underlying vadose zone, our high-fidelity model was designed to (1) reproduce field-scale observations, and (2) describe variably saturated water flows and root-water uptakes of crops as well as the tree. To overcome the lack of detailed information about root distribution, crown morphology, and soil heterogeneity, the high-fidelity model



**Fig. 4.** Schematic of the distribution of boundary conditions for the high-fidelity axisymmetric 2D model (A) and the low-fidelity 1D vertical low-fidelity model (B). The main differences are that: (1) the spatial root distribution is simplified in 1D by assuming a linear increase with depth, and (2) the entire soil surface in 1D is assumed to be within the dripline.

assumes that these aspects of the tree-soil domain are two-dimensionally axisymmetric. Deb et al., (2013) showed that this assumption is effective and accurate. The resulting pseudo-3D discretization uses a dense 2D finite-element mesh, and allows the modeler to infer the spatial variability of water fluxes and root-water uptake [(A) in Fig. 3].

In contrast, the low-fidelity model conceptualizes processes in the soil-tree domain as strictly one-dimensional [(B) in Fig. 3]. This strong simplification of the domain’s spatial variability reduces computing time, but risks biasing the calibration procedure. The present study mitigates this issue (at least partially) in two ways. We start by using the same theoretical framework for both models (high- and low-fidelity). Then, we correct the response of the low-fidelity model by using a multifidelity surrogate approach with an embedded response-surface emulator. In this way, it is possible to maximize the computational efficiency while maintaining the theoretical accuracy of the high-fidelity model.

To reduce the computational cost of the Bayesian analysis, the multifidelity approach that is used here combines the computationally efficient, low-fidelity 1D vertical model [(B) in Fig. 3 and Fig. 4] with an additive correction function to approximate the response of the computationally intensive high-fidelity, 2D axisymmetric model [(A) in Fig. 3 and Fig. 4] (Gano et al., 2006; Leary et al., 2003; Viana et al., 2009; Wu et al., 2020; J. Zhang et al., 2018). Specifically, the aggregated log-likelihood obtained from the high-fidelity model,  $L_h(\mathbf{u})$ , is approximated by adding a correction function,  $g(\mathbf{u})$ , to the aggregated log-likelihood that is calculated via the low-fidelity model,  $L_l(\mathbf{u})$ :

$$L_h(\mathbf{u}) = L_l(\mathbf{u}) + g(\mathbf{u}) \tag{10}$$

Because the exact form of  $g(\mathbf{u})$  is unknown, an approximation to it is built by using a Gaussian process that is based on the kriging technique, which is trained on a relatively low number of high- and low-fidelity model executions. Kriging, belonging to the class of Gaussian process emulators (Rasmussen & Williams, 2006; Sacks et al., 1989), combines a polynomial model with a localized deviation model that is based upon a spatial correlation of samples:

$$g(\mathbf{u}) = f(\mathbf{u}) + Z(\mathbf{u}) \tag{11}$$

where  $f(\mathbf{u})$  is a function that approximates the response surface through a set of points in the parameters’ space. The vector  $Z(\mathbf{u})$  is the

result of a stochastic process with zero mean and nonzero covariance. The parameters in  $Z(\mathbf{u})$  are optimized. For the sake of brevity, mathematical details about kriging are not reported here. Thorough theoretical descriptions of using the kriging method for surrogate analysis are given in Forrester et al. (2008) and Kennedy and O’Hagan (2001).

#### 2.4.2. Training and validation of the multifidelity surrogate

The preliminary training and validation phases verify the capability of the surrogate to accurately reproduce the response of the high-fidelity model. The training/validation procedure is iterative, as described below:

The Latin hypercube sampling generates a set of parameters (McKay et al., 1979), which is used to initially train the kriging-based correction function. The training sample size,  $s$ , is set based on the relation proposed by Jones et al. (1998) [eq. (12)]:

$$s = 10D \tag{12}$$

where  $D$  is the dimensionality of the parameters’ space, equal to 15 in the present study, thus leading to a total of 150 initial training sites. A *for* loop is used to iterate through the training samples, and calculate the aggregated log-likelihood [i.e., eq. (9)] for both the high and low-fidelity models and for each parameters’ set.

The training set is used to optimize hyperparameters of the kriging-based correction function, and obtain a first multifidelity surrogate. The surrogate is combined with the MCMC to estimate a first approximation of the parameters posterior distribution.

The final position of the chains (i.e., 100 solutions) is used to calculate the aggregated log-likelihood for both the original high-fidelity 2D model and the multifidelity surrogate.

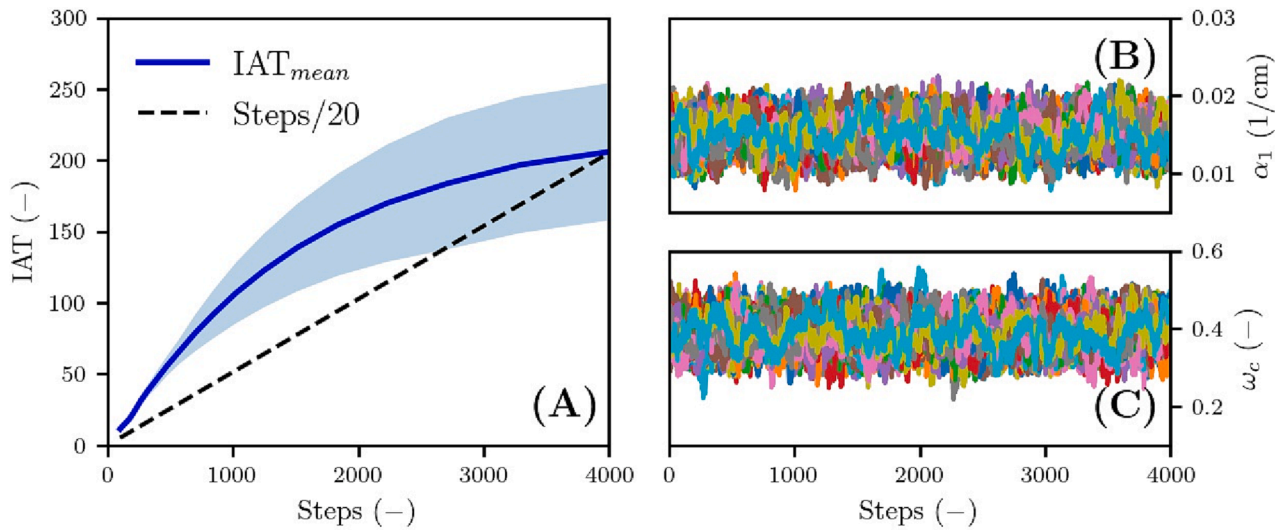
A dimensionless error metric,  $E$ , compares the response of the original model and the multifidelity surrogate:

$$E = \frac{\sum_{i=1}^K |L(\mathbf{u})_{high-fidelity} - L(\mathbf{u})_{multifidelity}|}{\sum_{i=1}^K |L(\mathbf{u})_{high-fidelity}|} \tag{13}$$

If the error metric is lower than 1%, it is assumed that the surrogate well approximates the response of the original model in high-likelihood regions and the validation is successful.

