

Reviewer 1

Dear Reviewer,

We would like to extend our thanks for your constructive review of our manuscript. Below we respond point by point to each of your comments. All changes in the manuscript and supplemental material documents are written in purple for clarity.

Comment 1: Use of colors in Figures, in particular Fig 1-2-3 : these figures are not very accessible to readers with color-vision deficiencies. Modifying the symbols used or working with more clearly distinguishable symbol fills offer an easy fix. See suggestions in Figure preparation guidelines offered on the EGU journals' website.

We thank the reviewer for pointing out this out. We revised all figures to improve accessibility for readers with color-vision deficiencies. Specifically, we replaced the original colour scheme with a colourblind-safe palette based on the Okabe-Ito design, as it ensures clear visual separation among regions. In addition, marker contrast was enhanced through consistent use of black edges. These changes were applied consistently throughout the manuscript.

Comment 2: L91 mentions that much of the presented have been exploited in previous publications, but Table 1 does not provide citations for many of the cruises where data were collected – does that mean e.g. that data from cruise 1-13 have not been published previously? This is not quite clear.

To clarify, Table 1 lists references that correspond to previously archived components of individual cruise datasets, rather than all studies that have used or interpreted these data. Data from many earlier cruises contributed to scientific publications but have not previously been archived as complete, quality-controlled datasets. The text has been revised to make this distinction explicit.

Comment 3: L184: total nitrogen: is this really total (particulate + dissolved) nitrogen, or should this be total dissolved nitrogen (sum of inorganic DIN species and DON)? The methods information in the supplement does not make me any wiser, since it just mentions it was measured on a TOC analyser but not whether or not samples were filtered and if so, on what type of filters

Samples were filtered through 0.45 μm (Millipore polycarbonate (MA) or Nuclepore cellulose nitrate membrane) filters prior to analysis and, therefore, the reported nitrogen concentrations represent the dissolved fraction (i.e. total dissolved nitrogen (DIN + DON)). The manuscript and the supplemental material have been revised to include the filtration procedures and terminology.

Comment 4: it might be useful to mention for each of the parameters which fraction of the data were flagged as questionable, and whether there are any patterns in this (e.g. from certain cruises, certain cruise days, etc.)

We agree that summarizing the distribution of quality flags improves transparency. We added a new table (Table 5) summarizing the number and proportion of flagged values (flag = 3) for each parameter across the dataset. No systematic patterns associated with specific cruises, regions, or sampling periods were identified. Flagged values are generally isolated and likely reflect individual outliers rather than systematic issues.

Comment 5: L327: “indicating the presence of unidentified alkalinity”: yes, or: a problem with the pH data or issues with carbonate system equilibrium constants used? The discussion on carbonate system inconsistencies is an important one, and also points out the difficulty in applying a systematic quality control procedure as done for the other parameters.

The text was revised to clarify that discrepancies in the carbonate system may arise from multiple sources, including uncertainties in pH measurements, the choice of equilibrium constants, and potential contributions from organic alkalinity, rather than attributing them solely to “unidentified alkalinity” (Fradette, 2025).

several of the plots show a couple of data that visually really jump out, and for which it's not clear to me why they were not flagged. For example:

Comment 6: Figure 8, DSi versus nitrate for the upper SLE has one datapoint well above the rest of the data.

This data point has now been assigned a QC flag of 3 (questionable) and removed from the figure for clarity.

Comment 7: Figure 9, AOU vs nitrite for Sffjord: one sample point deviates from all others.

This data point has now been assigned a QC flag of 3 (questionable) and removed from the figure for clarity.

Comment 8: Figures 12-13-16: 2 datapoints somewhat above and below 100m depth at Saguenay Fjord jump out with markedly higher salinity, TA, and $d^{18}\text{O-H}_2\text{O}$. That is internally consistent, but still very odd. Could this point to mislabeling or evaporation during sample storage?

These data points are internally consistent across multiple parameters but remain anomalous relative to surrounding observations. As the origin of these deviations cannot be definitively determined (potential sampling or analytical artefacts), their flag was left as is as it passed our systematic QC analysis.

Comment 9: Figure 13 pH_TS at Gulf of St-Lawrence: one exceptionally low pH seems highly unlikely.

This data point has now been assigned a QC flag of 3 (questionable) and removed from the figure for clarity.

