Advancing Non-invasive, Passive Measurement of Root Zone Soil Water Content at the Subfield Scale Using Gamma-ray Spectroscopy

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DAUGHERTY GLOBAL INSTITUTE
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Motivation for Estimating Soil Water Content (SWC) with Gamma-ray spectroscopy

"Developing correction algorithms for soil moisture content is one of the most urgent tasks for gamma-ray spectrometry research in the near future."
- Reinhardt and Herrmann, 2019

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Water management; Irrigation

Climate and hydrology modeling

Satellite product validation

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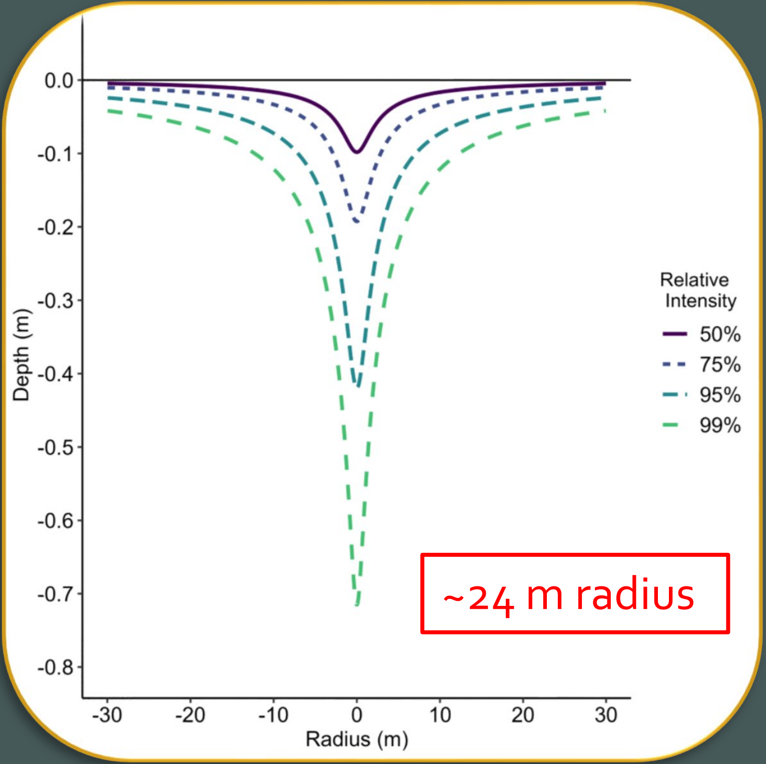

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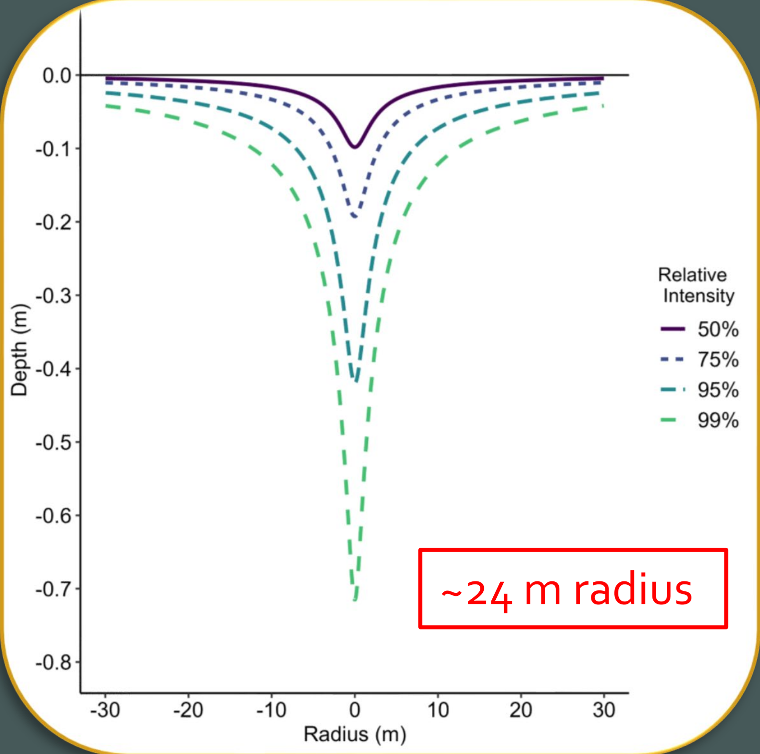

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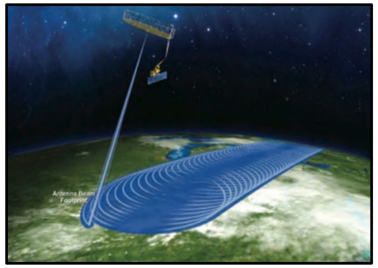
Context of current methods:

https://www.ictinternational.com/products/tdr-315/tdr-315l/

Time domain reflectometry (TDR)
$0.01\ cm^3\ cm^{-3}$ resolution
Point sensor

Cosmic-ray Neutron Sensor (CRNS)
< $0.03\ cm^3\ cm^{-3}$ RMSE
12 – 70 cm depth, ~ 200 m radius
Bogena et al., 2013; Franz et al., 2012

Soil Moisture Active Passive (SMAP)
$\pm 0.04\ cm^3\ cm^{-3}$
Top 5 cm, ~ 10 km resolution
Entekhabi et al., 2010

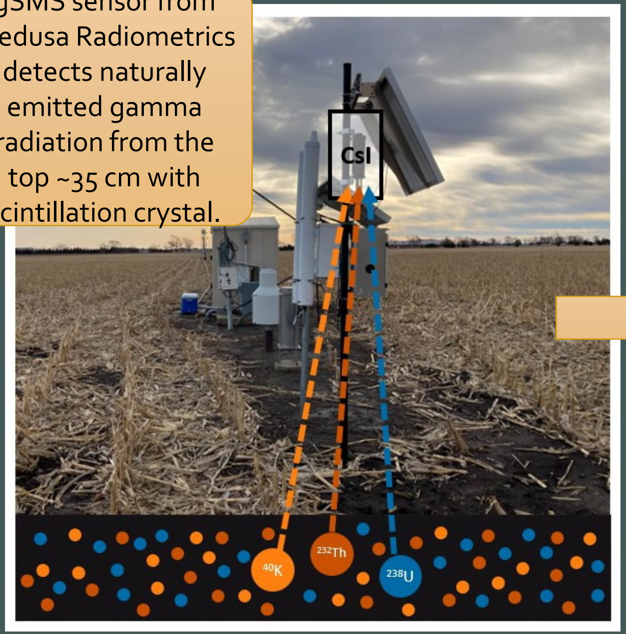


https://smap.jpl.nasa.gov/resources/39/smap-orbital-motion/

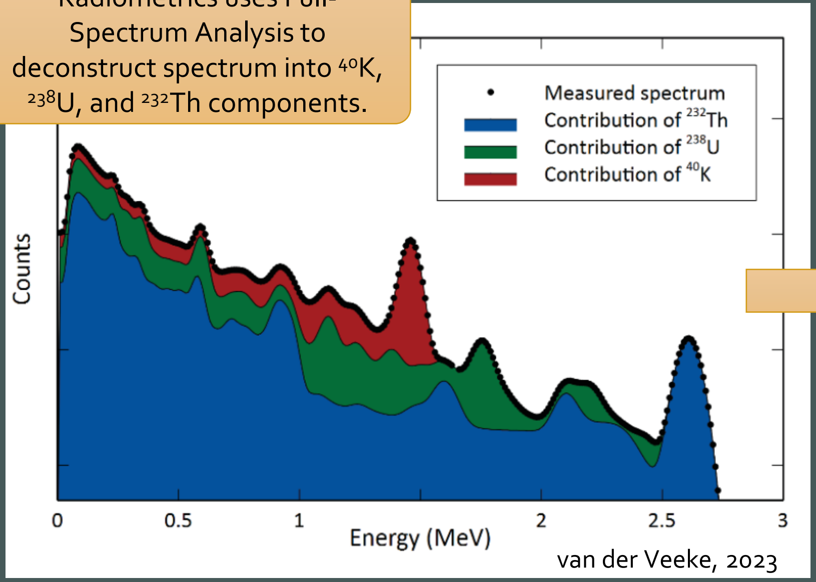
Target error: < $0.04\ cm^3\ cm^{-3}$ or 0.02 – 0.03 $g\ g^{-1}$ RMSE