If the error metric is higher than 1%, the posterior solutions are



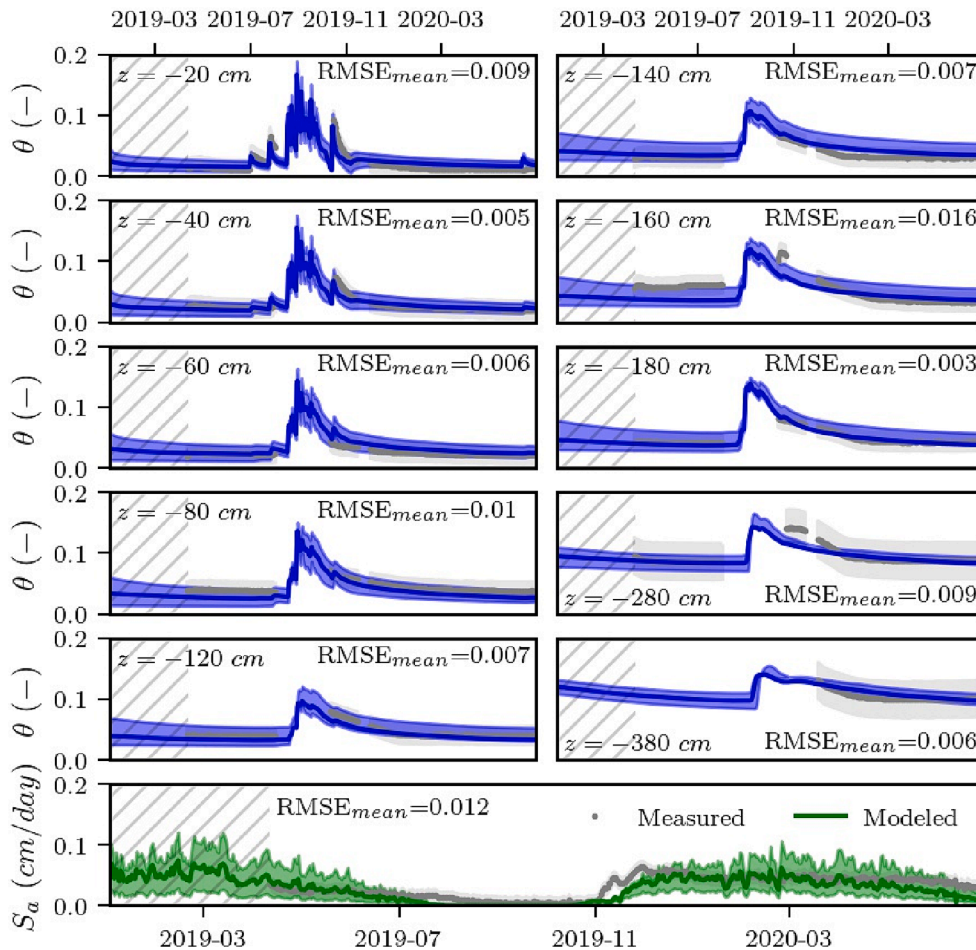


**Fig. 5.** Diagnostic plot of the MCMC algorithm, showing: (A) the average (blue solid line) and the standard deviation band of the integrated autocorrelation times (grey band) as a function of the number of algorithm steps. The black dashed line in (A) corresponds to the convergence threshold value of 20 IAT. (B) and (C) show the position of the chains in the ensemble as a function of the number of algorithm steps for the parameters  $\alpha_1$  and  $\omega_c$ , respectively (each colour indicates individual runs). (A) shows that IAT is reaching its true value asymptotically, and that the length of the chains has reached the threshold value of 20 IAT. (B) and (C) complement that information by highlighting the good mixing in the ensemble and the absence of any significant trend, as confirmed by the IAT analysis.

added to training set and the process restarts from step 2.

By iteratively adding posterior solutions to the training set (*active learning*) (Zhang et al., 2020), the training procedure guarantees that the surrogate well approximates high-likelihood areas in the parameters'

space. This, together with the initial well-spaced Latin hypercube sample, assures an efficient coverage of the parameters' space.



**Fig. 6.** Model calibration: a comparison between the model predictive uncertainty bands (blue and green areas); the mean posterior solution (solid lines); and measured values (grey circles) for sap flow ( $S_a$ ) and volumetric water contents ( $\theta$ ) at eight different depths. Predictive bands and the mean posterior solution were obtained by propagating the calculated High-Density Interval and mean solutions (Table 1), respectively, into the high-fidelity axisymmetric HYDRUS-2D model. The hatched areas indicate the model spin-up period, while the grey bands represent the sensor accuracy. Each plot shows the RMSE that was calculated from the mean soil hydraulic and root water uptake parameters, as taken from the parameter's posterior distributions (Table 1).

### 2.4.3. Model setup and boundary conditions

The previously described equations for water flow and root water uptake were solved using the finite-element model, HYDRUS (Šimůnek et al., 2016). More specifically, we used a non-standard version of HYDRUS model that can simulate root water uptake from two plant species (Faidherbia and crop rotation of groundnut and pearl millet) in 2D. The high-fidelity, axisymmetric 2D domain is discretized into 4,000 2D triangular elements, and the low-fidelity 1D vertical domains is discretized into 200 1D finite elements. Both models use a finer mesh near the soil surface in order to provide accurate simulations of pressure-head gradients that are induced by atmospheric conditions. Based upon preliminary soil-texture information, both models discretize the vadose zone profile into three separate soil horizons: (1) an upper soil layer from 0 to  $-100$  cm (i.e., to the 100 cm depth); (2) an intermediate soil layer between  $-100$  and  $-200$  cm; and (3) a deeper soil layer from  $-200$  to  $-600$  cm. In both models, the spatial distributions of the densities of crop and tree roots are constant in time. However, the spatial distributions are more detailed in the high-fidelity model than in the low-fidelity one. In particular, the high-fidelity model assumes that Faidherbia roots extend beyond the dripline area; that the root density is higher outside of the canopy; and that the root density increases with depth until the capillary fringe [(A) in Fig. 4] (Roupsard et al., 1999). At any distance from the tree, the root density of crops at the surface is assumed to increase linearly with depth, down to the maximum rooting depth of 100 cm. The simpler low-fidelity model, too, assumes that root densities of crops increase linearly with depth [(B) in Fig. 4], but also assumes that the distribution is the same for all distances from the tree.

Fig. 4 also shows the distribution of the boundary conditions (BCs) for the two models. The atmospheric boundary condition at the soil surface includes precipitation, potential soil evaporation, and potential transpiration. The pressure head at the soil surface cannot exceed (in absolute value) the minimum allowed pressure head,  $h_{crit}$ . No flux is allowed through the vertical sides of the transport domain due to symmetry. Finally, a Dirichlet-type variable head BC is set at the bottom of the domain to simulate measured water table fluctuations.

