Caravan-Qual: A global scale integration of water quality observations into a large-sample hydrology dataset

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Abstract

Protecting and improving surface water quality is contingent upon understanding the trends and spatial patterns in physical, biological, and chemical conditions and their underlying drivers. This requires observational data, spanning a diverse range of water quality constituents, coupled with contextual environmental data. Here we present the first global-scale integration of water quality into large-sample hydrology (named Caravan-Qual), combining ~70 million observations of 100 water quality constituents with streamflow measurements, meteorological forcing and catchment attributes covering the period 1980-2025. We envisage that the dataset can facilitate a diverse range of empirical analyses (e.g. spatio-temporal analysis across diverse regions, quantification of pollutant loadings and exports, concentration-discharge analysis), in addition to supporting development and evaluation of process-based and data-driven models for water quality prediction and management.

1. Background and summary

Hydrological monitoring is critical for the sustainable management of Earth's water resources, with data underpinning our understanding of natural processes in water systems and the impact of anthropogenic interventions. Furthermore, data is fundamental for the development, calibration and validation of process-based models, remote sensing and data driven approaches (e.g. machine learning) that both further our process understanding and support water resource management[1].

The last decade has seen a proliferation in efforts to compile, standardise and openly disseminate datasets spanning hundreds to thousands of catchments, driven by the emergence of *large-sample hydrology* (LSH) as a sub-discipline in hydrological sciences[2,3]. Many of these datasets have emerged following the CAMELS (Catchment Attributes and Meteorology for Large-sample Studies) framework first developed for the contiguous United States[4], with national implementations publicly available for Australia[5], Brazil[6], Chile[7], Denmark[8], France[9], Germany[10], Great Britain[11], India[12], Spain[13] and Switzerland[14]. Other noteworthy LSH datasets include the Hydrometeorological Sandbox - École de Technologie Supérieure (HYSETS)[15] and LArge-SaMple Data for Hydrology and Environmenal Sciences (LamaH) datasets for Central Europe[16] and Iceland[17].

Leveraging these national efforts, the *Caravan* initiative[18] has sought to harmonise and combine these datasets into a single, globally-applicable framework. Together with publicly available extensions (e.g. GRDC-Caravan[19]), *Caravan* currently contains accessible, consistently formatted and globally standardised daily streamflow data, together with associated meteorological forcing (e.g. precipitation, temperature)[20] and static attributes (e.g. land use, soils)[21], for ~25,000 catchments distributed globally. Such LSH datasets have already enabled novel applications in hydrological modelling, including the development of machine learning approaches for streamflow prediction[22].

Comparable advances have not (yet) been made for water quality research, for which the availability and accessibility of observational data lags considerably behind streamflow[23]. While national and regional water quality datasets exist, such as for the US[24], China[25] and the European Union[26], these datasets are typically inconsistent in aspects such as monitored water quality constituents, naming conventions and reporting units. Efforts to aggregate and standardise water quality data from these sources into global databases, such as the Global Freshwater Quality Database (GEMStat)[27], GLObal RIver CHemistry Database (GLORICH)[28] and Global River Water Quality Archive (GRQA)[29], provided new opportunities to examine water quality dynamics at regional to global scales. However, these datasets lack connections to catchment attributes and meteorological forcing data that are integral to other LSH datasets, while connections to observed streamflow measurements are also often lacking. Given the inextricable link between water quality and streamflow (e.g. dilution, mobilisation and transport), this represents a significant shortcoming of existing global water quality databases[30]. Recently, several national level datasets that include water quality have been developed, including for the USA (CAMELS-Chem)[30], Switzerland (CAMELS-CH-Chem)[31] and Germany (QUADICA)[32]. Nevertheless, the overall lack of water quality in large sample hydrology datasets represents a critical bottleneck for advancing our understanding of water quality dynamics at large scales.

Here, we present an open-access dataset (named *Caravan-Qual*) that combines observations of 100 water quality constituents (Table 1) with corresponding streamflow records, catchment attributes and meteorological forcing time series. To this end, we leverage a range of national to global water quality datasets, together with both data and open-source software associated with the *Caravan* initiative.

The current dataset includes >70 million river water quality observations from 137,373 monitoring stations (across 85,358 unique TDX-Hydro LINKNOs[33]), in addition to streamflow data from 25,839 gauge stations. *Caravan-Qual* covers the time period 1980 – 2025 and includes data located across all continents, albeit with a strong spatial bias towards North America (55% of observations) and Europe (27%) (Figure 1). The number of observations across all water quality constituents have generally increased over time (the decline in recent years are an artifact of reporting lags), with physical (e.g. water temperature, electrical conductivity) and chemical parameters (e.g. pH, dissolved oxygen) dominating in terms of number of measurements (Figure 2). It should also be noted that water quality data records are highly discontinuous across all constituents, with ~25% of monitoring stations having observations from only a single day, though some longer records do exist for most constituents (Figure 3).

This work represents the first attempt to bring water quality data into the large-sample hydrology paradigm at global scale, integrating water quality observations with catchment attributes, meteorological forcing and co-located streamflow data, and is envisaged to facilitate research into topics including:

- Spatio-temporal analysis of river water quality dynamics at regional to global scales.
- Investigation of the empirical relationships between (constituent-specific) water quality responses and hydrological, meteorological and catchment characteristics.
- The development and evaluation of process-based, hybrid and data-driven water quality models across diverse hydrological and climatic conditions.

It is also hoped that the open-access nature and standardised format of *Caravan-Qual*, together with an introductory Jupyter notebook, helps lower barriers to entry for researchers interested in water quality, while simultaneously promoting transparency and reproducible science within the field.

