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Structural limits and ill-posedness of soil water storage balance method for diagnosing root water uptake

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Abstract. Depth-resolved root water uptake (RWU) can be inferred through soil water storage balance (SWSB) from soil water content observations, yet their fundamental identifiability and robustness remain unclear. Using controlled numerical experiments with prescribed contrasting RWU profiles, we systematically evaluate the performance of SWSB-based RWU inversion under varying spatiotemporal aggregation and upper boundary conditions. Our results show that while accurate estimates can be obtained under idealized, error-free datasets, even modest uncertainties in soil hydraulic parameters (±10%) and soil water content measurements (±1%) lead to error amplification in RWU estimates by around 60-fold. Furthermore, the sensitivity analysis shows that SWSB-based RWU inversion is highly sensitive to soil water content, as it directly influences storage change (ΔV) and regulates the relationships between soil water content (θ) and pressure head (h), as well as saturated (k_s) and unsaturated (k) hydraulic conductivities. These findings highlight SWSB-based RWU inversion is fundamentally ill-posed and becomes non-identifiable under realistic uncertainties. Overall, this study delineates the conditions under which SWSB-based RWU inversion can be reliably applied and emphasizes the need for additional independent constraints.

1 Introduction

Root water uptake (RWU) plays a central role in regulating plant transpiration, drought resilience, and land-atmosphere feedback. The vertical distribution of RWU determines how plants access spatially heterogeneous soil water resources and how they respond to transient hydroclimatic conditions such as drying cycles and rainfall pulses (Couvreur et al., 2012; Gao et al., 2022; Sperry et al., 2002). Quantification of RWU profiles is therefore essential for understanding plant water-use strategies (Burks and Tumber-Dávila, 2025), ecosystem responses to climate variability (Carminati et al., 2026), and the partitioning of evapotranspiration (Yang et al., 2018).

A wide range of methods has been developed to quantify RWU profiles, including imaging-based techniques, process-based hydrological modeling, and stable isotope approaches. Imaging methods such as magnetic resonance imaging (MRI) can

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directly resolve fine-scale water uptake dynamics around roots, providing unique mechanistic insights into root-soil interactions (Postma et al., 2017). However, this approach is largely confined to small soil volumes and controlled laboratory conditions (Maeght et al., 2013). Process-based hydrological approaches infer RWU by introducing a sink term into Richards' equation and prescribing or calibrating its vertical distribution. The performance of this framework depends strongly on accurate parameterization of soil hydraulic properties and rooting characteristics, which often vary across species and environmental conditions and site-specificity (Mencuccini et al., 2019). Stable isotope methods estimate RWU by exploiting mass balance relationships between plant xylem water and soil water isotopic signatures across depth. It can constrain the depth origin of transpired water without explicitly modeling root hydraulics, but is limited by the substantial uncertainties arising from spatial heterogeneity, sampling artifacts, and the underdetermination of inverse mixing models (Barbeta et al., 2020; Dubbert et al., 2019).

Against this background, soil water storage balance (SWSB) approaches (also known as soil water balance, SWB) have attracted renewed attention due to their apparent parsimony and increasing data availability (Rickard et al., 2025). With the widespread deployment of soil water content sensor networks, high-frequency measurements of soil water content are now routinely available across spatial and temporal scales, making SWSB-based inference of RWU conceptually appealing (Lapides et al., 2025). Existing studies have combined SWSB formulations with Bayesian frameworks (Huang et al., 2023), Kalman filtering (Li et al., 2021), or other inverse modeling techniques (Guderle and Hildebrandt, 2015; Sakar et al., 2026; Zuo and Zhang, 2002) to estimate RWU profiles directly from soil water content measurements. These developments suggest that RWU profiles could be inferred from depth-wise soil water storage changes and flux divergences, potentially bypassing uncertainties associated with root trait.

However, inferring RWU from soil water storage balance is fundamentally an inverse problem that may be ill-posed, rendering the solution non-unique (Hupet et al., 2003). This is because RWU does not appear as an independently observed quantity but is inferred as a residual term after accounting for changes in soil water storage and interlayer fluxes, which are strongly coupled. Moreover, SWSB-based RWU inversion relies on differencing operations of soil water storage and on interlayer fluxes derived from soil hydraulic parameters via Darcy's law, both of which inherently amplify the uncertainty of approximated root water uptake fluxes. As a result, the inferred RWU profiles can be highly sensitive to uncertainties in soil hydraulic properties, errors in soil water content measurements, and accuracy of boundary conditions (e.g., evaporation). While recent studies implicitly assume these quantities to be sufficiently well constrained, the extent to which such uncertainties undermine the identifiability and robustness of SWSB-based RWU inversion remains largely unexplored.

Here, we hypothesize that SWSB-based RWU inversion is fundamentally ill-posed and non-identifiable under realistic conditions. We systematically assess the feasibility of SWSB-based RWU inversion using controlled numerical experiments. We first examine how spatial-temporal aggregations, root water uptake patterns, and boundary conditions (dry and wet)

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affect the estimation of RWU profiles. Then, a comprehensive sensitivity analysis is conducted to quantify the impact of soil hydraulic parameter uncertainty and observational errors in soil water content and upper boundary. By explicitly diagnosing when SWSB-based inversion becomes non-identifiable or unstable, our results provide a quantitative framework for interpreting RWU estimates derived from SWSB approaches and clarify the conditions under which such methods can, and cannot, be reliably applied.

2 Material and methods

2.1 Root water uptake proportions from soil water storage balance

For a one-dimensional vertical soil profile, internal soil water dynamics can be described by the continuity equation:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} - S \tag{1}$$

where θ is the volumetric soil water content, q is the vertical soil water flux, t denotes time, and z is soil depth (positive downward). The term S represents the sink term associated with root water uptake, expressed as a volumetric extraction rate per unit time.