Gamma-ray spectroscopy to Soil Water Content (SWC)

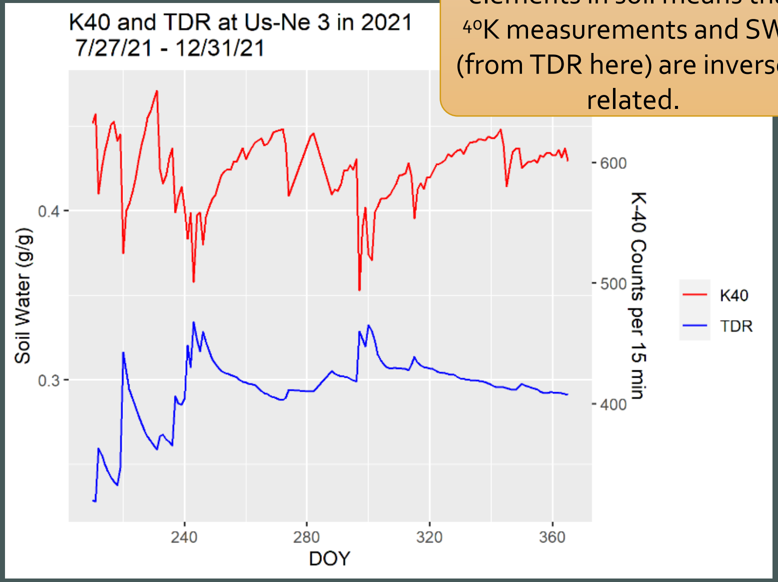
gSMS sensor from Medusa Radiometrics detects naturally emitted gamma radiation from the top ~35 cm with scintillation crystal.



Software from Medusa Radiometrics uses Full-Spectrum Analysis to deconstruct spectrum into ^{40}K, ^{238}U, and ^{232}Th components.



The high attenuating power of H^+ relative to all other elements in soil means that ^{40}K measurements and SWC (from TDR here) are inversely related.



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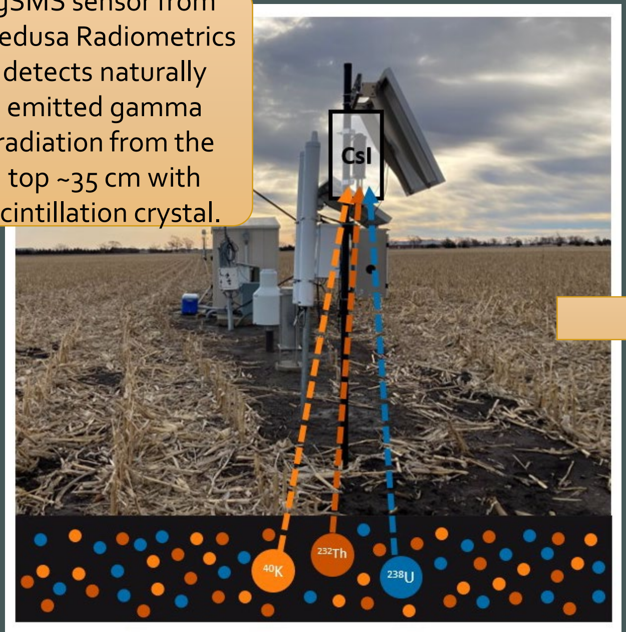

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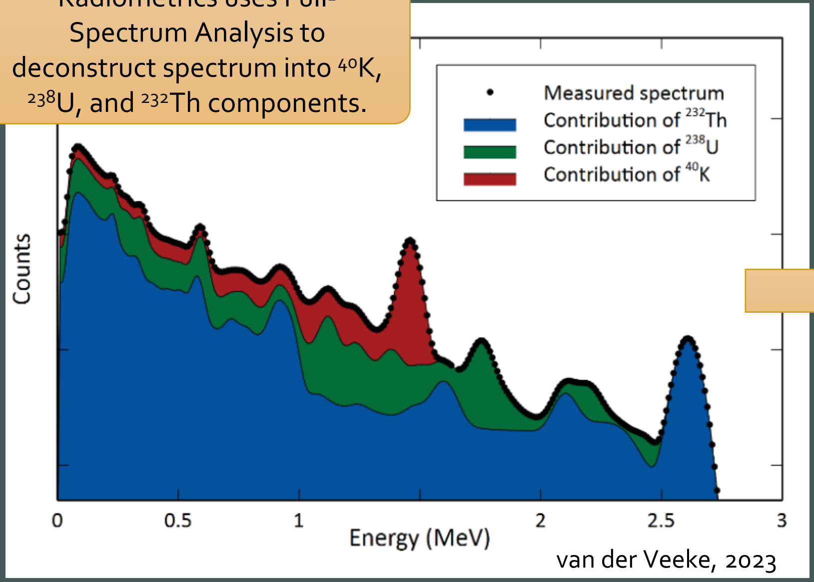

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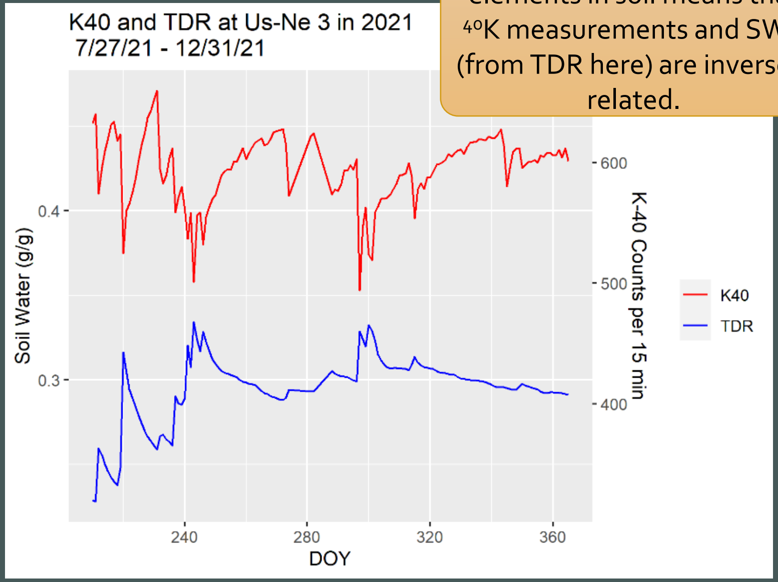


How do we estimate actual SWC from ^{40}K?

Theoretical equation exists, but with **limited field validation**

Correction for water in vegetation has been proposed, but only tested in a tomato field

"**Experimental proof under field conditions** (scattered radiation) **of attenuation coefficients** calculated from theoretical application of the Lambert–Beer law (collimated beam condition) **is still missing**." - Reinhardt and Herrmann, 2019

GOAL: Validate or **improve theoretical equation** and **offer insight on practical use** of the gSMS method using a robust empirical data set over a range of SWC and vegetation conditions.

Study area and sampling design

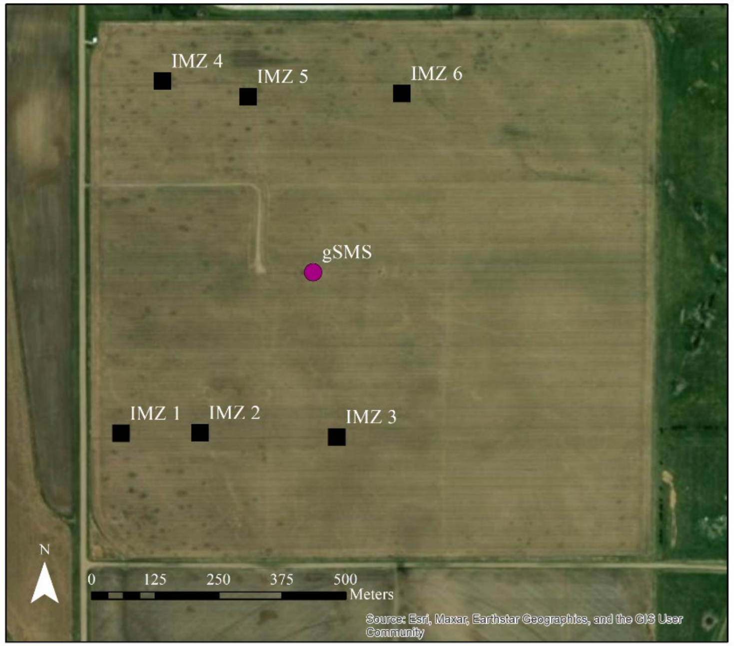


Figure 2. Locations of the gSMS and IMZ's in the field.