Comment 10: Figure 11 and corresponding text: provide regression info for water isotope relationships (rather than mentioning the slope is close to 8)

The revised manuscript includes regression statistics for the water isotope relationships. Specifically, the slope, intercept, and R^2 are now reported in the main text.

References

Fradette, C.: Evaluating Data Quality of Coastal Spectrophotometric pH Measurements: Implications for Ocean Acidification and Ocean Alkalinity Enhancement Research, Dalhousie University, Halifax, NS, 127 pp., 2025.

Reviewer 2

Dear Reviewer,

We would like to extend our thanks for your constructive review of our manuscript. Below, we respond point by point to each of your comments. All changes in the manuscript and supplemental material documents are written in purple for clarity.

Major comments:

Comment 1: In section 3, Data collection, please add the total number of data points in the description of the product. This section also lacks a more detailed description of the distribution of the data in depth in the water column (L. 168-170). Are there stations/regions with only surface samples or have all stations been sampled at different depths?

The number of samples per parameter and cruise was provided in Table 3 of the original manuscript. To improve clarity, we added an additional statement in Section 3 of the manuscript. Sampling depth coverage varies across cruises and regions, reflecting differences in sampling objectives and logistics. Whereas all regions include stations with depth-resolved sampling, at some stations sampling was limited to surface or near-surface measurements. Most stations, however, include full-depth CTD profiles with discrete sampling at multiple depths, whereas others consist of irregular or limited depth sampling. This variability has now been clarified in the revised text.

Comment 2: Consider adding a column for in-situ pH calculated from pH_TS_measured and for depth to the dataset.

A column for in-situ pH is already present in the dataset under the label “pH_TS_IS”. Depth information is provided through CTDPRES that serves as the standard vertical coordinate. Given the near-linear relationship between pressure and depth at these shallow depths, an additional depth variable was not included to avoid redundancy.

Comment 3: Please be consistent with the abbreviation for pH and choose one, as several are used in the manuscript and supplementary material (pH, pH_{TS}, pH_T) and it can be confusing.

Done. Once defined in Section 3, pH_{TS} is the only abbreviation used.

Comment 4: Consider adding a description of the results of the primary QC (number of flag=3, for which parameters etc).

We added a new table (see Table 5) and a description summarizing the number of flagged values by parameter to improve transparency.

Comment 5: In section 4.4, I understand that the authors want to use the same constants as used in GLODAP and CODAP-NA for consistency. However, these two data products don't have data in rivers or estuaries, and the data compilation presented here is based on data from a region strongly influenced by low-salinity waters. Therefore, as described in lines 284-289, the use of other constants, more suitable for low-salinity or cold waters, would have been more appropriate and would have allowed for a more in-depth discussion of the carbonate system parameters.

We agree that the choice of equilibrium constants can influence carbonate system calculations, particularly in low-salinity and estuarine environments. As noted in the manuscript, alternative formulations (e.g., Cai and Wang, 1998; Lueker et al., 2000; Waters et al., 2014) may provide improved agreement among carbonate variables under such conditions. The primary objective of this manuscript is, however, to compile and document a quality-controlled dataset, and we therefore adopted the same set of equilibrium constants as prescribed in best practice (Dickson et al., 2007) and used in other major data products (GLODAP, CODAP-NA). A systematic evaluation of alternative constant formulations and their impact on carbonate system calculations would be valuable, but would require a dedicated methodological study that is beyond the scope of this data description paper. The manuscript was revised to clarify this rationale and explicitly acknowledge this.

Comment 6: All the subsections of section 4.4 should be moved to another section. In these subsections, results of the qualitative QC are described, therefore they belong in a “Results and Discussion” section and not in “Methods”.

Also, please consider changing the data product code of the calculated carbonate variables to facilitate the use of the product (replace space by underscore and remove the brackets).

We acknowledge that some elements of qualitative QC evaluation are described alongside the methodological framework in Section 4.4. This structure, however, follows the conventions of data descriptor papers published in ESSD, where QC procedures and their outcomes are most often presented in tandem to provide transparency and context for the dataset. The intent of these subsections is not to present results in the traditional sense, but to document the behavior of the dataset under the applied QC framework, including known limitations and diagnostic patterns. Moving these sections to a separate “Results and Discussion” section would reduce the cohesion between the QC and its application. Regarding the data product variable names, we agree and have updated the naming convention for calculated variables (within the CSV but mentioned in the MS) to improve usability by replacing spaces with underscores and removing brackets (e.g., DIC(pH,TA) is now DIC_pHTA).

