Supplement 1: Summary of *in situ* investigations of soil water depth-profiles, bulk soil water isotopes, xylem water isotopes and transpired water isotopes (arranged by these four groups, within groups chronological order)

Author	*Environment / Location*	*Measured compartment*	*Method*	*Findings/ Recommendations Advantages (+) /Disadvantages (-)*
(Herbstritt et al., 2012)	Laboratory	Liquid water Soil column	• Material: gas permeable membrane (PP) • Soil type: sand • Push-through system, flow rate 200 ml/min with excess line, equilibrated with pure N_2 • Calibration: - liquid water standards injected - compared to vapor standards - correction for water vapor concentration - determination of fractionation factors - application in soil column experiment	• Fit equilibrium fractionation factors for each system (membrane effects) • Vapor concentration and temperature are highly correlated − Matric effects might have caused deviation of fractionation factors, not membrane effects + Temporal resolution of less than 1 min. for liquid water samples
(Soderberg et al., 2012)	Semiarid, Kenya	Soil water isotope depth-profiles	• Material: gas permeable membrane (Teflon) with open ending, packed with glass wool • Soil type: sandy loam • Pull-only system with additional dilution of 400 ml/min, diluted with ambient air • Calibration/Validation: No information provided	• Include soil water potential into Craig-Gordon model for soils + Includes modelling of results − Glass wool might fractionate − Condensation issue not addressed − Dilution with non-dried ambient air
(Volkmann and Weiler, 2014)	Humid (southwest Germany)	Soil water isotope depth-profiles Evolution of evaporation front	• Material: gas permeable membrane (PE) with mixing chamber • Soil type: clayey silt • Both push-trough (flow rate not specified) and pull-only (30-35 ml/min) systems used, dilution with pure N_2 • Calibration: - boxes filled with soil and equipped with gas probes, water content, EC, temperature, soil water potential sensors - isotope standards added to water content of 20 vol.-% - linear two-point calibration & quality control standard - correction for vapor-concentration dependence - liquid–vapor equilibrium after Majoube (1971) - normalization to VSMOW and drift correction • Validation: depth profiles using cryogenic vacuum extraction	• First successful field study and comprehensive investigation of *in situ* soil water isotopes + Very flexible system + Both stationary and mobile use + Both push-through and pull-only methods tested + Control of condensation via dilution directly in probe − Complex system − Expensive probes
(Rothfuss et al., 2015, 2013)	Laboratory	Soil water isotopes	• Material: gas permeable membrane (PP) • Soil type: fine sand • Push-trough system with excess tube; dry synthetic air flow of 25 ml/min at inlet, dilution with dry synthetic air after passage through soil • Calibration: - three standards prepared, added to dried soil and measured over a range of temperatures (8°C - 24°C) - constant water vapor concentration via dilution with dry synthetic air - drift correction and check for material changes of the soil gas probe • Validation: comparison to theoretically calculated vapor values	• Potential isotope-effects introduced via gas permeable probe (difference of theoretical and observed values for δ^2H_{vap}) • Uncertainties when using CG-model • Gas-permeable membranes can resolve rapid changes of isotope values + Linear correction for non-reached isotopic equilibrium + Water vapor concentration kept constant + Checked for equilibrium conditions − Test limited to laboratory conditions − Isotopic equilibrium not reached