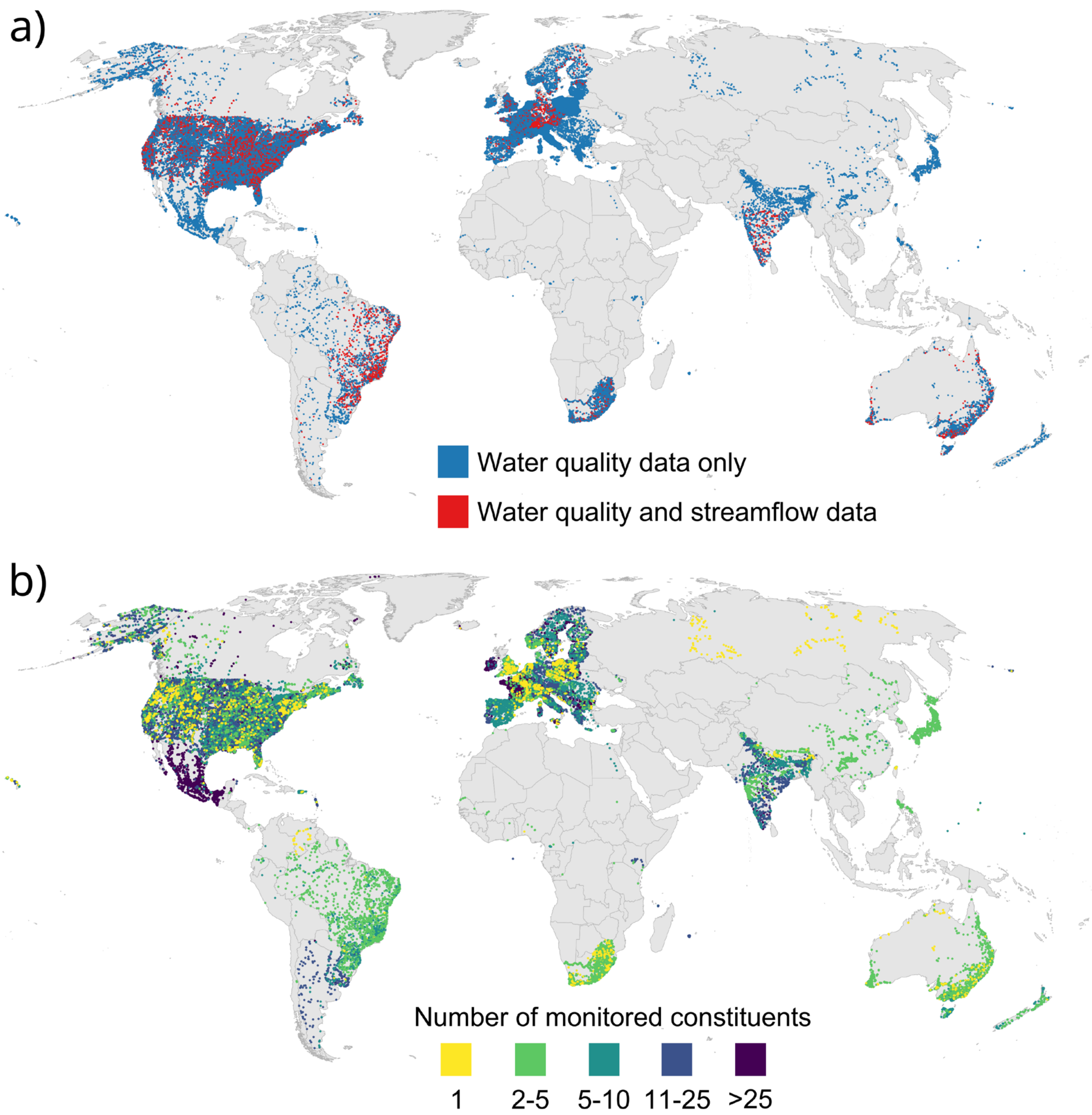

Figure 1. Spatial distribution of river water quality observations in *Caravan-Qual*. Panel **a)** displays the location of water quality monitoring stations, including and excluding streamflow data with a 10km distance threshold; whereas panel **b)** displays the number of water quality constituents monitored at each location.

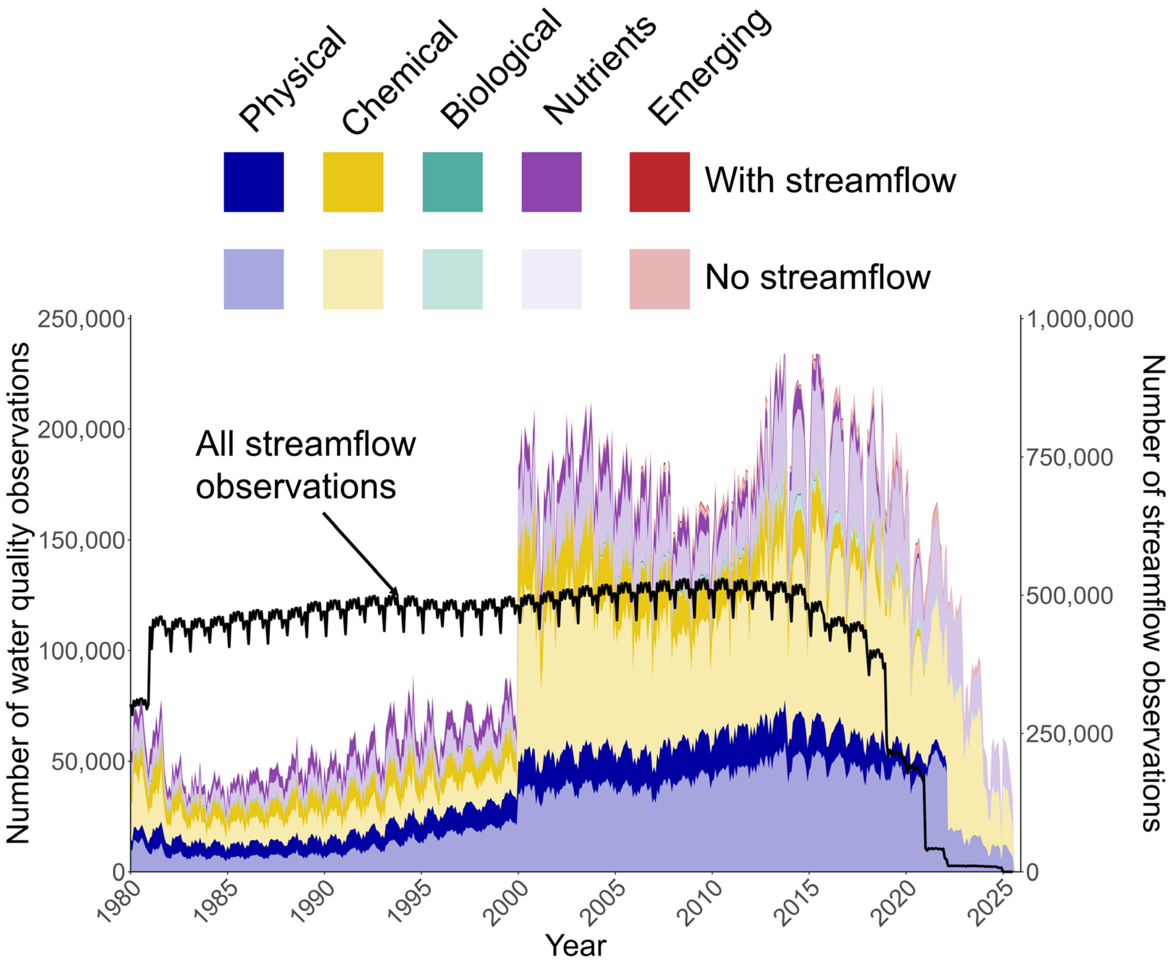

Figure 2. Temporal distribution of river water quality observations in the *Caravan-Qual* database. The plot displays the number of observations of water quality, with and without an associated streamflow measurement, aggregated per month across five key water quality groupings over 1980 – 2021 (see Table 1). The black line shows the total number of streamflow observations, aggregated per month.