Under the assumption that soil water content varies slowly over the considered time interval and that vertical fluxes can be approximated by layer-integrated values, Eq. (1) can be discretized in space and time to yield a layer-wise soil water storage balance：

$$\Delta V_i = Q_{i_{in}} - Q_{i_{out}} \tag{2}$$

where ΔV_i denotes the change in soil water storage of layer i over a given time interval $\Delta t = t_i^{final} - t_i^{initial}$; $Q_{i_{in}}$ and $Q_{i_{out}}$ are the cumulative inflow and outflow fluxes (m) of that layer during Δt.

The soil water storage of layer i is calculated as：

$$\Delta V_i^{final} = \Delta z_i \theta_i^{final} \tag{3}$$

$$\Delta V_i^{initial} = \Delta z_i \theta_i^{initial} \tag{4}$$

where Δz_i is the thickness of layer i; $\theta_i^{initial}$ and θ_i^{final} are the initial and final volumetric water contents, respectively.

For a N-layer soil column, the layer-wise water balance equations over a given time interval Δt can be written as

$$\Delta V_1 = P - E - D_1 - R_1 \ (For\ layer\ 1) \tag{5}$$

$$\Delta V_i = D_{i-1} - D_i - R_i \ (For\ layer\ i=2 \ldots N) \tag{6}$$

where P and E denote the total precipitation and evaporation over Δt, respectively. D_i represents the cumulative drainage flux from layer i to layer $i+1$ during Δt, and R_i is the total root water uptake from layer i over the same interval.

Estimation of interlayer drainage fluxes, D

The cumulative drainage flux D_i within the given period is approximated using the trapezoidal rule based on instantaneous Darcy fluxes evaluated at the initial and the final of the time interval:

$$D_i=\frac{\left(D_i^{initial}+D_i^{final}\right)\Delta t}{2} \tag{7}$$

Instantaneous fluxes at initial and final time point of the give time interval are computed according to Darcy's law:

$$D_i^{initial}= - \left(\frac{k_i^{initial}+k_{i+1}^{initial}}{2}\right)\left(\frac{h_i^{initial}-h_{i-1}^{initial}}{\Delta z}-1\right) \tag{8}$$

$$D_i^{final}= - \left(\frac{k_i^{final}+k_{i+1}^{final}}{2}\right) k_i^{final} \left(\frac{h_i^{final}-h_{i-1}^{final}}{\Delta z}-1\right) \tag{9}$$

For the bottom soil layer, a free-drainage lower boundary condition is assumed:

$$D_i^{initial} = k_i^{initial} \tag{10}$$

$$D_i^{final} = k_i^{final} \tag{11}$$

Soil hydraulic conductivity $k(\theta)$ and pressure head $h(\theta)$ are described using the Brooks-Corey model:

$$k(\theta)=k_{sat}\left(\frac{\theta-\theta_{res}}{\theta_{sat}-\theta_{res}}\right)^{\eta} \tag{12}$$

$$h(\theta)=h_e\left(\frac{\theta-\theta_{res}}{\theta_{sat}-\theta_{res}}\right)^{-\frac{1}{n}} \tag{13}$$

where θ_{sat} and θ_{res} are the saturated and residual water contents, respectively; k_{sat} is the saturated hydraulic conductivity; h_e is the air-entry pressure head; n is the pore-size distribution index; and η is a shape parameter approximated as $\eta = 2/n + 3$.

Estimation of root water uptake proportions

The cumulative root water uptake from each layer over the given period Δt is obtained by rearranging Eqs. (5)-(6):

$$R_1=P- E- D_1- \Delta V_1 \tag{14}$$

$$R_i= D_{i-1}-D_i- \Delta V_i \ (i=2 \ldots N) \tag{15}$$

The depth-wise root water uptake proportion of layer i is then calculated as

$$UP_i= \frac{R_i}{\sum_{i=1}^{n} R_i} \tag{16}$$

where $\sum_{i=1}^{n} R_i$ is the transpiration.

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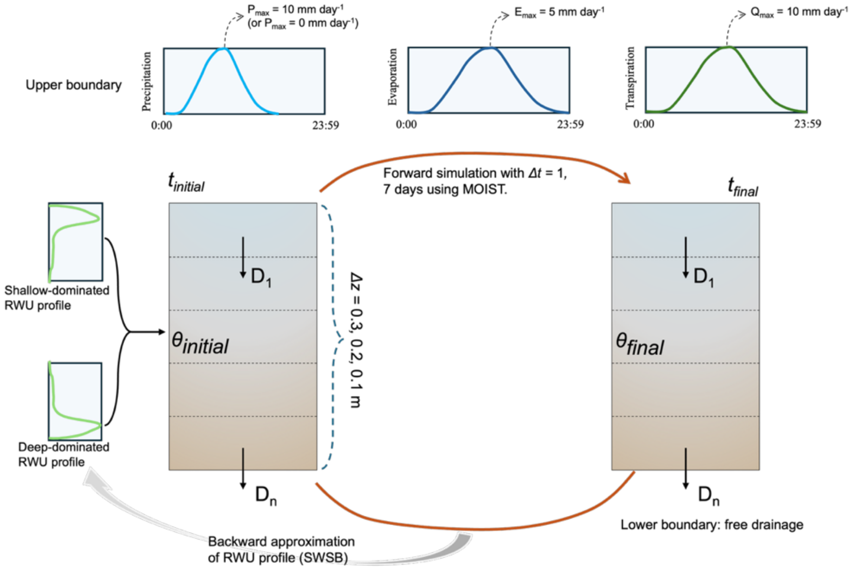
2.2 Method evaluation