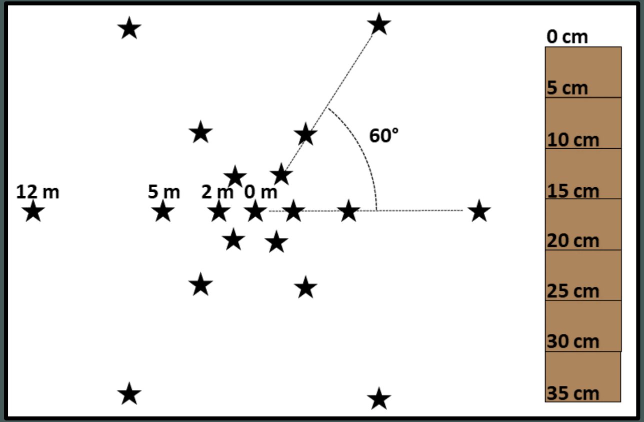


Figure 3. Sampling design for 19 profiles (★) within the gSMS footprint, which were sampled in 5 cm intervals down to 35 cm below the surface.

- Non-irrigated, no-till site in eastern Nebraska, United States
- Maize/soybean rotation, sandy clay loam
- Ameriflux and Long term agro-ecosystem research (LTAR) site
- 27 gravimetric water content samples between 5 Sept. 2021 and 23 Oct. 2023.
- 15-minute gSMS data processed to specific activity of ^{40}K and averaged over 4-hour periods
- Destructive biomass sampling from intensive measurement zones (IMZ's)
- 3 bulk density samples in 2023
- Chemical analysis for lattice water in 2023

Calibration Equation (in mass terms)

Total soil water ($\boldsymbol{\theta_{tot}}$) [g g^{-1}] $= \dfrac{\text{mass of water in } \textbf{pore space}, \text{ soil } \textbf{mineral structure}, \text{ and } \textbf{soil organic carbon}}{\text{mass of dry soil}}$

Pore space water (θ_g): gravimetric water content $\left(\text{Mass}_{\text{pore water}}/\text{Mass}_{\text{dry soil}}\right)$ [g g^{-1}]

Mineral structure or lattice water ($\theta_{lattice}$): water released between 105˚C and 1000˚C [g g^{-1}]

Soil organic carbon water (θ_{SOC}): molar equivalent of water in soil organic carbon [g g^{-1}]

$$\boldsymbol{\theta_{tot} = \left(\frac{I_0 * f(BWE)}{I_t} - 1\right)\frac{(\mu/\rho)_s}{(\mu/\rho)_w}} \qquad \textbf{(1)}$$

$\boldsymbol{I_0}$ = ^{40}K measurement in dry soil [Bq kg-1]

$\boldsymbol{I_t}$ = ^{40}K at measurement time [Bq kg-1]

$\boldsymbol{f(BWE)}$= a biomass correction factor in the form, $f(BWE) = (-0.0120 \pm 0.0001) * BWE + 1.0000$, where BWE is biomass water equivalence [mm] (the plant H_2O content expressed as a depth of water and estimated from drying and weighing destructive samples).

$\boldsymbol{(\mu/\rho)_s}$ = mass attenuation coefficient of soil (pure SiO_2) = 0.05257 cm^2 g^{-1} for 1.46MeV

$\boldsymbol{(\mu/\rho)_w}$ = mass attenuation coefficient of water = 0.05836 cm^2 g^{-1} for 1.46 MeV

Baldoncini et al., 2018; van der Veeke, 2023; Baldoncini et al., 2019

Dissatisfaction with the Calibration Equation

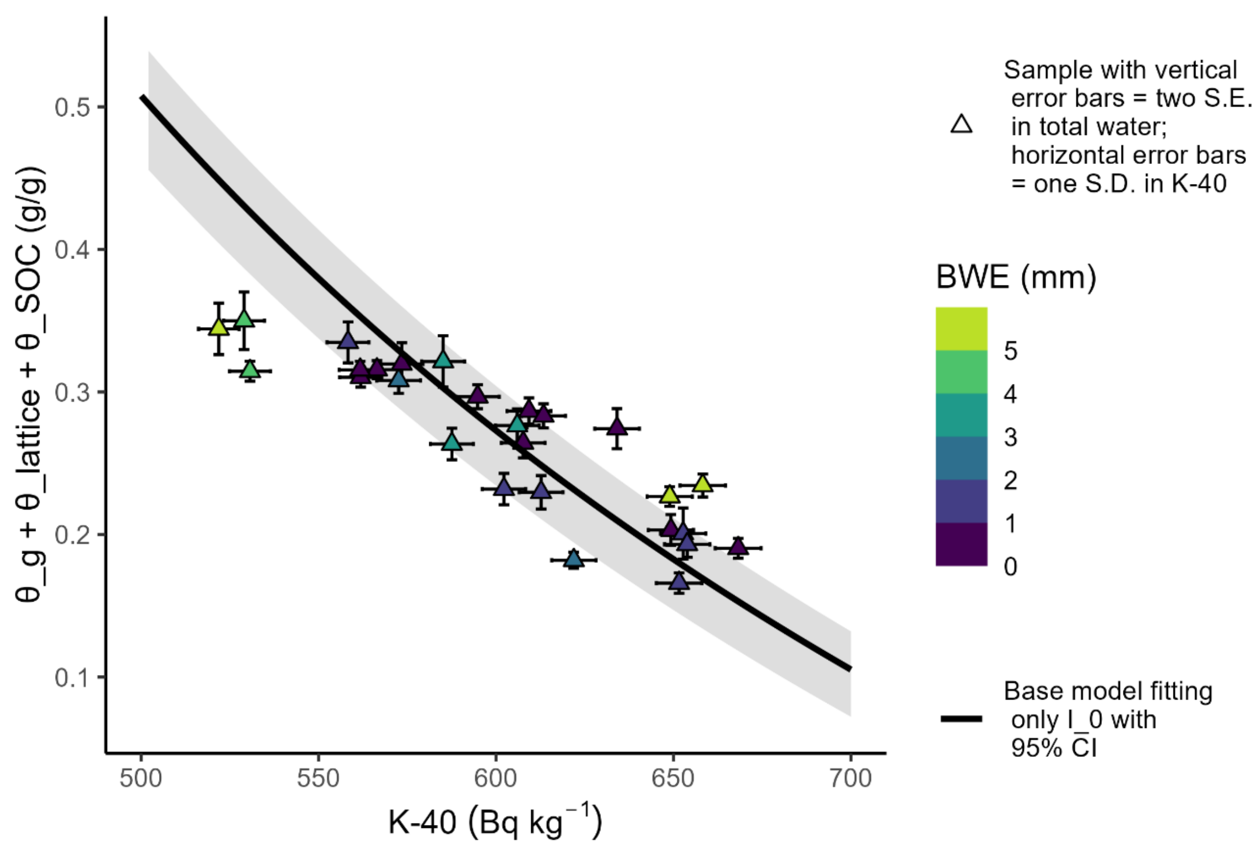
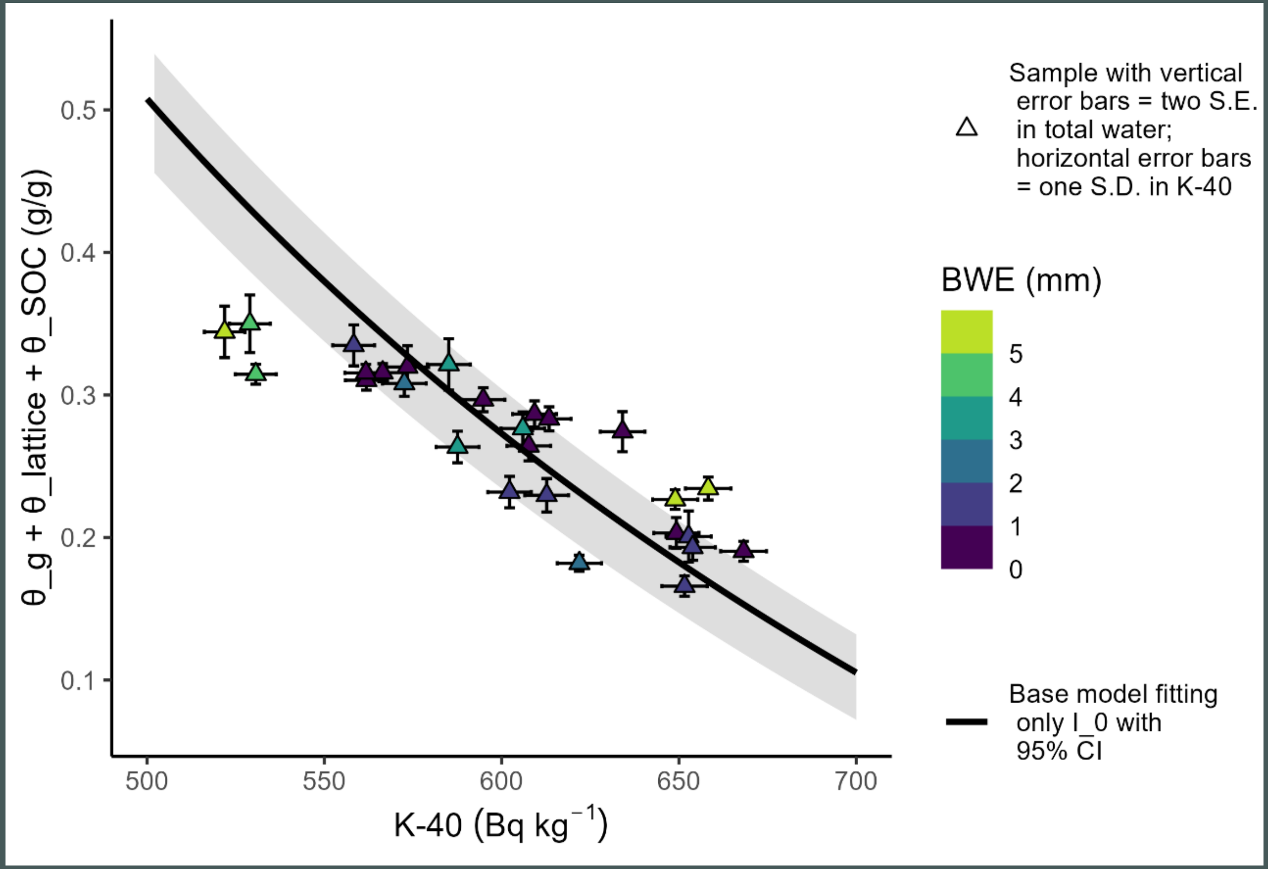