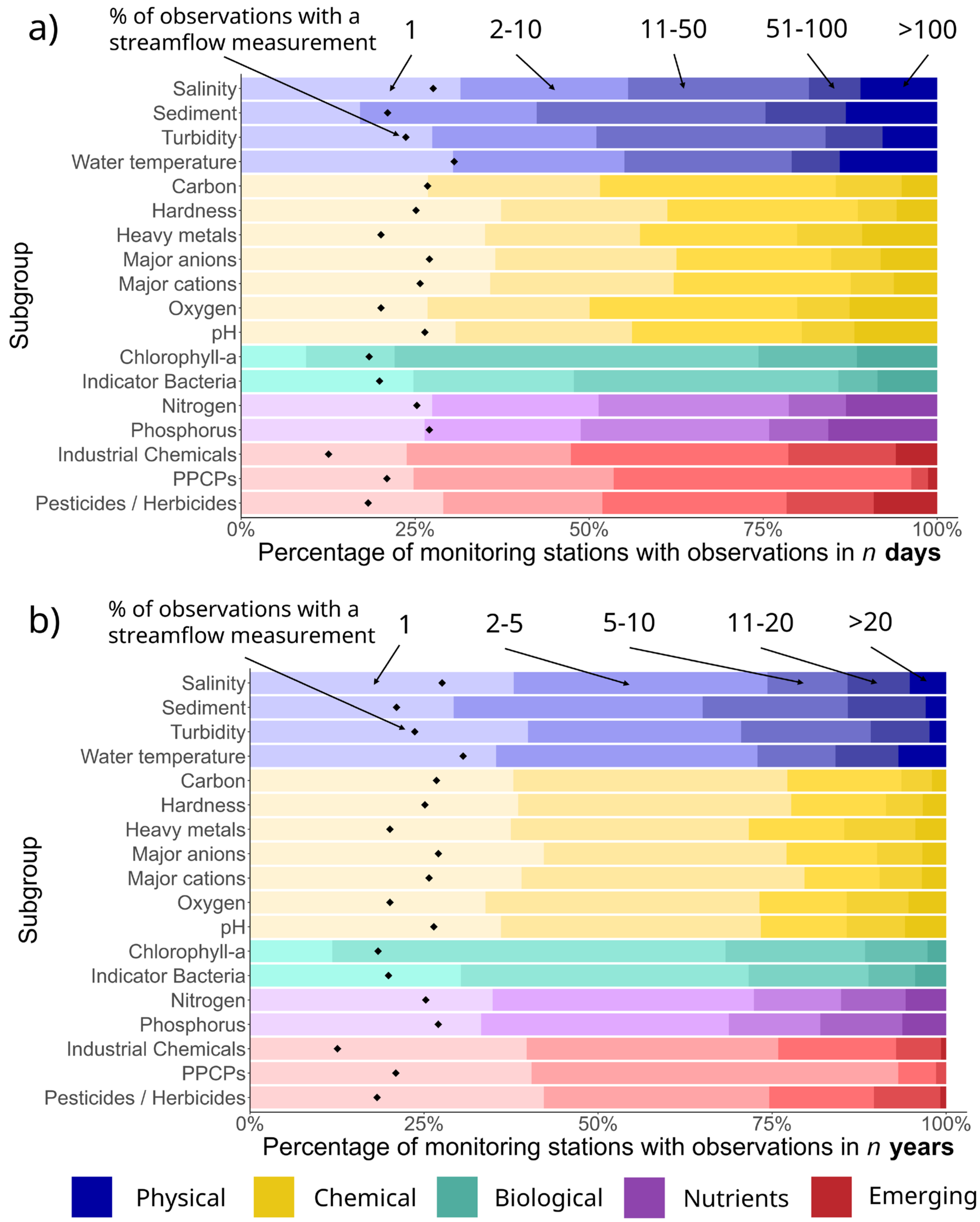

Figure 3. Aggregated statistics on the temporal availability of river water quality data per monitoring station in the *Caravan-Qual* database. Panel **a)** displays the percentage of river water quality monitoring stations with observations in *n* **days**, whereas panel **b)** displays the percentage of river monitoring stations with observations in *n* **years**, across 18 key water quality subgroups. Black dots display the percentage of observations that have an associated streamflow measurement (with a 10km distance threshold) per water quality subgroup.

2. Methods

2.1 Water quality data: sources

Water quality data in *Caravan-Qual* is compiled from several existing global, regional and national databases (Figure 4), all of which have fully open-access licenses that permit redistribution, including:

- **Global:** UNEP GEMS/Water Global Freshwater Quality Archive (GEMS)[27]
- **Global:** Global River Water Quality Archive (GRQA)[29]
- **Global:** GLObal River Chemistry (GLORICH) dataset[28], via[29]
- **Europe:** NORMAN EMPODAT[34]
- **Europe:** Waterbase WISE State of Environment (Waterbase)[26]
- **United States:** Water Quality Portal (WQP)[24]
- **China:** China National Environmental Monitoring Centre (CNEMC), via[25]
- **United Kingdom:** Department for Environment, Food and Rural Affairs (UK-EA)[35]
- **Canada:** Canadian Environmental Sustainability Indicators (CESI), via[29].
- **Switzerland:** National Surface Water Quality Monitoring Programme (NAWA), via[31]

A total of 100 water quality constituents are included, categorised into five groups and 18 sub-groups (Table 1), representing some of the most commonly monitored water quality constituents which are relevant for human activities and environmental health (Table 1). These constituents cover a large diversity in both source (e.g. primarily natural versus anthropogenic) and in-stream behaviour (e.g. conservative versus reactive transport). Note that these groupings serve only as an organisational framework; all individual constituents are included separately in *Caravan-Qual* with a unique constituent name and code (Table 1). The metadata of each water quality dataset was initially screened to identify the presence of and naming conventions used for each of the 100 target water quality constituents in *Caravan-Qual*, with all relevant observations systematically downloaded from each water quality dataset and mapped to a common nomenclature (Table 1).

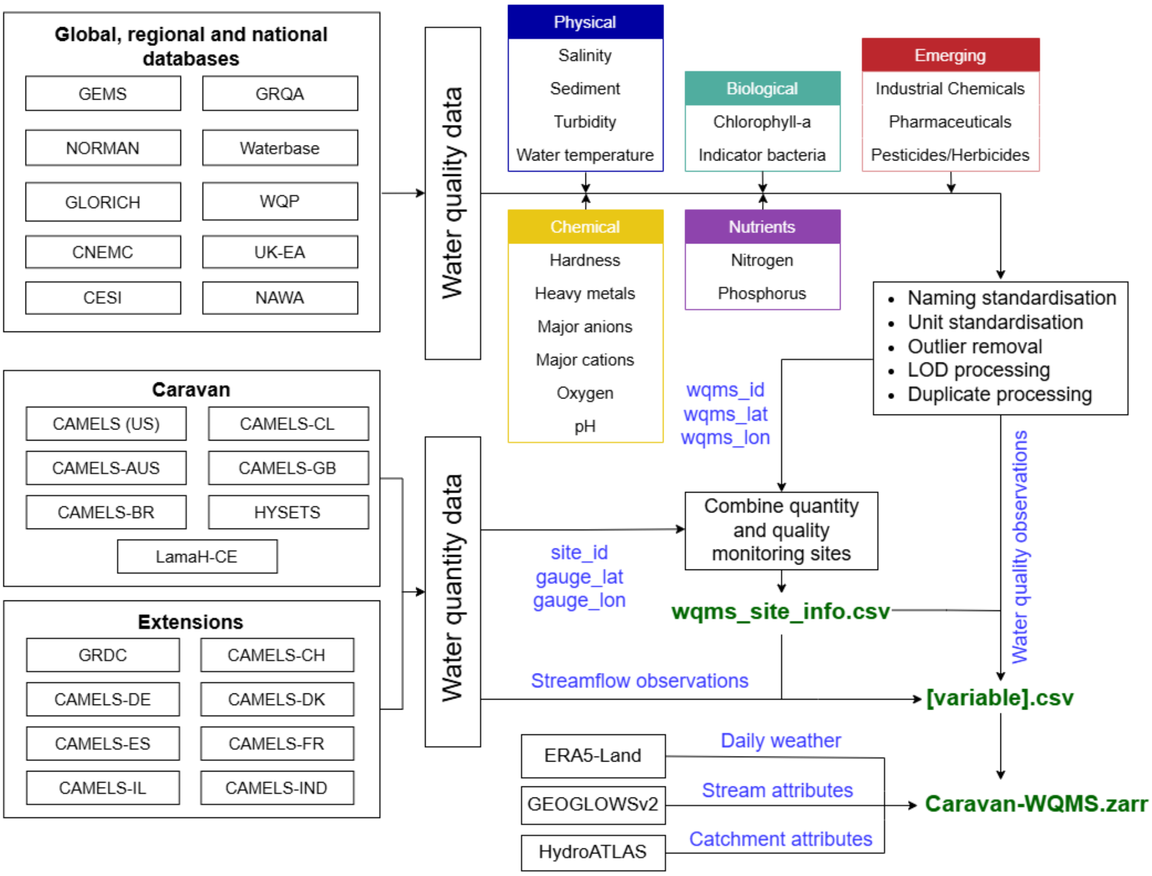

Figure 4. Methodological workflow for creating the *Caravan-Qual* database, highlighting the sources of water quality and streamflow data and the subsequent processing steps.

Table 1. Groupings, sub-groupings and constituents included in the *Caravan-Qual* dataset. Note that where constituents have multiple constituent codes, each code refers to a distinct form of that constituent.