Errors of SWSB-based RWU inversion typically arise from precipitation (*P*), evaporation (*E*), interlayer fluxes (*D*), and 125 changes in soil water storage (ΔV, computed from θ). Measurement errors in precipitation (P) are often assumed negligible, but not for *E* and ΔV (θ). By contrast, interlayer fluxes (*D*) cannot be observed directly and must be approximated numerically. Accordingly, our evaluation of SWSB-based RWU inversion focuses on two main error sources: (1) errors associated with the numerical estimation of interlayer fluxes (*D*), and (2) errors arising from measurements of evaporation (*E*) and soil water contents (θ). Consequently, we conducted a series of controlled numerical experiments using MOIST 130 model as a forward simulator of soil water dynamics. These experiments are designed to isolate numerical and parametric sources of uncertainty under idealized conditions with given RWU profiles as benchmarks (Figure 1).

2.2.1 Forward simulation

MOIST (Fu et al., 2025) is used to simulate vertical soil water flow and soil water profiles in a one-meter soil column. Soil hydraulic parameters are prescribed and assumed homogeneous within the profile. Initial soil water content profiles are 135 prescribed, and soil water dynamics are simulated under two upper boundary conditions: a dry scenario (P = 0 mm day^{-1}) and a wet scenario (P = 10 mm day^{-1}) (Figure 1); two temporal aggregation schemes: a daily time step (Δt = 1 day) and a weekly time step (Δt = 7 days), three spatial discretization schemes: Δz = 0.1, 0.2, and 0.3 m; and two prescribed root water uptake profiles: shallow-dominated and deep-dominated root water uptake (Figure 1).



140 **Figure 1. Conceptual framework of the numerical experiments used to evaluate soil water storage balance (SWSB)-based root water uptake (RWU) inversion. A one-dimensional soil column, with prescribed soil hydraulic properties (θ_{sat} = 0.35 m^3 m^{-3}, θ_{res} = 0.01 m^3 m^{-3}, k_{sat} = 1.23 × 10^{-7} m s^{-1}, n = 0.22, h_e = -0.193 m), is discretized with multiple layer thicknesses (Δz = 0.3, 0.2, 0.1 m), driven by time-varying upper boundary fluxes (precipitation, evaporation, and transpiration) and two types of prescribed RWU profiles (shallow-dominated and deep-dominated). Forward simulations generate soil water content profiles at the initial ($\theta_{initial}$)**

and final (θ_{final}) time points, along with internal fluxes such as interlayer drainage (*D*) under various temporal steps (daily and weekly). These quantities are then used as inputs to the SWSB framework to approximate internal fluxes and invert depth-resolved RWU.

To represent realistic intra-day variability, precipitation, evaporation, and transpiration are prescribed as sinusoidal functions over each day (Figure 1), ensuring that daily totals are conserved while allowing sub-daily fluxes to vary continuously. This design mimics the typical diurnal patterns of evaporation and episodic rainfall without introducing stochastic noise, thereby maintaining an error-free benchmark framework.

2.2.2 Errors associated with the numerical estimation of interlayer fluxes

Using interlayer soil water fluxes simulated by the MOIST model, we evaluated the accuracy of the trapezoidal rule for estimating temporally integrated drainage fluxes between adjacent soil layers (Eq. 7). For each layer interface, cumulative percolation over a given time interval is computed directly from MOIST outputs and compared with the corresponding trapezoidal approximation (Eq. 7). The trapezoidal approximation is further used to estimate interlayer drainage fluxes (*D*), which serve as a key input to the SWSB method for inferring root water uptake profiles. To explicitly assess how errors in *D* propagate into RWU estimates, we performed parallel inversions using (1) trapezoidal-approximated fluxes and (2) benchmark fluxes obtained directly from MOIST. This comparison enables isolation of the impact of numerical approximation errors in *D* on RWU inversion performance.

Subsequently, the MOIST-simulated initial and final soil water content profiles, together with prescribed boundary fluxes and known soil hydraulic parameters (Figure 1), are used as inputs to the SWSB inversion framework to estimate RWU profiles. RWU is expressed as layer-wise uptake proportions, ensuring comparability across scenarios with different absolute uptake magnitudes. The accuracy of the inverted RWU profiles is quantified using the Earth Mover's Distance (EMD) to quantify the discrepancy between the inferred and true RWU profiles. For a discretized soil profile with N layers, let $u = (u_1, \ldots, u_N)$ and $v = (v_1, \ldots, v_N)$ denote the benchmark and SWSB inverted RWU proportions, respectively, with $\sum u_i = \sum v_i = 1$. The EMD is computed as

$$\mathrm{EMD} = \sum_{i=1}^{N} \left| \sum_{j=1}^{i} \left(u_j - v_j \right) \right| \Delta z \tag{17}$$

where Δz is the layer thickness. This metric explicitly accounts for the vertical structure of RWU distributions by penalizing both magnitude differences and their displacement along the soil profile.

By combining (i) numerical evaluation of interlayer flux estimation, (ii) SWSB-based inversion of RWU profiles, and (iii) quantitative error metrics under controlled conditions, this method evaluation framework allows a systematic assessment of when and why SWSB-based RWU inversion succeeds or fails. Importantly, all numerical tests are conducted under error-free conditions unless otherwise stated, so that any observed instability or failure reflects intrinsic limitations of the inversion structure rather than observational noise.

2.2.3 Sensitivity analysis

The analyses presented in Section 2.2.2 are conducted under idealized conditions, in which only the method uncertainty that compute interlayer drainage fluxes (D) on RWU inversion is evaluated. Other sources of uncertainty, such as soil water content measurements, boundary fluxes (e.g., evaporation), and soil hydraulic parameters, are assumed to be error-free. In practical applications, however, these quantities are subject to unavoidable uncertainties, which may introduce inconsistencies in the layer-wise water balance and propagate into RWU estimates.

