Supplement of Atmos. Meas. Tech., 18, 2607–2618, 2025
https://doi.org/10.5194/amt-18-2607-2025-supplement

Atmospheric Measurement Techniques
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EGU

Supplement of

Simple water vapor sampling for stable isotope analysis using affordable valves and bags

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Supplement:

Table S1: Specifications of the gas sample bags used (18€ excl. VAT, https://www.samplebags.eu/product/multi-layer-foil-bags-single-stainless-steel-fitting/).

Specifications: Multi-Foil sampling bags	
Multi-Foil sample bag with protective 5-layer barrier:	
Layer	Material
1.	386.08 µm gauge nylon (outer layer)
2.	Metalized aluminum
3.	Polyethylene
4.	8.89 µm aluminum foil
5.	50.8 µm polyethylene (inner layer)
Additional Information:	
Total film thickness	0.10922 mm
Water vapor transmission rate (WVTR)	< 0.00465 g / m² / d
O_2 transmission rate (MOCON)	1.55 cm³ / m² / d
Tensile strength (ASTM D88283, A)	1.687368 kg / cm² 2.249824 kg / cm² (MD*) 1.827982 kg / cm² (CD**)
Breaking strength (GRABFED 191)	29.9371 kg 36.741 kg (MD*) 34.473 kg (CD**)
Bursting strength (FTMS 191C, 5122)	4.991797 kg / cm²
Puncture strength (FTMS 101C, 2065.1)	> 151.71 kPa
Maximum operating temperature	82 °C
Minimum operating temperature	-30 °C
Fittings	Stainless steel

* MD = machine direction ** CD = cross direction

Table S2: Differences during the storage experiment for M22 and L22 with all storage durations (Overall differences: M22: - 0.5 ‰ ± 0.5 for $\delta^{18}O$ and 0 ‰ ± 1.6 for $\delta^{2}H$; L22: - 0.1 ‰ ± 1.1 for $\delta^{18}O$ and 2.8 ‰ ± 4.9 for $\delta^{2}H$).

	M22		L22	
Storage duration [d]	$\delta^{18}O$ [‰]	$\delta^{2}H$ [‰]	$\delta^{18}O$ [‰]	$\delta^{2}H$ [‰]
1	– 0.5 ± 0.7	– 0.7 ± 1.3	– 0.9 ± 0.4	0.4 ± 2.6
3	– 0.7 ± 0.3	– 0.4 ± 1.6	0.1 ± 0.5	8.9 ± 2
7	– 0.3 ± 0.2	1 ± 1.7	1.1 ± 1.1	- 0.9 ± 1.9

Table S3: Z-scores during the storage experiment for M22 and L22 with all storage durations (Overall differences: M22: - 1.2 ‰ ± 1.2 for $\delta^{18}O$ and 0 ‰ ± 0.6 for $\delta^{2}H$; L22: 0.3 ‰ ± 2.7 for $\delta^{18}O$ and 1.4 ‰ ± 2.5 for $\delta^{2}H$).

	M22		L22	
Storage duration [d]	z-score $\delta^{18}O$	z-score $\delta^{2}H$	z-score $\delta^{18}O$	z-score $\delta^{2}H$
1	– 1.2 ± 1.8	– 0.3 ± 0.6	– 2.2 ± 0.9	0.2 ± 1.3
3	– 1.8 ± 0.7	– 0.2 ± 0.8	0.4 ± 1.3	4.4 ± 1
7	– 0.7 ± 0.5	– 0.5 ± 0.8	2.6 ± 2.8	- 0.5 ± 0.9

Figure S1:

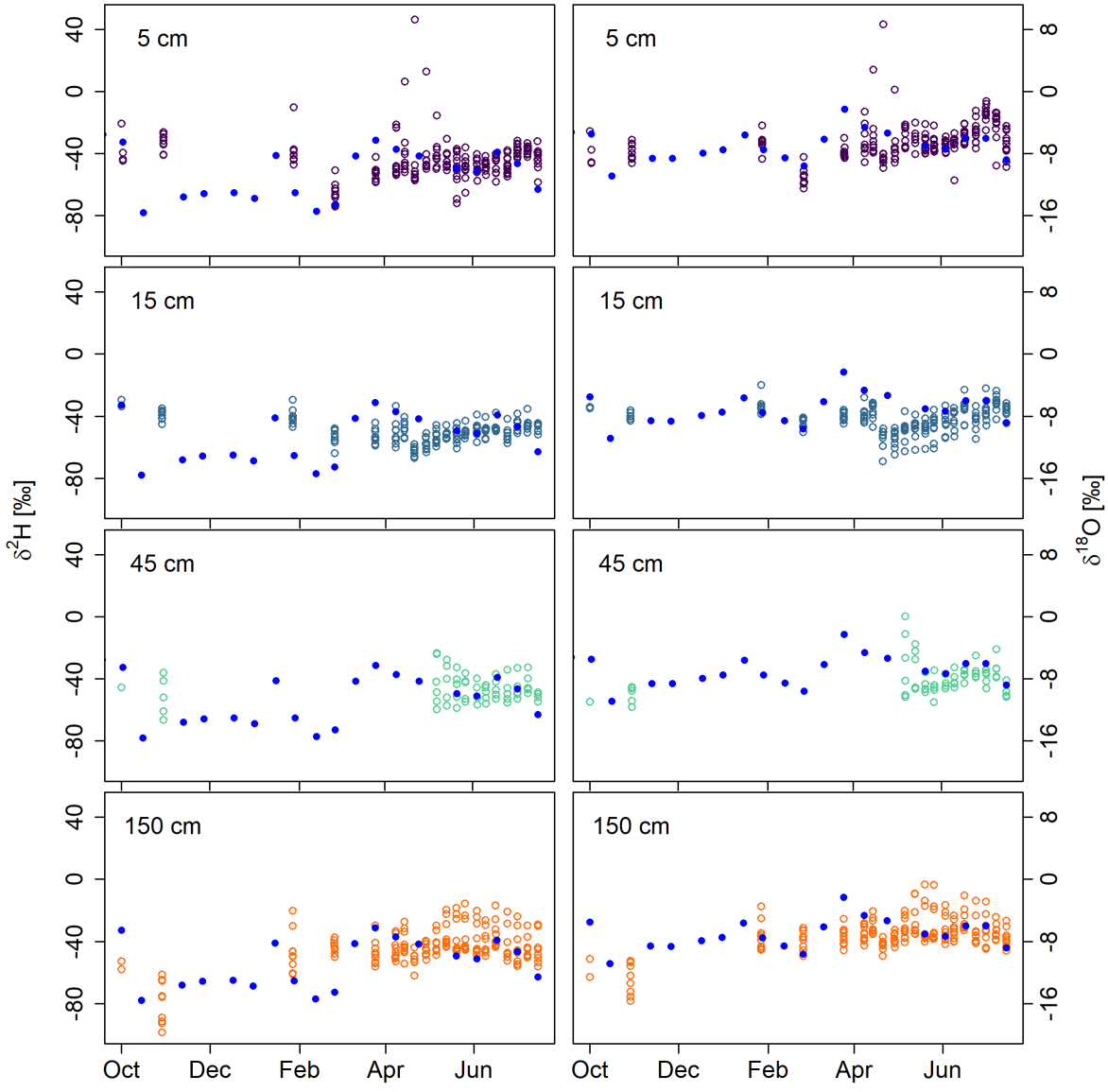

Figure S1: Field measurements using bags over an entire winter wheat growing season at four different depths and bulk precipitation samples of two weeks (blue).

Experiment S2: High isotope difference re-use test

To test the reusability of the gas bags for a wide range of isotopic samples, and thus different applications, another reusability test was performed with large isotopic differences. For this purpose: (a) an initial standard (L23) was filled into new gas bags and stored for one day and then measured, (b) the bags were flushed with dry air 10 times, (c) the opposite standard (H23) was filled into the bags and measured after one and three days.

