Stable water isotopes in landscapes: big data & ML opportunities to respond to current challenges on water resources under environmental change

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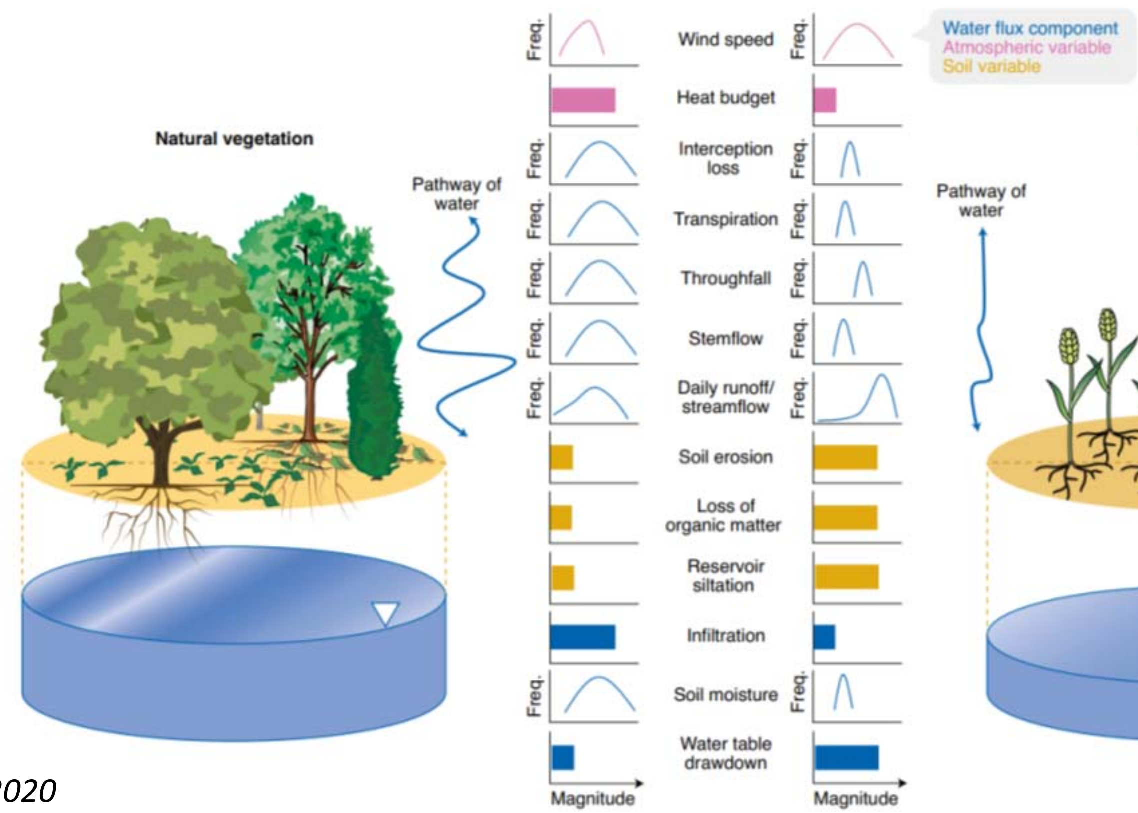
Northern Rivers Institute

Challenges of environmental change on water resources

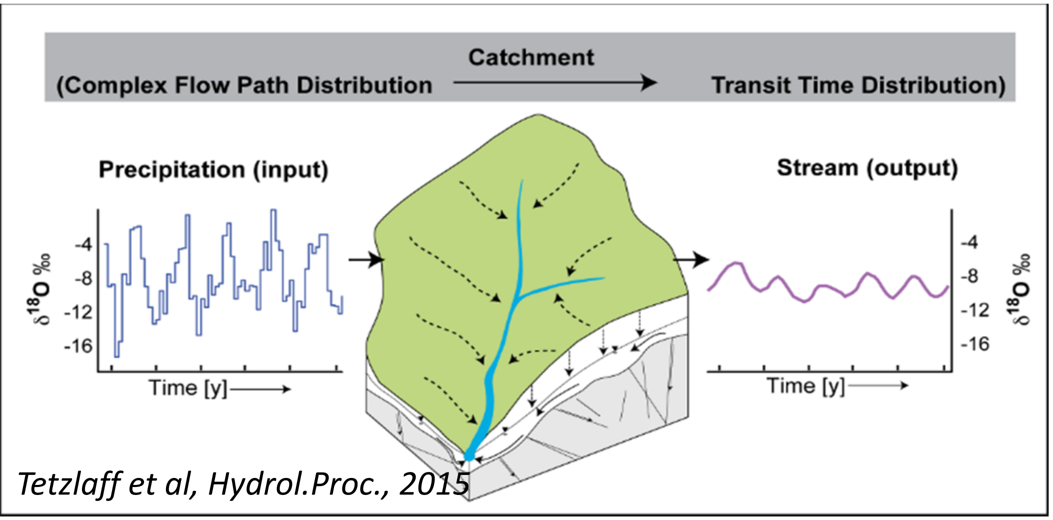
- Climate extremes: heavy rain events and droughts
- Landuse changes: intensification, deforestation, hydropower
- “Homogenization in the water cycle”: Changes in water balance
- Water security
- Water pollution

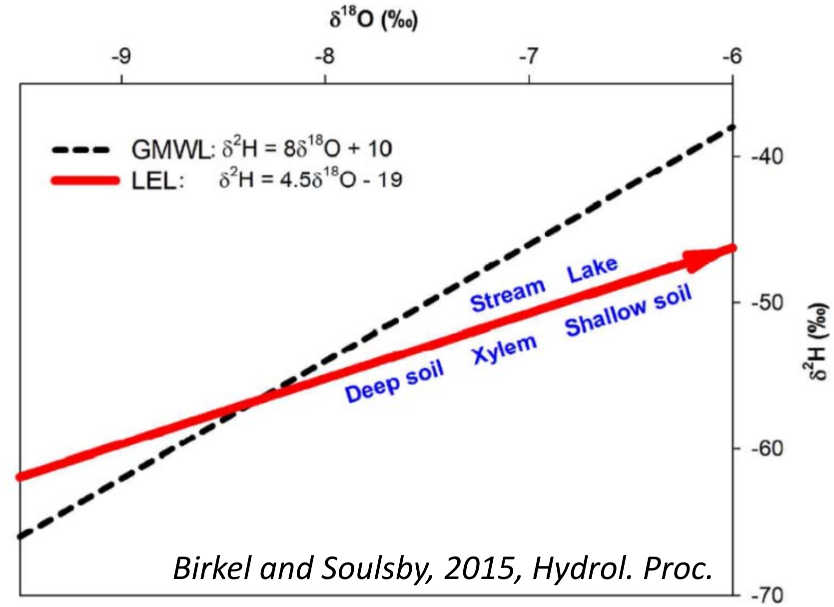


Levia et al., Nature Geoscience, 2020

Utility of water isotopes in catchment hydrology

Input-output relationships to quantify ages





Damping reflects amount of stored water in soils & groundwater that is **mixing** with incoming water

Evaporation and **fractionation**: Deviation (*change in slope*) compared to MWL of water samples (stream, soils, plant xylem water etc)

A timeline of benchmark tracer publication in hydrology

L. 5, NO. 2 WATER RESOURCES RESEARCH APRIL :

1969

Determination of the Ground-Water Component of Peak Discharge from the Chemistry of Total Runoff

GEORGE F. PINDER AND JOHN F. JONES

Nova Scotia Department of Mines, Halifax, Nova Scotia

Abstract. The ground-water component of stream discharge may be determined from the chemical characteristics of the stream water. A chemical mass-balance is used to relate total, direct, and ground-water runoff. To solve the mass-balance equation, it is necessary to estimate the chemical composition of the ground-water and direct-runoff components. The solute concentration of ground water is determined from total runoff during baseflow; the chemical characteristics of direct-runoff are estimated from samples of total runoff collected from selected locations in a basin during peak discharge periods. In three small watersheds in Nova Scotia ground-water runoff constituted from 32 to 42% of peak discharge for the period of analysis.