To further quantify how these errors propagate through the SWSB-based RWU inversion, we performed a global sensitivity analysis using the Sobol variance decomposition framework under conditions of coarse spatial discretization (three soil layers) and a short integration interval (Δt = 1 day). This combination represents the most favorable scenario for the trapezoidal approximation, as interlayer fluxes within the short time step are close to linear variations, thereby satisfying the underlying assumptions of the trapezoidal method. The Earth Mover's Distance (EMD) is used as the response variable (computed at a daily scale), as it provides a robust metric for quantifying distributional differences between prescribed and estimated layer-wise uptake proportions.

Three cases are considered in the sensitivity analysis:

Case 1: Soil hydraulic parameter error only

In this scenario, errors are introduced exclusively through soil hydraulic parameters, including θ_{sat}, θ_{res}, n, h_e, and k_{sat}. Each parameter is perturbed independently within ±10% of its reference value. This range is selected as a conservative yet realistic estimate of parameter uncertainty, given that soil hydraulic properties are known to be spatially heterogeneous and difficult to measure accurately, even under controlled conditions. Parameters such as saturated hydraulic conductivity (k_{sat}) are often reported to vary by one to two orders of magnitude across small spatial scales (Ahmadisharaf et al., 2024; Vereecken et al., 2016), making ±10% a lower-bound estimate of uncertainty in practice. This scenario isolates the intrinsic sensitivity of the SWSB inversion to hydraulic parameter uncertainty alone.

Case 2: Measurement and forcing data error

In the second scenario, error is introduced only through observational and forcing data. Initial and final soil water content profiles are perturbed by random multiplicative noise of ±1%, representing realistic sensor error. This range is consistent with the reported accuracy of commonly used soil water sensors, such as time-domain reflectometry (TDR) and capacitance-based probes, which typically exhibit errors of 1%-3% volumetric water content under field conditions (Bogena et al., 2021; Topp et al., 1980). In addition, soil evaporation is perturbed by ±5% to reflect errors associated with evaporation

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measurement or modeling, which can arise from aerodynamic assumptions, energy balance closure, and partitioning of evapotranspiration (Stoy et al., 2019; Wilson et al., 2002). By excluding hydraulic uncertainty, this scenario isolates the impact of data-related errors on SWSB inversion performance.

Case 3: Combined parameter and data errors

The third scenario represents a realistic application setting, in which both soil hydraulic parameters (±10%) and observational data (±1% soil water content, ±5% evaporation) are uncertain simultaneously. This combined scenario is designed to evaluate the global sensitivity and structural robustness of the SWSB inversion under practical conditions, where multiple sources of uncertainty interact nonlinearly. In real-world applications, soil hydraulic properties are rarely known with high precision, and measurement or estimation errors in soil water and boundary fluxes are unavoidable. Therefore, this case provides a stringent test of the practical applicability of SWSB-based RWU inversion.

For each case, Sobol sensitivity indices are estimated using Monte Carlo sampling. A total of 10,000 realizations is generated for each analysis to ensure convergence of both first order (S_i) and total-effect (ST_i) indices. The first-order Sobol index (S_i) quantifies the contribution of an individual parameter to the variance of EMD, assuming all other parameters are fixed, while the total-effect index (ST_i) measures the overall contribution of a parameter, including all higher-order interaction effects with other variables. Together, these indices allow discrimination between dominant individual drivers and interaction-dominated uncertainty propagation in the SWB inversion. Additionally, an EMD threshold of 0.01 is adopted as the criterion for successful RWU inversion. This threshold is determined based on prior numerical experiments, which indicated that RWU profiles become noticeably distorted when EMD exceeds 0.01. Accordingly, the success rate is defined as the proportion of EMD values below this threshold.

3 Results

3.1 Impact of interlayer flux representation on SWSB-based RWU inversion

The EMD values of SWSB-based RWU estimates under different soil discretization, hydrological conditions, and uptake patterns are shown in Figures 2a-2d. When interlayer fluxes are approximated using the trapezoidal rule, RWU estimation errors increase systematically with the number of soil layers under both dry (Figures 2a and 2c) and wet conditions (Figures 2b and 2d). This is particularly pronounced for longer integration intervals (7-day) and finer spatially discretization, where EMD values increase markedly from approximately 0.001 at 3 layers to 0.03 at 10 layers. In the 10-layer discretization, the inferred RWU profiles even exhibit negative uptake values (e.g., Figures 2f, 2p, 2v, 2bb), indicating a clear breakdown of the inversion under fine discretization. This can be attributed to that the trapezoidal rule assumes linear variation of fluxes between initial and final time points, which becomes increasingly inadequate for representing nonlinear soil water dynamics

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over longer integration periods and thinner layer thicknesses (e.g., Figures 2u, 2v, 2aa, 2bb).