Group	Subgroup	Constituent	Constituent code(s)	Units
Physical	Salinity	Electrical Conductivity	EC	uS/cm
		Total Dissolved Solids	TDS	mg/l
	Sediment	Total Suspended Solids	TSS	mg/l
	Turbidity	Turbidity	Turbidity	NTU
	Water temperature	Water Temperature	TEMP	deg C
Chemical	Carbon[1]	Dissolved Carbon	DC; DIC; DOC	mg/l
		Particulate Carbon	PC; PIC; POC	mg/l
		Total Carbon	TC; TIC; TOC	mg/l
	Hardness	Total Hardness	Hardness-Tot	mg/l
	Heavy metals[2]	Arsenic	As-Dis; As-Tot	ug/l
		Cadmium	Cd-Dis; Cd-Tot	ug/l
		Chromium	Cr-Dis; Cr-Tot	ug/l
		Copper	Cu-Dis; Cu-Tot	ug/l
		Iron	Fe-Dis; Fe-Tot	ug/l
		Lead	Pb-Dis; Pb-Tot	ug/l
		Mercury	Hg-Dis; Hg-Tot	ug/l
		Nickel	Ni-Dis; Ni-Tot	ug/l
		Potassium	K-Dis; K-Tot	mg/l
		Zinc	Zn-Dis; Zn-Tot	ug/l
	Major anions[2]	Chloride	Cl-Dis; Cl-Tot	mg/l
		Fluoride	F-Dis; F-Tot	mg/l
		Hydrogencarbonate	HCO3	mg/l
	Major cations[2]	Calcium	Ca-Dis; Ca-Tot	mg/l
		Magnesium	Mg-Dis; Mg-Tot	mg/l
		Manganese	Mn-Dis; Mn-Tot	ug/l
	Oxygen[3]	Biochemical oxygen demand	BOD; BOD5; BOD7	mg/l
		Chemical oxygen demand	COD; CODCr; CODMn	mg/l
		Dissolved oxygen	DO	mg/l
		Dissolved oxygen saturation	DOSAT	%
	pH	pH	pH	-
Biological	Chlorophyll-a	Chlorophyll-a	Chl-a	ug/l
	Indicator bacteria	Escherichia Coli	EColi	cfu/100ml
		Fecal Coliform	FC	cfu/100ml
		Total Coliforms	TotColi	cfu/100ml

Nutrients	Nitrogen[4]	Dissolved nitrogen	DIN; DKN; DON	mg/l
		Particulate nitrogen	PN; PON	mg/l
		Total nitrogen	TAN; TDN; TIN; TKN; TN; TON	mg/l
		Nitrite	NO2N	mg/l
		Nitrate	NO3N	mg/l
		Nitrate-nitrite	NOxN	mg/l
		Ammonia-nitrogen	NH3N	mg/l
		Ammonium nitrogen	NH4N	mg/l
	Phosphorus[5]	Dissolved phosphorus	DIP; DOP	mg/l
		Particulate phosphorus	POP	mg/l
		Total phosphorus	TDP; TIP; TOP; TP; TPP; TRP	mg/l
Emerging	Industrial Chemicals	Benzene	Benzene	ug/l
		PFOA	PFOA	ug/l
		PFOS	PFOS	ug/l
		Trichloroethene	Trichloroethene	ug/l
	Pharmaceuticals and personal care products (PPCPs)	Amoxicillin	Amoxicillin	ug/l
		Atenolol	Atenolol	ug/l
		Caffeine	Caffeine	ug/l
		Carbamazepine	Carbamazepine	ug/l
		Diclofenac	Diclofenac	ug/l
		Ibuprofen	Ibuprofen	ug/l
		Metoprolol	Metoprolol	ug/l
		Naproxen	Naproxen	ug/l
		Propranolol	Propranolol	ug/l
		Sulfamethoxazole	Sulfamethoxazole	ug/l
		Triclosan	Triclosan	ug/l
	Pesticides/ Herbicides	Atrazine	Atrazine	ug/l

[1]Various forms of carbon are included: DC = dissolved organic carbon; DIC = dissolved inorganic carbon; DOC = dissolved organic carbon; PC = particulate carbon; PIC = particulate inorganic carbon; POC = particulate organic carbon; TC = total carbon; TIC = total inorganic carbon; TOC = total organic carbon ; [2]The extensions "-Dis" and "-Tot" in constituent codes are used to distinguish between dissolved and total forms, respectively, of chemical constituents (where applicable) ; [3]BOD5 and BOD7 refer to the biological oxygen demand after 5 and 7 days, respectively; [4]Various forms of nitrogen are included: DIN = dissolved inorganic nitrogen; DKN = Dissolved Kjeldahl Nitrogen; DON = Dissolved Organic Nitrogen; PN = Particulate Nitrogen; PON = Particulate Organic Nitrogen; TAN = Total Ammonia Nitrogen; TDN = Total Dissolved Nitrogen; TIN = Total Inorganic Nitrogen; TKN = Total Kjeldahl Nitrogen; TN = Total Nitrogen; TON = Total Organic Nitrogen; [5]Various forms of phosphorus are included: DIP = Dissolved Inorganic Phosphorus; DOP = Dissolved Organic Phosphorus; POP = Particulate Organic Phosphorus; TDP = Total Dissolved Phosphorus; TIP = Total Inorganic Phosphorus; TOP = Total Organic Phosphorus; TP = Total Phosphorus; TPP = Total Particulate Phosphorus; TRP = Total Reactive Phosphorus.

2.2 Water quality data: processing and harmonisation

Obtaining water quality data for many constituents and from multiple sources presents processing and harmonisation challenges, including (aforementioned) naming conventions, but also related to reporting units, outliers and detection limits[29,36].

Data processing was implemented in two stages. Individual datasets are first pre-processed independently to remove observations without specific geographical (e.g. latitude and longitude) and temporal (e.g. DD/MM/YYYY) information. Measurement units are harmonised to a target unit per water quality constituent (Table 1), following the procedure described for GRQA[29], while observations with missing or incompatible units were dropped.

All (remaining) observations are subsequently combined into a unified dataset for post-processing. Individual water quality monitoring sites are identified on the basis of unique coordinate pairs (at 5 decimal places), and were assigned a unique id ("wqms_id"). Outliers are detected and removed, initially for all sites based on physically plausible limits (defined per water quality constituent), followed by application of the interquartile range method (IQR, with a threshold of 5xIQR) to each water quality monitoring site independently (only where n_obs > 10). This conservative threshold was chosen to remove extreme anomalies but preserve legitimate high values, given that 1) quality control procedures were likely already applied to source datasets; and 2) an additional filtering to physically plausible limits is also applied. Observations reported as below detection limits (left censored data; i.e. "<") were processed using Regression on Order Statistics (ROS) for stations meeting data availability requirements (at least five detected values; less than 50% of the measurements below detection limit) and otherwise substituted with half of the detection limit[37]. Finally, exact duplicates (i.e. identical wqms_id, date and observation) were removed, with distinct observations from the same wqms_id and date averaged to a single representative daily value. Technical validation of the procedure for processing and harmonising water quality data is provided in Section 4.1.

This structure enables modular updates to *Caravan-Qual,* for example, the dataset can be extended with additional water quality or streamflow data without having to reprocess the whole dataset.

2.3 Streamflow data: sources

Streamflow data in *Caravan-Qual* is compiled by aggregating observations contained in *Caravan*[18] with various datasets that have subsequently been released (Figure 4). The open-access datasets that are included are:

- CAMELS (US)[4], via[18]
- CAMELS-AUS[5], via[18]
- CAMELS-BR[6], via[18]
- CAMELS-CL[7], via[18]
- CAMELS-GB[11], via[18]
- HYSETS[15], via[18]
- LamaH-CE[16], via[18]
- LamaH-Ice[17]
- GRDC-Caravan[19]
- CAMELS-CH[14], via[31]
- CAMELS-CZ[38]
- CAMELS-DE[10]
- CAMELS-DK[8]
- CAMELS-ES[13]
- CAMELS-FR[9]
- CAMELS-IL[39]
- CAMELS-IND[12]

Diverging from *Caravan*, streamflow data is converted to $m^3 s^{-1}$ (opposed to mm day^{-1}) as volumetric discharge is arguably more suitable for water quality applications (e.g. load estimation, concentration-discharge relationships). Nevertheless, catchment areas are included in metadata to allow users to easily convert between units if desired.

2.4 Integrating water quality and streamflow data

Water quality monitoring stations are spatially matched to streamflow gauges to integrate water quality and streamflow observations (Figure 5). To this end, a multi-directional river network was derived for GEOGLOWSv2[40], which itself is derived from the TDX-Hydro dataset[33], to allow both upstream and downstream traversal. An additional variable ("merged_LINKNO") was computed from GEOGLOWSv2, which provides a common identifier for connected river segments ("LINKNO") where there is no associated change in stream order ("strmOrder"). Both water quality monitoring stations and gauge stations were snapped to the nearest point on this river network, constrained to the "LINKNO" whose catchment polygon contained the station coordinates. Water quality monitoring stations are paired with the nearest (upstream or downstream) streamflow gauge on the same "merged_LINKNO", with along-stream distance included in the metadata to support flexible distance filtering. Technical validation of the approach for matching water quality and streamflow observations is provided in Section 4.2.

