

Danish groundwater $p\text{CO}_2$: a multi-decadal national data set

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Abstract

This data set provides a comprehensive assessment of groundwater partial pressure CO_2 ($p\text{CO}_2$) across Denmark, spanning more than three decades (1988–2024). Using groundwater chemistry data from the national borehole database, Jupiter, $p\text{CO}_2$ levels were calculated and compared using two distinct approaches: (1) geochemical modelling via PHREEQC; and (2) simplified carbonate equilibria using only pH and alkalinity. While the latter is widely used for its simplicity, the PHREEQC method offers more accurate estimates by accounting for ionic strength and complexation. Despite Denmark's extensive public archive of groundwater chemistry, $p\text{CO}_2$ values have remained largely unavailable to the scientific community due to data complexity. This data set addresses this data gap through rigorous cleaning and the flagging of potentially contaminated samples to ensure high data fidelity. The resulting long-term, large-scale overview is essential for elucidating the role of groundwater in the carbon cycle and its spatiotemporal dynamics. Furthermore, these data establish critical baseline conditions necessary for monitoring and protecting groundwater resources in the context of the future CO_2 injection and storage in deep geological reservoirs.

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Abbreviations

DGU: Danish Geological Survey
DOC: Dissolved organic carbon
GRUMO: National Groundwater Monitoring Program
IC: Ion Chromatography
ICP-OES: Inductively Coupled Plasma – Optical Emission Spectroscopy
LOD: limit of detection
MS: Mass Spectrometry
MST: Ministry of Environment
 $p\text{CO}_2$: partial pressure of CO_2
TA: measured total alkalinity

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Tabular abstract

Geographical coverage	Denmark
Temporal coverage	1989–2024
Subject(s)	Geochemistry and geochronology, Soils and biogeochemistry
Data format(s)	Calculated geochemical data in xlsx format.
Sample collection and analysis	Calculated using PHREEQC and carbonate equilibria based on groundwater chemistry data
Parameters	Field measured pH, alkalinity, % charge balance error, $p\text{CO}_2$, concentrations of B, NH_4 , Si, Total P, DOC and HS^-
Related publications	None
Potential application(s) for these data	Defining baseline of groundwater $p\text{CO}_2$ prior to CO_2 injection for geological storage. Basic research on groundwater's role in terrestrial carbon cycle.

1 Introduction

Although sensors for direct measurement of aquatic partial pressure of CO_2 ($p\text{CO}_2$) are available, their high cost limits their employment, particularly in large-scale national monitoring networks. Instead, $p\text{CO}_2$ is generally derived indirectly from water chemistry. A common and simple approach involves estimating $p\text{CO}_2$ from alkalinity and pH using the following equation (Eq. 1):

$$p\text{CO}_2 = \frac{[\text{HCO}_3^-] \cdot 10^{-\text{pH}}}{K_H \cdot K_{a1}} \quad (1)$$

where K_H represents Henry's Law Constant for CO_2 (3.4×10^{-2} mol/L/atm at 25°C), and K_{a1} is the first dissociation constant of carbonic acid ($10^{-6.35}$ at 25°C).

This approach assumes that the measured total alkalinity (TA) is predominantly composed of bicarbonate (HCO_3^-) and carbonate (CO_3^{2-}) ions, and the contributions of non-carbonic alkalinity such as N-alkalinity (NH_4^+), S-alkalinity (HS^- and S^{2-}), Si-alkalinity (HSiO_3^- and SiO_3^{2-}), B-alkalinity (B(OH)_4^-), P-alkalinity (H_3PO_4 , HPO_4^{2-} , and PO_4^{3-}), and organic acid (Org^-) are negligible (Eq. 2; Stumm & Morgan 1996):

$$\begin{aligned} \text{Total Alkalinity (TA)} = & \left[\text{HCO}_3^- \right] + 2 \left[\text{CO}_3^{2-} \right] + \left[\text{OH}^- \right] - \left[\text{H}^+ \right] \\ & + \left[\text{NH}_3 \right] + \left[\text{HS}^- \right] + 2 \left[\text{S}^{2-} \right] + \left[\text{HSiO}_3^- \right] \\ & + 2 \left[\text{SiO}_3^{2-} \right] + \left[\text{B(OH)}_4^- \right] - \left[\text{H}_3\text{PO}_4 \right] \\ & + \left[\text{HPO}_4^{2-} \right] + 2 \left[\text{PO}_4^{3-} \right] + \left[\text{Org}^- \right] \quad (2) \end{aligned}$$

While this simplification is valid for most neutral fresh-water conditions, it can lead to an overestimation of $p\text{CO}_2$ in environments where non-carbonic alkalinity is high, such as organic-rich, acidic conditions or highly reduced conditions (Stumm & Morgan 1996; Abril *et al.* 2015).

