Data Article

∼14 000 years of geochemical and isotopic data from Lake Simcoe, Canada

R.M. Doyle\textsuperscript{a, b}, N. Bumstead\textsuperscript{a}, C.F.M. Lewis\textsuperscript{c}, F.J. Longstaffe\textsuperscript{a, *}

\textsuperscript{a} Department of Earth Sciences, Biological and Geological Sciences, The University of Western Ontario, 1151 Richmond St N, London, ON N6A 5B7, Canada
\textsuperscript{b} AMGC Research Group, Vrije Universiteit Brussel, Pleinlaan 2, Brussels 1050, Belgium
\textsuperscript{c} Geological Survey of Atlantic Canada, Bedford Institute of Oceanography, Box 1006, 1 Challenger Drive, Dartmouth, Nova Scotia, B2Y 4A2, Canada

**ARTICLE INFO**

**Article history:**
Received 20 July 2022
Revised 9 August 2022
Accepted 10 August 2022
Available online 14 August 2022

**Dataset link:** Geochemical and isotopic analyses of a ∼14 000 year old sediment core collected from Lake Simcoe, Canada (Original data)

**Keywords:**
Ostracods
Laurentian Great Lakes region
Glacial meltwater
8.2ka event
Holocene
Pleistocene-Holocene transition
Lake Algonquin

**ABSTRACT**

This dataset contains measurements of modern water and ancient core materials from Lake Simcoe, the fourth largest lake wholly in Ontario, Canada. These data consist of: (i) oxygen, hydrogen and carbon isotope (δ\textsuperscript{18}O, δ\textsuperscript{2}H and δ\textsuperscript{13}C) compositions for modern water samples; (ii) physical measurements of one piston core, PC-5; (iii) δ\textsuperscript{13}C and δ\textsuperscript{18}O values of ostracods collected from PC-5, and (iv) δ\textsuperscript{13}C and δ\textsuperscript{18}O values of ancient DIC and water, respectively, inferred from item (iii). Physical measurements performed on core PC-5 include magnetic susceptibility, mineralogy and grain size. Mass accumulation rates are also reported. These data will be of interest to those aiming to better characterize the timing and pathway of meltwater flow during and following deglaciation of the Laurentide Ice Sheet in the Laurentian Great Lakes region. These data will also be useful to researchers investigating the influence of deglaciation on the oxygen and carbon isotope systematics of ancient lake environments. A discussion of these data is available in “A ∼14 000-year record of environmental change from Lake Simcoe, Canada” [1].

**DOI of original article:** 10.1016/j.quascirev.2022.107667
* Corresponding author.

E-mail address: flongsta@uwo.ca (F.J. Longstaffe).
Social media: @lake_nerd (R.M. Doyle), @O_isotopist (F.J. Longstaffe)

https://doi.org/10.1016/j.dib.2022.108541

2352-3409/Crown Copyright © 2022 Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/)
Specifications Table

