– READ ME FIRST – Data Set Documentation

Accompanying document to:

New water fractions and transit time distributions at Plynlimon, Wales, estimated from stable water isotopes in precipitation and streamflow

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Data archive

These data sets are made publicly available for use in education and research. The data sets are attached to the accompanying manuscript as supplemental information, and are also be archived at www.envidat.ch.

Those who use these data in published work should cite:

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Disclaimer

These data are provided "as is", with no guarantee that they are free of errors or omissions. Those who use the data contained herein do so entirely at their own risk, and are solely responsible for determining their suitability for any particular purpose. The authors and their respective employers make no warranty, express or implied, including warranties of merchantability and fitness for a particular purpose, with respect to any information or data contained in this distribution package. The authors and their respective employers assume no legal liability for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed herein and do not represent that use of such information, apparatus, product or process would not infringe on privately owned rights.

Raw data archive

The archived data include a raw data archive and quality-controlled data. The Raw Data Archive (denoted by column headers with "RDA" at the end of each variable name) contains the raw measurements as reported by the laboratory. This raw data archive is provided for completeness of documentation, and also in the interests of full transparency concerning data editing that has been subsequently applied. The raw data archive also provides the opportunity to go back to the original data in case new information emerges suggesting that interesting real-world phenomena may have been inadvertently edited out. However, *the raw data archive should not be used for routine analyses,* because the raw data include some values that are believed to be substantially in error (see comments in the data tables). Instead, routine analyses should use the edited version of the data, where to the greatest extent possible, problematic data values have been corrected or excluded.

Sampling and analysis procedure

For details on the sampling and analysis procedure, please refer to the main manuscript and its supplemental material.

Column headers of data sets

The following table explains the column headers of 7-hourly and weekly stable water isotope data collected at Plynlimon, Wales, UK.

The data sets are provided as separate, tab-delimited .txt files.

Column Header	**Explanation**	**Relevant for precipitation (P) or streamwater (Q) sample?**	**Weekly and/or 7-hourly data?**
sample_ID	Continuous numbering of samples at each site. The numbering does not necessarily start at 1, since the data sets are subsets of the longer solute data sets recorded at 7-hourly and weekly intervals.	P, Q	W, 7
Unique Code	Same as sample ID, but with site identifier	P, Q	7
Site	Site identifier (see below)	P, Q	W, 7
Site Name	Full name of site	P, Q	W
Date_Time yyyy.mm.dd HH:MM	The time that the sample was collected. Stream samples are instantaneous grab samples collected at the given time. For rainfall samples, the time stamp corresponds to the end of the sampling interval for precipitation sampling, and the sample period is usually the interval between the previous sample collection Date_Time and the current one. Note that the precipitation chemistry data of Neal et al. (2013b) use a different timestamp convention, in which precipitation samples are labeled according to the time that each sampling interval began (rather than ended). Format: yyyy.mm.dd HH:MM	P, Q	W, 7
Volume-weighted mean sampling time yyyy.mm.dd HH:MM	For stream samples: the sampling time. For rainfall samples: the average sampling time, where each hour is weighted by the hourly rainfall recorded by the Carreg Wen automatic weather station (AWS). During gaps in the Carreg Wen AWS record, the Tanllwyth AWS was used. Where both AWS's had data gaps, the average of all other working AWS's at Plynlimon was used. If no rainfall was recorded within the sampling interval, the mean sampling time is assumed to be the mean of the interval. Format: yyyy.mm.dd HH:MM	P, Q	W, 7

Precip sampling starts yyyy.mm.dd HH:MM	The time stamp corresponds to the time at which the precipitation sampling started. This time usually corresponds to the time the previous precipitation sampling ended. Format: yyyy.mm.dd HH:MM	P	7
Precip sampling ends yyyy.mm.dd	The time stamp corresponds to the time stamp at which the precipitation sampling ended. This is equivalent to the time given in the column Date_Time. Format: yyyy.mm.dd HH:MM	P	7
Yr	Year extracted from Date_Time	P, Q	W, 7
Month	Month extracted from Date_Time	P, Q	W, 7
Day	Day of the month extracted from Date_Time	P, Q	W, 7
Time HH:MM	Time (HH:MM) extracted from Date_Time	P, Q	W, 7
Date yyyy.mm.dd	Date (yyyy.mm.dd) extracted from Date_Time	P, Q	W, 7
Year	Date_Time as decimal year	P, Q	W, 7
Year_mean_sampling	Volume-weighted mean sampling time as decimal year	P, Q	W, 7
water flux (mm/hr)	Discharge or rainfall converted to mm/hr	P, Q	W, 7
log_flow	Log10 of water flux (mm/hr)	P, Q	W, 7
Cl mg/l	Chloride concentration in mg/l	P, Q	W, 7
delta_18O	Oxygen-18 relative to VSMOV [‰]	P, Q	W, 7
delta_2H	Deuterium relative to VSMOV [‰]	P, Q	W, 7
Stream flow (Cumecs)	Discharge in m^3/s	Q	W, 7
Runoff (mm/15min)	Discharge in mm/15min, converted from flow cumecs using catchment area (see below)	Q	W, 7
Rainfall (mm)	Cumulative rainfall between precipitation sampling starts and precipitation sampling ends	P	W, 7
Notes	Remarks on samples collected (error notes etc)	P, Q	W, 7
Type	“input” (precipitation sample) or “stream” (streamwater sample)	P, Q	W, 7
Description	Description of sampling location	P, Q	W, 7
Sample yes/no	Sample collected? (This refers to sampling in general and provides information on whether solute data is available for this time point. Information specifically on isotope sampling is provided in the next column.)	P, Q	7
Isotope sample yes/no	‘yes’ if an isotope sample was taken, else ‘no’	P, Q	7