WATER RESOURCES RESEARCH

1975

Subsurface Flow From Snowmelt Traced by Tritium

J. MARTINEC

Federal Institute for Snow and Avalanche Research, Weissfluhjoch, Davos, Switzerland

An explanation is offered of the apparent discrepancy between the small velocities of subsurface flow and the watershed response. Environmental tritium in the hydrological cycle provided evidence for a new insight into the runoff mechanism. By this concept the quick reaction of outflow to a massive groundwater recharge is brought to agreement with the long residence time of the infiltrated water.

Importance of old (pre-event) water

Journal of Hydrology, 43 (1979) 45—65 45

[2] 1979

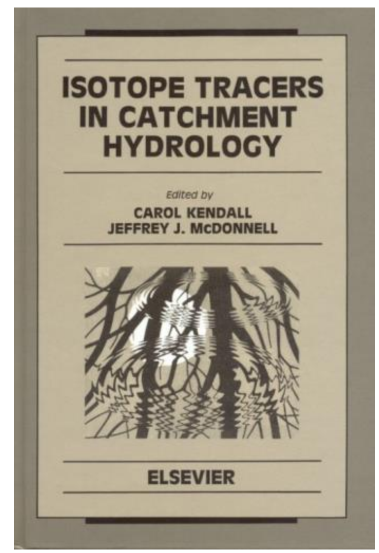
THE ROLE OF GROUNDWATER IN STORM RUNOFF

MICHAEL G. SKLASH and ROBERT N. FARVOLDEN

Department of Geology, University of Windsor, Windsor, Ont. N9B 3P4 (Canada)
Department of Earth Sciences, University of Waterloo, Waterloo, Ont. N2L 3G1 (Canada)

(Accepted for publication April 25, 1979)

1998



Origins of tracer-aided models

Hydrological Processes

Article

1988

Chloride in precipitation and streamwater for the upland catchment of river severn, mid-wales; some consequences for hydrochemical models

Colin Neal, Nils Christophersen, Richard Neale, Christopher J. Smith, Paul G. Whitehead, Brian Reynolds

First published: April/June 1988 | https://doi.org/10.1002/hyp.3360020206 | Cited by: 66

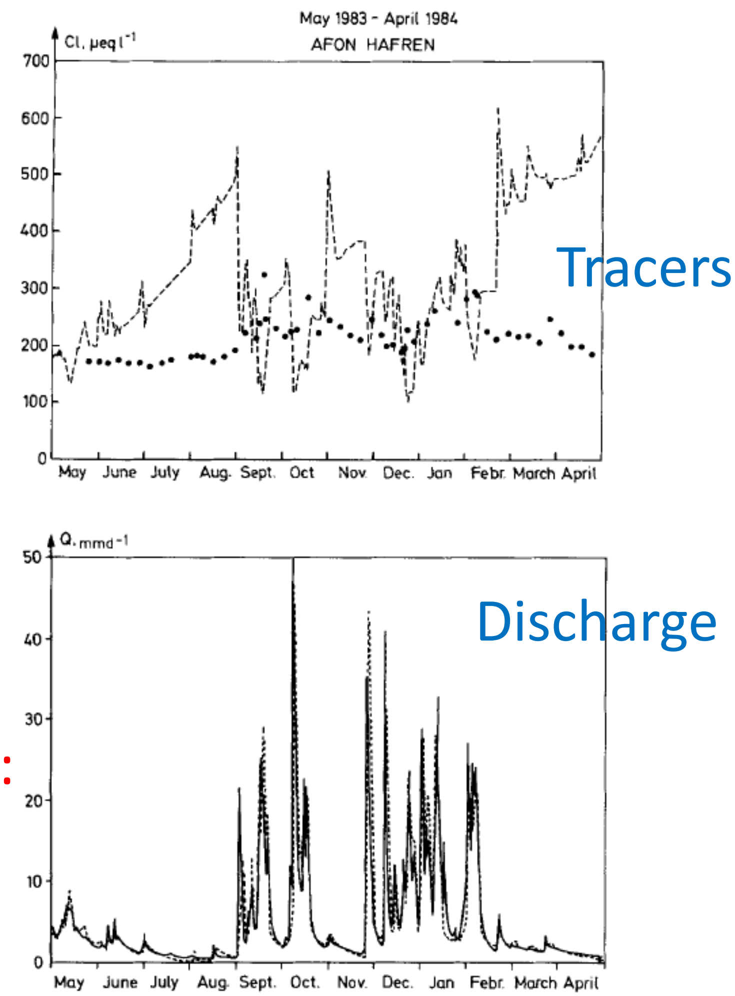
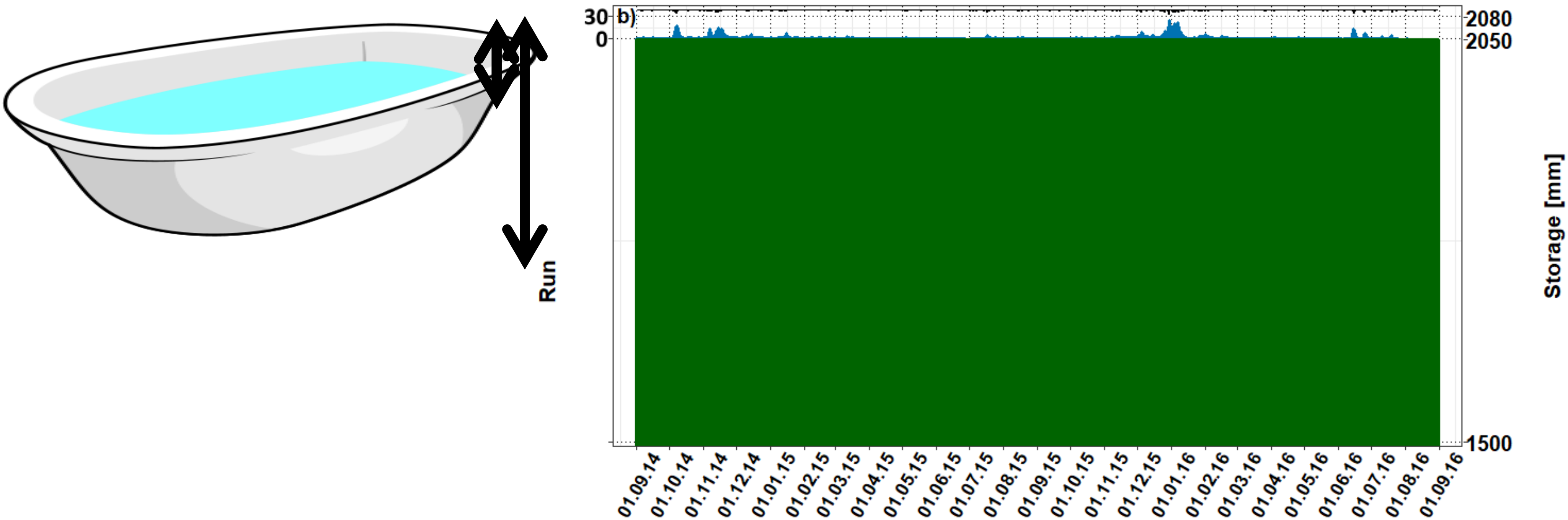


Figure 6. Upper panel: Observed (●) and daily simulated (dashed line) Cl concentrations for the Afon Hafren for the period May 1983–April 1984
Lower panel: Daily observed (full line) and daily simulated (dashed line) hydrograph

Discharge simulations good, but model failed to:

- Characterise storage
- Conceptualise mixing
- Represent flow paths and fluxes

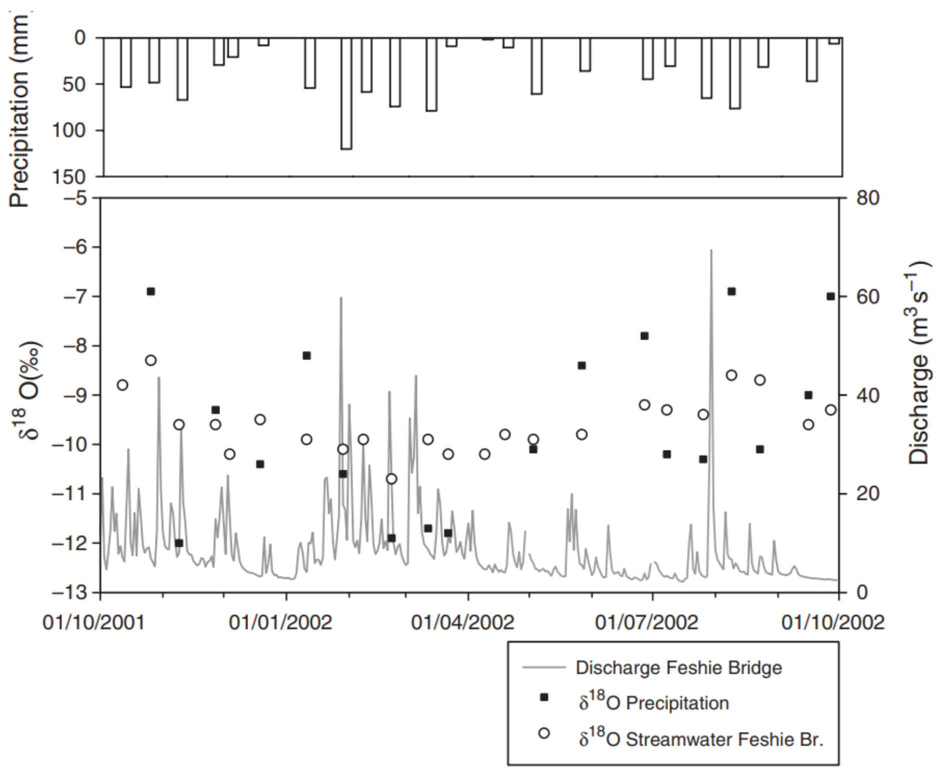
Total catchment storage >> flow variation



Large isotope damping: storage is 3 orders of magnitude larger than flow

The past: weekly data & coarse spatial resolution

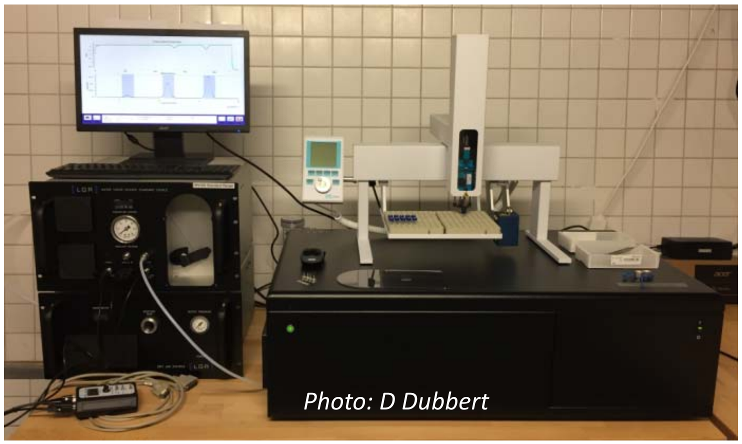
Samples were “simply” expensive



Soulsby et al., Hydrol. Proc, 2006

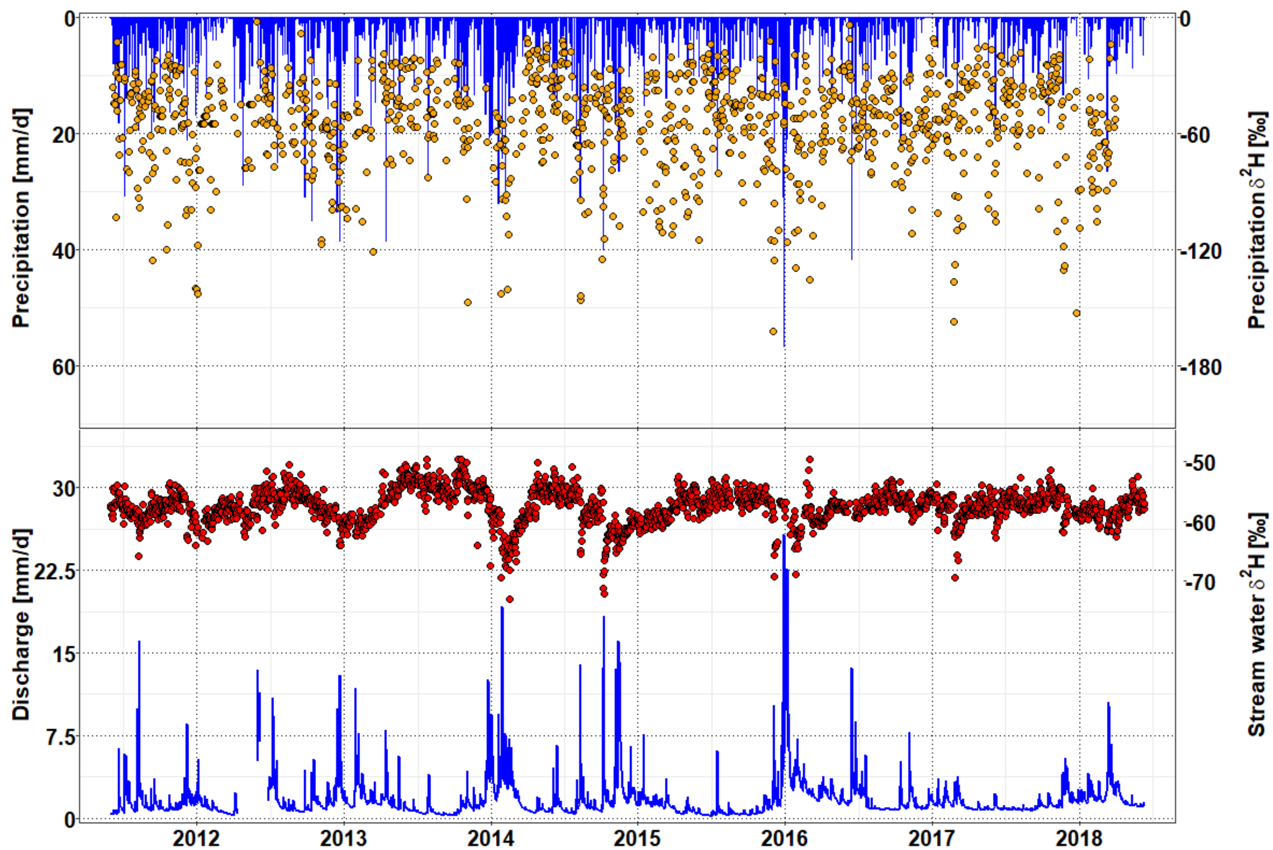
Photo T Goldhammer

Recently: Step change through "Big data" from long-term high resolution tracer data