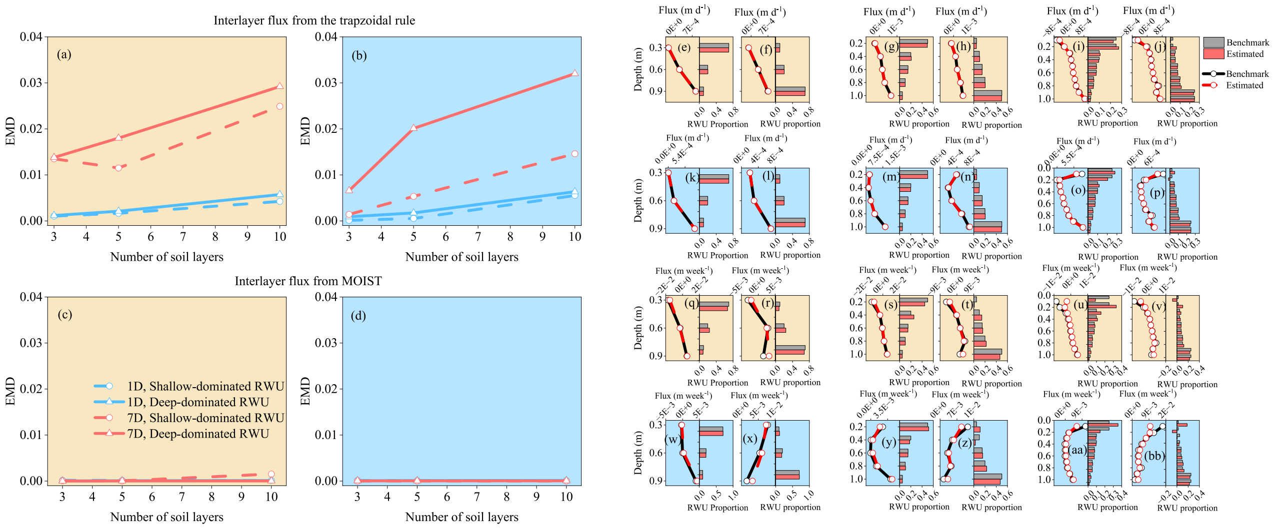

Figure 2. Impact of interlayer drainage flux estimation on the accuracy of SWSB-based RWU inversion. Panels a and b are root water uptake (RWU) estimation error, quantified by the Earth Mover's Distance (EMD), as a function of soil discretization (number of layers) under dry (yellow filled) and wet (blue filled) conditions, respectively, when interlayer fluxes are approximated using the trapezoidal rule. Results are shown for different temporal resolutions (Δt = 1 and 7 days) and benchmark RWU patterns (shallow-rooted and deep-rooted). Panels c and d are same as panels a and b but using interlayer fluxes directly obtained from the MOIST model. Panels e to bb are comparison of interlayer fluxes and corresponding RWU profiles derived from trapezoidal approximation and MOIST simulations under dry (yellow filled) and wet (blue filled) conditions, respectively.

By contrast, when drainage fluxes are taken directly from the MOIST (Figures 2c-2d), RWU estimation errors remain consistently low across all discretization levels, generally on the order of 10^{-3}. Moreover, EMD values show little sensitivity to the number of soil layers, regardless of hydrological condition, integration interval, or uptake pattern (almost straight lines in Figures 2c and 2d). This indicates that, when the soil water balance is accurately closed at each layer, the SWSB framework can reliably recover RWU profiles.

Overall, these results demonstrate that SWSB-based RWU inversion is fundamentally constrained by the accuracy of layer-wise water balance closure. When interlayer drainage fluxes are numerically approximated, RWU estimates remain reliable only under short integration intervals (e.g., daily) and coarse vertical discretization (e.g., 3 layers). Increasing the number of soil layers or extending the integration interval leads to the accumulation of flux approximation errors, which propagate and amplify in the inferred RWU profiles.

3.2 Sensitivity of SWSB to parameter and data uncertainties

Results from Section 3.1 indicate that accurate layer-wise water balance closure is critical for reliably recovering RWU profiles. In practical applications, however, soil water balance in each layer is further affected by uncertainties in

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measurements (e.g., evaporation and soil water content) as well as in soil hydraulic parameters used for interlayer flux estimation. The sensitivity analysis presented in this section aims to systematically evaluate how uncertainties in soil hydraulic parameters, soil water content observations, and boundary fluxes propagate through the SWSB framework and influence the accuracy and stability of RWU inversion.

When only uncertainties from soil hydraulic parameters are considered (Case 1), the sensitivity indices (S_i and ST_i) of pore-size distribution index (n) are very close and the largest among all soil hydraulic parameters (Table 1), indicating that its influence on RWU inversion is predominantly driven by its main (first-order) effect, with negligible interaction effects with other parameters. This behavior is expected, as n controls both the θ-h relationship and the k-θ relationship (Eqs. 12 and 13), thereby directly affecting the estimation of hydraulic gradients and unsaturated hydraulic conductivity, and ultimately the calculation of interlayer fluxes.

Additonally, the success rates (SR) of RWU inversion are approximately 0.3 and 0.6 for shallow- and deep-dominated RWU patterns, respectively (Table 1). This suggests that, when accounting for uncertainties in soil hydraulic parameters, the performance of SWSB-based RWU inversion deteriorates substantially. The higher success rate for inverting deep-dominated RWU profiles can be attributed to the depth-dependent propagation of parameter uncertainty. Near the soil surface, parameter uncertainty interacts with precipitation and evaporation, increasing variability in the water balance and obscuring the RWU signal. By contrast, deeper layers are less affected by upper boundary fluxes, resulting in a simpler signal structure and improved identifiability.

Table 1. Sobol sensitivity indices (Si, STi) and inversion success rates (SR) for SWB-based RWU estimation under Δz = 0.3 m and Δt = 1 day, for shallow- (Sh) and deep-dominated (De) RWU patterns under dry (Dr) and wet (We) upper boundary conditions. Sensitivity analyses consider uncertainties in soil hydraulic parameters, observations (soil water content and evaporation), and their combination. Large total-effect indices (STi) relative to first-order indices (Si) indicate strong parameter interactions and structural instability of the inversion, particularly under combined uncertainties. The success rate (SR) is defined as the fraction of realizations with EMD < 0.01 (based on 10,000 runs).