Figure 4. The experimental relationship between total water - the sum of gravimetric water content (θ_g), lattice water ($\theta_{lattice}$), and soil organic carbon (θ_{SOC}) - and ^{40}K compared to the relationship predicted by the calibration equation without a biomass correction (black line) and the corresponding 95% confidence interval.

Dissatisfaction with the Calibration Equation



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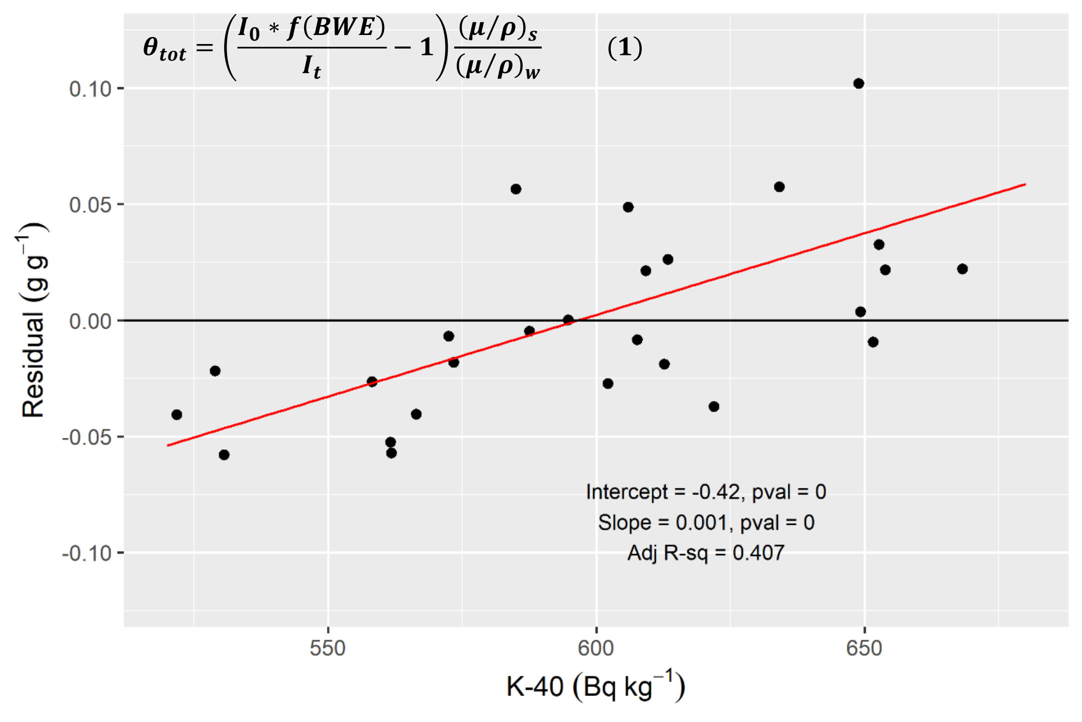


Figure 5. Residuals of the calibration equation with the biomass correction included and I_0 is fit to the data show a significant linear trend (p-value < 0.001) with respect to ^{40}K.

RMSE* *(g g⁻¹)	***R^2***	***Adj R^2***	***I_0* *(Bq kg⁻¹)***	***$(\mu/\rho)_s$* *(cm² g⁻¹)***	***$(\mu/\rho)_w$* *(cm² g⁻¹)***
0.046	0.258	0.157	793	0.0526	0.0584

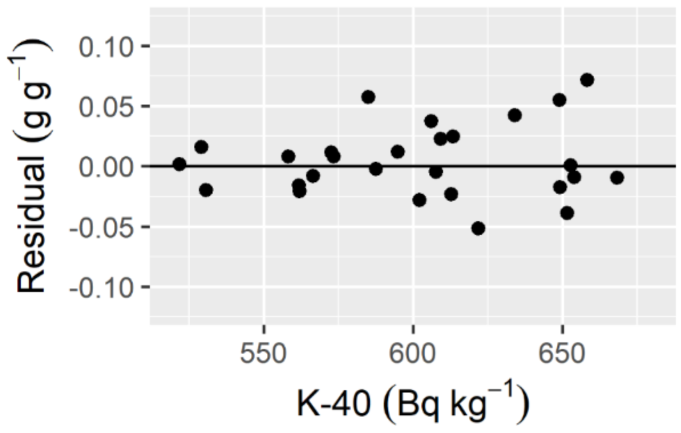
Adjust mass attenuation to eliminate trend in residuals

- Linear trend in the residuals can be eliminated by introducing a fitted parameter to create an "effective mass attenuation coefficient":