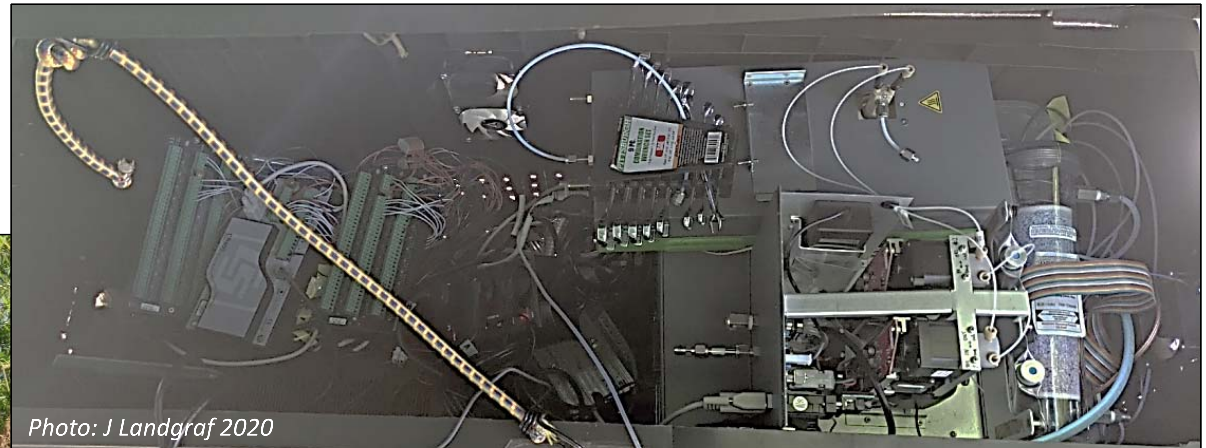


Laser analysers: basis for long-term high resolution tracer time series

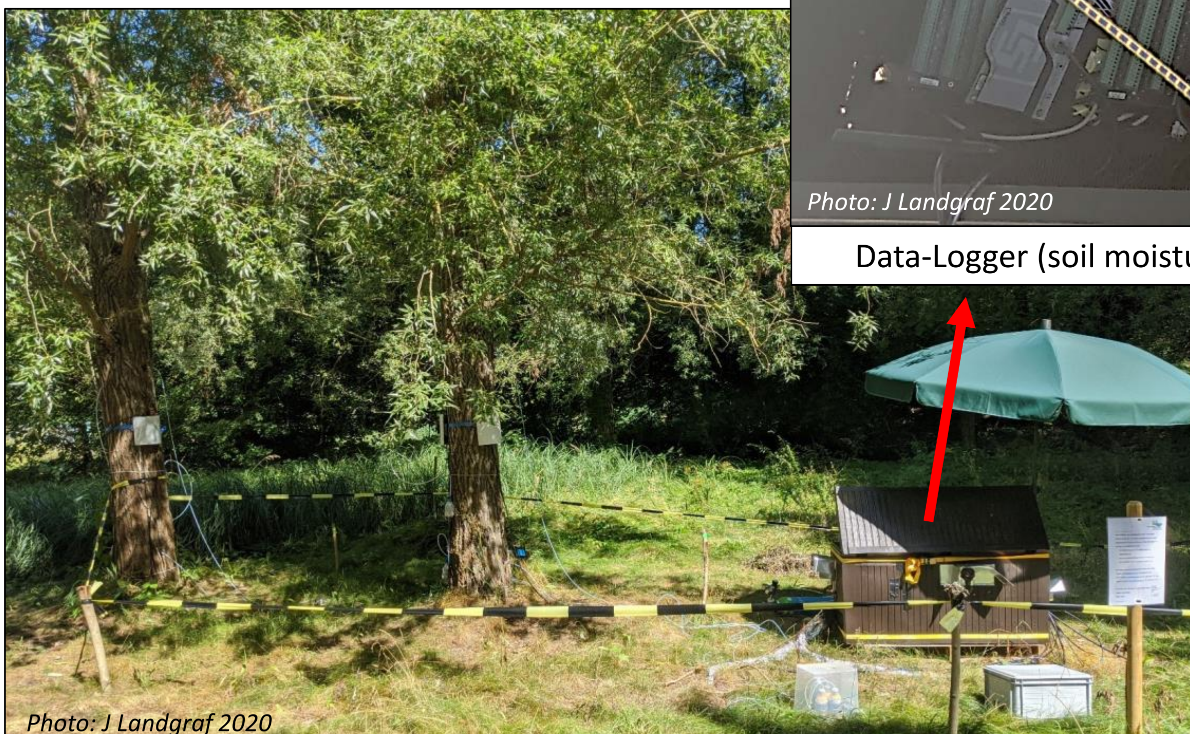
7 yrs daily isotopes from the Bruntland Burn experimental catchment



In-situ tracer data: it looks easier than it is!



Data-Logger (soil moisture/ temperature)   Picarro vaporizer



Northern Willow   Southern Willow   Pit A   Laser-Box   Pit B

- Complex setup
- Daily maintenance & troubleshooting
- Vast amount of data

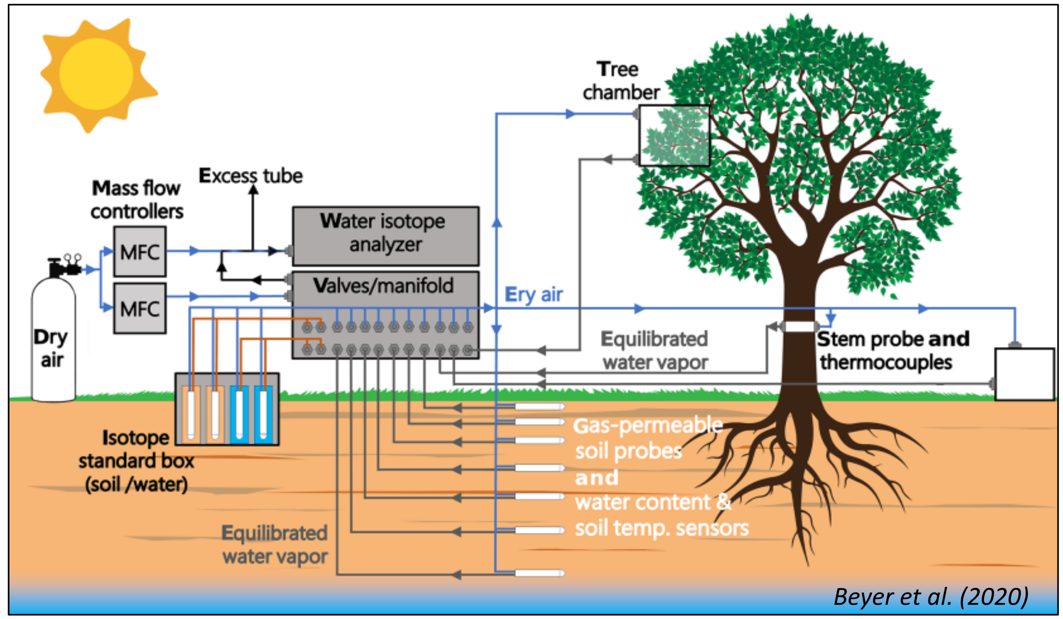
PhD project Jessica Landgraf

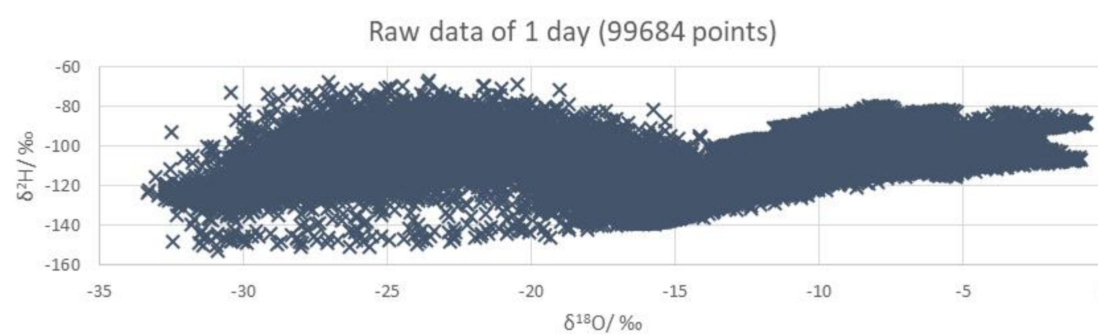
In-situ tracer data: very quickly REALLY BIG data & detailed insights into temporal high-resolution processes