To mitigate these limitations, geochemical modelling such as PHREEQC (Parkhurst & Appelo 2013) is employed. Unlike the simple carbonate equilibria approach, PHREEQC treats alkalinity as an input parameter that includes both carbonate and non-carbonate alkalinity. It computes $p\text{CO}_2$ comprehensively by accounting for ionic strength, ion speciation, charge, and mass balance. Furthermore, the calculated charge balance error can serve as diagnostic tool for analytical quality, ensuring the robustness of the resulting estimates (Pötter *et al.* 2021).

In Denmark, despite the availability of extensive, long-term groundwater chemistry records, the carbonate system has historically received limited attention, as monitoring efforts have prioritised agricultural contamination. Furthermore, the inherent complexity of the national database requires specific expertise to extract reliable $p\text{CO}_2$ estimates. This study presents a nationwide $p\text{CO}_2$ data set for Danish groundwater calculated via PHREEQC, provided alongside estimates derived from (Eq. 1) for comparative analysis.

2 Data sources

All available groundwater chemistry data were retrieved from the national borehole database, Jupiter (Hansen & Pjetursson 2011; Fig. 1), in April 2024. The data set primarily comprises samples collected under the Danish National Groundwater Monitoring Program (GRUMO; Thorling *et al.* 2025), supplemented by the Groundwater Quality Control of abstraction wells for public water supply program (Boringskontrol; Miljø og Ligestillingsministeriet 2025) and various ad-hoc independent projects.

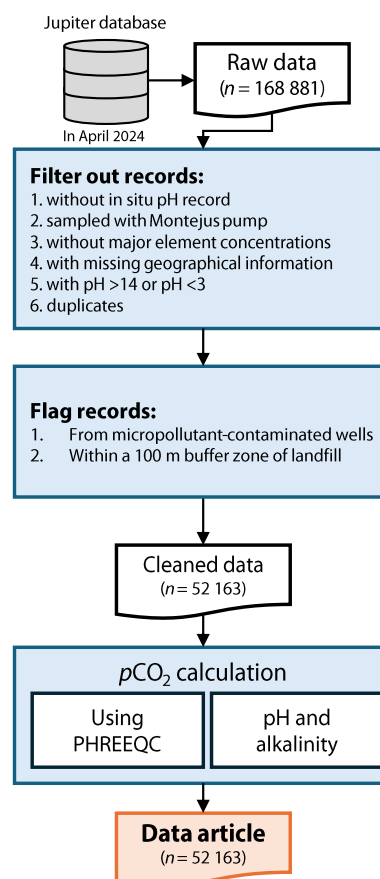


Fig. 1 Flow chart of data processing and $p\text{CO}_2$ calculation.

3 Analytical methods

Groundwater samples were analysed by various accredited commercial laboratories around Denmark. While analytical techniques have evolved over the past three decades, data continuity and quality have been maintained through standardised national protocols and regulations for groundwater sampling and laboratory analysis (Thorling 2023; Miljøstyrelsen 2025).

In accordance with these standards, pH is typically measured on-site using a closed flow cell connected to the pump and hose to ensure stability and minimise atmospheric CO_2 exchange. Alkalinity is determined by potentiometric acid titration, including Gran titration or other standardised titrimetric methods. For elemental analysis, major and minor elements as well as trace metals are analysed using Inductively Coupled Plasma – Optical Emission Spectroscopy (ICP-OES) or Mass Spectrometry (MS). Anions are quantified using Ion Chromatography (IC). Additionally, dissolved silicate and sulphide are determined using colorimetric and spectrophotometric methods, respectively.