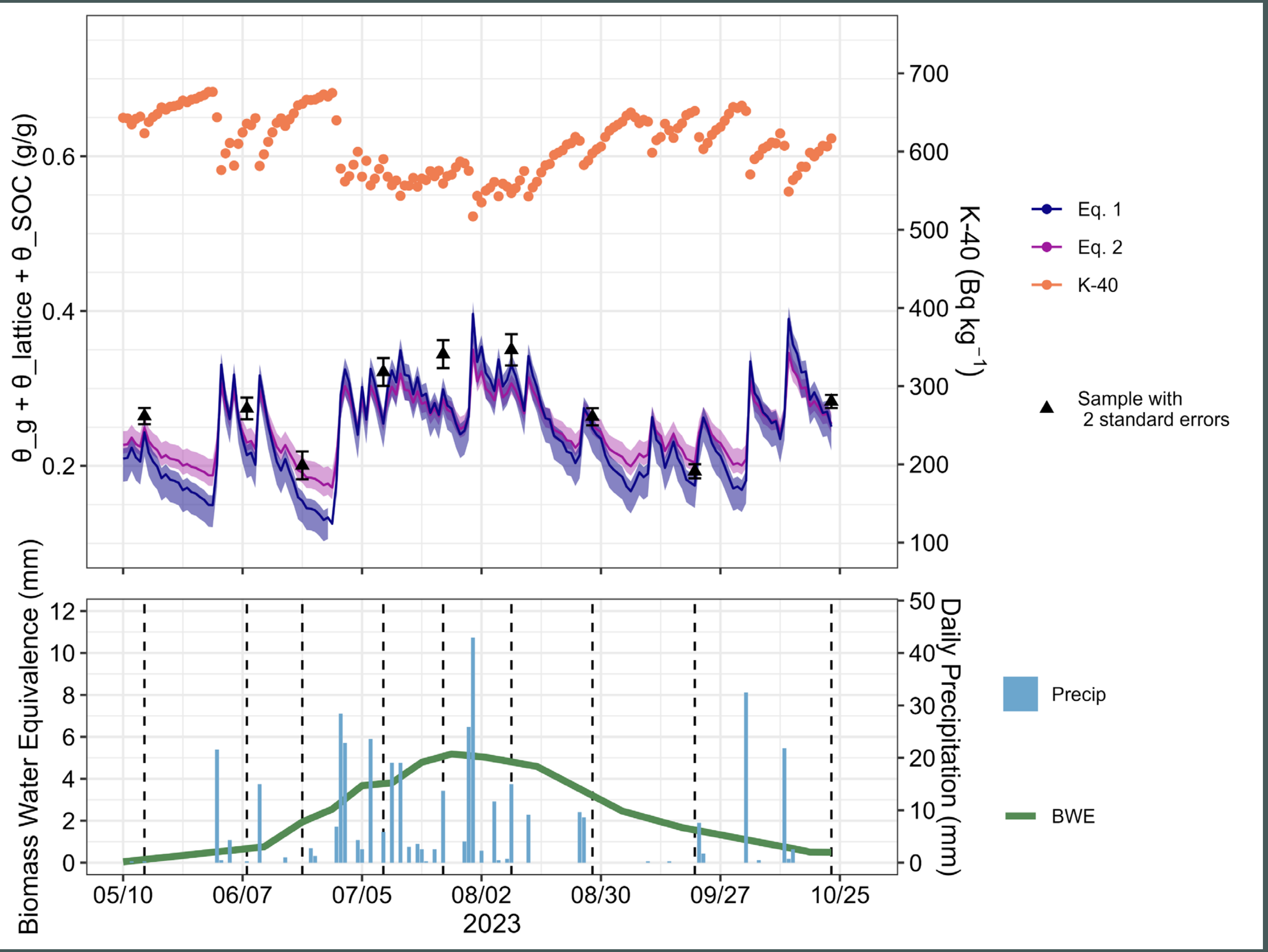
$$\theta_{tot} = \left(\frac{I_0 \cdot (-0.012 * BWE + 1)}{I_t} - 1\right)\frac{(\mu/\rho)_s}{(\mu/\rho)_w} * \boldsymbol{a} \quad (2)$$

Table 1. Results of model fitting using shuffled complex evolution algorithm (sceua function in the R package, rtop v. 0.6-6). Validation statistics are calculated using leave-one-out cross-validation. Parameters fit to the data are bolded and denoted with (*). The literature (SiO_2) value for $(\mu/\rho)_s$ = 0.05257 cm² g⁻¹, and the value for water is $(\mu/\rho)_w$ = 0.05836 cm² g⁻¹ at the ^{40}K peak energy.

RMSE (g g⁻¹)	R^2	Adj R^2	I_0 (Bq kg⁻¹)	$(\mu/\rho)_s$ (cm² g⁻¹)	$(\mu/\rho)_w$ (cm² g⁻¹)	a
0.032	0.640	0.550	**935***	0.0526	0.0584	**0.56***



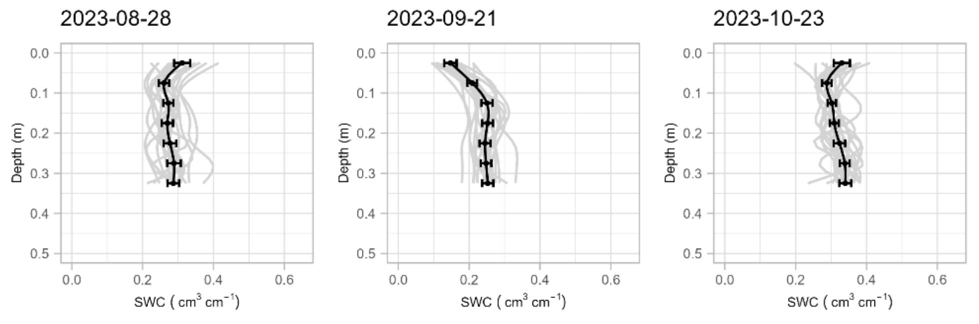
Visualize model performance



Eq. 1: $\theta_{tot} = \left(\frac{I_0 \cdot (-0.012 * BWE + 1)}{I_t} - 1 \right) \frac{(\mu/\rho)_s}{(\mu/\rho)_w}$

Eq. 2: $\theta_{tot} = \left(\frac{I_0 \cdot (-0.012 * BWE + 1)}{I_t} - 1 \right) \frac{(\mu/\rho)_s}{(\mu/\rho)_w} * a$

Typical soil moisture profiles sampled



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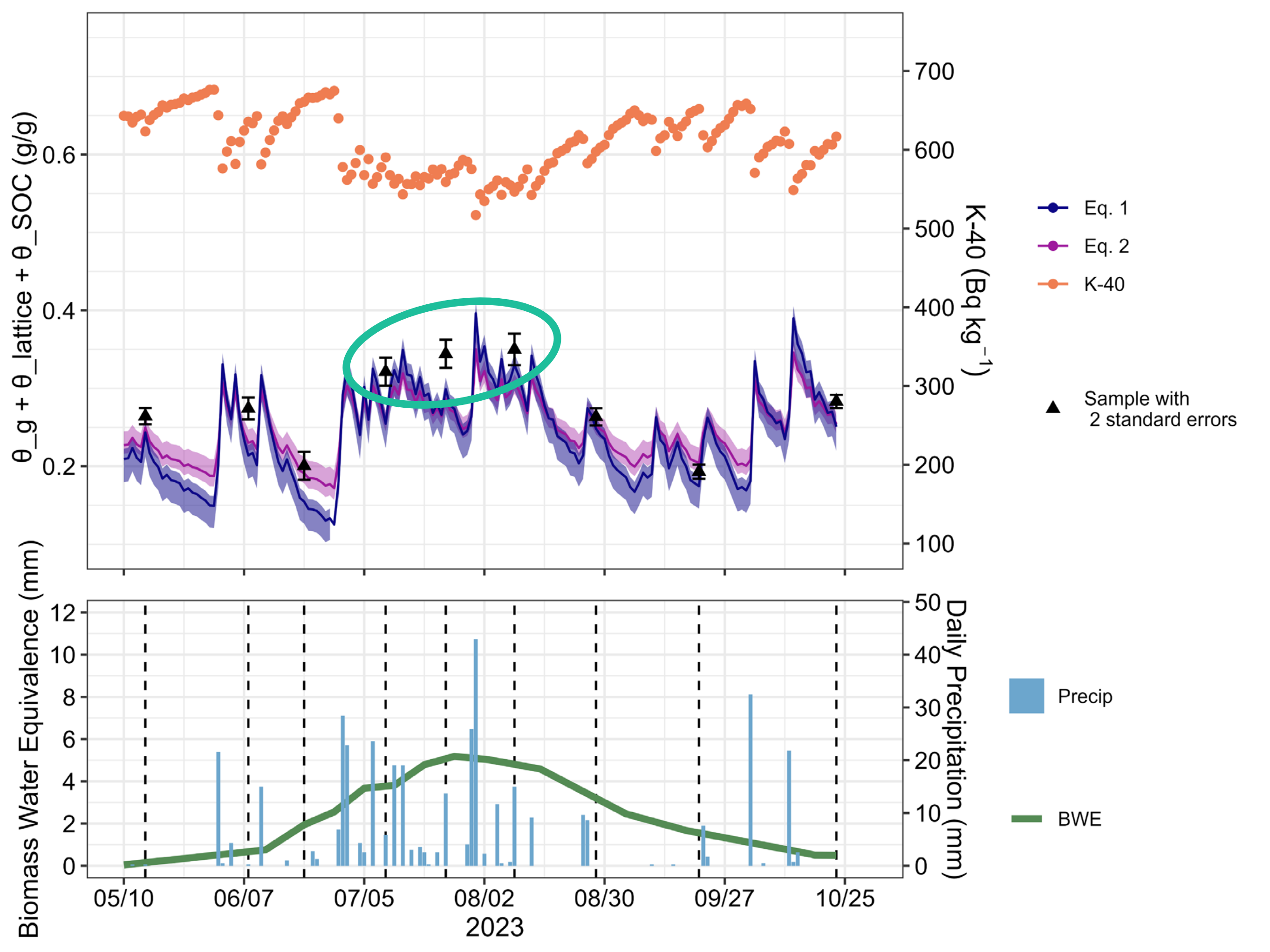