In-situ isotope optimal setup

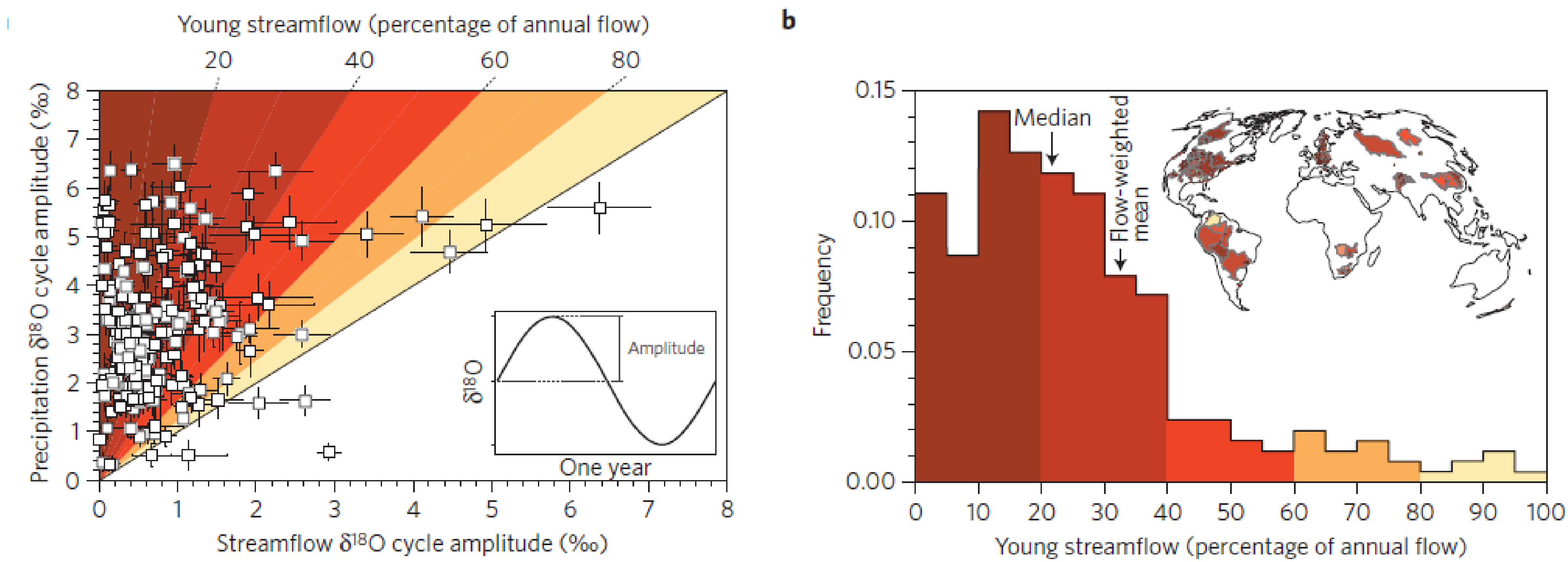
- Soil probe
- Stem probe
- Tree chamber
- Dry air for flushing
- Isotope standards
- Water isotope analyser

Data point roughly every second over weeks or months





Generalisation at global scale: spatially BIG data

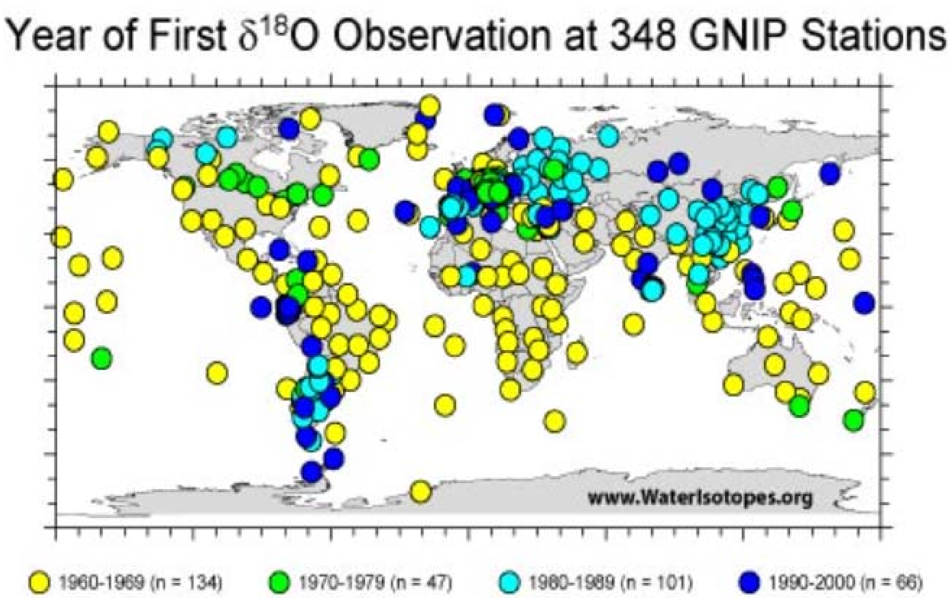


Jasechko et al., 2017, Nature (Geosciences)

High proportion of young water during high flows
But aquifers with old water dominate during low flows
Subsequent work: VERY old water often disconnected from surface waters

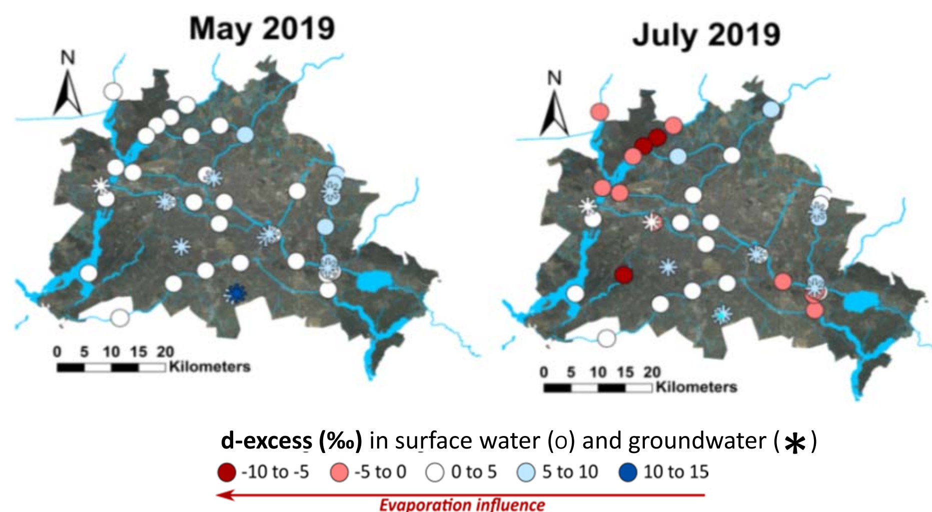
Networks and metadata bases of isotopes for spatial big data

Precip GNIP IAEA



Waterisotopes.org

- Rivers GNIR IAEA
- Global data set of vapour isotopes
- …
- Regional or "local" maps/ data bases: landscapes, catchments, cities…



Kuhlemann et al., HP, 2020

Challenges of HAVING big data

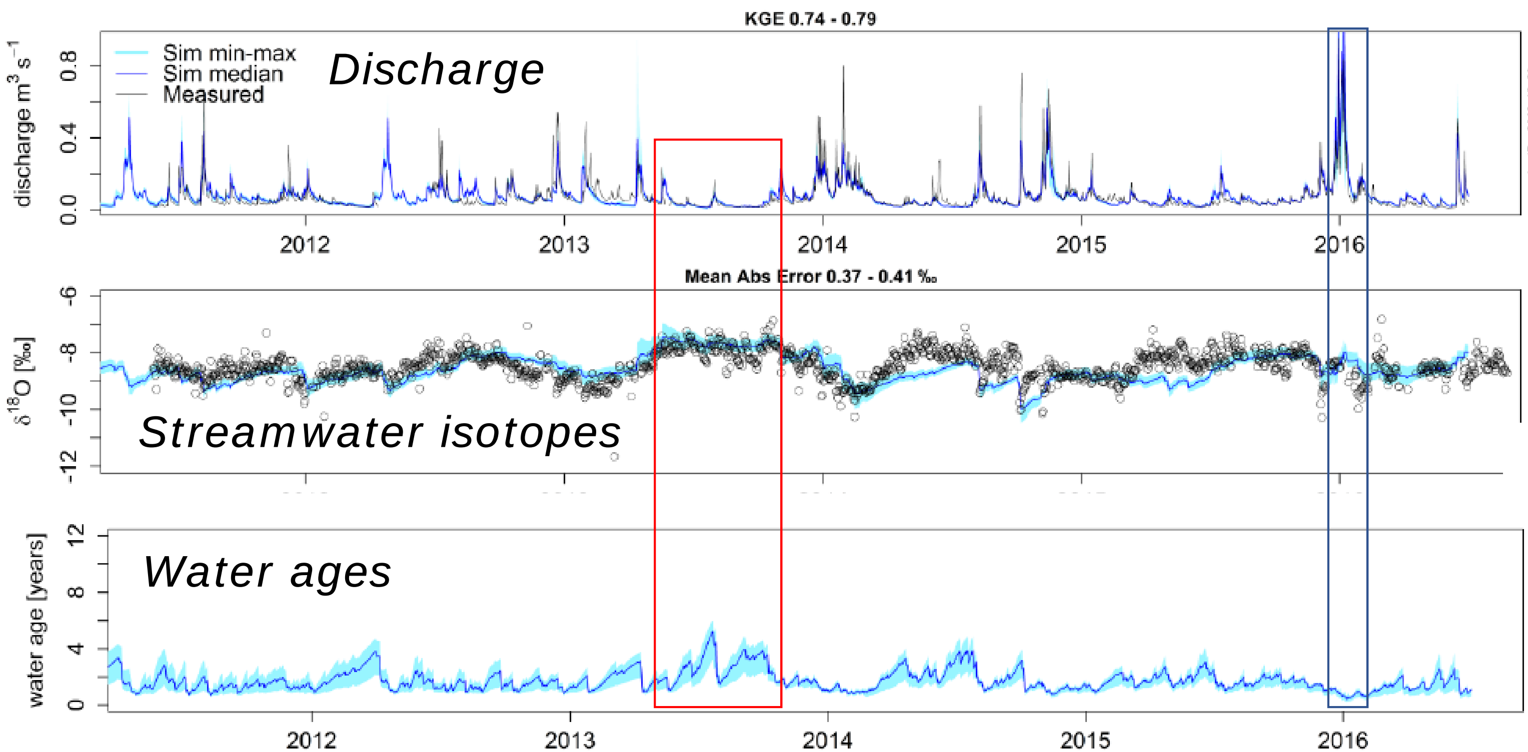
Vetting and/or interpreting big data is not trivial:

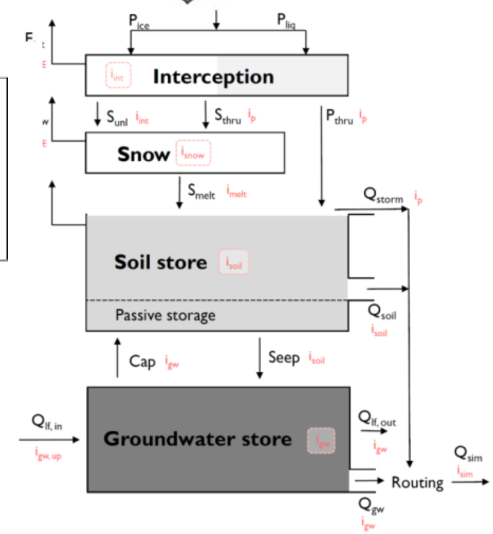
- Some patterns being revealed that have never been seen before
- Patterns might ‘suggest’ new processes & revealing un-knowns
- New data force us to ask ***what do these mean***?
- Many potential artifacts or analytical challenges exist

- Emergence of new processes – this will impact MODELS
- Need to re-think established assumptions, mechanisms, best practices, best analyses

Slide inspired by Todd Dawson

New generation of tracer-aided models: explicit incorporation of mixing volumes and storage



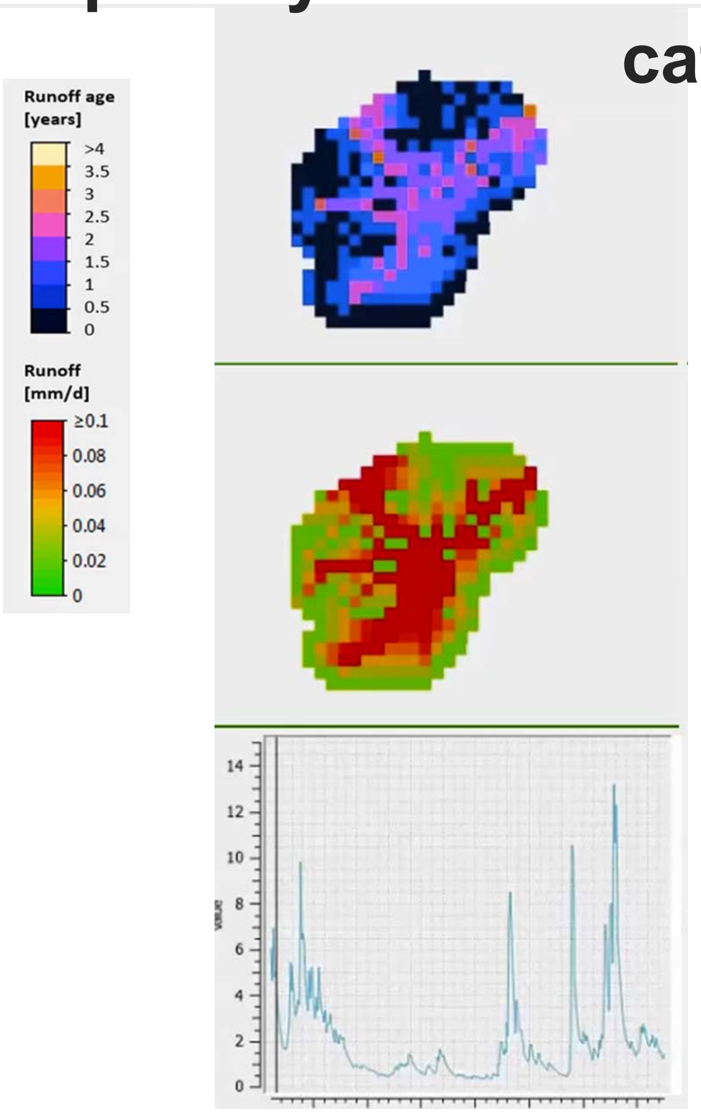


Soulsby et al., WRR, 2015

van Huijgevoort et al., HP, 2016

Ala-Aho P, et al. (2017) Hydrology and Earth System Sciences (HESS).

Spatially distributed estimation of water ages at the catchment scale



Age

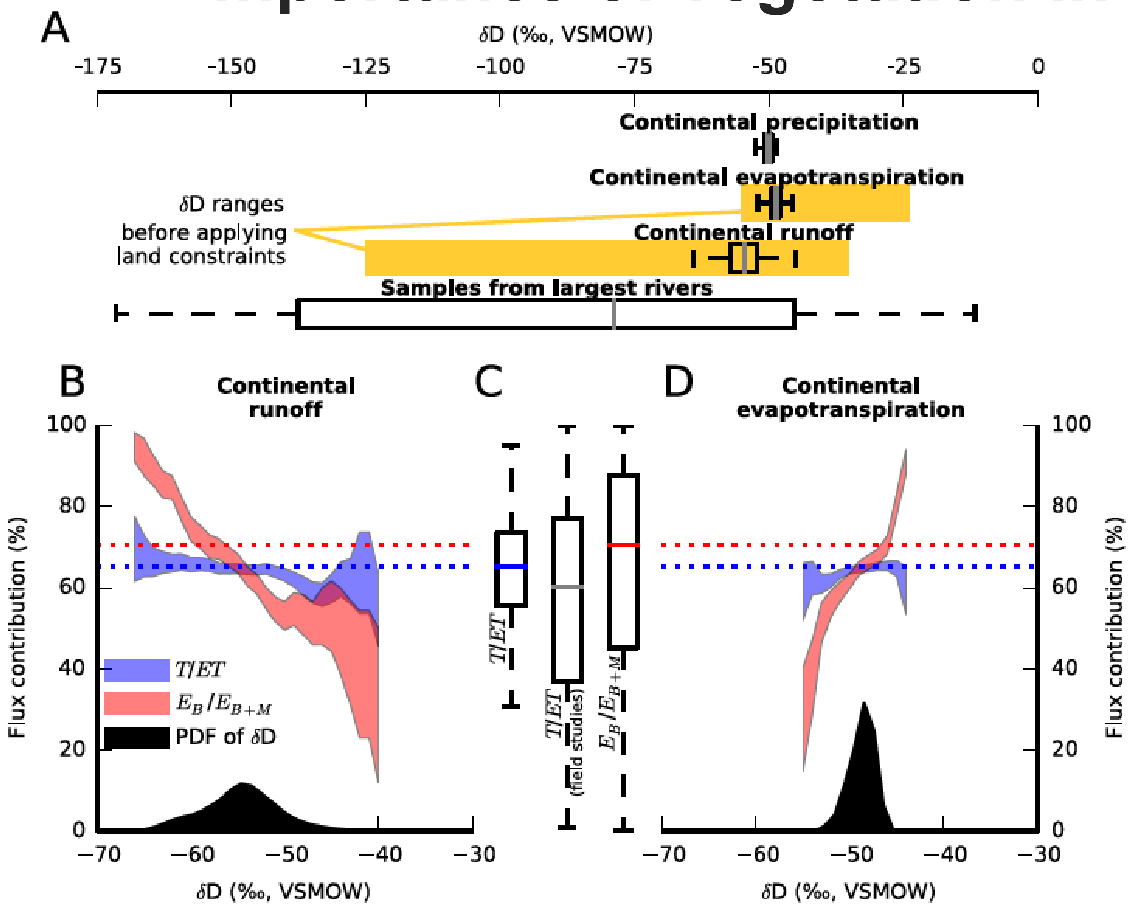
Runoff

Stable isotope tracers:

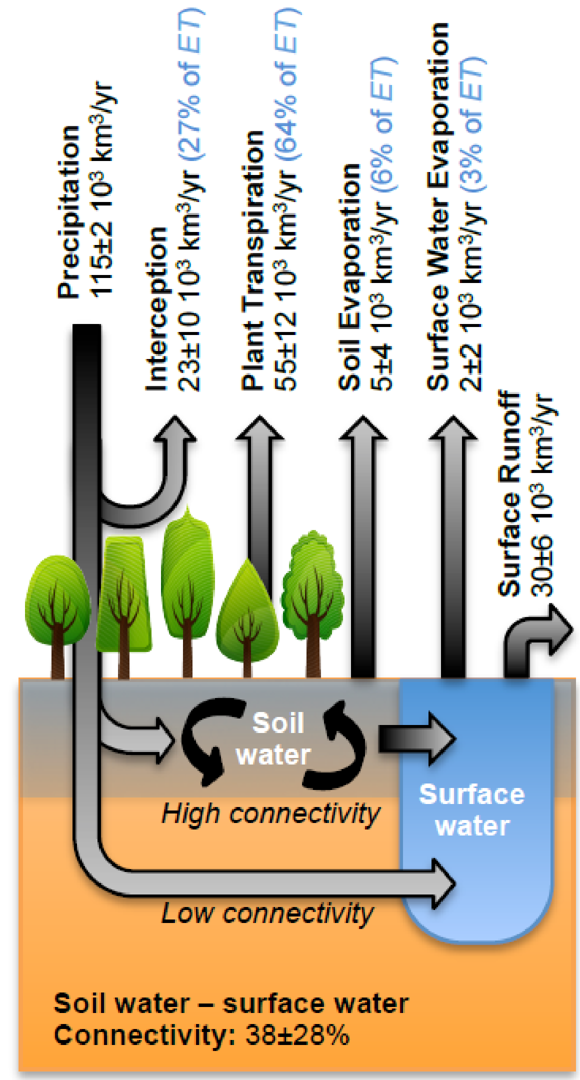
- To estimate ages
- To estimate total storage
- As diagnostics of model states

Ala-Aho P, et al. (2017) Hydrology and Earth System Sciences (HESS).

Importance of vegetation in tackling env. change



Good et al. (2015), Science



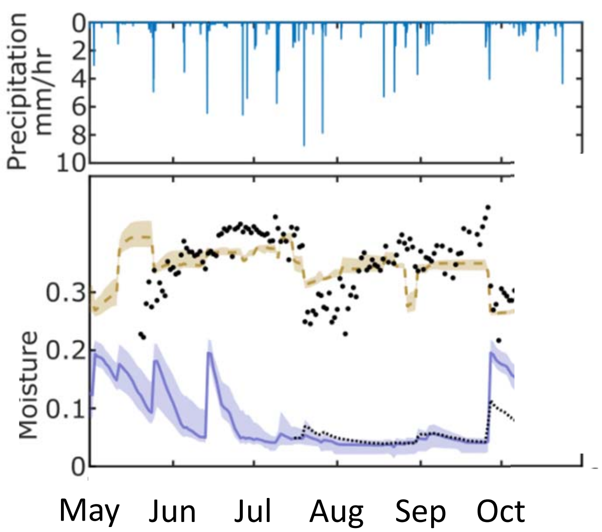
T >> annual runoff from world's rivers

Tracking fluxes & isotopes in landscape compartments using tracer-aided ecohydrological models

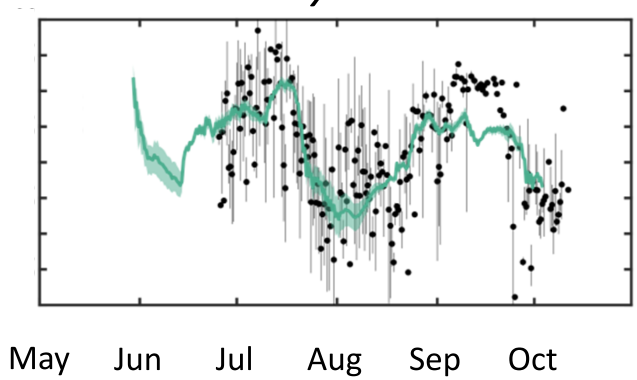
Physically-based modelling captures dynamics of soil moisture, isotopes in soil & plant xylem water & sources of plant water

Estimation of water ages of different compartments: Very young inferred water age in shallow soil

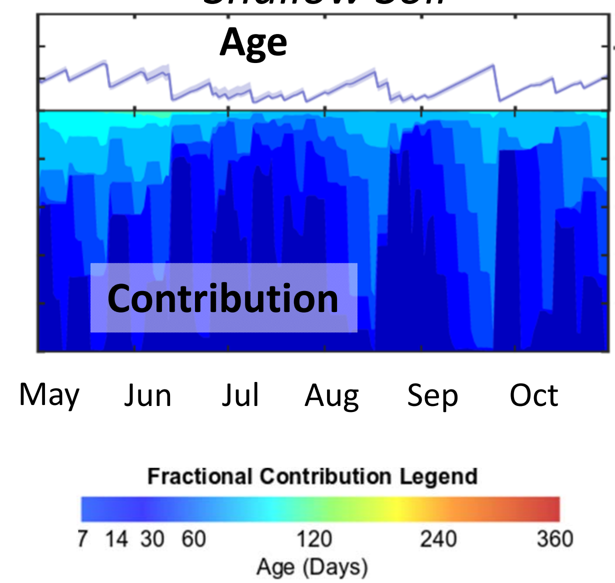
Soil



Xylem



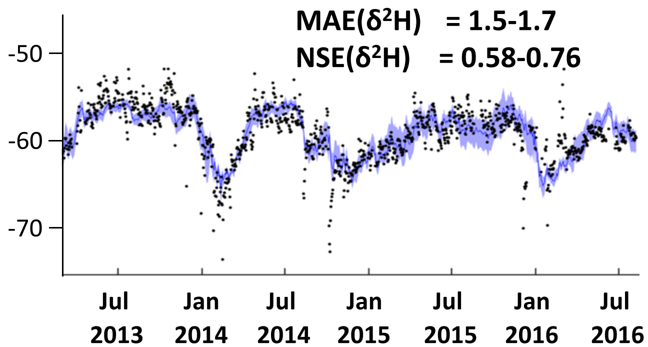
Shallow Soil



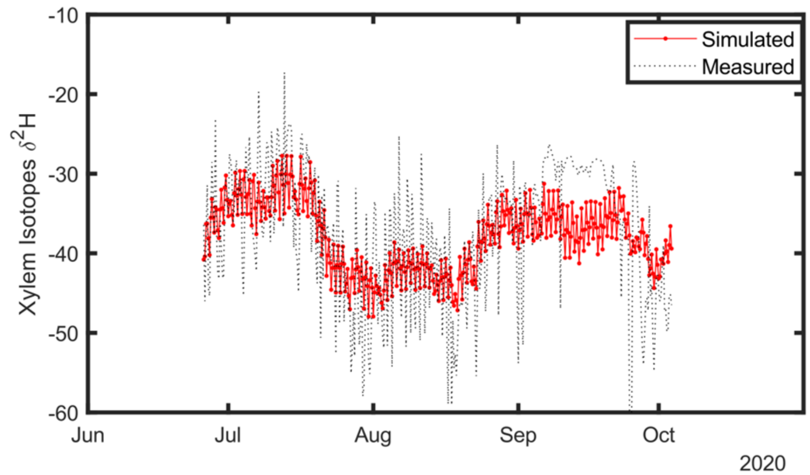
Smith et al., Biogeosciences Discussion.