| Subject          | Geochemistry and Petrology, Environmental Science |
|------------------|---------------------------------------------------|
| Specific subject area | Isotopic and geochemical data from lake sediments, including ostracods. |
| Type of data     | .xlsx and .docx files                               |
| How the data were acquired | Modern water samples from Lake Simcoe were analyzed using (i) a Picarro® L2120-i δ²H and δ¹⁸O Analyser and (ii) a Thermo Scientific™ GasBench® II connected to a Thermo Scientific™ Delta plus XL™ continuous flow isotope ratio mass spectrometer (IRMS) and a heater block equipped with a CombiPal® autosampler. ostracods collected from sediment core PC-5 were analyzed using (i) a Micromass MultiPrep®, device coupled to a VG Optima®, dual-inlet isotope ratio mass spectrometer (IRMS) or (ii) a Thermo Scientific™ GasBench® II interfaced with a Thermo Scientific™ Delta plus XL™ continuous flow IRMS. Sediment core PC-5 was analyzed using the following instruments: (i) a Malvern Mastersizer®, 2000 laser grain-size analyzer, (ii) a GEOTEK®, multi-sensor core logger (MSCL) and (iii) a Rigaku High Brilliance Rotating Anode X-ray Diffractometer. |
| Data format      | Raw.                                               |
| Description of data collection | All samples were collected from Lake Simcoe. The water samples were collected at various depths in the lake from May 2009 to November 2011. All other data originate from sediment core PC-5 collected from the deepest, flattest part of the lake in June 2007. |
| Data source location | Lake Simcoe, Ontario, Canada, 44.4873, –79.4169 |
| Data accessibility | [2] R.M. Doyle, N. Bumstead, C.F.M. Lewis, F.J. Longstaffe. Geochemical and isotopic analyses of a ~14 000 year old sediment core collected from Lake Simcoe, Canada. Zenodo (2022) https://doi.org/10.5281/zenodo.6959403. |
| Related research article | [1] R.M. Doyle, N. Bumstead, C.F.M. Lewis, F.J. Longstaffe. A ~14 000-year record of environmental change from Lake Simcoe, Canada, Quat. Sci. Rev. 292 (2022) 107667, doi:https://doi.org/10.1016/j.quascirev.2022.107667. |

Value of the Data

- These data may be compared with other proxy archives in the Laurentide Great Lakes region of North America to better characterize the timing and pathway of meltwater flow following deglaciation of the Laurentide Ice Sheet.
- These data are useful to researchers investigating the influence of deglaciation on the oxygen and carbon isotope systematics of ancient lake environments.
- These data could also be used as a baseline for relative temperature change in southern Ontario.
- These data are beneficial to researchers interested in contextualizing the recent eutrophication of Lake Simcoe against a backdrop of natural variation.

1. Data Description

These data include the stable isotope ratios (δ¹⁸O, δ²H and δ¹³C) of modern water from Lake Simcoe, as well as the stable isotope ratios (δ¹⁸O and δ¹³C) of ostracods in core sediments from
Lake Simcoe. Physical measurements of sediment core PC-5 (e.g., grain size, magnetic susceptibility, mineralogy) are also provided. For plots of these data, refer to Doyle and colleagues [1]. This dataset is contained in one Microsoft Excel file:

LakeSimcoeData.xlsx – one data table containing all analytical measurements, including: (i) δ18O, δ13C and δ2H of modern waters; (ii) ostracod assemblages from core PC-5; (iii) δ18O and δ13C of ostracod valves in core PC-5; (iv) δ18O and δ13C of ancient water and DIC, respectively, are inferred from isotopic analyses of ostracod valves and are also reported in this datasheet.

2. Experimental Design, Materials and Methods

Analysis of δ2H and δ18O of modern waters: Unfiltered water samples were removed from the refrigerator and left to sit until they warmed to room temperature. 1 mL of water was pipetted into a 2 mL glass vial for analysis. Analysis of δ2H and δ18O of modern waters using a Picarro® L2120-i δ2H and δ18O Analyser – Calibration of δ2H and δ18O to VSMOW was achieved using LSIS standards Heaven (accepted δ2H: +88.7‰; accepted δ18O: −0.27‰) and LSD (accepted δ2H: −161.8‰; accepted δ18O: −22.57‰). Analytical accuracy and precision were evaluated using LSIS standards MID (accepted δ2H: −108.1‰; accepted δ18O: +13.08‰) and EDT (accepted δ2H: −56‰; accepted δ18O: −7.27‰). The δ2H results for MID and EDT were −108.00 ± 0.67‰ (n = 35) and −54.68 ± 1.17‰ (n = 111), respectively, which compare well with accepted values and expected reproducibility. The δ18O results for MID and EDT were −13.01 ± 0.14‰ (n = 35) and −7.22 ± 0.18‰ (n = 111), respectively, which compare well with accepted values and expected reproducibility. The accepted values for all LSIS standards were determined previously by direct calibration to a VSMOW- and SLAP-scale.