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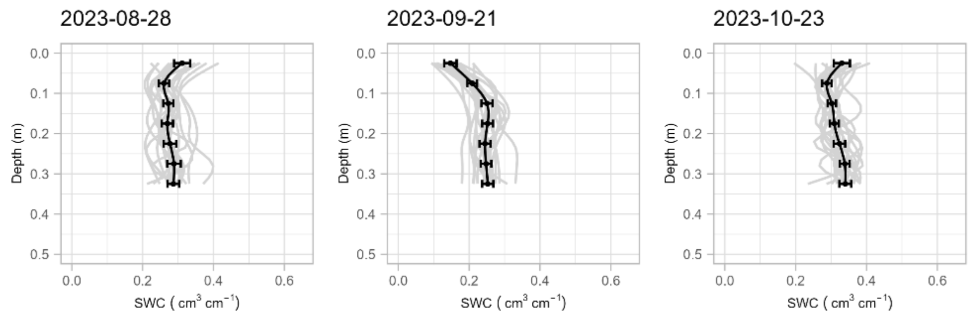
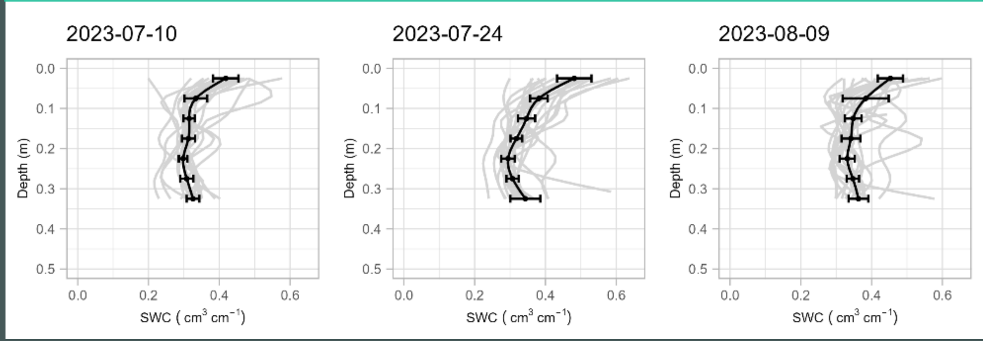


Samples collected within 4 hours of precipitation events. Even though calibration samples were depth weighted, an error persists.



What sample size is needed to fit the calibration equation?

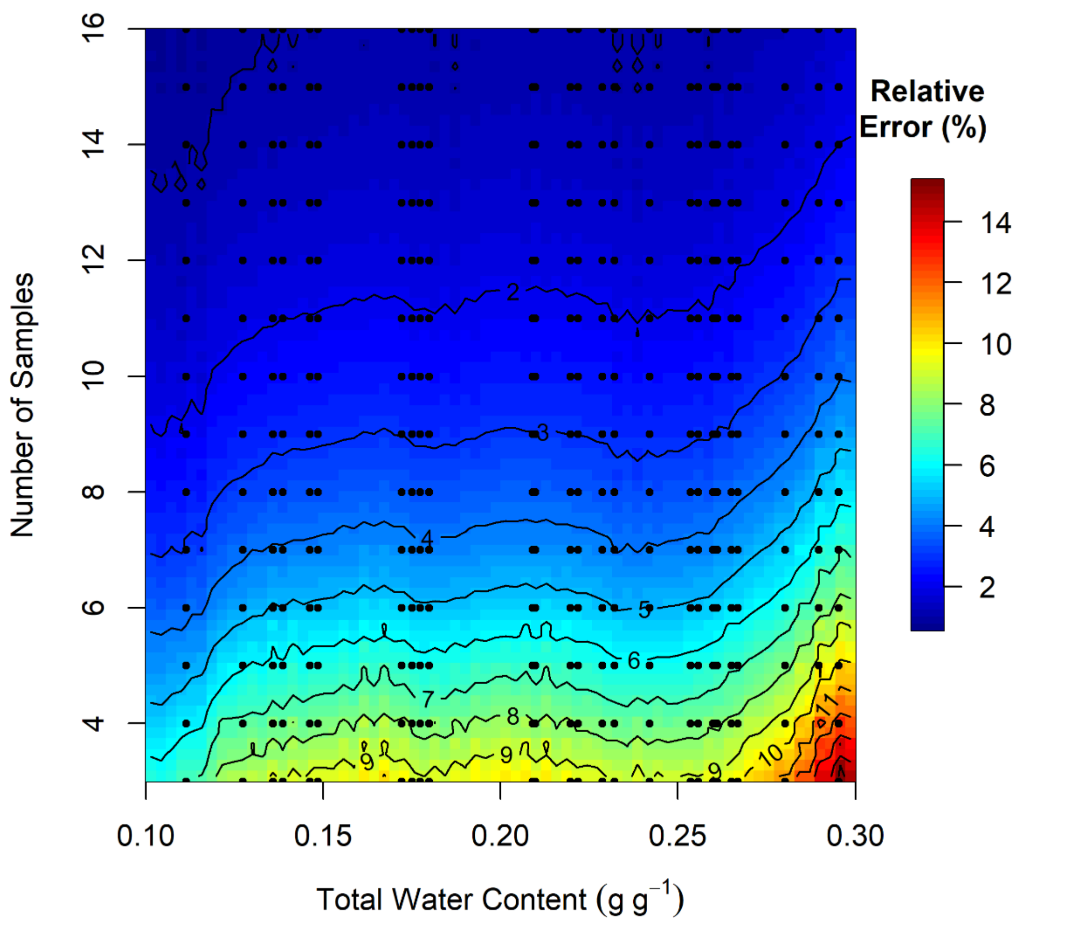


Figure 6. Relative error in total water content (θ_{tot}) calculated from the number of sample profiles indicated on the vertical axis compared to θ_{tot} calculated using all 19 sample profiles. The image was generated by smoothing and interpolating the sample relative error values shown by the black dots.