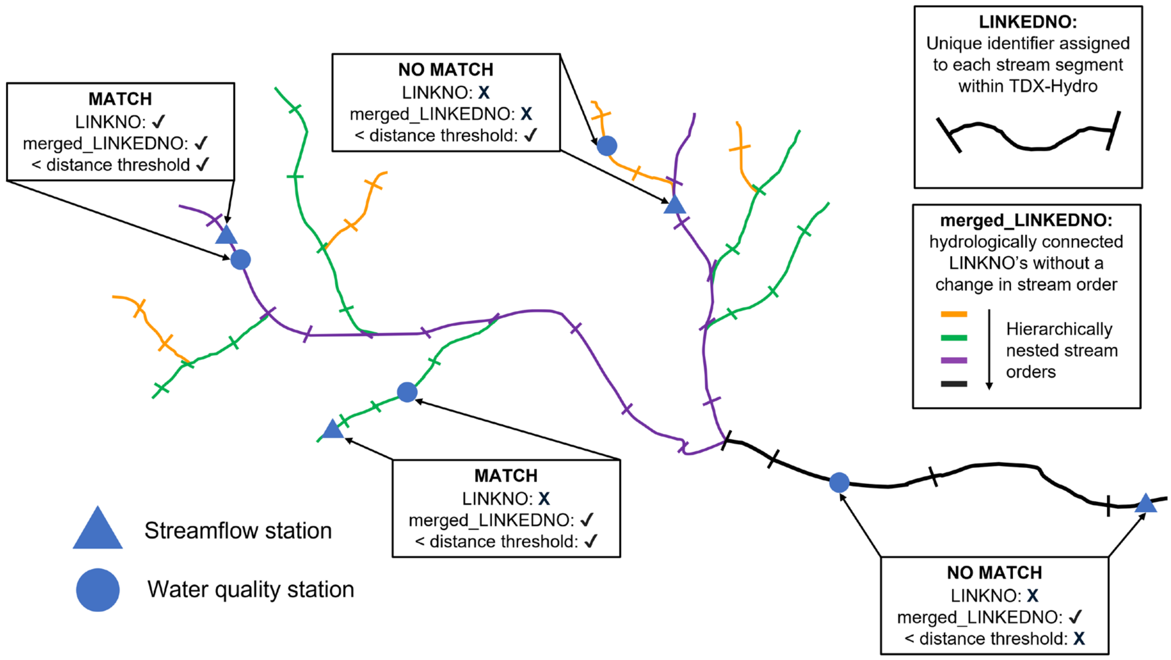

Figure 5. Methodological workflow for matching water quality monitoring stations with streamflow gauges.

2.5 Deriving meteorological forcing and catchment attributes

Meteorological forcings and catchment attributes are derived for all water quality monitoring stations using open-source software developed for *Caravan*[18], which requires lumped upstream catchment polygons per monitoring station. As upstream polygons are not commonly provided in water quality datasets, these were derived using GEOGLOWSv2[40] by identifying the LINKNO catchment polygon containing each water quality monitoring station and then subsequently aggregating all upstream contributing polygons through recursive network traversal. Additional stream attributes are also derived from GEOGLOWSv2 (Table 2). Technical validation of the delineation of lumped upstream catchments is provided in Section 4.3.

Meteorological forcing is derived from ERA5-Land[20] for 23 variables (Table 3), while catchment attributes are derived from HydroATLAS[21] (Table 4). The approaches for deriving these data is extensively described and validated by *Caravan*[18], with the only deviation being that potential evaporation is estimated from ERA5-Land variables using the FAO's Penman-Monteith equation (instead of directly using ERA5-Land potential evaporation) due to data quality issues[41].

Table 2. Stream attributes included in *Caravan-Qual*. All variables are processed directly from GEOGLOWSv2, which itself is derived from TDX-Hydro.

Stream attributes	Description
LINKNO	A river ID number unique to the TDXHydro delineation.
strmOrder	The Strahler stream order
DSContArea	The total drainage area upstream of the most downstream point (i.e. the outlet) of this segment.
TDXHydroRegion	The original TDX regional group number
TopologicalOrder	The topological order of a stream
LengthGeodesicMeters	Geodesic length (in meters) of the river segment
TerminalLink	The TDXHydroLinkNo of the eventual outlet
musk_k	The Muskingum k parameter
musk_x	The Muskingum x parameter

Table 3. Meteorological variables included in *Caravan-Qual*. All variables are processed directly from ERA5-Land using open-source *Caravan* code, with the exception of potential evaporation which is estimated using the FAO's Penman-Monteith equation.

Feature (variable name)	Aggregation	Unit
Air temperature (temperature_2m)	Daily min/max and mean	°C
Dew point temperature (dewpoint_temperature_2m)	Daily min/max and mean	°C
Eastward wind component (u_component_of_wind_10m)	Daily min/max and mean	ms^{-1}
Net thermal radiation at the surface (surface_net_thermal_radiation)	Daily min/max and mean	Wm^{-2}
Northward wind component (v_component_of_wind_10m)	Daily min/max and mean	ms^{-1}
Potential evaporation (potential_evaporation)	Daily sum	mm/day
Precipitation (total_precipitation)	Daily sum	mm/day
Shortwave radiation (surface_net_solar_radiation)	Daily min/max and mean	Wm^{-2}
Surface pressure (surface_pressure)	Daily min/max and mean	*kPa*

Table 4. Catchment attributes included in *Caravan-Qual*. All variables are processed directly from HydroATLAS using open-source *Caravan* code.

Group	Description (HydroATLAS name)	Aggregation	Unit
Hydrology	Natural discharge (dis_m3_p[mn, mx,yr])	annual min/max/mean	m^3 s^{-1}
	Land surface runoff (run_mm_syr)	spatial mean of sub-basin runoff	*mm*
	Inundation extent (inu_pc_s[mn, mx, lt])	annual min/mean and long-term max	%
	Limnicity - percent lake area (lka_pc_sse)	spatial extent	%
	Lake Volume (lkv_mc_usu)	at reach pour point	10^6 m^3
	Reservoir volume (rev_mc_usu)	at reach pour point	10^6 m^3
	Degree of regulation (dor_pc_pva)	index at reach pour point	
	River area (ria_ha_ssu)	at reach pour point	*hectares*
	River volume (riv_tc_ssu)	at reach pour point	10^3 m^3
	Groundwater table depth (gwt_cm_sav)	spatial mean	*cm*
Physiography	Elevation (ele_mt_s[av, mn, mx])	spatial mean/min/max	*m* above sea level
	Terrain slope (slp_dg_sav)	spatial mean	° (x10)
	Stream gradient (sgr_dk_sav)	mean of reach segments	*dm*/*km*
Climate	Climate zones from GEnS (clz_cl_smj)	spatial majority	classes (n = 18)
	Climate strata from GeNS (cls_cl_smj)	spatial majority	classes (n = 125)
	Air temperature (tmp_dc_s[01–12, mn, mx, yr])	monthly mean, annual mean/min/max	°*C* (x10)
	Precipitation (pre_mm_s[01–2, yr])	monthly mean, annual mean	*mm*
	Potential evapotranspiration (pet_mm_s[01–12, yr])	monthly mean, annual mean	*mm*
	Actual evapotranspiration (aet_mm_s[01–12, yr])	monthly mean, annual mean	*mm*