(Gangi et al., 2015)	Laboratory	Soil water and carbon dioxide $\delta^{18}O$	• Material: gas permeable membrane (PP) • Soil type: fine sand • Push-trough system with excess tube; dry synthetic air flow of 85 ml/min at inlet, dilution with dry synthetic air after passage through soil • Validation: comparison to theoretically calculated and modelled values	• No fractionation due to tubing for δ18O • Combined measurements of oxygen isotopologues in soils and atmospheric carbon dioxide + modelling involved (MuSICA) − No field testing
(Gaj et al., 2016)	Semi-arid (Namibia)	Soil water isotope depth-profiles Evolution of evaporation front	• Material: gas permeable membrane (PP) • Soil type: medium sand • Pull-only at 95 to 110 ml/min, pre-flushing of probes using dry air; system changeable to push-through • Calibration: - four standards prepared in oven-dried soil material; 5 ml of standard solution added - drift and memory correction, quality control - conversion of the corrected vapor to respective liquid water isotopic compositions • Validation: depth profiles using cryogenic vacuum extraction	• First successful *in situ* study in semi-arid environment • Recommendations: - Organic contamination should be investigated further - Increase probe length under dry conditions - Use heating/dilution to avoid condensation - Further development of calibration strategies for clay-rich soils. + calibration in soil media + water vapor concentration controlled by sampling time + calculated influence radius for pull-only method and air volumes sampled − Not corrected for water vapor concentration − Strong deviations in upper soil layer
(Pratt et al., 2016)	Humid (Canada)	Waste rock mining site unsaturated zone isotopes	• Material: HDPE tubes with 50-mm stainless steel mesh filter • Soil type: coarse textured sand tailings dyke • Pull-only, 30 ml/min, no dilution or flushing • Calibration: - 10ml of liquid water standards added to Ziploc bag - correction for water vapor concentration - conversion of the corrected vapor to respective liquid water isotopic compositions • Validation: comparison to bag equilibration method	• Direct *in situ* measurement of natural, water stable isotope profiles thick unsaturated mine waste is challenging • Bag equilibration as alternative • General agreement to samples collected in equilibration bags for some depths − Strong deviations in most depths
(Oerter et al., 2019, 2017; Oerter and Bowen, 2017, 2019)	Desert/Arid (Utah, United States)	Soil water isotope depth-profiles	• Material: gas permeable membrane (PP) • Soil type: coarse textured sand tailings dyke • Push-trough system with excess tube; dry N_2 for flushing and dilution; flow of 60 ml/min; dilution flow of 20 ml/min • Calibration: - oven dried (105°C for >12 h) soil material at 7%, 18%, 26% GWC (g water g^{-1} soil), n = 18 calibration standards (3 soil depth groups (7% to 11% clay content) × 3 GWC contents × 2 water types) - multi-linear regression for one-step correction of water isotope data derived from standards, variables used: clay content, water content, water vapor isotope value - CO_2 spectral interference correction • Validation: depth profiles using cryogenic vacuum extraction and bag equilibration	• Throughput rates greater than $7h^{-1}$ • Accuracy of the method to be equivalent to direct headspace equilibration and vacuum extraction techniques • measurement duration of ~5 min is typically sufficient to achieve >2 min of stable H_2O and δ^2H and $\delta^{18}O$ measurements • Most complete approach in terms of calibration and setup + water vapor concentration kept constant (20.000 ppm) + calibration carried out in same media as measured (=soil) + one-step calibration with different soil types and water contents; calibration can easily be extended to more variables

				- Effect of changing environmental conditions (temperature) not addressed, issue of condensation not addressed at all
(Kühnhammer et al., 2019)	Laboratory	Water isotopes across soil column and in plant transpiration	• Material: gas permeable membrane (PP) and throughflow plant chamber • Soil type: silt loam • Plant species: *Centaurea jacea* (herbaceous) • Push-trough system with excess tube; dry synthetic air flow of 50 ml/min at inlet, dilution with dry synthetic air • Calibration: - two soil standards with gas permeable membranes integrated into automated system - calibration equation developed by Rothfuss et al (2013), drift correction, correction for effect of wvmr • Validation: - comparison of calculated liquid values with water added to soil column - agreement between soil and transpiration isotope values in dual isotope space - comparison root water uptake profiles and changes in soil water content	• Data set of 48 days monitoring isotopic changes in soil and plant water uptake + error propagation to estimate realistic value for measurement precision + combined continuous *in situ* measurement across soil profile and in plant transpiration + check for isotopic steady-state in plant transpiration + root water uptake modelling including additional parameters − No check for isotopic equilibrium in soil measurements − Not easily transferable to the field
Dubbert et al., 2013	Semi-arid (Portugal)	Evaporation bulk water isotopes	• Material: Custom build soil chamber • Soil type: loamy sand • Open gas exchange system following the design of Pape et al. (2009) • Calibration: - liquid injection of 3 standards - water vapor concentration dependency from 5000-30000 ppmv considered	• First data set observing soil evaporation *in situ* under field conditions • Sensitivity analysis of the Craig and Gordon model for input parameters • Different conditions monitored (bare soil, root ingrowth, vegetated soil) • High impact of vegetation cover and root ingrowth on isotopic signature of soil evaporation
Quade et al. 2018	Laboratory	Evaporation bulk water isotopes	• Material: Custom build soil chamber • Soil type: silty loam • Keeling plot approach • Calibration: - Vapor equilibration standards in the same soil as the experimental column	• Evaluating temporal dynamics of the kinetic fractionation factor • αK values within the range reported in the literature • prevalence of turbulent water vapor transport under water-saturated soil conditions and at soil water content significantly lower than saturation
(Volkmann et al., 2016)	Humid (Southern Germany	Xylem water isotopes	• Material: gas permeable membrane (PE) with mixing chamber • Plant species: deciduous maple trees (*Acer campestre L.*; 9m tall, 0.2m in diameter at breast height and 30m^2 of crown projected area) • Mixed system; dry N_2 provided in throughflow line, set at the flow rate induced by laser spectrometer (30-35 ml/min); dilution with N_2 directly in probe; pre-flushing of system for 120s • Calibration: - three standards, headspace measured; conversion of xylem vapor values using Majoube equation and measured temperatures in tree • Validation:	• First study of *in situ* measured xylem water isotopes • *In situ* monitoring of xylem water isotopes is feasible, but complicated • Good precision and repeatability, but accuracy needs to be improved • Longer-term study needed • Issue of organic contamination needs to be addressed + Condensation avoided via dilution directly in probe − No check if equilibration conditions were reached in probe − Partially large discrepancies between extracted values and in situ measured data − Complicated