4 Data cleaning and quality control

The extracted data set underwent a rigorous filtering process to ensure the reliability of the groundwater $p\text{CO}_2$

calculations. Initially, records lacking TA measurements and erroneous in-situ pH values (defined as <3 or >14) were excluded. A primary concern in $p\text{CO}_2$ estimation is the high susceptibility of groundwater to degassing during sampling, as it is typically supersaturated relative to the atmosphere. The sampling method significantly influences this risk. Specifically, the Montejus pump, which is efficient for narrow or short-screened wells, uses pressurised N_2 gas to lift water. This method can strip dissolved CO_2 from the sample. Consequently, all samples collected via Montejus pumps were removed from the data set.

The data set was further refined by removing records based on the following criteria:

1. Absence of major cations (Ca^{2+} , Mg^{2+} , Na^+ , and K^+) and anions (NO_3^- , SO_4^{2-} , and Cl^-) analyses
2. Missing geographical coordinates or depths to the screen intervals
3. Duplicates

Finally, environmental contamination, particularly from organic pollutants, can substantially affect the inorganic system in groundwater. Rather than excluding these samples, we implemented a flagging system to alert users to potential biases. This allows researchers to decide whether to include these records based on their specific study goals. Samples were flagged if they were collected from boreholes identified by Danish Ministry of Environment (MST) as impacted by micro-organic pollutants or located within a 100 m buffer zone from a known landfill. After following this quality control and flagging process, the final cleaned data set comprised 52 163 records (Fig. 1).

5 $p\text{CO}_2$ calculations

5.1 Geochemical modelling (PHREEQC)

Geochemical modelling was performed using PHREEQC to calculate $p\text{CO}_2$ based on the comprehensive groundwater chemistry data in the cleaned data set. Beyond TA and pH, the model incorporated nutrient species (NO_3^- , NO_2^- , NH_4^+ and total P), major ions (e.g., Ca^{2+} , Mg^{2+} , Na^+ , K^+ , Cl^- , SO_4^{2-} , Si) and a suite of minor ions (e.g., B, Sr^{2+} , Ba^{2+}), and trace metals (e.g., Fe, Al, Mn). The temperature was set at 10°C to represent Danish groundwater conditions.

While non-carbonate alkalinity elements such as silicate, sulphide and B were measured at much lower frequencies than major elements, their impact on the carbonate system was assessed as insignificant. Given that nearly all groundwater samples exhibited a pH below nine, where dissolved Si exists primarily as neutral silicic acid, the contribution of the Si-alkalinity is negligible. Similarly, the concentrations of B, S, NH_4^+ and P were significantly lower than TA, confirming their minimal contributions to TA (Fig. S1 in Supplementary Material).

Our PHREEQC calculations did not include organic acids because GRUMO does not include organic acids in the analyses. Since dissolved organic carbon (DOC) is part of the program, we estimated the contribution of organic acids to TA based on an empirical relationship (Eq. 3) between DOC and total organic acid (HA_T) in natural waters (Morel *et al.* 1993):

$$\text{HA}_T (\text{eq L}^{-1}) = 10^{-2} \times \text{DOC} \left(\text{g} \cdot \text{C} \cdot \text{L}^{-1} \right) \quad (3)$$

While DOC in Danish groundwater varied between non-detectable and 970 mg/L (mean: 2 mg/L), the ratio of estimated HA_T to TA was less than 0.05 in 97% of the samples (Fig. S1), indicating insignificant contributions of organic acids in most cases.

Before calculation, values reported below the limit of detection (LOD) were converted to half of the detection limit (LOD/2). To handle the large-scale national data set, a custom Python routine was developed to automate the PHREEQC calculations (Dideriksen 2025).

5.2 $p\text{CO}_2$ estimates using carbonate equilibria

For comparison with the PHREEQC results, $p\text{CO}_2$ was estimated using the simple carbonate equilibria approach, assuming TA is dominated by carbonate species. In this simplification, HCO_3^- is derived from TA and the measured pH is follows:

$$\text{TA} \approx [\text{HCO}_3^-] + 2[\text{CO}_3^{2-}] + [\text{OH}^-] - [\text{H}^+] \quad (4)$$

Given that CO_3^{2-} is related to HCO_3^- by the second dissociation constant (K_{a2}),

$$[\text{CO}_3^{2-}] = \frac{K_{a2} \times [\text{HCO}_3^-]}{[\text{H}^+]} \quad (5)$$

$$\text{HCO}_3^- = \frac{\text{TA} - [\text{OH}^-] + [\text{H}^+]}{1 + \frac{2 \times K_{a2}}{[\text{H}^+]}} \quad (6)$$

Once the HCO_3^- concentration was determined, $p\text{CO}_2$ was calculated (using Eq. 1). All equilibrium constants ($K_H = 5.1 \times 10^{-2}$; $K_{a1} = 10^{-6.45}$; $K_{a2} = 10^{-10.49}$) were adjusted to 10°C (Harned & Scholes 1941; Harned & Davis 1943; National Institute of Standards and Technology [NIST] 2025).