	Global aridity index (ari_ix_sav)	spatial mean	index value (x10)
	Climate moisture index (cmi_ix_s[01–12, yr])	monthly mean, annual mean	index value (x10)
	Snow cover extent (snw_pc_s[01–12, mx, yr])	monthly mean, annual max/mean	% cover
Land Cover	Land cover classes (glc_cl_smj)	spatial majority	classes (n = 22)
	Land cover extent (glc_pc_s[01–22])	spatial mean	% cover
	Potential natural vegetation classes (pnv_cl_smj)	spatial majority	classes (n = 15)
	Potential natural vegetation extent (pnv_pc_s[01–15])	spatial mean	% cover
	Wetland classes (wet_cl_smj)	spatial majority	classes (n = 12)
	Wetland extent (wet_pc_s[01–09, g1, g2])	spatial mean	% cover & grouping
	Forest cover extent (for_pc_sse)	spatial mean	% cover
	Cropland extent (crp_pc_sse)	spatial mean	% cover
	Pasture extent (pst_pc_sse)	spatial mean	% cover
	Irrigated area extent (equipped) (ire_pc_sse)	spatial mean	% cover
	Permafrost extent (prm_pc_sse)	spatial mean	% cover
	Protected area extent (pac_pc_sse)	spatial mean	% cover
	Terrestrial biomes (tbi_cl_smj)	spatial majority	classes (n = 14)
	Terrestrial ecoregions (tec_cl_smj)	spatial majority	classes (n = 846)
	Freshwater major habitat types (fmh_cl_smj)	spatial majority	classes (n = 13)
	Freshwater ecoregions (fec_cl_smj)	spatial majority	classes (n = 426)
Soils & Geology	Clay fraction in soil (cly_pc_sav)	spatial mean	%
	Silt fraction in soil (slt_pc_sav)	spatial mean	%
	Sand fraction in soil (snd_pc_sav)	spatial mean	%

	Organic carbon content in soil (soc_th_sav)	spatial mean	tonnes/hectare
	Soil water content (swc_pc_s[01–12, yr])	monthly mean, annual mean	%
	Lithological classes (lit_cl_smj)	spatial majority	classes (n = 16)
	Karst area extent (kar_pc_sse)	spatial mean	% cover
	Soil erosion (ero_kh_sav)	spatial mean	*kg/hectare/yr*
Anthropogenic	Population count (pop_ct_usu)	at reach pour point	count (thousands)
	Population density (ppd_pk_sav)	spatial mean	people per km^2
	Urban extent (urb_pc_sse)	spatial mean	% cover
	Nighttime lights (nli_ix_sav)	spatial mean	index value (x100)
	Road density (rdd_mk_sav)	spatial mean	m/km_2
	Human footprint (hft_ix_s[93,09])	spatial mean for 1993 & 2009	index value (x100)
	Gross domestic product (gdp_ud_sav)	spatial mean	USD ($)
	Human development index (hdi_ix_sav)	spatial mean	index value (x1000)

3. Data records

The full *Caravan-Qual* dataset[42] is available at https://doi.org/10.24416/UU01-S8QW8O. *Caravan-Qual* is provided in Zarr format, a cloud-optimised format that enables chunked compression, lazy loading and rapid querying of spatial or temporal subsets[43]. The dataset is structured as follows:

- Caravan-Qual.zarr
    - **Dimensions:** time (daily timesteps from 1980-01-01 to 2025-09-30); wqms_id (water quality monitoring station identifier); gauge_id (streamflow gauge identifiers) and LINKNO (river reach identifiers).
    - **Station metadata:** spatial metadata per wqms_id (wqms_lat, wqms_lon, country_name, hydrobasin_level12, merged_LINKNO) and gauge_id (gauge_lat, gauge_lon).
    - **Observational data**: water quality observations for multiple parameters (see constituent codes in Table 1), indexed by wqms_id and time. Streamflow observations (streamflow), indexed by gauge_id and time.
    - **Catchment and river network attributes:** static catchment attributes derived from HydroATLAS (see Caravan[18]) and stream attributes from GEOGLOWSv2 (see Table 2). Indexed by LINKNO.
    - **Weather data**: daily meteorological data from ERA5-Land (see Table 3), indexed by LINKNO and time.
- Caravan-Qual_linkages.parquet
    - A metadata table (stored in Parquet format) that provides linkages between water quality monitoring stations and their corresponding streamflow gauge identifiers, catchment attributes and meteorological forcing. This file also contains detailed metadata per water quality monitoring station, combined and per individual water quality constituent, including the number of observations, start and end date of monitoring and the number of observation years. This structure enables efficient querying of the entire dataset (based, for example, on geographical, temporal or water quality criteria) without iterating through all data files.
- wqms_site_info.csv
    - Basic metadata for each water quality monitoring station, indexed by station identifier (wqms_id). Contains geographic coordinates (wqms_lat, wqms_lon), the associated river segment identifier (LINKNO), in addition to the co-located streamflow gauge identifier (gauge_id) and distance between the monitoring station and gauge (gauge_distance_km).
- auxiliary/
    - Contains all data required for extending *Caravan-Qual*, such as the GEOGLOWSv2[40], HydroATLAS[21] and the raw (unprocessed) water quality data.

For broader accessibility, a lite version of *Caravan-Qual* is available: https://doi.org/10.5281/zenodo.17787066[44]. This includes the water quality observations, in addition to all catchment and streamflow attributes, but linked to monthly (instead of daily) weather variables. Furthermore, all water quality observations are provided here as comma separated values per constituent (i.e. [constituent].csv), including linked streamflow measurements (in $m^3 s^{-1}$, within a 10km distance threshold).

4. Technical validation

4.1 Processing water quality data

Extensive processing was applied to the raw water quality observations that comprise *Caravan-Qual*, including the removal of duplicate observations, averaging of multiple observations with different values from the same day, outlier detection and removal and procedures for dealing with left-censored observational data (see Section 2.2). To assess the impact of these processing steps on the final dataset, the proportion of observations affected by each processing step is displayed (Figure 6). Furthermore, the impact of these processing steps on water quality time series is illustrated for example monitoring stations (Figure 7).

Across all subgroups, 90% of raw water quality observations are retained, with ~4% of observations excluded due to exact duplicate removal, ~1% due to outlier detection and 5% of observations removed when averaging multiple observations from the same date. Retention rate across the different subgroups was relatively stable, ranging from 83.2% (Herbicides) to 96.1% (Chlorophyll-a). Approximately 7% of observations were flagged as below detection limits, with ~2% of observations processed using the ROS method and ~5% using direct substitution. The need for this processing was highly unequal across water quality subgroupings, being particularly high for industrial chemicals (~65% of observations), pesticides/herbicides (~58%) and pharmaceuticals (~31%), as well as certain heavy metals (e.g. Mercury, Lead and Chromium).