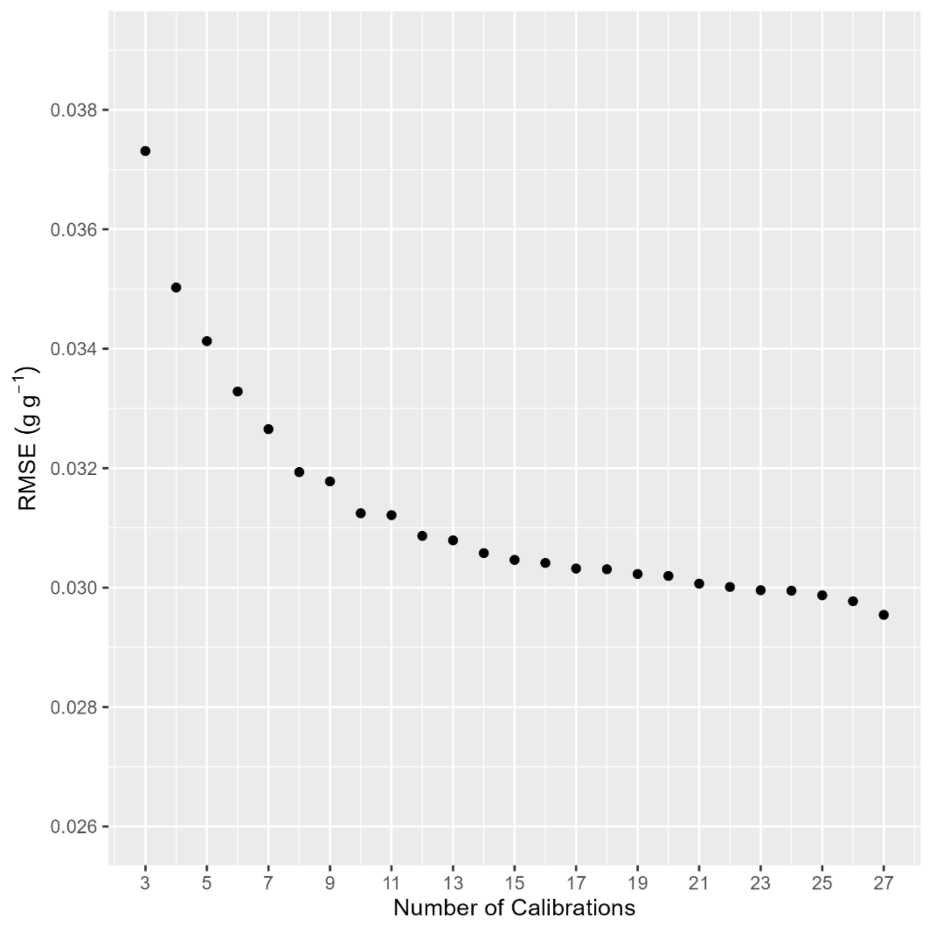


Figure 7. Root mean squared error (RMSE) in predicting total water content for all 27 samples, using an equation calibrated with the number of calibrations on the horizontal axis, using 10/19 profiles. Results are shown for Equation 2 (2 fitted parameters).

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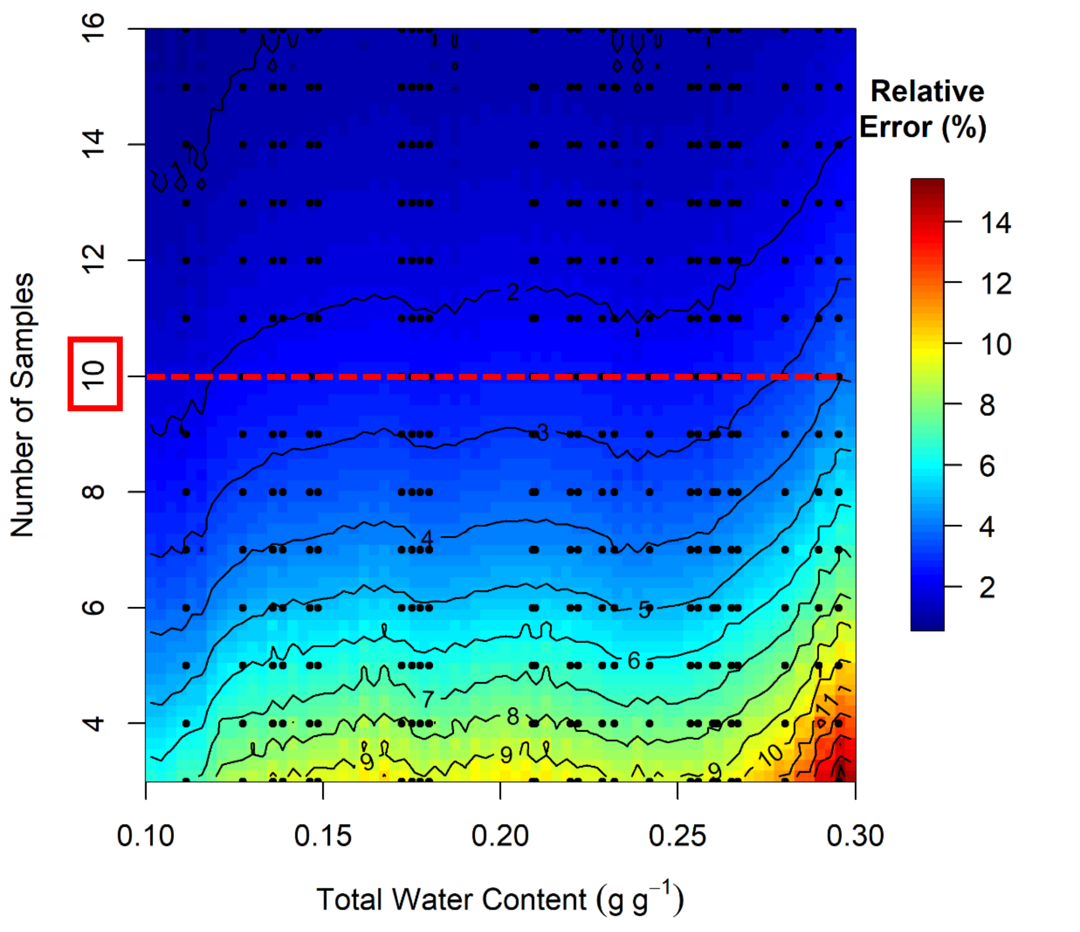

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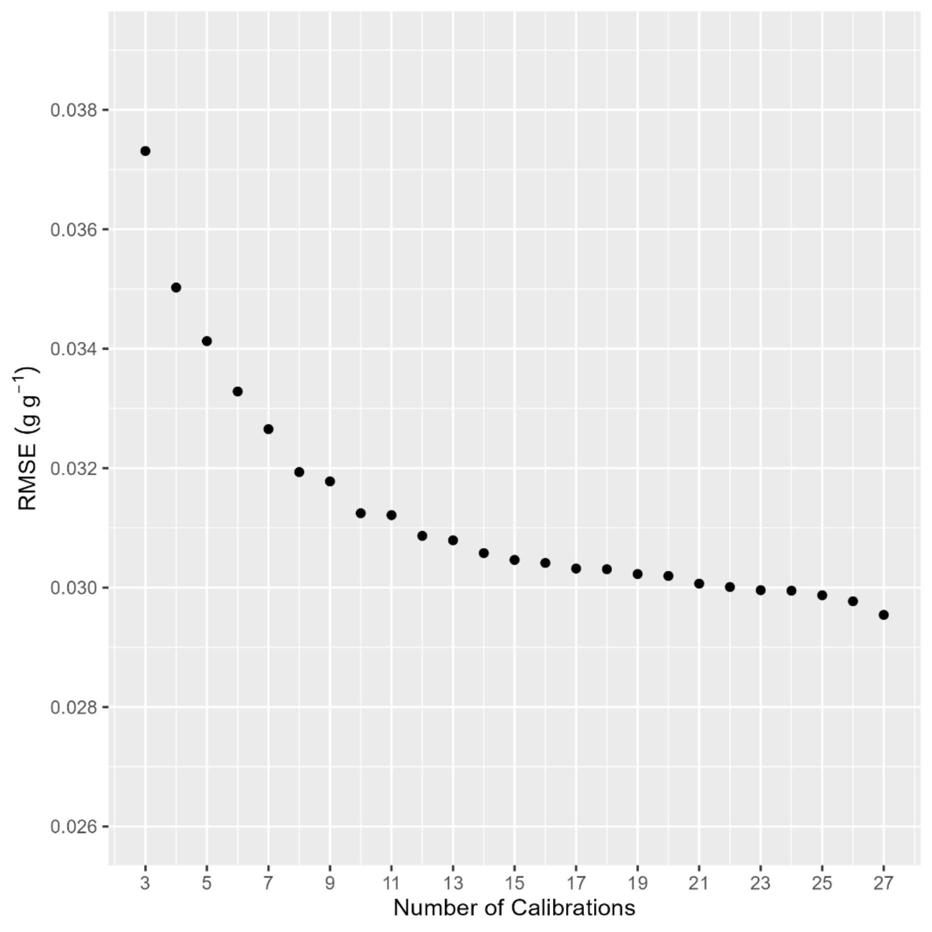