6 Data description and main features

6.1 Data structure

The data set is structured to provide both the calculated $p\text{CO}_2$ values and the necessary geospatial and groundwater chemical metadata for future uses. Each record is characterised by five primary data categories: (1) identifiers; (2) spatial and temporal information;

(3) groundwater chemistry metadata; (4) calculated $p\text{CO}_2$ values; and (5) quality flags (Table 1).

For identifiers, the data set provides two well identification numbers (DGUNR and BORID), screen identifier (INDTNR), and unique sample IDs (PROVEID). A unique feature of the Jupiter database is the dual-identification system for boreholes. Each borehole is assigned with both a Danish Geological Survey (DGU) number (DGUNR) and a Borehole ID (BORID). The DGU number is official and traditional nomenclature, and is the standard for searching the Jupiter database; however, the inclusion of dots and spaces makes it prone to formatting errors during data processing. Whereas BORID is a unique integer-based serial number assigned internally by the Jupiter database. In this data set, the BORID is used as primary key for data management and joining tables to ensure computational integrity, while the DGUNR is retained to ensure compatibility with official records and manual database queries.

For the spatial and temporal information, X and Y coordinates (XUTM32EUREF89 and YUTM32EUREF89) within the EUREF89 UTM 32N system, depths to the screen top and bottom (INDTTOP and INDTBUND, respectively), and sampling dates (PROVEDATO) were provided (Table 1). Groundwater chemistry metadata include in-situ pH (pH) and TA (HCO_3^-). Where available, concentrations of non-carbonate alkalinity elements such as B, NH_4^+ , Si, P, DOC and HS^- were included. Below-LOD values are shown as negative of LODs. $p\text{CO}_2$ values estimated using both approaches – using PHREEQC

($p\text{CO}_2_{\text{atm}}$) and the carbonate equilibria ($p\text{CO}_2_{\text{atm_CS}}$) – were also included in this file. Finally, quality flags such as landfill buffer zones (Landfill_Flag) and microorganic pollutants (MD_MFS_Flag) were flagged as '1'. The percentage errors of charge balance (pct_err) from the PHREEQC calculation are also provided in the data set as a measure of analytical quality.

6.2 Charge balance error as a data quality indicator

Water is electrically neutral; therefore, the charge of solutes in water should be balanced. When the charge is not balanced, this can be an indication of errors in data such as analytical uncertainty or mistakes in entry or recording. In general, $\pm 5\%$ of charge balance errors are considered as an acceptable range (Pötter *et al.* 2021), and 92% of our data ($n = 48\,502$) showed charge balance error within this range (Fig. 2a). Data outside this range should be used with caution.

6.3 $p\text{CO}_2$ calculated using PRHEEQC vs. carbonate equilibria

Our data set presents $p\text{CO}_2$ values calculated with both PHREEQC and the carbonate equilibria (Eq. 1). Although these two values show a strong positive correlation, the values estimated using the carbonate equilibria were about 22% higher than those by PHREEQC (Fig. 2b). This consistent difference may be attributed to ion-pairing of HCO_3^- with other major cations such as Ca^{2+} and Na^+ ,

Table 1 Attributes and their descriptions of the groundwater $p\text{CO}_2$ data.