	ShDr			ShWe			DeDr			DeWe		
	S_i	ST_i	SR	S_i	ST_i	SR	S_i	ST_i	SR	S_i	ST_i	SR
θ_{sat}	2.4E-02	2.2E-02	0.28	1.6E-02	2.2E-02	0.33	2.6E-02	2.5E-02	0.61	2.2E-02	2.8E-02	0.60
θ_{res}	4.6E-05	8.4E-06		5.1E-05	8.1E-06		-1.1E-03	6.8E-04		8.1E-04	5.4E-04	
n	1.6E-01	1.7E-01		1.4E-01	1.3E-01		2.2E-01	2.6E-01		1.0E-01	9.5E-02	
h_e	3.5E-02	3.1E-02		2.9E-02	2.9E-02		4.2E-02	5.7E-02		1.7E-02	1.9E-02	
k_{sat}	5.7E-02	6.7E-02		7.8E-02	6.8E-02		1.2E-02	1.2E-02		2.1E-02	1.8E-02	
θ	3.2E-04	1.4E-01	0.17	-4.1E-03	1.5E+00	0.18	5.2E-03	2.2E+00	0.26	4.8E-03	1.2E+02	0.20
E	4.8E-04	2.1E-02		-4.7E-03	8.6E-01		7.8E-03	1.6E+00		1.4E-01	1.2E+00	
θ_{sat}	1.6E-03	5.2E+00	0.09	-3.6E-03	2.1E+00	0.12	-4.9E-04	8.5E-01	0.22	1.1E-08	1.4E-06	0.19
θ_{res}	-2.5E-05	8.5E-04		-5.3E-05	3.8E-01		-2.9E-04	4.3E-01		-1.7E-09	3.2E-07	
n	-1.3E-04	5.3E-05		1.6E-05	2.2E-03		1.1E-05	1.2E-04		7.8E-08	1.2E-09	
h_e	8.6E-05	1.4E-05		-1.8E-04	6.2E-04		-1.3E-05	2.9E-04		-2.8E-08	1.9E-10	
k_{sat}	5.4E-04	4.7E-02		2.6E-02	1.4E+01		-4.7E-04	9.0E-01		1.3E-08	3.5E-06	
θ	4.1E-02	1.7E+00		2.0E-02	4.5E+00		1.2E-04	1.4E+01		4.3E-06	1.8E-06	
E	9.8E-04	2.2E-01		6.5E-03	6.4E-01		-5.2E-04	9.4E-01		-1.9E-07	1.2E-06	

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Moreover, introducing measurement uncertainties (θ and E) alone (Case 2) leads to a pronounced degradation in inversion performance (Table 1). The success rates (*SR*) decrease substantially, by approximately 40% and 60% for shallow- and deep-dominated RWU scenarios, respectively, compared to Case 1. At the same time, the total sensitivity indices (ST_i) are consistently larger than the corresponding first-order indices (S_i), indicating strong interaction effects among measurement-related variables. Notably, the ST_i of θ is generally the largest among all variables, suggesting that soil water content is the dominant factor controlling RWU inversion performance.

Lastly, when uncertainties in both soil hydraulic parameters and measurements are considered simultaneously (Case 3), the success rates decline to their lowest levels (approximately 0.1 and 0.2 for shallow- and deep-dominated uptake patterns, respectively) (Table 1). In addition, the total sensitivity index (ST_i) of the $\theta_{initial}$ becomes further amplified, indicating that SWSB-based RWU inversion is most sensitive to θ, with strong interaction effects among variables. This is consistent with Case 1: when θ is error-free, the dominant source of uncertainty arises from the hydraulic parameter n, which simultaneously affects the relationships between θ and h, as well as between k and k_{sat}. When uncertainty in θ is introduced, however, it directly perturbs these relationships, thereby amplifying its influence on RWU inversion.

Overall, SWSB-based RWU inversion is highly sensitive to realistic uncertainties in both soil water content observations and soil hydraulic parameters. The combined effects of residual amplification, measurement error propagation, and parameter compensation lead to a rapid loss of robustness and identifiability. The low success rate (~ 0.15) suggests that reliable estimation of depth-resolved RWU is unlikely to be achieved using soil water balance alone.

4. Discussion

Estimating root water uptake (RWU) from soil water contents using the soil water storage balance (SWSB) framework has long been regarded as an attractive alternative to fully mechanistic inverse modelling, due to its conceptual simplicity, low computational cost (Liao et al., 2025; Sakar et al., 2026), and independence from prior knowledge of root water uptake profiles (Li et al., 2021). In its discrete form, the SWSB equations attribute changes in soil water storage (ΔV) to the combined effects of inflow and outflow. However, our numerical analysis demonstrates that this formulation is intrinsically ill-posed when used for inverse estimation of layer-wise RWU.

The fundamental difficulty arises because RWU is not directly observed but inferred as a residual term after differencing several quantities. Specifically, ΔV is computed as the difference between initial and final soil water content measurements over a given period and is further combined with other flux components to solve for root water uptake. As a result, inversion of RWU from soil water content observations involves successive differencing operations that make the problem highly

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sensitive to small errors. In this framework, compensating interlayer fluxes can easily overshadow the RWU signal (Tarantola, 2005), leading to unstable solutions of root water uptake profiles (Fu et al., 2026; Hupet et al., 2003).