			- comparison with vacuum-extracted xylem cores measured with IRMS	
(Marshall et al.)	Greenhouse	Xylem water isotopes	• Material: hole drilled through the stem of a tree, Swagelok connections on both sides (airtight); flush with acetone to avoid pitch and resin production • Plant species: Pine trees (*Pinus sylvestris* L. and *Pinus pinea* L.); first experiment: cut-stem tree; second experiment: intact-root experiment • First experiment: pull-only with ~35-40 ml/min and flush of system manually when needed; second experiment: push-through with 80 ml/min of dry air (diving air), 5min pre-flush and 15 min measurement time • Calibration: - four standards, headspace measured; conversion of xylem vapor values using Majoube equation and measured temperatures in tree • Validation: - comparison to source water isotope values	• Novel approach for measuring xylem water isotopes • Method requires testing for different tree species and under different environmental conditions + *In situ* monitoring of xylem water isotopes of natural abundances is possible + No gas-permeable membranes are required + No influence of organic contamination observed + fundamental aspects of *in situ* studies thoroughly evaluated by modelling − Systems needs to be simplified − possibility of liquid water reaching water vapor analyser if tree shows strong defence mechanism or 'backflow' of water occurs
Wang et al., 2013	Great Plains, Oklahoma, USA	Evaporation bulk water isotopes Transpiration water isotopes Evapotranspiration water isotopes	• Material: modified commercial soil chamber, commercial plant chamber, custom build ET chamber • Soil type: not provided • Plant species: *Bromus arvensis L., Vicia sativa L., Solanum carolinense L., Euphorbia dentata Michx., Tridens flavus (L.) Hitchc.* • Keeling plot approach • Calibration: Liquid injections	• Testing chamber based bare soil observations vs modelled by Craig and Gordon model and impact on ET partitioning • Difference between approaches on T/ET • Demonstrate necessity for uniform partitioning approach
(Wang et al., 2012)	Laboratory, arid (Kenia)	Transpiration water isotopes	• Material: custom build transpiration chamber, OA-ICOS • Plant species: *Spathiphyllum spp*, *Acacia spec.* • Open gas exchange system • Calibration: - verification of set up using a dew point generator - liquid injections to calibrate the laser spectrometer	• First publication of in-situ transpiration measurements + Observation of transit from non-steady state to isotopic steady state − Limited data set − Complex set up
(Simonin et al., 2013)	laboratory	Transpiration water isotopes	• Material: fully automated leaf gas exchange system (MPH1000, Licor 7600); Laser spectrometry • Plant species: Citrus, Tobacco • Open gas exchange system • Calibration: - Liquid water standards injected spanning the observed isotopic range - Concentration dependencies 3000-24000 ppmv	• Exposed leaves to changes in environmental conditions • Non-steady state effects dominate transpiration of both species • Even when leaves are already physiologically transpiring in steady state + Evaluated the rate of change in leaf water, determined leaf water turn-over time
(Dubbert et al., 2014)	Semi-arid (central Portugal)	Transpiration water isotopes	• Material: Custom build branch chamber, Laser spectrometer • Plant species: cork oak (*Quercus suber L.*) • Open gas exchange system • Calibration: - liquid injection of 3 standards - concentration dependency from 5000-30000 ppmv	• Diurnal courses of isotopic signatures of transpiration during different seasons • Dominance of non-steady state effects • Sensitivity analysis of the Craig and Gordon/Dongmann based model
(Song et al., 2015)	Laboratory	Transpiration water isotopes	• Material: Fully automated leaf gas exchange system (Licor 7600), Laser spectrometer	• Adapting existing non-steady state leaf water model to cuvettes, where delta atm is influenced by delta T

			• Plant species: Cotton • Calibration: - liquid injection, following Simonin et al., 2013	