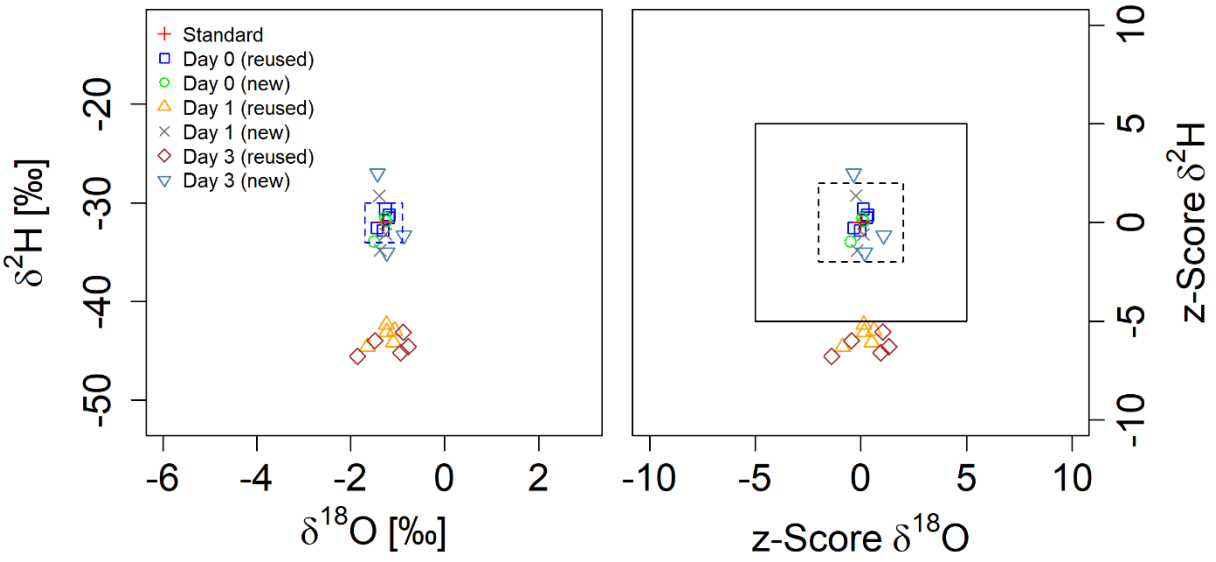

Figure S2: High isotope difference re-use test with L23 as the initial standard followed by H23. Sample bags were stored in the laboratory under stable conditions and measured after one and three days.

Since the isotopic range in the field reusability experiment was relatively narrow (< 20 ‰ for δ^2H between first and second sampling), we additionally performed a small experiment using two laboratory standards with higher differences in isotopic signatures (difference 76.2‰ in δ^2H): we stored our standard L23 in the bags for one day, rinsed them 10 times, and filled them with the opposite standard H23 (see Fig. S2). Directly after bag filling, results were unaffected for both $\delta^{18}O$ and δ^2H. While storing did not have an effect on the $\delta^{18}O$ signature a clear but consistent effect was visible after one day regarding δ^2H, which, contrary to the results of Herbstritt et al. (2023), did not increase over time (three days storage). Since this effect is stable over three days of storage and we know the previous sample signature, this effect may be correctable like the moist conditioning approach described by Herbstritt et al. (2023). Therefore, we recommend reusing bags according to the presented approach (10x rinsing and ideally similar samples for reused bags) only for natural abundance measurements.

Handling Recommendations:

Our measurements over an entire cultivation period provided many insights into the handling of the described gas bag approach:

- Regarding the described dry **air supply box**, the use should always be tested for the specific application, as a very high flow rate combined with very humid air could greatly affect the duration of possible use.
- Using the **gas bags**, the manufacturer states that the valves should not be opened more than one turn (Sense Trading B.V., personal communication, 2024). However, our experience has shown that a quarter to half opening is already sufficient to fill the gas bags reliably. If the gas bags are opened too wide, leaks may occur, and the sample may be contaminated. In addition, great care must be taken not to fill the bags more than 90% to avoid material damage (as specified by the manufacturer). On the other hand, a larger sample is recommended to reduce any effect on the sample.
- When using the **bags in the field**, it is necessary to record the source temperature at the corresponding depth during the measurement to be able to convert the isotopic signature of the soil water from vapor to liquid. In addition, it should be ensured that there is no liquid water in the soil probes, e.g. by flushing with dry air beforehand. Furthermore, it is advantageous to fill the bags in a protected box to avoid large temperature differences in the bag during filling (e.g. due to solar radiation in summer) and reduce the risk of damage to the gas bag, e.g. from sharp plant parts. The same applies to transport.
- When **reusing the bags**, it was important that 1) the bags were rinsed ten times with dry air, 2) the additional connection including valve was built and 3) the bags and their valves (especially the seals) were regularly checked for damage.
- The **subsequent measurement in the laboratory** was easy to perform, but the combination of the vapor storage method with in situ probes following the approaches of Rothfuss et al. (2013) or Marshall et al. (2020) requires that the temperature in the laboratory is higher than the source temperature during the measurement. Otherwise, condensation will occur in the bag, which can greatly distort the measurement result.