Isotope bottle acidified	‘yes’ if isotope split was taken from an acidified sample bottle, otherwise ‘no’. Rows without isotope samples are empty. If the isotope bottle was acidified, deuterium values in column delta_2H are adjusted for the offset of 0.68 ‰ observed between acidified and un-acidified samples (for more details see the main manuscript and the supplemental information to the manuscript).	P, Q	7
Dry deposition affected (yes/no)	‘yes’ if the sample is likely affected by dry deposition and chloride concentrations should be treated with care, ‘no’ if the dry deposition effect is likely negligible (caution: dry-deposition affected chloride samples have NOT been excluded from the chloride data set).	P	7
Dry_interval	Hours since last rainfall	P	7
Day_of_week	Day of week the sample was taken	P, Q	7
Trip	Number of trip (up to 24 bottles per carousel; one fill of carousel = one trip). Trip numbering ends after trip 99, when 7-hourly solute sampling at Upper Hafren and Carreg Wen was suspended.	P, Q	7
Bottle_in_trip	Number of bottle in trip/in carousel. Bottles were filled in order 1-24.	P, Q	7
air fraction in isotope bottle	Some sample bottles had visually obvious head space when they were opened for isotope analysis, despite having been filled completely at the time of original sampling. This column indicates the fraction of head space compared to the total sample bottle volume. (affected samples are included in the RDA isotope values, but not the final values)	P, Q	W
Cl mg/l RDA	Chloride concentration in mg/l – Raw Data Archive	P, Q	W, 7
delta_18O RDA	Oxygen-18 relative to VSMOV – Raw Data Archive	P, Q	W, 7
delta_2H RDA	Deuterium relative to VSMOV – Raw Data Archive	P, Q	W, 7

Site Identifier and Catchment Area

Identifier	Site Name	Location Code[1]	Latitude Datum (WGS84)	Longitude Datum (WGS84)	Altitude (m a.s.l.)	Catchment area (km^2)	Note
CR	Carreg Wen	C	52.4826	-3.7263	575	n.a.	Sampling site for rainfall samples
UHF	Upper Hafren	G	52.4879	-3.7269	550	1.22	Sampling site for streamwater samples
LHF	Lower Hafren	B	52.4754	-3.7052	352	3.58	Sampling site for streamwater samples
TAN	Tanllwyth at Tanllwyth Bridge	AD	52.4745	-3.7073	356	0.916	Sampling site for streamwater samples

[1] Following publication of weekly data in Neal et al. (2013a), https://catalogue.ceh.ac.uk/documents/44095e17-43b0-45d4-a781-aab4f72da025.

Further details on spatial extents and spot heights, as well as a digital terrain model are available from the Center of Ecology & Hydrology: https://catalogue.ceh.ac.uk/documents/91961a0f-3158-4d00-984d-91eb1e03e8bd.

Available solute data sets

This file contains additional explanation to the data sets of weekly and 7-hourly stable water isotope data collected at Plynlimon, Wales, UK. These data sets are embedded in longer-term data collection efforts that have previously been published. Streamwater chemistry analyses are available weekly from 1983-2011 at up to five catchments, and bi-weekly thereafter. Streamwater chemistry is also available at 7-hourly resolution between 2007-2009 at Upper and Lower Hafren. Please refer to these data sets for solute data.

Weekly solute data sets and documentation:

- Neal, C., Reynolds, B., Norris, D., Kirchner, J. W., Neal, M., Rowland, P., Wickham, H., Harman, S., Armstrong, L., and Sleep, D.: Three decades of water quality measurements from the Upper Severn experimental catchments at Plynlimon, Wales: an openly accessible data

resource for research, modelling, environmental management and education, Hydrol. Process., 25, 3818-3830, https://doi.org/10.1002/hyp.8191, 2011.

- Neal, C., Kirchner, J., and Reynolds, B.: Plynlimon research catchment hydrochemistry, NERC Environmental Information Data Centre, https://doi.org/10.5285/44095e17-43b0-45d4-a781-aab4f72da025, 2013a.
- Norris, D. A., Harvey, R., Winterbourn, J. M., Hughes, S., Lebron, I., Thacker, S. A., Lawlor, A. J., Carter, H. T., Patel, M., Keenan, P. O., Pereira, M. G., Cosby, B. J., Reynolds, B., Grant, S. J., Pomeroy, I., Hinton, C., Spinney, K., Peters, T. D., and Callahan, B.: Plynlimon research catchment hydrochemistry (2011-2016), NERC Environmental Information Data Centre, https://doi.org/10.5285/794c609b-da62-4a42-a4c1-267219865bb1, 2017.

7-hourly solute data sets and documentation:

- Neal, C., Reynolds, B., Rowland, P., Norris, D., Kirchner, J. W., Neal, M., Sleep, D., Lawlor, A., Woods, C., and Thacker, S.: High-frequency water quality time series in precipitation and streamflow: From fragmentary signals to scientific challenge, Sci. Total Environ., 434, 3-12, https://doi.org/10.1016/j.scitotenv.2011.10.072, 2012.
- Neal, C., Kirchner, J., and Reynolds, B.: Plynlimon research catchment high-frequency hydrochemistry data, NERC Environmental Information Data Centre, https://doi.org/10.5285/551a10ae-b8ed-4ebd-ab38-033dd597a374, 2013b.
- Neal, C., Reynolds, B., Kirchner, J. W., Rowland, P., Norris, D., Sleep, D., Lawlor, A., Woods, C., Thacker, S., and Guyatt, H.: High-frequency precipitation and stream water quality time series from Plynlimon, Wales: an openly accessible data resource spanning the periodic table, Hydrol. Process., 27, 2531-2539, https://doi.org/10.1002/hyp.9814, 2013c.