## 3. Results and discussion

### 3.1. Model calibration

#### 3.1.1. MCMC diagnostic

The surrogate training required, in total, 250 runs of the high-fidelity axisymmetric HYDRUS-2D model to reduce the surrogate approximation error ( $E$ ) to 0.94%. The validated multifidelity surrogate was then used for the Bayesian inference via the MCMC algorithm, which required 4,000 steps, and a total of 400,000 surrogate model evaluations, to achieve the IAT convergence threshold [(A) in Fig. 5]. The mean acceptance fraction was 0.19, which is considered to be a satisfactory value if the posterior distribution is multivariate Gaussian (Gelman et al., 2004). The satisfactory performance of the sampler is further demonstrated by the good mixing of the chains in the ensemble [(B) and (C) in Fig. 5], and is proven statistically by the average ESS value ( $=637$ ; Table 1).

It must be emphasized that performing 400,000 simulations with the high-fidelity axisymmetric HYDRUS-2D model would require approximately 90 days on the available computer (Intel CITM) i7-8750H CPU 2.20 GHz, RAM 16 GB). In contrast, only four days were necessary to complete the Bayesian analysis with the multifidelity surrogate.

#### 3.1.2. Model predictive checks

Fig. 6 shows a comparison between the model predictive uncertainty bands (blue and green areas); mean posterior solutions (solid lines); and measured values (grey circles) of sap flow ( $S_a$ ) and volumetric water contents ( $\theta$ ) at eight different depths. The predictive bands and the mean posterior solutions were obtained by propagating the calculated High-Density Intervals (HDIs) and mean solutions, respectively (Table 1),

into the high-fidelity axisymmetric HYDRUS-2D model. The results indicate that the model reproduces, with satisfactory accuracy and low predictive uncertainty, both the water distribution in the soil and the actual transpiration dynamics during the calibration period. Although the deviation between modelled and predicted volumetric water contents increases with depth, the error remains limited, as confirmed by the root mean square errors (RMSEs) calculated for the mean solution from the parameters' posterior distributions.

The predicted sap flows exhibit a time-shift error, especially during November 2019 and January 2020. Those periods coincide with the end of the rainy season and Faidherbia's re-greening period. The time shift can be partially attributed to inconsistencies between the actual sap flow and the measured LAI, which the model used to partition evapotranspiration fluxes. In particular, the underestimation of the actual sap flows may be the numerical result of the underestimated LAIs, which in turn led the model to predict low potential transpiration fluxes. We also note that the macroscopic root water uptake approach used in HYDRUS approximates the actual transpiration process only conceptually. In contrast, sap-flow measurements are a good—albeit imperfect—indicator of transpiration (Meinzer et al., 2004). Therefore, the model's time-shift error appears to be a consequence of the nature of the LAI data, rather than an indication of deficiencies in the models.

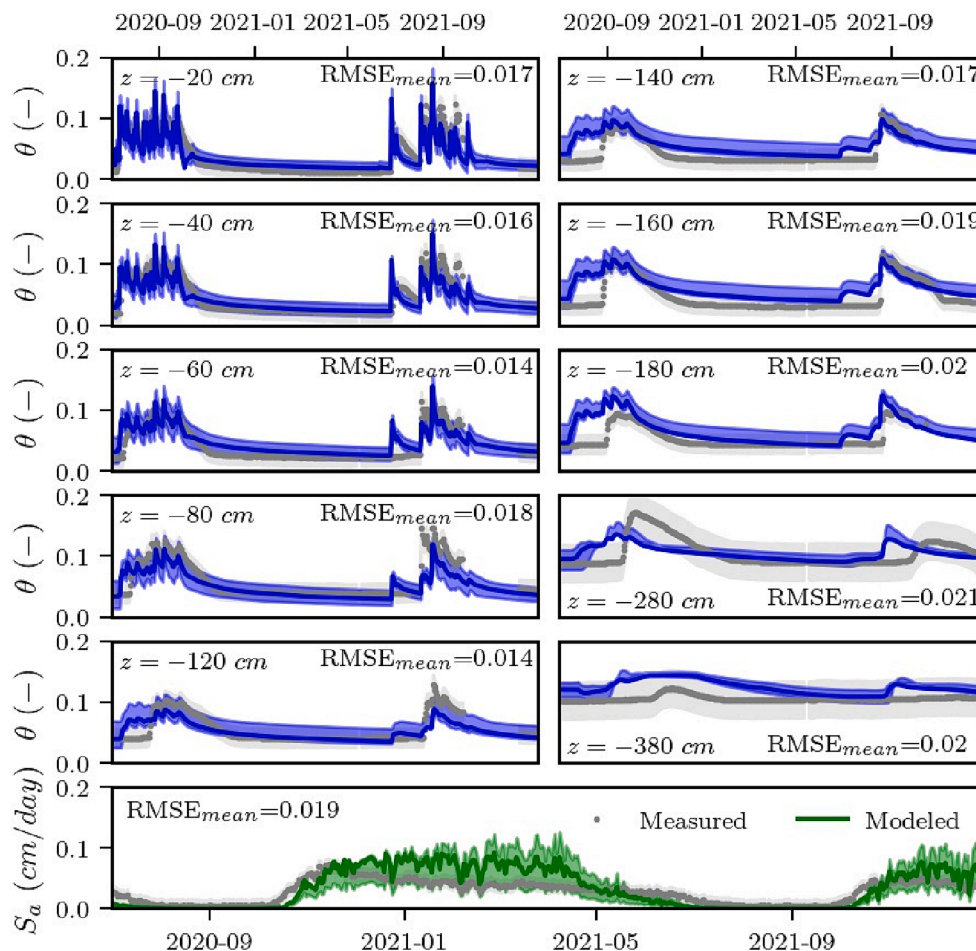
In summary, the model interprets the dynamics of Faidherbia's transpiration well, and the model predictive checks (on the whole) do not indicate significant systematic discrepancies between model predictions and observations (Gelman et al., 2004). Thus, results from the calibration phase suggest that the model can explain the underlying hydrological processes satisfactorily.

#### 3.1.3. Assessment of the parameters

The calculated mean, and 3% and 97% High-Density Intervals (HDIs) of the parameters' posterior distributions are reported in Table 1. They indicate that the inverse problem is well-posed, with an acceptable level of uncertainty. HDIs are generally narrow, except for the saturated soil water contents ( $\theta_s$ ) and hydraulic conductivities ( $K_s$ ), which have larger uncertainties. Those uncertainties can be partially explained by the limited range of the volumetric water contents (measured during 2019–2021), which never approached the saturated values. Thus, those measurements were mainly informative of the dry end of the retention and conductivity curves.