Comment 7: In general, in section 4.4.1 to 4.4.4, further quantification of the uncertainties related to the measurement methods, choice of constants and organic alkalinity contribution is needed to fully understand the errors and limitations associated with the calculation of pH and other carbonate system variables from pH. In light of all these uncertainties, I wonder whether it is possible to discuss the internal consistency of the carbonate system parameters based on this method.

We agree that uncertainties associated with measurement methods, the choice of equilibrium constants, and potential contributions from organic alkalinity influence carbonate system calculations, particularly in estuaries. The primary objective of this manuscript is, however, to compile and document a quality-controlled observational dataset, rather than to provide a full uncertainty analysis or to resolve carbonate system internal consistency. The comparisons presented in Section 4.4 are therefore intended to illustrate patterns in the dataset, identify broad offsets, and provide completeness in the description of the data. Quantitative uncertainty analysis, including propagation of analytical precision, constant selection, and organic alkalinity contributions, is outside the scope of this paper. Carter et al. (2024) highlights the complexity of such approaches, hence why a dedicated study would be necessary to tackle this issue. Nevertheless, it is an important avenue for future work for those using this dataset. To address the reviewer’s concern, we clearly describe the diagnostic nature of these evaluations and explicitly acknowledge sources of uncertainty and limitations.

Comment 8: L. 301-302: Here you find that the calculated pH is underestimated compared to the measured values. Can you elaborate on this result regarding the influence of the use of Lueker et al (2000) constants for the calculation and the mention on lines 188-189 that these constants lead to a possible overestimation of pH (the opposite of what is found here).

This is an insightful comment. We agree that the apparent discrepancy between the expected influence of the Lueker et al. (2000) constants and the observed bias in calculated pH warrants clarification. Whereas Sulpis et al. (2020) states that the use of the Lueker formulation may lead to an overestimation of pH in surface samples (and underestimation of pCO₂) at lower temperatures (<8 °C), the direction and magnitude of offsets between calculated and measured pH are not controlled by equilibrium constants alone. It is also important to note that Sulpis et al. (2020) evaluated uncertainty for a subset of equilibrium constants and in surface water only, and therefore may not capture the full range of variability present in this dataset. They may also reflect uncertainties in measurements, inconsistencies among parameters (e.g., sampling and storage), and potential contribution from organic alkalinity. This has been explored in previous publications in this region (e.g., Delaigue et al., 2020; Dinauer and Mucci, 2017, 2018; Fradette, 2025; Minor and Brinkley, 2022; Mucci and Jutras, 2026) and should be addressed in future work.

Comment 9: L. 305-309: Elaborate on the methodological source of uncertainty. Which samples or cruises are affected? Please quantify the uncertainty related to the measurement methods and add it here or in the supplementary when the uncertainty and precision of each method is developed. And are these data flagged as questionable if the measurement uncertainty is high?

The dataset presented here is a compilation of measurements collected over multiple decades and across numerous research programs. All data were originally QCed at the instrument level by the contributing laboratories prior to inclusion in this synthesis. Analytical uncertainties, precision, and methodological details for each parameter are

provided in the Supplementary Material (Sect. S3), based on the original analytical protocols and associated references. These uncertainties are not associated with specific cruises or subsets of the dataset but instead represent the expected variability of a multi-source data product. QC in this study was applied at the compiled dataset level, focusing on consistency checks, vertical structure, and property-property relationships.

Comment 10: L. 309-313: Please quantify the uncertainties related to the choice in the carbonic acid dissociation constants and the possible impact of organic alkalinity on the calculation.

We acknowledge that uncertainties associated with the choice of carbonic acid dissociation constants and the contribution of organic alkalinity can influence calculations, particularly at low-salinity. A quantitative assessment of these effects is, however, beyond the scope of this data description paper, as it would require a dedicated sensitivity analysis of carbonate system parameters. This limitation is now explicitly acknowledged in the Section 4.4 for the manuscript.