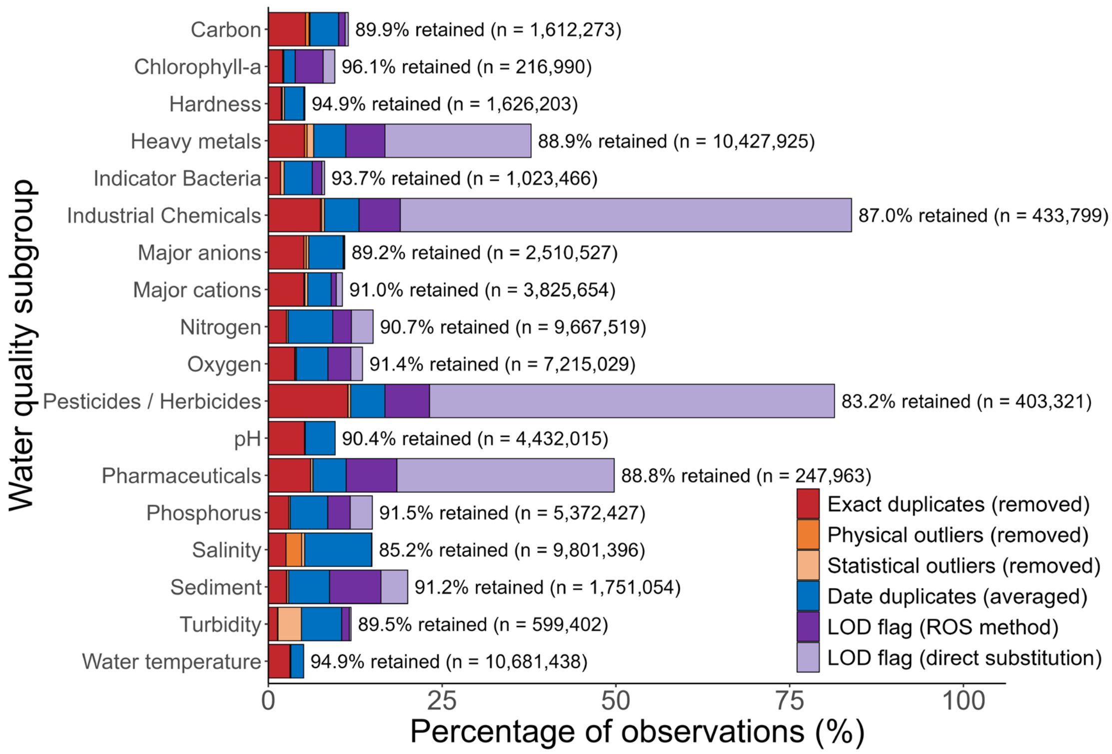

Figure 6. Validation of the water quality processing procedure in *Caravan-Qual*, displaying statistics (aggregated per water quality subgroup) of the percentage of observations which underwent processing steps (e.g. duplicate processing, outlier removal). The percentage stated per bar refers to the percentage of raw water quality data that is retained in the processed version, with the number in brackets displaying the number of observations per water quality subgroup after processing.

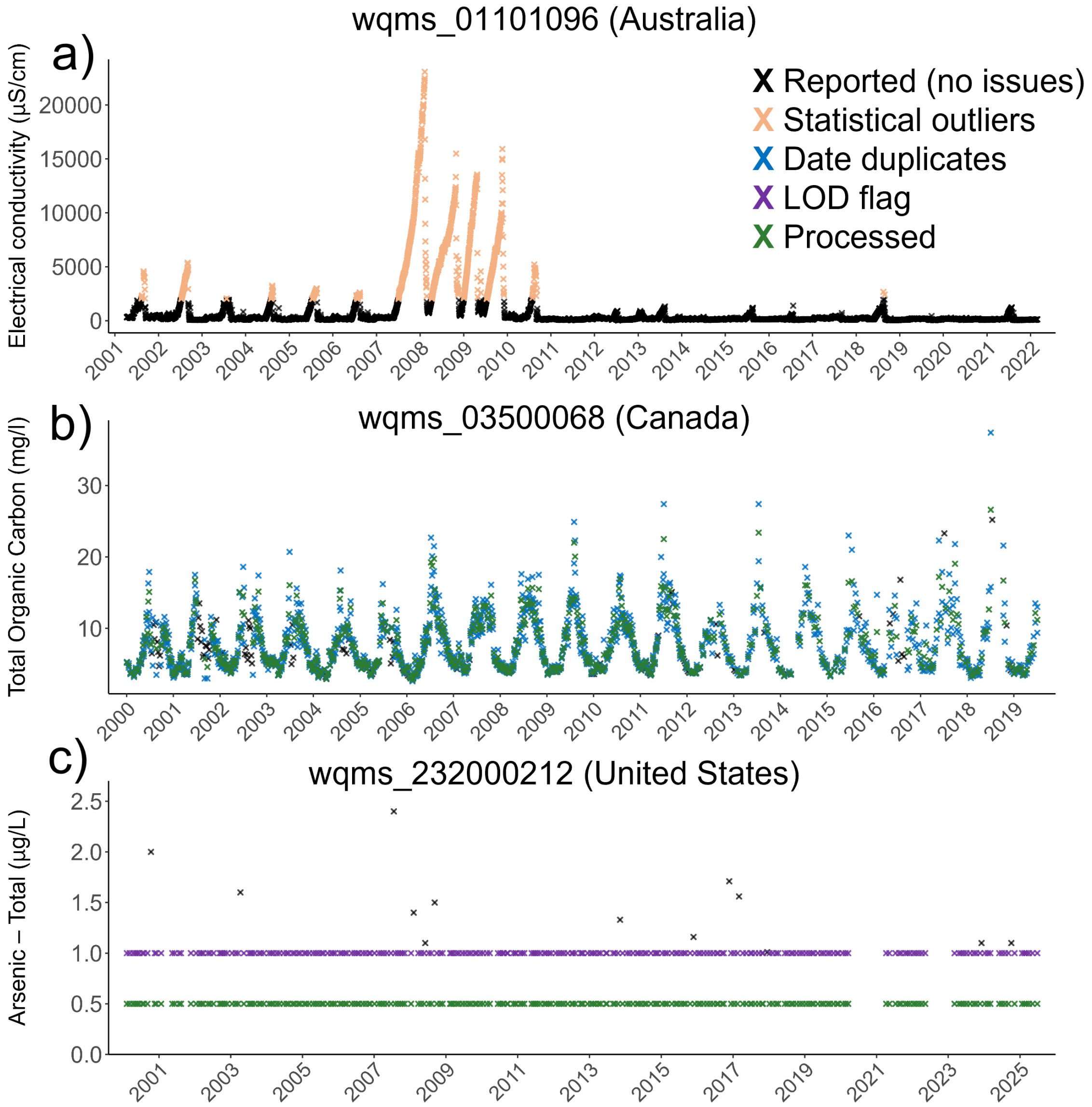

Figure 7. Validation of the water quality processing procedure in *Caravan-Qual*, displaying example time-series plots for individual water quality monitoring stations where different processing steps were applied, including **a)** the removal of outliers; **b)** the processing of multiple observations with different values on the same date; and **c)** the processing of left-censored (i.e. observations reported with a Limit of Detection [LOD] flag) water quality data.

4.2 Delineation of lumped catchments

To validate the accuracy of the catchment delineation method developed for *Caravan-Qual*, a spatial comparison against catchment boundaries from proximate streamflow gauges is used – given that co-located water quality monitoring stations and streamflow gauges should represent (largely) identical upstream catchment areas.

9,237 water quality monitoring station-streamflow gauge pairs within a 100m threshold are evaluated (Figure 8). Delineated catchment areas for water quality stations showed strong agreement with reported streamflow gauge areas (R^2 = 0.93), with a median area ratio (i.e. streamflow gauge area/water quality station area) of 0.98 (Figure 8a). Furthermore, the spatial overlap of catchments are high, with a median Intersection over Union (IoU) value of 0.94 (Figure 8b). 79% of stations (7,319) have a IoU value exceeding 0.8, with 9% (805) having a value less than 0.4. Overall, these results demonstrate that the method developed for *Caravan-Qual* can reliably delineate catchment boundaries for water quality monitoring stations, which are subsequently used for the derivation of catchment characteristics and meteorological data.