The relatively high estimated values of  $K_s$  might be explained by the finding of Lu et al. (2020) that in coarse soils, tree roots can increase  $K_s$  up to 1,085% by inducing the formation of macropores. Therefore, the high  $K_s$  values that we found suggest that in the area of study, macropore formation and/or preferential flow was occurring in the root zone. This behaviour was already observed by Bargaues Tobella et al. (2014), who investigated the effect of scattered trees upon soil infiltrability in an agroforestry parkland in Burkina Faso. In that study, dye-tracer experiments demonstrated that preferential flow and infiltrability were significantly higher under Shea trees' canopies than in the surrounding open areas. In particular, the joint action of tree roots and high organic-matter contents from litter inputs increases the macroporosity, thus creating preferred pathways for water flow. Moreover, the potential effect of other occurring mechanisms, such as stemflow and film flow along roots (Nikodem et al., 2010), are not properly accounted in the model, but lumped in the soil hydraulic parameters. Nevertheless, the relatively high uncertainty in the estimation of  $K_s$  suggests that more specific measurements are required to better characterize the hydraulic behaviour of the system.

Overall, estimated soil hydraulic parameters are consistent with the measured soil textural composition, in that the parameters reproduce the hydraulic properties of a highly permeable sandy soil whose fine fraction increases with depth. The corresponding decrease of the coarse material is reflected in the lower value of the shape parameter,  $n_3$ , for the deeper soil layer, which contains more clay (2.9–5.5%) and silt (29.3–34.7%), but less sand (67.8–59.8). Estimated saturated water



**Fig. 7.** Model validation: comparisons between the model predictive uncertainty bands (blue and green areas), the mean posterior solution (solid lines); and (grey circles) measured sap flow ( $S_a$ ) and volumetric water contents ( $\theta$ ) at eight different depths. Predictive bands and the mean posterior solution were obtained by propagating the calculated High-Density Interval and mean solutions (Table 1), respectively, into the high-fidelity axisymmetric HYDRUS-2D model. Each plot shows the corresponding RMSE that was calculated by using the mean values of soil hydraulic and root water uptake parameters, as taken from the parameters' posterior distributions (Table 1).

contents ( $\theta_s$ ) range between 0.2 and 0.45, which would be typical for the soil that is investigated in the present study.

More interesting are the root water uptake parameters. The value of the estimated root adaptability factor,  $\omega_c$ , indicates that root water uptake is moderately compensated. This finding supports the hypotheses of Roupsard et al. (1999); Roupsard et al. (2022) about the phreatophytic behaviour of *Faidherbia*. In particular, results from the calibration procedure indicate that roots are able to meet the transpiration demand by extracting more soil water via the less-stressed part of the roots, until  $\omega_c$  reaches a value between approximately 0.31 and 0.48. At that point, the roots as a whole start to experience some stress. Deb et al. (2013) used a similar value of  $\omega_c$  to simulate the compensated root water uptake of a Pecan tree. In another study, Wang et al. (2022) showed how a  $\omega_c$  value between 0.3 and 0.7 led to optimal results when simulating transpiration dynamics of the phreatophyte *Tamarix ramosissima*.

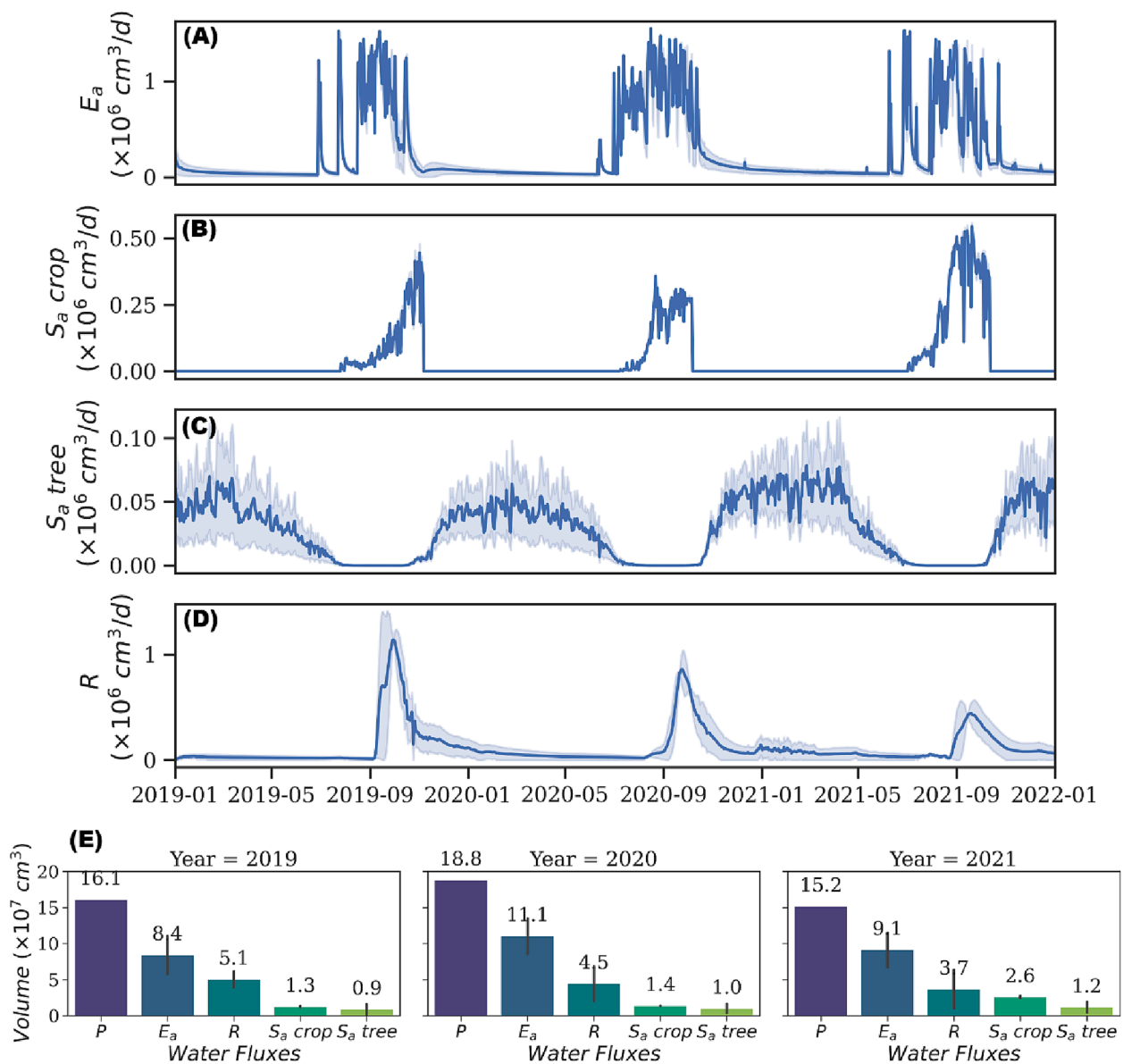
The estimated pressure head at which the root water uptake is reduced by 50% ( $h_{50}$ ) is relatively low (in absolute value): it ranges from  $-140.1$  to  $-54.5$  cm. Similar values were used by Yin et al. (2018) to simulate transpiration patterns in the phreatophyte *Salix matsudana*. Our  $h_{50}$  values, together with the estimated value of the shape parameter  $p$ , suggest that the model treats the uptake reduction as essentially a step function: under moderately wet conditions, the actual and potential transpiration are close (according to the model), but they will diverge as the pressure head increases (in absolute value) and soil pores desaturate (Skaggs et al., 2006a). This prediction is physically realistic for sandy soils (Zhu et al., 2009) like the one investigated in the present study.