ML (*e.g. Neural Network*) to predict isotopes time series

Stream isotopes



Plant Xylem isotopes

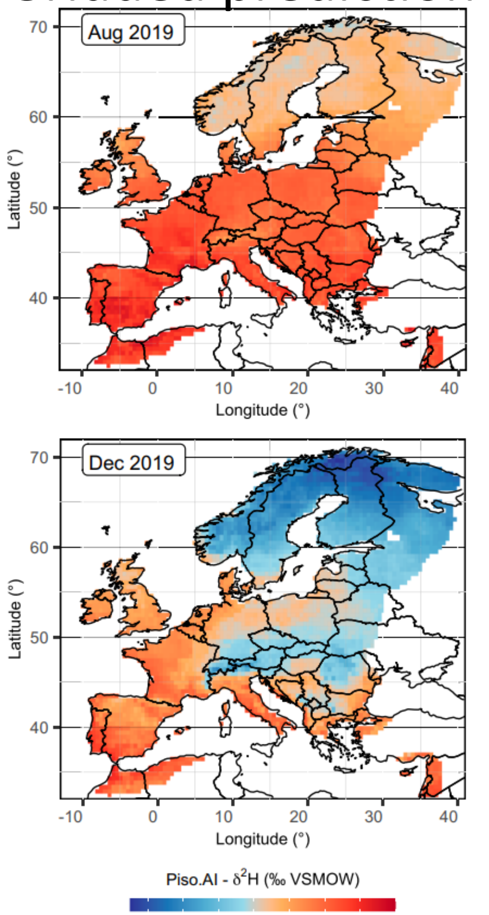


- Use of LSTM: faster set-up and run time
- Helped confirm some processes (or measurements) not integrated in models

Slides from Aaron Smith (talks on Wed in WG Water/Environment)

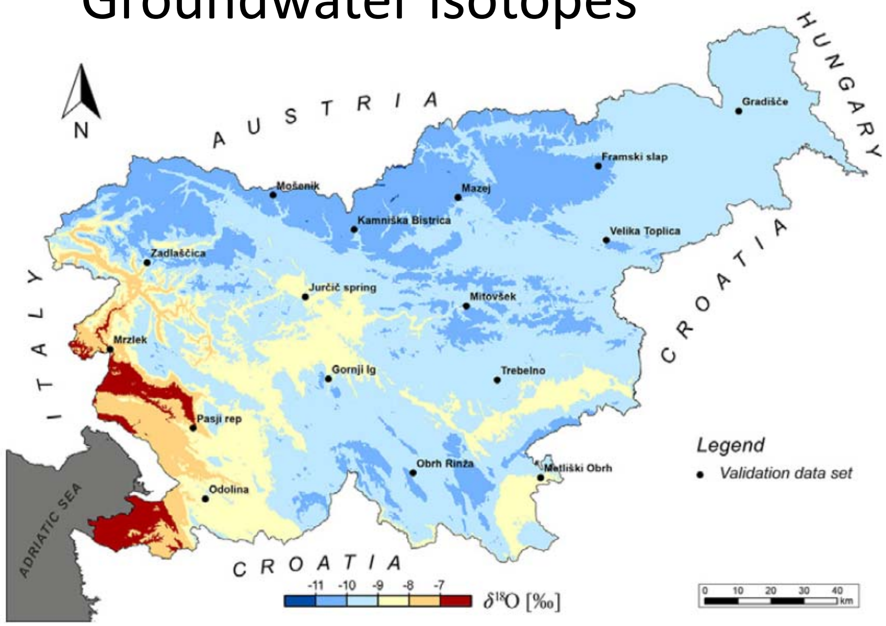
ML to predict isotopes spatially: spatial mapping of…

Gridded prediction for precip δ²H



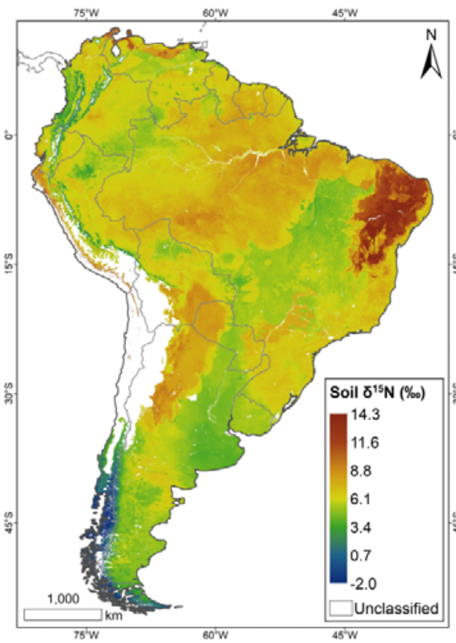
Nelson et al., 2021, PNAS

Groundwater isotopes



Cerar et al. 2018

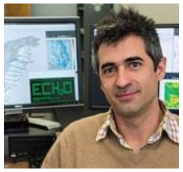
Soil isotopes



Sena-Souza et al. 2020

Opportunities for AI/ML

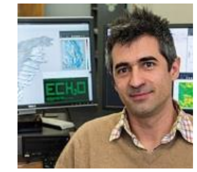
Thanks to M. Maneta for Input



- Combining high-frequency & high spatial resolution data to cope with increasing pressures on water resources
- Extracting patterns from images & time series can assist in classification of distinct hydrological modes (more meaningful inter-comparisons between periods / locations with previously undetected similarities)
- Reduction of model complexity (*from high computational cost to faster runs)*
- Predictions in “un-sampled” catchments via similarity detection & information transfer (*e.g. through neural networks*)
- Bias correction of data & improved parameter regionalization / simulation for spatially-explicit hydrologic models
- Improved data gap filling

Limitations for Big data & ML

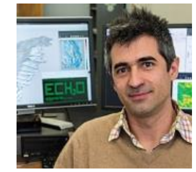
Thanks to M. Maneta for Input



- Water isotopes: data ownership / Data accessibility
- Data limitations: not enough data, variabilities, uncertainties
- Sparse datasets: more traditional analysis (classification, regression methods) with stronger constraining assumptions might perform better
- New patterns / processes: correct interpretation (process-based knowledge) required

- ML methods = black boxes, interpretation of hidden information is difficult
- ML & Big Data: require LOTS of data for deep learning methods to *learn (*particularly for isotope hydrology as usually more "modest" in size)
- Lot of "pre-processing" of parameters (*e.g. identify optimal No of hidden layers (depth of the network), No of neurons per layer, type & length of input features*) with little to no guidance on adequate values
- Adjustments often via trial & error (tremendous & frustrating time sink)
- Can lead to flawed extrapolation or predictions & poor generalization power

Some potential future directions of ML
(in hydrology / water stable isotopes)



Thanks to M. Maneta for Input

- Compared to other Sciences (e.g atmospheric sciences) hydrology has not yet seen wide application of ML methods - plenty of opportunities for advancement & discovery
- Linking ML & process-based knowledge / analysis
- Integrating novel types of field observations (e.g. *in-situ*) into local to regional models is a new research frontier
- “Physics-aware” ML: While ML is excellent at approximating processes & predicting outcomes - predictions do not necessarily respect basic physical laws that are foundations in hydrology *(e.g. conservation of mass or conservation of energy):* new methods need to consider encoding physical laws in learning process

Summary

- Stable water isotopes: from a specialist sub-field to major data source for innovation in hydrology
- Driven by increasingly cheap & flexible analytical tools
- Used to test hypotheses about complex multi-scale hydrological processes e.g. mixing interactions between various storage, fluxes and ages
- Means to help calibration and/or testing of hydrological models
- Need to consider plant-soil-atmosphere interactions and human impacts on water partitioning

- Cross-road now: Big data providing new insights at a range of scales while also providing new types of data for models
- New patterns & processes observed but clear challenges