4.1 Amplification of ill-posedness under flux approximation

Our virtual simulations have confirmed that SWSB based RWU inversion is sensitive to flux estimation errors. Errors in interlayer flux estimation arise from the numerical approximation itself. Most existing studies that infer RWU using SWSB in combination with Richards' equation implicitly assume that approximated interlayer fluxes are either error-free or sufficiently accurate during the inversion period (Jackisch et al., 2020; Lai et al., 2023; Li et al., 2021). However, no matter how sophisticated the numerical scheme is (e.g., higher-order approximations, MCMC, or Kalman filtering; (Li et al., 2021)), such approaches cannot overcome the fundamental limitation that fluxes are approximated rather than independently observed. This interpretation can be supported by our virtual experiments, which show that under rainfall conditions, drainage fluxes can be estimated more accurately than under dry conditions, yet the inferred RWU profiles exhibit larger errors (e.g., Figures 2u and 2v). This apparent paradox indicates that improved numerical accuracy in flux estimation does not necessarily translate into improved RWU inversion. Instead, it reflects a shift in the underlying information structure of the system, where rainfall reduces the relative contribution of RWU to soil water storage dynamics. As a result, the inversion becomes increasingly sensitive to small inconsistencies, which is consistent with the structural ill-conditioning of RWU inferred as a residual term.

Neglecting interlayer flux errors may result in substantial misinterpretation of RWU profiles, potentially leading to misleading conclusions regarding plant water use strategies or drought responses. For example, under weekly integration and wet conditions, the inverted RWU profiles exhibit an apparent concentration of uptake in the shallow soil layers (e.g., Figures 2aa and 2bb). This pattern could be interpreted as enhanced reliance on topsoil water following precipitation (Sprenger et al., 2025). However, forward simulations show no corresponding change in the benchmark RWU profile, indicating that this apparent shallow uptake is spurious. Instead, it arises as a compensatory artifact required to satisfy the soil water balance under mismatches in drainage and storage. Consequently, such inversion artifacts may be misinterpreted as physiological plant responses, whereas they in fact reflect numerical compensation for unresolved fluxes errors.

Together, these results indicate that flux approximation errors do not merely introduce numerical inaccuracies, but fundamentally alter the information content of the inversion, thereby amplifying its structural ill-posedness.

4.2 Propagation of soil water content uncertainty in SWSB-based RWU inversion

The analysis in Section 4.2 indicates that errors in interlayer flux estimation primarily originate from uncertainties in soil water content. Our sensitivity analysis further shows that, when both hydraulic parameter and measurement uncertainties are considered, SWSB-based RWU inversion is most sensitive to soil water content. with perturbations as small as ±1% being sufficient to amplify RWU estimation errors by approximately 60 times. This is consistent with the findings of Guderle and Hildebrandt (2015), who reported relative RWU errors approaching 800% when both sensor precision and calibration errors are considered.

Soil water content influences RWU inversion through two primary pathways. First, errors in soil water content directly affect the estimation of soil water storage changes (ΔV), which constitute a key component of the SWSB framework. Because RWU is inferred as a residual of storage change and flux divergence, even small biases in soil water content can propagate into ΔV and lead to substantial errors in the estimated uptake. This effect is particularly pronounced when RWU represents only a small fraction of the overall water balance, as the residual becomes highly sensitive to inconsistencies among the contributing terms.

Second, soil water content errors propagate into interlayer flux estimation through the nonlinear transformation between water content and pressure head, as well as saturated and unsaturated hydraulic conductivity, through soil water retention functions (Brooks and Corey, 1964; van Genuchten, 1980), which are then used to compute fluxes through Darcy's law. Since soil hydraulic parameters are well known to be highly variable (Vereecken et al., 2016), even small errors in soil water content can be significantly amplified when translated into pressure head, particularly within the nonlinear range of the retention curve. These amplified errors further propagate into flux estimates, leading to disproportionately large uncertainties in interlayer fluxes and, consequently, in RWU inversion (as confirmed by our sensitive analysis, Table 1). This coupled error propagation mechanism further exacerbates the ill-posedness of the RWU inversion.

It is important to emphasize that the errors of soil water contents introduced in our analysis are already conservative. For example, commonly used soil water content sensors such as the Acclima TDR315N and Campbell Scientific CS650/655 report nominal accuracies of approximately ±2% and ±1%, respectively (manufacturer specifications; see also Bogena et al., 2021), with potentially larger errors under field conditions. These uncertainty levels indicate that sensor-induced errors alone are sufficient to drive substantial deviations of the SWSB-inverted root water uptake profiles from the true uptake pattern. Although previous studies have attempted to mitigate these issues through sensor calibration or smoothing techniques (e.g., Zuo and Zhang, 2002), such approaches primarily reduce noise but do not introduce new independent information into the inversion.

If measurement errors are strictly systematic and time-invariant, their influence on soil water storage changes (ΔV) may be limited, as storage is computed from differences between successive observations and constant biases tend to cancel out. By contrast, random or time-varying errors can propagate directly into storage estimates, substantially degrading RWU inversion. In practice, however, it remains difficult to determine whether measurement errors are predominantly systematic or random under field conditions, as sensor performance is influenced by factors such as temperature, soil heterogeneity, and calibration drift (Robinson et al., 2008). This ambiguity further complicates the interpretation of inversion results and highlights an inherent limitation in SWSB-based approaches. One possible way forward is to simultaneously measure both soil water content and matric potential, thereby reducing reliance on parameterized retention relationships. However, soil water potential sensors themselves can be subject to substantial uncertainties and practical limitations in field deployment (Bittelli, 2010). Therefore, whether such approaches can effectively improve RWU inversion remains an open question and warrants further investigation.

4.3 Role of boundary conditions in controlling RWU identifiability

Although the sensitivity analysis indicates that evaporation (E) exerts a weaker influence than soil water content, upper boundary fluxes (P and E) fundamentally control the identifiability of RWU by regulating the signal-to-noise ratio of RWU within soil water storage dynamics. In essence, boundary conditions determine whether RWU signals can be distinguished from other competing fluxes in the soil water balance.