It must be emphasized that because this study presents the first detailed simulation (to our knowledge) of *Faidherbia*'s phreatophytic behaviour, it is not possible to make meaningful comparisons between

our estimated root water uptake parameters and those from other existing studies on *Faidherbia*. However, comparisons with the existing literature on other phreatophytes, as well as the discussion about the physical meaning of the root water uptake parameters, suggest that the model provides a good approximation of *Faidherbia*'s macroscopic behaviour of and its influence upon water fluxes in the vadose zone.

#### 3.1.4. Model validation

To validate the high-fidelity 2D axisymmetric HYDRUS-2D model, we propagated into it the parameters' estimated posterior distributions (Table 1). Fig. 7 shows a comparison between the model-predictive-uncertainty bands (blue and green areas); the mean posterior solution (solid lines); and measured values (grey circles) of sap flow ( $S_a$ ) and volumetric water contents ( $\theta$ ) at eight different depths. The model predictive performance generally remained satisfactory, but the bias was greater than during the calibration period. This observation is confirmed by the RMSE values that were calculated for the mean solution from the parameters' posterior distributions. Those values now range between 0.014 and 0.021  $\text{cm}^3 \text{cm}^{-3}$  for the volumetric water content, and reach 0.019  $\text{cm day}^{-1}$  for the sap flow. While the model approximates water distribution well in the upper soil horizons, the deviation between model predictions and measurements is greater for deeper soil layers. In particular, the model seems to systematically anticipate the arrival of the moisture front for  $z < -100$  cm, while still reproducing the peak timing and soil drying well for  $-100 \text{ cm} < z < -200$  cm. This result suggests an imperfect modelling of the soil-wetting process—a deficiency that can be partially explained by the higher frequency of soil-drying data in the calibration dataset (Fig. 6). Nor is it possible to rule out possible effects of soil heterogeneity, macropore



**Fig. 8.** Water flux partitioning as predicted by the high-fidelity axisymmetric HYDRUS-2D model: daily time series of water volume in (A) actual evaporation ( $E_a$ ); (B) non-compensated root water uptake of the crops (i.e.,  $S_a \text{ crop}$  when the roots adaptability factor  $\omega_c = 1$ ); (C) compensated root water uptake of the tree (i.e.,  $S_a \text{ tree}$  when the roots adaptability factor  $\omega_c = 0.39$ ); (D) groundwater recharge ( $R$ ); and (E) yearly water budget. The uncertainties of the model parameters that were derived from the Bayesian analysis are propagated into the water fluxes as the error band for the daily series and the error bar for the yearly water budget.

flow, and measurement inaccuracies. More evident is the model's overestimation of the sap flow (compared to during the calibration phase), although the transpiration pattern is again well reproduced.

The fitting could probably have been improved through a different apportioning of computation time between the calibration and validation periods (e.g., by extending the calibration and shortening the validation), as well by making the model more detailed (e.g., increasing the soil layering). However, greater detail would have increased the computational cost of the analysis by increasing both the dimensionality of the inverse problem and the complexity of the multifidelity surrogate training. Overall, results from the validation phase do not provide grounds for rejecting the model. Instead, the model's predictive performance remains satisfactory for the purpose of the analysis, which is to understand water fluxes in the vadose zone below *Faidherbia* trees.

### 3.1.5. Hydrological interpretation of water fluxes

The interpretations that follow are based upon results from the validated high-fidelity axisymmetric HYDRUS-2D model, using the

parameters' estimated posterior distributions.

### 3.1.6. Partitioning of the water fluxes

A study of Fig. 8 shows that the model predictive uncertainty is low, except for the actual transpiration of *Faidherbia* ( $S_a \text{ tree}$ ) and the groundwater recharge ( $R$ ). The uncertainty of these parameter is attributable to the relatively high uncertainties of the root parameters themselves.

The predicted daily actual evaporation fluxes ( $E_a$ ) are low during the December-to-June dry seasons (mean:  $6.6 \pm 0.4 \times 10^4 \text{ cm}^3 \text{ d}^{-1}$ ). These  $E_a$  values are representative of second-stage evaporation, during which high pressure heads at the surface limit the upward water fluxes. Conversely, the model predicts higher  $E_a$  values during the wet seasons, as expected because of the moister soil conditions. Specifically, the average predicted  $E_a$  for the wet season is  $5.32 \pm 1.0 \times 10^5 \text{ cm}^3 \text{ d}^{-1}$ , and the maximum (which occurs during rainy days) is  $1.55 \pm 0.7 \times 10^6 \text{ cm}^3 \text{ d}^{-1}$  [(A) in Fig. 8].

Wet seasons are also the times when local farmers practice the

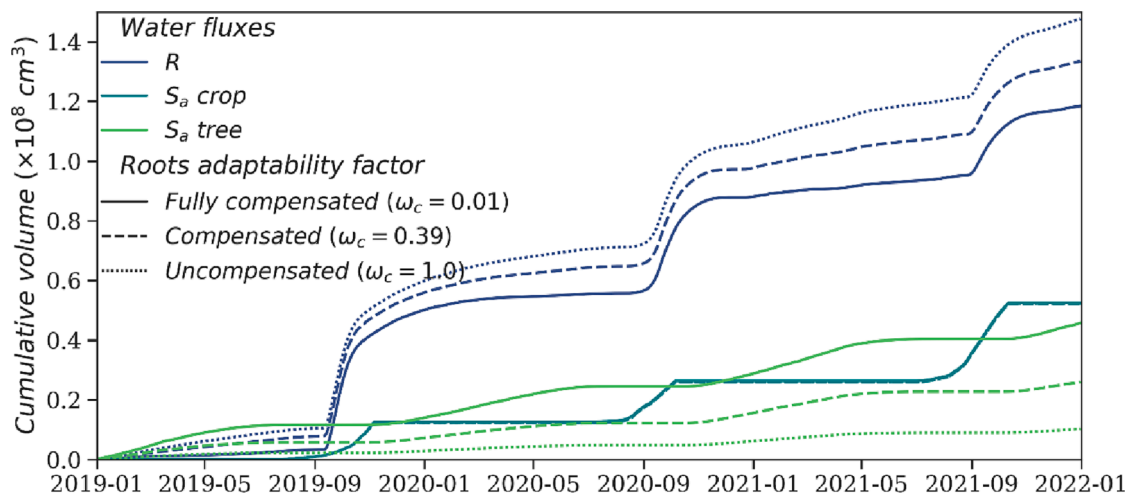


Fig. 9. (From the high-fidelity axisymmetric HYDRUS-2D model.) Time dependence of cumulative water volumes that are recharged ( $R$ ), transpired by crops ( $S_a$  crop), and transpired by *Faidherbia* ( $S_a$  tree) when *Faidherbia*'s root water uptake is compensated ( $\omega_c = 0.39$ , based on calibration results), fully compensated ( $\omega_c = 0.01$ ), and uncompensated ( $\omega_c = 1.0$ ).