Analysis of δ13C DIC of modern waters: For samples, five drops of 100% concentrated orthophosphoric acid were added to the bottom of the glass vials, which were then septum-sealed and flushed with He for 5 min. One (1) mL of sample was then injected into the flushed vial using a 1 mL syringe. The vials were reacted in the GasBench® heater block at 35 °C overnight prior to isotopic measurements. The produced gas was then transported automatically to the IRMS using an autosampler. For each standard, 0.25 mg was weighed into the bottom of a glass vial, and the vial was placed in a horizontal position. Concentrated orthophosphoric acid (100%) was then added to the top of the vial such that the acid was separated from the standard powder. A septum cap was then attached to the vial and tightened. Next, the vial was flushed with He for 5 min at room temperature. The vial was then turned upright, thus allowing the acid to react with the standard powder. The vial was then immediately placed in the GasBench® heater block overnight reacting at 35 °C. The evolved gas was then automatically transferred to the IRMS using an autosampler. Analysis of δ13C DIC of modern waters was conducted using a Thermo ScientificTM GasBench® II coupled to a Thermo ScientificTM DeltaPlus XL™ IRMS. Calibration of δ13C to VPDB was achieved using NBS-18, NBS-19 and Suprapur. Accuracy and precision of analyses were evaluated using the δ13C of WS-1. The δ13C results for WS-1 were 0.80 ± 0.11‰ (n = 5), which compare well with accepted values and expected reproducibility.

Analysis of δ13C and δ18O of ostracods: To collect ostracods, each interval of sediment was first wet-sieved. The sieved material and ostracods were separated under a binocular microscope using statically charged camel hairs. Ostracod valves were then identified and cleaned with bleach to remove organic material adhered to the valves. The δ13C and δ18O of most ostracods were measured using a Micromass MultiPrep® coupled to a dual-inlet VG Optima® Isotope Ratio Mass Spectrometer (IRMS). Calibration of δ13C to VPDB was achieved using NBS-19 (accepted value: δ13C = +1.95‰) and Suprapur (accepted value: −35.28‰). Accuracy and precision of analyses were evaluated using the δ13C of NBS-18 (accepted value: −5.0‰) and LSIS standard WS-1 (accepted value: +0.76‰). The δ13C results for NBS-18 and WS-1 were −5.01 ± 0.07‰ (n = 41) and +0.72 ± 0.08‰ (n = 14), respectively, which compare well with accepted values and expected reproducibility. Calibration of δ18O to VSMOW was achieved using
NBS-19 (accepted value: +28.65‰) and NBS-18 (accepted value: +7.20‰). Analytical accuracy and precision were evaluated using Suprapur (accepted value: +13.25‰) and WS-1 (accepted value: +26.23‰). The δ¹⁸O results for Suprapur and WS-1 were +13.28 ± 0.17‰ (n = 35) and +26.20 ± 0.11‰ (n = 14), respectively, which compare well with accepted VSMOW-SLAP calibrated values and expected reproducibility. The δ¹³C and δ¹⁸O of all remaining ostracods were measured using a Thermo Scientific™ GasBench® II coupled to a Thermo Scientific™ Delta-plus X™ IRMS. Calibration of δ¹³C to VPDB was achieved using NBS-19 and Suprapur. Accuracy and precision of analyses were evaluated using the δ¹³C of NBS-18 and WS-1. The δ¹³C results for NBS-18 and WS-1 were −4.99 ± 0.12‰ (n = 8) and +0.91 ± 0.28‰ (n = 6), respectively, which compare well with accepted values and expected reproducibility. Calibration of δ¹⁸O to VSMOW was achieved using NBS-19 and NBS-18. Analytical accuracy and precision were evaluated using Suprapur and WS-1. The δ¹⁸O results for Suprapur and WS-1 were +13.30 ± 0.34‰ (n = 8) and +26.03 ± 0.71‰ (n = 6), respectively, which compare well with accepted values and expected reproducibility. Methods for converting the δ¹³C and δ¹⁸O to estimates of δ¹³C_DIC and δ¹⁸O_Lake water are provided in the main research article [1].