This effect is evident in the contrasting inversion performance between shallow- and deep-dominated RWU profiles. For shallow-dominated cases, near-surface soil moisture dynamics are simultaneously influenced by precipitation, evaporation, infiltration, and root water uptake. These fluxes are often of comparable magnitude, which obscures the RWU signal and makes it difficult to isolate during inversion (Carrera et al., 2005; Doherty and Hunt, 2009). As a result, RWU becomes poorly identifiable. By contrast, deep-dominated RWU profiles exhibit substantially higher inversion success rates. In these cases, root water uptake in surface layers is relatively small, while deeper layers account for most of the uptake. Because deeper soil layers are not directly affected by atmospheric boundary fluxes, their water balance is governed by fewer competing processes, primarily inter-layer fluxes and RWU. This reduced process complexity leads to a clearer signal structure, improving the separability and identifiability of RWU. This implies that changes in boundary forcing conditions can fundamentally alter the composition of storage signals, thereby determining whether RWU remains identifiable within the soil water balance.

These findings are consistent with inverse modelling theory, which shows that strong boundary forcing amplifies the propagation of measurement and model errors into inferred internal fluxes (Liao et al., 2025; Vrugt, 2016), and help explain why improved numerical accuracy in flux approximation under wet conditions does not necessarily translate into improved RWU inversion (Fu et al., 2026).

Overall, the success of SWSB-based RWU inversion is governed not only by soil water content observations and flux estimation accuracy, but more fundamentally by the information content and separability of RWU signals within the soil water balance, which are controlled by boundary conditions.

4.4 Implications and limits for practical RWU estimation

Our results do not imply that approximating root water uptake from soil water storage balance concepts is fundamentally flawed; rather, they delineate strict limits on the information that can be reliably extracted from soil water content observations alone. Under highly idealized conditions, such as short integration windows (quasi-steady-state conditions), absence of rainfall, and negligible measurement uncertainty, SWSB-based approaches can approximate cumulative interlayer fluxes reasonably and may provide acceptable estimates of RWU profiles (Figure 2). This interpretation is consistent with earlier studies that focused on extended dry periods or exploited sub-daily soil water dynamics to separate vertical flow and root uptake based on temporal structure (Cai et al., 2018; Guderle and Hildebrandt, 2015).

However, the apparent success reported in previous studies is conditional on strong (and often implicit) assumptions, including accurately known soil hydraulic properties, negligible measurement errors, and favorable boundary conditions (e.g., Huang et al., 2023; Li et al., 2021). Our results indicate that these assumptions are not merely technical conveniences but critical prerequisites for identifiability. Once these assumptions are relaxed, SWSB-based RWU inversion rapidly collapses into an interaction-dominated regime. Consequently, RWU becomes effectively non-identifiable when inferred solely from soil water balance constraints, consistent with the non-uniqueness commonly encountered in tracer-aided mixing problems (Popp et al., 2025). In this sense, SWSB-based RWU inversion should be regarded not as a standalone diagnostic tool, but as a conditional inference framework whose reliability critically depends on the information content of the soil water balance.

Based on these findings, several practical guidelines can be proposed for the application of SWSB-based RWU inversion. The method should be restricted to conditions where the RWU signal constitutes a substantial fraction of the soil water balance, which is more likely under dry periods with minimal precipitation. Short integration intervals (e.g., daily or sub-daily) and coarse vertical discretization are recommended to reduce numerical errors and limit error accumulation during inversion. Attention should be given to measurement uncertainty in soil water content, as even small errors (on the order of 1%) can lead to substantial amplification of RWU estimation errors. Under conditions where rainfall dominates soil water dynamics or where uncertainties in measurements and parameters are significant, SWSB-based inversion should be applied with caution, and resulting RWU estimates should be interpreted as qualitative rather than quantitative diagnostics.

To improve the robustness of RWU estimation, SWSB-based approaches should be complemented with additional independent constraints, such as transpiration measurements, root distribution information, or tracer-based methods (hydrogen and oxygen stable isotopes), which can help reduce equifinality and enhance parameter identifiability (Fu et al., 2024; Ogle et al., 2014).

5. Conclusion

This study systematically evaluated the robustness and identifiability of root water uptake (RWU) inferred from soil water storage balance (SWSB) under realistic sources of uncertainty. Our results demonstrate that SWSB-based RWU inversion performs reliably only under near quasi-steady-state conditions. Deviations in RWU estimates are primarily driven by errors in interlayer flux estimation, which arise from both numerical approximation schemes and uncertainties in soil hydraulic parameters.

The sensitivity analysis further reveals that RWU inversion is highly sensitive to soil water content, as it simultaneously governs storage dynamics and mediates the relationships among key hydraulic variables. In addition, boundary conditions exert a critical control on inversion behaviour by modulating the signal-to-noise ratio of RWU within soil water storage dynamics. Under dry conditions, partial identifiability may be achieved under highly idealized assumptions. While under wet conditions, rainfall-driven infiltration dominates soil water storage changes, masking the RWU signal. This leads to an apparent reduction in sensitivity that coincides with deteriorating inversion performance, reflecting a loss of identifiability rather than improved robustness.

These findings do not imply that soil water balance approaches are invalid; rather, they highlight fundamental limits on what can be reliably inferred from soil water content observations alone. Robust estimation of RWU in field conditions therefore requires additional independent constraints or complementary observations beyond soil water content measurements.

Code and Data availability

The data used in this study is generated by MOIST model and the model can be accessed from https://zenodo.org/records/8397416.

Author contributions

Conceptualization: HF, BS, and WZ; Method development: HF; Data collection, simulation, analyzation, and visualization: HF; Writing and revision: HF, BS, and WZ.

Competing interests

None

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