rainfed rotation of groundnut (as they did in 2019 and 2021) and pearl millet (in 2020). The simulated daily actual transpiration of those crops,  $S_a$  crop, ranges from  $5.7 \pm 0.0 \times 10^3$  to  $8.2 \pm 1.7 \times 10^4$   $\text{cm}^3 \text{d}^{-1}$  in the early growing stage (late July, early August), versus  $1.72 \pm 0.0 \times 10^4$  to  $5.4 \pm 0.02 \times 10^5$   $\text{cm}^3 \text{d}^{-1}$  during the vegetative stage (September). Predicted values of  $S_a$  crop are higher under groundnut (max:  $4.95 \pm 0.45 \times 10^5$   $\text{cm}^3 \text{d}^{-1}$ ; mean:  $0.52 \pm 0.03 \times 10^5$   $\text{cm}^3 \text{d}^{-1}$ ) than under pearl millet (max:  $3.58 \pm 0.01 \times 10^5$   $\text{cm}^3 \text{d}^{-1}$ ; mean:  $0.37 \pm 0.08 \times 10^5$   $\text{cm}^3 \text{d}^{-1}$ ). This outcome is the result of groundnut's higher LAI. The partitionings of  $E_a$  and  $S_a$  crop, as derived from the high-fidelity 2D model, are similar to those which Diongue et al. (2022b) computed via HYDRUS-1D for location at the study area that are outside of the trees' radius of influence (i.e., > 30 m away from any tree).

The predicted seasonal variations of *Faidherbia*'s actual transpiration ( $S_a$  tree) are opposite to those of the crops, as is consistent with the species' reverse phenology. *Faidherbia*'s predicted flux becomes negligible during the rainy season, but increases after the onset of leafing. Specifically, *Faidherbia*'s predicted flux is around  $1.48 \pm 0.56 \times 10^2$   $\text{cm}^3 \text{d}^{-1}$  in late September and early October, and the maximums (mean:  $5.17 \pm 3.75 \times 10^4$   $\text{cm}^3 \text{d}^{-1}$ ) occur during January-February. Interestingly, the onset of leafing of this phreatophyte species is paced with the groundwater recharge rate,  $R$  (Roupsard et al., 2022), which varies from  $0.44 \pm 0.15 \times 10^6$   $\text{cm}^3 \text{d}^{-1}$  in 2021 to  $1.14 \pm 0.01 \times 10^6$   $\text{cm}^3 \text{d}^{-1}$  in 2019 [(C) and (D) in Fig. 8].

The model predicts that at the annual scale,  $E_a$  is the main component of the water balance, ranging from  $8.4 \pm 2.6 \times 10^7$   $\text{cm}^3 \text{y}^{-1}$  in 2019 ( $=52.3 \pm 16.4\%$  of the year's total precipitation,  $P$ ) to  $11.1 \pm 2.4 \times 10^7$   $\text{cm}^3 \text{y}^{-1}$  in 2020 ( $=58.7 \pm 13\%$  of  $P$ ). The second-largest component is  $R$ , which varied between  $3.7 \pm 2.7 \times 10^7$   $\text{cm}^3 \text{y}^{-1}$  in 2021 ( $=24.4 \pm 17.6\%$  of  $P$ ) and  $5.1 \pm 1.1 \times 10^7$   $\text{cm}^3 \text{y}^{-1}$  in 2019 ( $=31.3 \pm 7.1\%$  of  $P$ ) [(D) in Fig. 10]. The fluxes  $S_a$  crop and  $S_a$  tree are the smallest components.  $S_a$  crop ranged from  $1.3 \pm 0.1 \times 10^7$   $\text{cm}^3 \text{y}^{-1}$  ( $7.8 \pm 0.7\%$  of  $P$ ) in 2019 to  $2.6 \pm 0.1 \times 10^7$   $\text{cm}^3 \text{y}^{-1}$  ( $17.2 \pm 1.0\%$  of  $P$ ) in 2021.  $S_a$  tree was even smaller:  $8.8 \pm 7.2 \times 10^6$  to  $1.2 \pm 0.7 \times 10^7$   $\text{cm}^3 \text{y}^{-1}$ , corresponding to  $5.5 \pm 4.5$  to  $7.7 \pm 4.9\%$  of  $P$ .

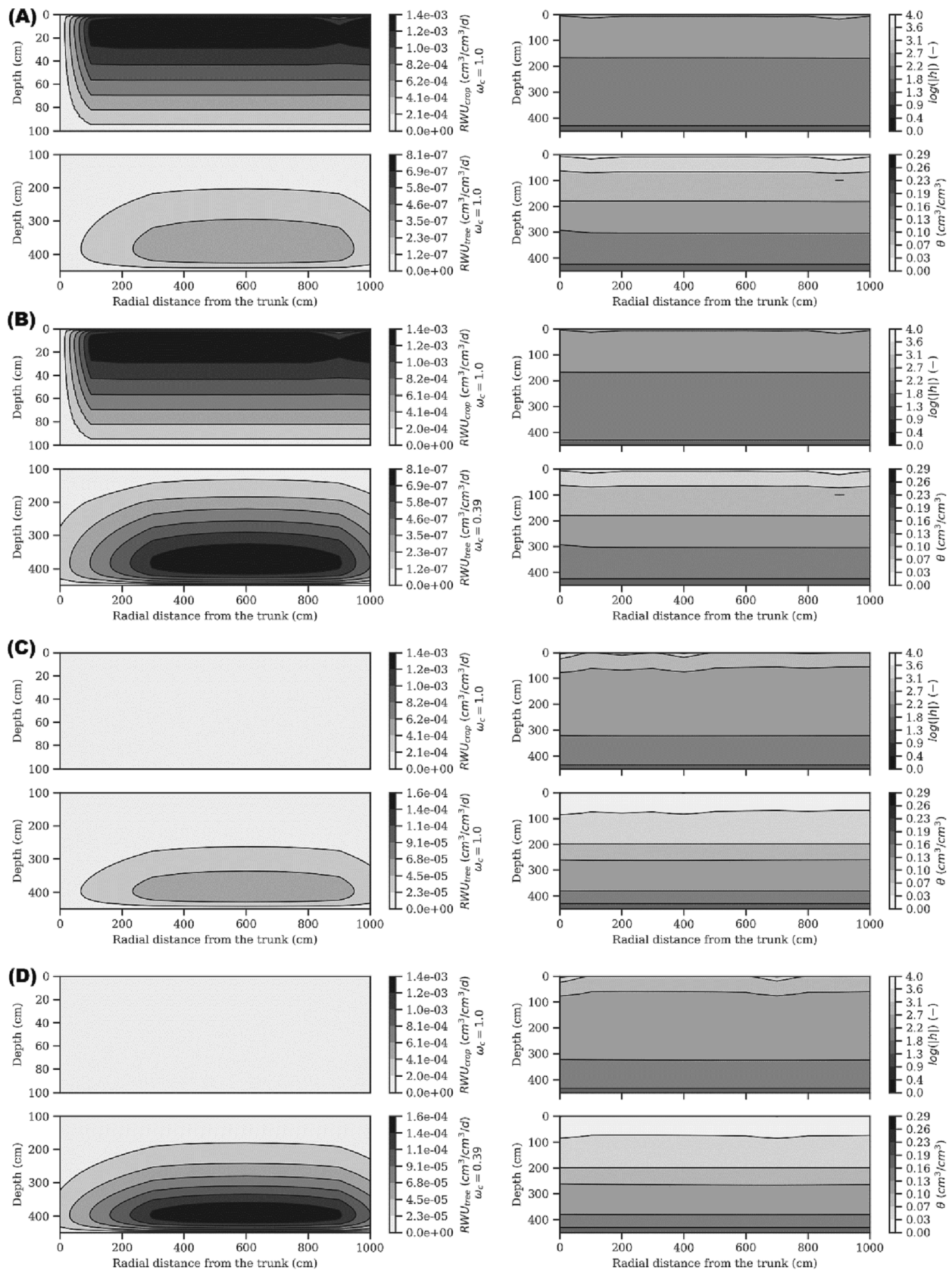
Groundwater recharge rates ( $R$ ) predicted by the high-fidelity axisymmetric HYDRUS-2D model are higher than those which have been reported for other semiarid regions (e.g., Boumaiza et al., 2021; Gaj et al., 2016; Koeniger et al., 2016; Skrzypek et al., 2019). The predicted rates are also higher than those calculated for Senegal's Groundnut Basin by researchers who used unsaturated-zone approaches (e.g., profiles of chloride, deuterium, and tritium in soil water). For example, Edmunds and Gaye (1994); Gaye and Edmunds (1996), who