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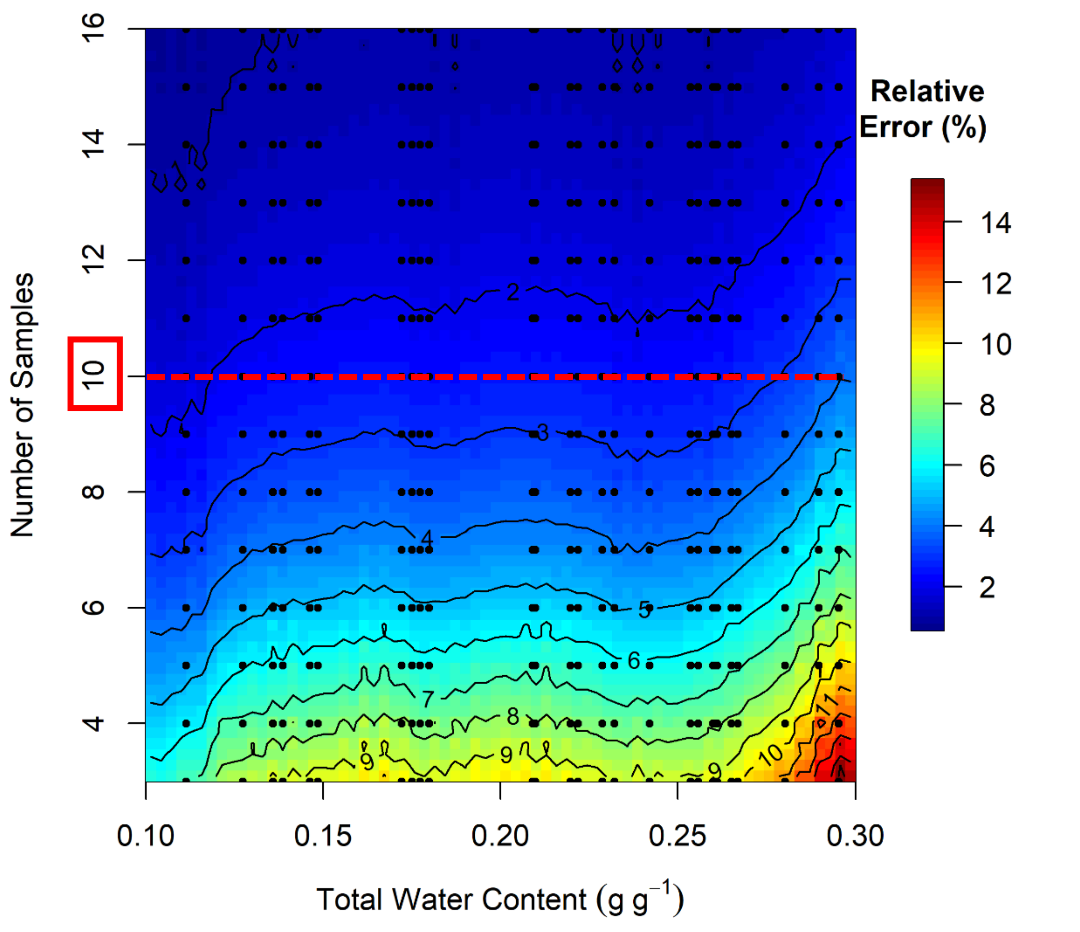

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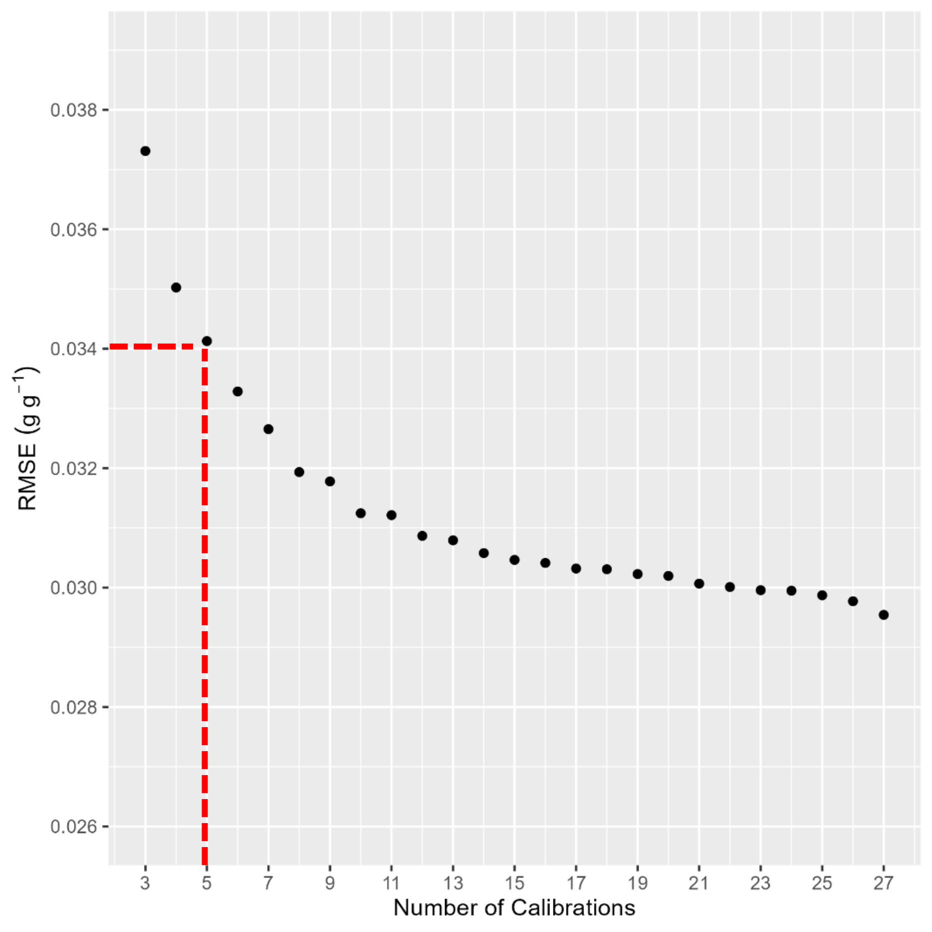

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Limitations and Strengths for the Future

- Limited to a single field site
  - Vegetation types beyond maize and soybean
  - Other soils
- The need for ~5 calibrations limits the method to dedicated research contexts
- Calibrating multiple parameters poses challenges to spatial mapping
- Physical substantiation for adjusting mass attenuation coefficients

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- gSMS accuracy ranks near other SWC methods (~ 0.03 g g^{-1})
- Same biomass water correction factor appears appropriate in tomato, maize, and soybean
- Small detectors and data processing software available
  - Cost similar to cosmic-ray neutron (~ $10K)
- Cosmic-ray Neutron research trajectory as a blueprint:
  - Parameter prediction based upon known site characteristics to reduce number of calibrations
  - Monte Carlo simulations for footprint size, heterogenous landscapes, biomass correction factors non-row crops

Takeaways

- Parameters $(\mu/\rho)_s$ and $(\mu/\rho)_w$ are important in quantifying θ_{tot} from ^{40}K
- Vegetation water correction factor is sufficient for maize and soybean at our field site.
- **Recommendations** for gSMS calibration based upon our field site:
  - ✓ 10 profiles in the gSMS footprint
  - ✓ 5 calibrations
  - ✓ Use a calibration equation that fits I_0 and mass attenuation
- **Future research** should aim to:

1) Improve physical understanding of gamma-ray attenuation under field conditions
2) Reduce number of calibrations required

Thank you!

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- Support provided by the Daugherty Water for Food Global Institute at the University of Nebraska.

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