Column in database	Description	Units	Type
DGUNR	DGU number. Official names of boreholes	-	Text
BORID	Borehole id on the Jupiter database	-	numerical
INDTNR	Screen id number	-	numerical
XUTM32EUREF89	X coordinate in the UTM zone 32 projection, reference to the European Reference Frame 1989 (ETSR89/EUREF89)	m	numerical
YUTM32EUREF89	Y coordinate in the UTM zone 32 projection, reference to the European Reference Frame 1989 (ETSR89/EUREF89)	m	numerical
INDTTOP	Depth to the top of the screen	m	numerical
INDTBUND	Depth to the bottom of the screen	m	numerical
PROVEID	Sample id number	-	numerical
PROVEDATO	Sampling date	-	Date
Landfill_Flag	Within a 100 m buffer zone from landfill sites. 1 = within and 0 = outside	-	Logical
MD_MFS_Flag	Contaminated with micropollutants. 1 = polluted and 0 = not polluted	-	Logical
$p\text{CO}_2_{\text{atm}}$	$p\text{CO}_2$ calculated using PHREEQC	atm	numerical
HCO_3^-	Alkalinity measured by the Gran titration method	mg/L	numerical
pH	In-situ pH measurement	-	numerical
B	Boron concentration	$\mu\text{g/L}$	numerical
NH_4^+	Ammonium + Ammonia concentration	mg/L	numerical
Si	Si concentration	mg/L	numerical
Total_P	Total P concentration	mg/L	numerical
DOC	Dissolved organic carbon	mg/L	numerical
HS^-	HS^- concentration	mg/L	numerical
pct_err	Percent error of charge balance	%	numerical
$p\text{CO}_2_{\text{atm_CS}}$	$p\text{CO}_2$ from carbonate system equilibria	atm	numerical

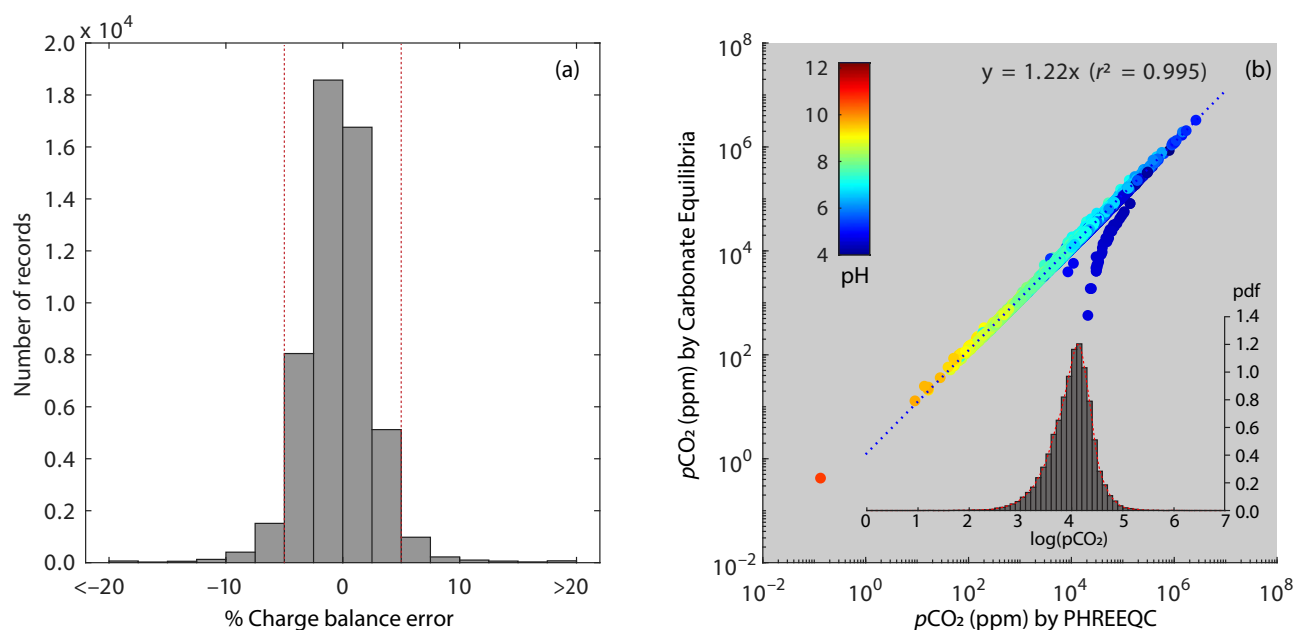


Fig. 2 Histogram of % charge balance error (a) and comparison of $p\text{CO}_2$ (ppm) values calculated by PHREEQC vs. carbonate equilibria after excluding % charge balance errors outside the threshold ($\pm 5\%$; b). The red vertical lines in (a) mark the threshold. A histogram of $\log(p\text{CO}_2, \text{ppm})$ calculated by PHREEQC is shown in (b). The Y-axis of the histogram was normalised to a probability density function (pdf).

which PHREEQC accounts for but the simplified equation does not.