Grain-size analysis of PC-5: Grain-size analysis of samples from each core was performed using a Malvern Mastersizer® 2000 laser grain-size analyzer hosted in the Control and Crystalization of Pharmaceuticals Laboratory (CCPL) at The University of Western Ontario.

In preparation for grain-size analysis, samples from PC-5 were disaggregated and treated with 15 mL of 0.3% bleach at 65 °C for at least 24 h to remove organic matter. The bleach was then removed by repeatedly rinsing each sample with distilled water. Finally, 10 mL of sodium hexametaphosphate solution, a dispersing agent, was added to each sample and samples were analyzed using the Mastersizer®.

Analysis of the magnetic susceptibility (MS) of PC-5: Prior to the analysis of MS, sediment core PC-5 was rinsed with distilled water and gently scraped horizontally using a spatula. MS was assessed using a GEOTEK® multi-sensor core logger (MSCL) in the Lake and Reservoir Systems Research Facility (LARS) at The University of Western Ontario.

Analysis of sediment mineralogy of PC-5: Samples from PC-5 were freeze-dried and homogenized using a rubber mortar and pestle. The sample was then mounted onto an Al-backpack holder or a glass front-pack holder and analyzed using a Rigaku, high brilliance, rotating-anode X-ray diffractometer equipped with a graphite monochromator and CoKα radiation produced at 45 kV and 160 mA. Samples were scanned from 2° to 82° 2θ at a scanning rate of 10° 2θ/min. The abundance of each mineral was estimated using the background-subtracted peak height of its most intense diffraction. Crystallinity differences were account for using a form factor of x1, except for the (001) diffractions of kaolinite (x2), chlorite (x2) and illite (x4).

Ethics Statement

This work did not involve human subjects, animal experiments, or data collected from social media platforms. The manuscript adheres to Elsevier's ethics in publishing standards.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Geochemical and isotopic analyses of a ~14 000 year old sediment core collected from Lake Simcoe, Canada (Original data) (Zenodo).
CRediT Author Statement

R.M. Doyle: Conceptualization, Writing – original draft, Writing – review & editing, Methodology, Formal analysis, Visualization; N. Bumstead: Conceptualization, Investigation, Methodology, Writing – review & editing; C.F.M. Lewis: Writing – review & editing; F.J. Longstaffe: Supervision, Conceptualization, Writing – review & editing, Resources, Project administration, Funding acquisition.

Acknowledgments

We thank Chip Heil Jr, Brad Hubeny (and others at the University of Rhode Island) and Reba Macdonald who were instrumental in the collection of the Lake Simcoe cores. We thank the Natural Sciences and Engineering Council of Canada (FJL), the Canada Foundation for Innovation (FJL), the Canada Research Chairs Program (FJL) and The Lake Simcoe Region Conservation Authority (NB) for financial support of this research, and the staff of The Laboratory for Stable Isotope Science (LSIS) at the University of Western Ontario for their dedicated assistance with the analytical work. Thank you to the Lake and Reservoir Systems Research Facility (LARS), especially Dr. Katrina Moser and Erika Hill, for their help analyzing the magnetic susceptibility of PC-5. This is LSIS contribution # 396 (RMD, NB, FJL) and Contribution # 20210691 of the Lands and Minerals Sector of Natural Resources Canada (CFML).

Supplementary Materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2022.108541.

References

[1] R.M. Doyle, N. Bumstead, C.F.M. Lewis, F.J. Longstaffe, A ~14 000-year record of environmental change from Lake Simcoe, Canada, Quat. Sci. Rev. 292 (2022) 107667, doi:10.1016/j.quascirev.2022.107667.
[2] R.M. Doyle, N. Bumstead, C.F.M. Lewis, F.J. Longstaffe, Geochemical and isotopic analyses of a ~14 000 year old sediment core collected from Lake Simcoe, Canada, Zenodo (2022), doi:10.5281/zenodo.6959403.