Comment 11: L. 331-334: Move this paragraph at the beginning or the end of this section 4.4.2 as it is currently in the middle of two paragraphs describing regional specifications and as it affects both paragraphs. Moreover, please quantify the uncertainty in the calculation of TA as it is calculated from pH. Same for line 353 with DIC.

This paragraph was repositioned to improve the flow and clarity of Section 4.4.2. Regarding uncertainty in calculated TA and DIC, we have clarified that these estimates are subject to combined uncertainties from input parameter measurements (pH, TA, DIC), equilibrium constant selection, and potential contributions from organic alkalinity. Again, a full propagation of uncertainty is beyond the scope of this paper.

Comment 12: In section 4.5, Lines 406 to 412 and 418 to 434 describe results and discussion of the QC and not methods. They should be moved to another section. The same is true for sections 4.6 and 4.7 where some paragraphs should stay in method and others should be moved in a “results and discussion” section.

As stated above, we recognize that some elements of the visual interpretations are presented alongside the description of methods. This structure, however, follows previous conventions, where QC procedures and their outcomes are documented together. These sections are intended to describe the data behavior in response to the QC framework rather than present results in the traditional sense.

Comment 13: The section 5 contains repetitions from previous paragraphs (example: L. 533 to 537 with lines L. 177, 199-200, and L. 208-214). Please rephrase or consider removing the repetition.

Redundant text was eliminated, reduced or rephrased in Section 5.

Comment 14: For Figures 12 to 17, if no description of these figures is made in the paper, they should be removed from the main manuscript.

Figures 12-17 are retained as they provide visual documentation of post-QC data distributions across regions and parameters, an integral component of dataset transparency and description. This type of visualization is consistent with other data product descriptions published in ESSD and allows for the visualization of the QCed profiles.

Comment 15: Most of section 6 has already been described in subsections of section 4. To avoid repetition, I suggest to move the paragraphs describing results and discussion that I highlighted earlier in the “method” to this “discussion and validation” section and to review them with the information already in this section 6.

We acknowledge that some descriptions appear in both Sections 4 and 6. Rather than relocating sections, we reduced redundancy and clarified their distinct roles. Section 4 focuses on the application and outcomes of the QC procedures and associated diagnostics, while Section 6 synthesizes these outcomes in the context of dataset validation and interpretation. To improve clarity, we added an introductory statement to Section 6 and included cross-references to Section 4 where appropriate.

Comment 16: The section 6.4 “Data limitations” would benefit from further discussion and quantification of the limitations of the data compilation, measurement methods and QC.

Section 6.4 was expanded to more explicitly describe the limitations of the dataset. In particular, we clarify the uneven spatial and seasonal sampling, variability in parameter availability across cruises, and the multi-source nature of the compilation. We also note that measurement uncertainties reflect those reported by the original data providers and are therefore heterogeneous across the dataset. Whereas these limitations are inherent to a large observational synthesis such as this one, they are explicitly described to support the use of this dataset.

Minor comments:

Comment 1: 167: provide instead of provides.

Done.

Comment 2: 196-197: Repetition of L. 149-150.

Lines 196-197 were removed to avoid repetition.

Comment 3: 202: “Both discrete samples and CTD...” This sentence can be removed as the parameters included in the dataset were already described previously in the last paragraph of section 3.

Done.

Comment 4: 211-213: Consider adding a map with the location of the three Channel areas in the supplementary material.

This is a good suggestion. A map showing the location of the three channel regions and landmarks of interest were added to the supplementary material (Fig. S1). This figure is reproduced from our previous publication in *Ocean Science* (Nesbitt et al., 2025) and included to provide spatial context for the regional definitions used in this dataset.

Comment 5: 233: Where do the regional reference profiles come from? Please add a citation or any relevant information about these profiles.

The term “regional reference profiles” refers to the ensemble of observations within each defined region in this dataset, rather than an external reference. Profiles were evaluated in the context of the broader distribution of measurements within each region to identify deviations in structure or consistency. The text was revised accordingly and “regional reference profiles” is now referred to as “regionally aggregated profiles” derived from the full dataset.