A specific group of samples showed greater differences between two methods. These samples were characterised by low pH (4–5) and alkalinity values below the LOD (1 mg/L as HCO_3^-). For these samples, $p\text{CO}_2$ was estimated by converting TA values to LOD/2, and they are shown as negative of LODs in the data set. Further, at these low values, non-carbonate contributions to alkalinity that may or may not have been measured could potentially be more important—for example DOC or HPO_4^{2-} . So, values with $\text{TA} < \text{LOD}$, marked as negative values, are highly uncertain and should be used with caution.

6.4 An overview of groundwater $p\text{CO}_2$

The mean of groundwater $p\text{CO}_2$ in Danish aquifer was 9772 ppm ($\log[p\text{CO}_2, \text{ppm}] = 3.99$) after excluding data with the charge balance errors outside the $\pm 5\%$ range (Fig. 2b). This is approximately 24 times higher than the atmospheric level (Fig. 2b). Our data also showed that groundwater $p\text{CO}_2$ varies over seven orders of magnitude (<1 to 2 640 200 ppm). Lower than 1 ppm values ($n = 3$) were found under highly alkaline conditions (pH = 10.7–12.2) with moderate to high TA (96–542 mg/L as HCO_3^-). Six samples were estimated to have $p\text{CO}_2$ greater than 1 atm. These samples are predominantly from the landfill buffer zones with a pH range 5–6 (mean: 5.4), an alkalinity range 205–1880 mg/L as HCO_3^- (mean: 632), and a DOC range 1–68 mg/L (mean: 15). According to the empirical relationship between

HA_T and TA (Eq. 3), the organic acid contribution to TA was estimated to be less than 2%. Therefore, these exceptionally high $p\text{CO}_2$ values may result from active microbial processes in the contaminated sites, leading to the buildup of gas pressure within the aquifers.

The groundwater $p\text{CO}_2$ data covers the entire country (Fig. 3a) with a depth range of 0–378 m (Fig. 3b). Most records are from shallow groundwater (<50 m below the land surface), and the frequency of measurement decreases with increasing depth (Fig. 3b). Groundwater $p\text{CO}_2$ concentrations generally decreased with increasing depth (Fig. 3b). This trend may be because the aquifer transitions into a closed system, where CO_2 is consumed during silicate and carbonate weathering processes without being replenished from the soil zone.

In total, 13 501 screens are included in the data set. Due to multiple reformation and revision of the GRUMO, the temporal coverage varies significantly across the country. As the monitoring program primarily focuses on agricultural contamination, parameters such as nitrate are sampled more frequently than carbonate species. The sample frequency for TA was higher during the 1990s, with samples collected one to four times a year. In the following years, the frequency decreased to once every 1–3 years. Water supply wells are typically sampled every 3–5 years, and wells at polluted sites are often sampled only for a short period. Approximately 38% of the screens were sampled for only a single year across the entire period (Fig. 3c). Only 147 screens have been measured 20 or more times for TA over the monitoring periods, and these measurements do not