studied chloride profiles at 15 separate sites and tritium profiles at two sites, showed that  $R$  averaged 5% of  $P$  in northern Senegal's Louga region, where the annual precipitation is around 290  $\text{mm y}^{-1}$ . Similarly, Diongue et al. (2022a) found that the average  $R$  in the Groundnut Basin during 2021 was less than 2% of  $P$ , based upon stable-isotope profiles of bulk soil water.

To understand why the  $R$  values predicted by the model are higher than those from unsaturated-zone approaches, it is important to note that the latter approach postulates that none of the recharge occurs via localized (focused) paths such as tree-induced macropores. Instead, the unsaturated-zone approach assumes that all of the recharge occurs diffusely, from soil water that percolates through the vadose-zone matrix by advection-dominated flow. Therefore, the model's high  $R$  values highlight the potential impact of *Faidherbia* roots in generating paths for localized recharge (Bargués Tobella et al., 2014; Ilstedt et al., 2016). This impact is consistent with results reported recently by Bargués-Tobella et al. (2020). These authors, who assessed deep drainage in the openings among trees, report that deep drainage in smaller openings (where the soil is more likely to contain root-induced macropores) is >10 times higher than in openings whose centres are >22 m distant from the nearest tree trunk. Thus, Bargués-Tobella et al. (2020) highlight the decisive role that tree cover plays in promoting recharge by increasing macropore flow and deep percolation, especially near the tree trunk.

### 3.1.7. Effect of root adaptability upon the water budget

To further investigate the influence of root adaptability factors ( $\omega_c$ ) upon the water budget, the validated high-fidelity 2D model was used to calculate and compare  $S_a$  crop,  $S_a$  tree, and  $R$  under conditions in which *Faidherbia*'s root water uptake (RWU) was (variously) compensated ( $\omega_c = 0.39$ ; a value that is based upon calibration results, and used as baseline), fully compensated ( $\omega_c = 0.01$ ), and uncompensated ( $\omega_c = 1.0$ ). The tree's cumulative transpiration (the line labelled  $S_a$  tree in Fig. 9) is significantly influenced by  $\omega_c$ , with values ranging from  $1.03 \times 10^7$   $\text{cm}^3$  in uncompensated conditions to  $2.60 \times 10^7$   $\text{cm}^3$  for compensated RWU. Transpiration remains high ( $4.58 \times 10^7$   $\text{cm}^3$ ) and similar to potential rates in fully compensated condition, resulting in increases of 43.2 and 77.6% compared to compensated and uncompensated root water uptake, respectively. This large increase is due to the low water-holding capacity of sandy soils, such as the one investigated in the present study. Some authors have reported that the enhanced compensated uptake occurs after significant water depletion, or after distribution of water stress over the soil profile (Deb et al., 2013; Šimůnek & Hopmans, 2009). For example, Deb et al. (2013) reported that the



**Fig. 10.** Spatial-distributions of pressure head ( $h$ ), soil water content ( $\theta$ ), and root water uptakes of the pearl millet crop and tree ( $RWU_{crop}$  and  $RWU_{free}$ , respectively) as derived from validation of the high-fidelity axisymmetric HYDRUS-2D model. Plots in (A) and (B) are the distributions at the onset of Faidherbia's leafing (Oct. 6–10–2020). The plots in (A) show the distributions that occur without compensation ( $\omega_c = 1.0$ ). Those in (B) show the distributions that occur with compensation for Faidherbia ( $\omega_c = 0.39$ ). The plots in (C) and (D) are for the time of maximum leaf density (Feb. 26–02–2020). The plots in (C) show the distributions that occur without compensation ( $\omega_c = 1.0$ ). Those in (D) show the distributions that occur with compensation for Faidherbia ( $\omega_c = 0.39$ ).

compensated RWU of pecan trees increased by only 8% compared to the uncompensated RWU. The small magnitude of that increase was attributed to the water-holding capacity of the orchard's silty clay loam soil. Still, the increase was sufficient to avoid severe water stress during the growing season.

In the present study, the compensated RWU had no significant impact upon the crop's cumulative transpiration ( $S_{a\text{ crop}}$  in Fig. 9), which decreased by only 0.2% under fully compensated condition. This result is due to *Faidherbia*'s reverse phenology, because of which the tree competes very little for water with adjacent crops. Conversely, increased RWU by *Faidherbia* in the fully compensated condition results in lower groundwater-recharge rates, with the cumulative value decreasing by 12.7% and 24.7%, respectively, compared to uncompensated and compensated RWU. This result suggests that root water uptake has an appreciable but moderate effect upon recharge fluxes. At the same time, *Faidherbia* can alter and potentially increase recharge fluxes through root-induced changes in the soil's hydraulic behaviour.