References

- Cai, W.-J. and Wang, Y.: The chemistry, fluxes, and sources of carbon dioxide in the estuarine waters of the Satilla and Altamaha Rivers, Georgia, *Limnology and Oceanography*, 43, 657–668, <https://doi.org/10.4319/lo.1998.43.4.0657>, 1998.
- Carter, B. R., Sharp, J. D., Dickson, A. G., Álvarez, M., Fong, M. B., García-Ibáñez, M. I., Woosley, R. J., Takeshita, Y., Barbero, L., Byrne, R. H., Cai, W.-J., Chierici, M., Clegg, S. L., Easley, R. A., Fassbender, A. J., Fleger, K. L., Li, X., Martín-Mayor, M., Schockman, K. M., and Wang, Z. A.: Uncertainty sources for measurable ocean carbonate chemistry variables, *Limnology and Oceanography*, 69, 1–21, <https://doi.org/10.1002/lno.12477>, 2024.
- Delaigue, L., Thomas, H., and Mucci, A.: Spatial variations in CO₂ fluxes in the Saguenay Fjord (Quebec, Canada) and results of a water mixing model, *Biogeosciences*, 17, 547–566, <https://doi.org/10.5194/bg-17-547-2020>, 2020.
- Dickson, A. G., Sabine, C. L., and Christian, J. R.: Guide to Best Practices for Ocean CO₂ Measurements., North Pacific Marine Science Organization, <https://doi.org/10.25607/OBP-1342>, 2007.
- Dinauer, A. and Mucci, A.: Spatial variability in surface-water *p*CO₂ and gas exchange in the world’s largest semi-enclosed estuarine system: St. Lawrence Estuary (Canada), *Biogeosciences*, 14, 3221–3237, <https://doi.org/10.5194/bg-14-3221-2017>, 2017.

Dinauer, A. and Mucci, A.: Distinguishing between physical and biological controls on the spatial variability of $p\text{CO}_2$: A novel approach using OMP water mass analysis (St. Lawrence, Canada), *Marine Chemistry*, 204, 107–120, <https://doi.org/10.1016/j.marchem.2018.03.007>, 2018.

Fradette, C.: Evaluating Data Quality of Coastal Spectrophotometric pH Measurements: Implications for Ocean Acidification and Ocean Alkalinity Enhancement Research, Dalhousie University, Halifax, NS, 127 pp., 2025.

Lueker, T. J., Dickson, A. G., and Keeling, C. D.: Ocean $p\text{CO}_2$ calculated from dissolved inorganic carbon, alkalinity, and equations for K_1 and K_2 : validation based on laboratory measurements of CO_2 in gas and seawater at equilibrium, *Marine Chemistry*, 70, 105–119, [https://doi.org/10.1016/S0304-4203\(00\)00022-0](https://doi.org/10.1016/S0304-4203(00)00022-0), 2000.

Minor, E. C. and Brinkley, G.: Alkalinity, pH, and $p\text{CO}_2$ in the Laurentian Great Lakes: An initial view of seasonal and inter-annual trends, *Journal of Great Lakes Research*, 48, 502–511, <https://doi.org/10.1016/j.jglr.2022.01.005>, 2022.

Mucci, A. O. and Jutras, M.: Seasonally-variable surface-water CO_2 gradients and fluxes along the Gulf and St. Lawrence Estuary (Quebec, Canada), *Marine Chemistry*, 276, 104637, <https://doi.org/10.1016/j.marchem.2026.104637>, 2026.

Nesbitt, W. A., Stevens, S. W., Mucci, A. O., Gerke, L., Tanhua, T., Chaillou, G., and Wallace, D. W. R.: The coupled oxygen and carbon dynamics in the subsurface waters of the Gulf and Lower St. Lawrence Estuary and implications for artificial oxygenation, *Ocean Science*, 21, 2179–2195, <https://doi.org/10.5194/os-21-2179-2025>, 2025.

Sulpis, O., Lauvset, S. K., and Hagens, M.: Current estimates of K_1^* and K_2^* appear inconsistent with measured CO_2 system parameters in cold oceanic regions, *Ocean Science*, 16, 847–862, <https://doi.org/10.5194/os-16-847-2020>, 2020.

Waters, J., Millero, F. J., and Woosley, R. J.: Corrigendum to “The free proton concentration scale for seawater pH”, [MARCHÉ: 149 (2013) 8–22], *Marine Chemistry*, 165, 66–67, <https://doi.org/10.1016/j.marchem.2014.07.004>, 2014.