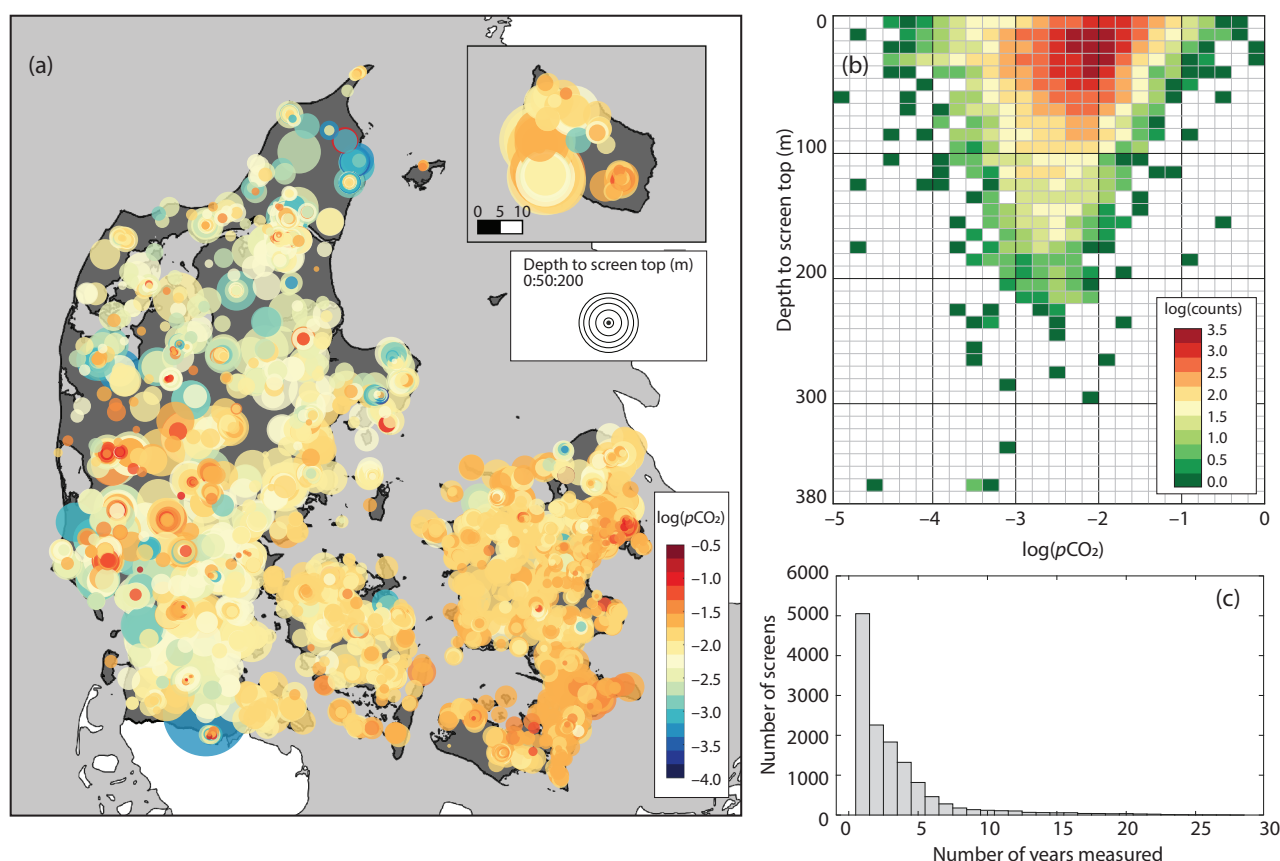


Fig. 3 National map of groundwater $p\text{CO}_2$ (atm) by PHREEQC (a). The map shows screens measured at least five times over the entire monitoring period. The $p\text{CO}_2$ values are shown by colour. The circle size shows the depth to the top of the screen. (b) Heatmap of $p\text{CO}_2$ (atm) with depth to the screen top. (c) histogram of number of years measured at the screen level.

necessarily occur in consecutive years. This heterogeneity reflects the historical evolution of the monitoring network and its sampling density over the past three decades.

6.5 Data applications and implications

Inland waters such as lakes, streams, and wetlands have emerged as a significant yet often unaccounted CO_2 source of terrestrial ecosystems (Raymond *et al.* 2013). While groundwater represents one of the largest terrestrial carbon storages and is typically characterised by high $p\text{CO}_2$ compared to the atmosphere (Curtis Monger *et al.* 2015), its specific contribution to the global carbon cycle has not received sufficient attention. This national, long-term data set of groundwater may contribute to a better understanding of the role groundwater plays in terrestrial carbon cycles as well as the transfer of carbon from land to the ocean.

In addition, as the use of the deep subsurface for applications such as carbon capture and storage (CCS) develops rapidly, it is critical to establish robust baselines of groundwater chemistry. These baselines are essential for monitoring the integrity of captured CO_2

and protecting groundwater as a valuable drinking water resource. Groundwater $p\text{CO}_2$ may be a primary indicator of activities affecting groundwater quality. Therefore, our data play an important role in defining natural variabilities of groundwater $p\text{CO}_2$, which is necessary to detect anomalous signals and potential leakage in groundwater systems.

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Additional information

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Author contributions

HK: conceptualisation, methodology, formal analysis, visualisation, writing-original draft, and writing-review & editing; LT: Data curation, methodology, and writing-review & editing; RJ: Conceptualisation, methodology, supervision, and writing-review & editing

Competing interests

The authors declare no competing interest.

Additional files

Three supplementary files are available at <https://doi.org/10.22008/FK2/UHONBF>. These include: Groundwater_pCO₂.xlsx, Readme.txt and Supplementary_Figure (Figure S1).

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