### 3.1.8. Spatial distribution of the root water uptake

To gain further insight into the strategies that *Faidherbia* employs to mitigate water stress, the validated model was used to investigate how the root adaptability factor ( $\omega_c$ ) affects spatial RWU patterns at two times of the year: during October (when *Faidherbia* begins its leafing, at the end of the cropping season), and in February (the time of maximum leaf density, and therefore peak transpiration demand). The 2D-contour plots in Fig. 10 show that during both periods, the compensated and uncompensated root uptakes from trees ( $RWU_{tree}$ ) vary not only with soil depth, but also with radial distance from the tree trunk. The model's output also shows that in early October (6–10-2020), when pearl millet crop is in its maturity stage, then harvested a few days later,  $\omega_c$  does not affect root uptake from crops ( $RWU_{crop}$ ). At that time,  $RWU_{crop}$  averages  $9.28 \times 10^{-4} \text{ cm}^3 \text{ cm}^{-3} \text{ d}^{-1}$ . According to results from the model, the amount of water extracted by pearl millet follows the millet's assumed root-length distribution. Specifically,  $RWU_{crop}$  is a function of depth, exclusively: at any given depth, it is the same at all distances from the tree, except within a few cm of the trunk. Moreover,  $RWU_{crop}$  is highest at the surface, and decreases linearly with depth.

During the same period (early October, 6–10-2020), *Faidherbia*'s transpiration demand is low, and the soil is still relatively wet due to ongoing redistribution of preceding rainfall infiltration. *Faidherbia* roots do not experience severe water stress at this time, but extract water at higher rates in the deep layers, especially outside of the dripline area. This result is consistent with *Faidherbia*'s root-length distribution, which is denser outside the tree canopy. The  $RWU_{tree}$  rates are minimal near the tree trunk and in the upper soil layer, but increase gradually with depth from 100 cm downward. The highest values occur within the 350–450 cm soil layer at radial distances > 300 cm. The rates decrease again in the capillary fringe. The magnitude and pattern of  $RWU_{tree}$  rates for compensated uptake (mean:  $1.99 \times 10^{-7} \text{ cm}^3 \text{ cm}^{-3} \text{ d}^{-1}$ ) and uncompensated uptake ( $0.77 \times 10^{-7} \text{ cm}^3 \text{ cm}^{-3} \text{ d}^{-1}$ ) vary slightly during early October, particularly with soil depth [(A) and (B) in Fig. 10]. Indeed, to compensate the water stress, roots extract water at higher rates in the deep layers thanks to the combined effect of (1) higher root density, and (2) wetter soil and lower pressure head gradient, compared to the shallow layer.

The spatial pattern of  $RWU_{tree}$  in February differs substantially from October's due to soil drying, which is induced by the limited holding capacity of the sandy media and the higher transpiration demand of *Faidherbia*. In addition, roots experience more water stress in February than during October, and the magnitudes of  $RWU_{tree}$  are higher: the mean compensated RWU is  $2.98 \times 10^{-5} \text{ cm}^3 \text{ cm}^{-3} \text{ d}^{-1}$ , and the mean uncompensated RWU is  $1.17 \times 10^{-5} \text{ cm}^3 \text{ cm}^{-3} \text{ d}^{-1}$ . Hence, the depth distribution of  $RWU_{tree}$  is driven not only by the most densely-rooted soil layers, but also by the soil-water conditions. These hydrological behaviours of *Faidherbia* confirm its suitability for Sahelian agroforestry: Because of its reverse phenology, *Faidherbia* extracts comparatively

little water throughout the cropping season, making this tree only a minor competing species (for water) with the adjacent crops. (Note that  $\omega_c$  has no significant effect upon  $RWU_{crop}$ .) Furthermore, the study area's low-density stands of *Faidherbia* consume less than 10% of  $P$ , and use deep water to mitigate water stress.

## 4. Summary and conclusions

The main goal of this study was to provide further insights into the hydrological impact of *Faidherbia* in arid areas, by combining diverse experimental data and mechanistic modelling. To overcome the computational bottleneck, a multifidelity surrogate-based approach was adopted. The proposed surrogate merges a one-dimensional, low-fidelity description of the vadose zone beneath *Faidherbia* (HYDRUS-1D), with a kriging-based correction function to emulate the response of a high-fidelity, two-dimensional axisymmetric representation of the domain (HYDRUS-2D). After training and validation, a probabilistic framework based upon Bayesian inference is used to calibrate the surrogate and to inversely estimate soil hydraulic and root water uptake parameters. The comparison between model predictions and observations confirms the good predictive accuracy and limited predictive uncertainty of the model during calibration as well as validation, and thus supports the use of multifidelity surrogates as an efficient tool for reducing the computational cost of calibrating mechanistic models.

The values of the surrogate-based estimated soil hydraulic and root water uptake parameters suggest that *Faidherbia* induces changes in the soil hydraulic properties. These values also confirm the phreatophytic behaviour of *Faidherbia*. In particular, the high values calculated for the saturated hydraulic conductivities ( $K_s$ ) in all soil horizons support the existence of macropore-related and/or root-induced preferential flow, which increases recharge rates significantly. This finding has been reported in other studies, but should be further investigated by performing comprehensive measurements of the root distribution and morphology, combined with tracer experiments to provide more-informative data for calibrating models. These data would make possible a robust comparison, via Bayesian modelling, in which the current unimodal Richards-based description of the water flow is tested against dual-domain or gravity-driven formulations that better describe preferential and macropore flow. By identifying the most appropriate model structure, such a comparison might confirm and assess the magnitude of these root-induced fast flows, thus further strengthening the findings of the present study, which indicates that of *Faidherbia* has a net positive effect upon the hydrological balance of arid areas. These detailed mechanistic analyses should be theoretically complemented by a watershed hydrological modelling to have a broader understanding of water fluxes in the agroforestry parkland.

### CRedit authorship contribution statement

**Djim M.L. Diongue:** Conceptualization, Writing – original draft, Investigation. **Giuseppe Brunetti:** Formal analysis, Writing – original draft, Methodology. **Christine Stumpp:** Supervision, Writing – review & editing. **Frederic C. Do:** Supervision, Writing – review & editing. **Olivier Rouspard:** Supervision, Writing – review & editing. **Didier Orange:** Supervision, Investigation. **Waly Faye:** Investigation. **Sidy Sow:** Investigation. **Christophe Jourdan:** Investigation. **Serigne Faye:** Supervision, Resources.

### Declaration of Competing Interest

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.

## Data availability

Data will be made available on request.

## Acknowledgments

D.M.L. Diongue received funding from CIRAD/IRD/EDEQUE, and is grateful to all Sophy's members for their warm hospitality during his stay in Vienna. Faidherbia-Flux received grants from EU-LEAP-Agri (RAMSES II), EU-DESIRA (CASSECS), EU-H2020 (SustainSahel), AGROPOLIS and TOTAL Foundations (DSCATT), CGIAR (GLDC). We are deeply grateful to the people of Sob-Niakhar, in particular I. Diouf, A. Diouf, and R. Diatte. We thank Prof. Jirka Simunek from University of California, Riverside for sharing with us the non-standard version of the HYDRUS model to simulate the effect of two vegetations. The « Laboratoire des Moyens Analytiques » (UAR IMAGO—LAMA certified ISO9001:2015), at IRD (« Institut de Recherche pour le Développement ») analysed the soil samples in Dakar (<http://www.imago.ird.fr/moyens-analytiques/dakar>). We also thank Dr. James Smith (<https://mx.link-edin.com/in/james-smith-1b195047>) who revised the English.

## Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jhydrol.2023.129717>.

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