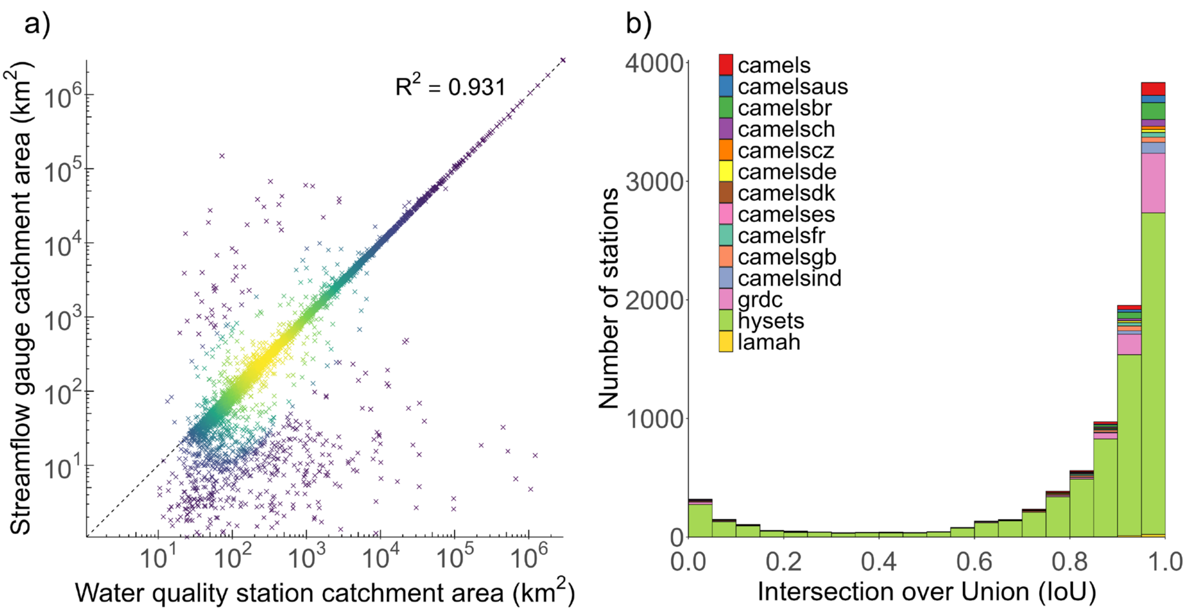

Figure 8. Validation of catchment delineation for water quality monitoring stations using co-located streamflow gauges. Panel **a)** displays a comparison of catchment areas for water quality monitoring stations (*Caravan-Qual* approach) and streamflow gauges (reported in streamflow datasets) located within 100m. The dashed line represents 1:1 agreement, with point density displayed using colour gradient. Panel **b)** displays the distribution of Intersection over Union (IoU) values quantifying spatial overlap between delineated and reported catchment polygons.

4.3 Linking water quality (wqms_id) and streamflow (gauge_id) observations

To validate the procedure for matching water quality monitoring stations with streamflow gauges in *Caravan-Qual*, we cross-checked our assignments for 631 water quality stations previously matched in CAMELS applications (516 from *CAMELS-Chem*[14]; 115 from *CAMELS-CH-Chem*[31]) (Figure 9). Our automated approach achieved a 99.7% agreement rate with those datasets, successfully identifying the same water quality-gauge station pairs in 629 of 631 cases. Just two water quality stations that were matched with streamflow gauges in *CAMELS-Chem* were not matched in our approach, while no water quality stations were matched to a different gauge station than as reported in *CAMELS-Chem* or *CAMELS-CH-Chem* (Figure 9). While the vast majority of these water quality monitoring stations are co-located with streamflow gauges (547 stations within 1m distance), water quality stations were also successfully matched with streamflow gauges at less proximate distances, including 46 water quality monitoring stations located between 1-10km from the gauge station. Overall, this high level of agreement demonstrates the reliability of our approach for linking water quality monitoring stations and streamflow gauges, and therefore is applicable to the broader *Caravan-Qual* dataset. Nevertheless, we provide users with the flexibility to define their own distance thresholds for matching water quality stations with streamflow gauges. Table 5 demonstrates how streamflow coverage varies with distance threshold, from 9.8% of stations (19.7% of observations) matched within a 1km radius to 32.7% of stations (42.8% of observations) with a more permissive threshold of 50km.

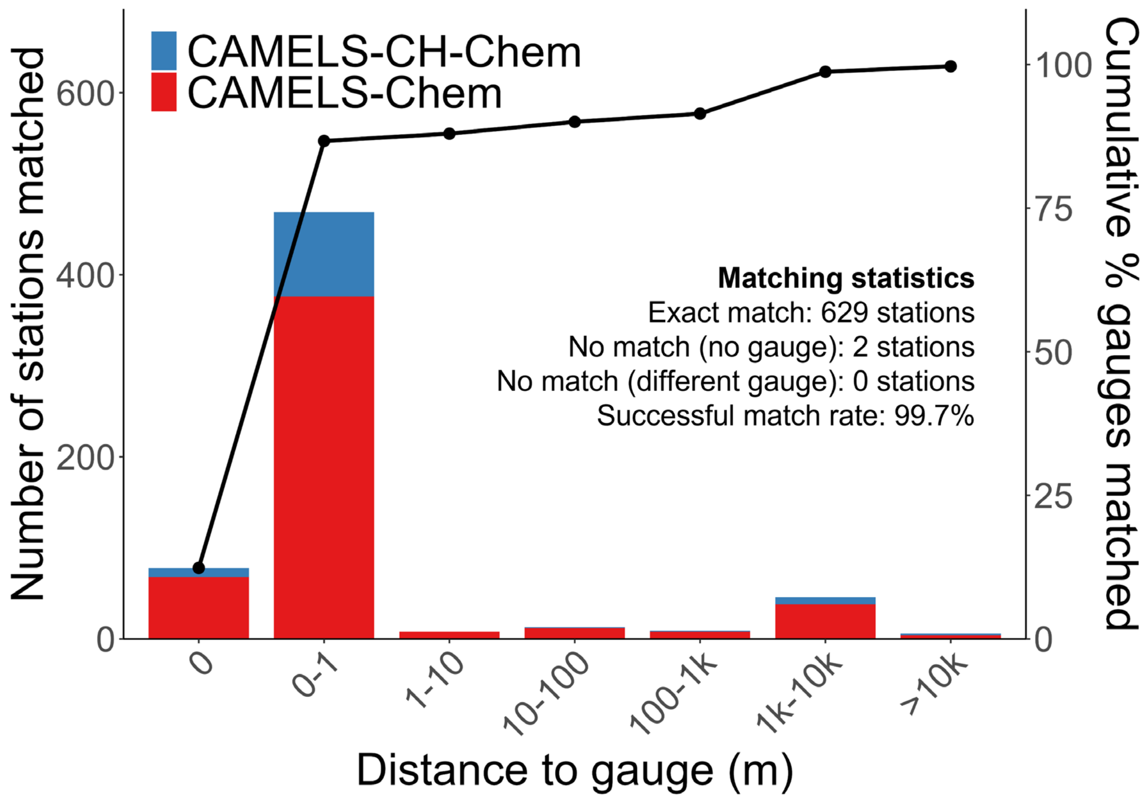

Figure 9. Validation of water quality monitoring station to gauge station matching procedure developed for *Caravan-Qual* against reference datasets (*CAMELS-Chem* and *CAMELS-CH-Chem*).

Table 5. Linkages between water quality and streamflow stations and observations when considering different distance thresholds for matching.

Distance	Water quality stations with matched gauge station (%)	Water quality observations with matched streamflow (%)
< 1km	9.9%	19.7%
< 5km	16.0%	25.9%
<10km	21.5%	31.1%
<25km	29.1%	38.8%
<50km	32.8%	42.9%

Usage notes

- Significant efforts have been made into retrieving water quality and streamflow data from across the world, but certain regions (e.g. Sub-Saharan Africa, Middle East and North Africa) are still severely underrepresented. *Caravan-Qual* is designed in such a way to be extendable, either with new streamflow measurements or water quality observations, and it is our hope that the dataset can continue to grow as more data becomes available with an open and redistributable license.
- The dataset is accompanied by an interactive Jupyter notebook to provide a user-friendly entry point for researchers seeking to leverage this resource. This can be accessed at: https://github.com/SustainableWaterSystems/Caravan-Qual.
- To a large degree, the validity of the water quality data is dependent upon the individual procedures and reporting practices from the monitoring institutes. Water quality data are subject to multiple sources of uncertainty, including analytical measurement error, transcription and reporting mistakes, and intentional censoring of values.

Code availability

The code that was used to produce the *Caravan-Qual* dataset is available through Zenodo[44] and in a project homepage at: https://github.com/SustainableWaterSystems/Caravan-Qual. The original *Caravan* code is available through Zenodo[45] and in a project homepage at: https://github.com/kratzert/Caravan/.

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Author contributions

The research was conceptualized by ERJ, who also led the data processing, analysis, interpretation and wrote the manuscript. FK processed the meteorological data and participated in planning the scope and structure of the dataset. MTHvV supervised the project and secured the funding. All authors contributed towards and approved the manuscript.

Competing interests

The contact author has declared that none of the authors has any competing interests.

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