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Merged and harmonized data for the atlas of lake sediment geochemistry of western Labrador and northeastern Quebec

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Abstract

Geochemical data for 21 678 lake-sediment samples, analysed for 53 elements by ICP-MS after aqua-regia digestion, were compiled to create an atlas of surficial geochemistry. Statistical tests and plots of the combined data, after the application of levelling functions, where necessary, show that the differences that previously existed between analyses employing digestions of varying strengths can be largely compensated for. Using this combined dataset, integrated geochemical maps for an area of almost 300 000 km^2 were published, revealing many large-scale geochemical features. These features are related to the rocks of the Paleoproterozoic 'Labrador Trough', part of the New Quebec Orogen, or to the relative amounts of organic and inorganic clastic material in the lake sediment. The release of the merged data sets is expected to provide assistance with geological mapping of this large area, as well as providing a stimulus for mineral exploration. By providing data in several formats, including the original raw data as well as levelled and/or smoothed data for some elements, we hope to encourage the use of these data and the development of new methods for exploratory data analysis and visualization.

Introduction

Lake-sediment samples from northeastern Québec (16,167 sites) and adjacent Labrador (5,511 sites) were collected between 1978 and 1997 (Fig. 1). In some areas of Québec (over the Labrador Trough), samples were collected at higher densities (Fig. 1). Furthermore, different geochemical analytical procedures were followed in the two regions. In order to create a combined dataset, the Labrador samples were re-analyzed by a commercial laboratory using the same *aqua regia* digestion as had been used for the Québec samples, followed by the determination of 53 elements by inductively coupled plasma-mass spectrometry. The merging of these two sets of analytical data enabled the creation of regional geochemical maps released in 2018 in GSC Open File 8348for a contiguous area in northeastern Canada of almost 300,000 km^2 (McCurdy et al., 2018).

This release of data for 21,678 sites in Labrador and Québec comprises unlevelled and unsmoothed ('raw') data for all elements, levelled data for Ag, Cd, Hg and Zn, smoothed data for all elements except Ag, Cd, Hg, and Zn, and levelled and smoothed data for Ag, Cd, Hg and Zn (Table 1). These four individual datasets are in separate worksheets in Appendix B – Geochemical Data.xlsx, an MS-Excel® file. The methods of nearest-neighbour and quantile regression were used to establish similarities and differences between samples in the two areas, and to derive levelling functions for Ag, between the samples collected on either side of the Québec-Labrador border, and also to alleviate discontinuities within the Québec dataset itself for the other three elements. To extract the 'signal' from typically rather 'noisy' geochemical data, a 'moving-median' smoothing algorithm was applied (Amor et al., 2016). For detailed descriptions of methods used to harmonize data ('levelling' and 'smoothing') see Amor (2015), Amor et al., 2016) and Amor et al., (2019).

Table 1. Three data files were derived from the original 'raw' data compiled for the geochemical atlas, including an intermediate file comprising levelled data for Ag, Cd, Hg and Zn. All four datasets are included in Appendix B –Geochemical Data.

Dataset	**Elements**
Raw Data	All elements

Levelled and Unsmoothed Data	Ag, Cd, Hg, Zn
Smoothed Data	All elements except Ag, Cd, Hg, Zn
Levelled and Smoothed Data	Ag, Cd, Hg, Zn

This release of data at several processing stages is aimed at stimulating mineral exploration and encouraging the use of these data and the possible development of new methods for exploratory data analysis and visualization.

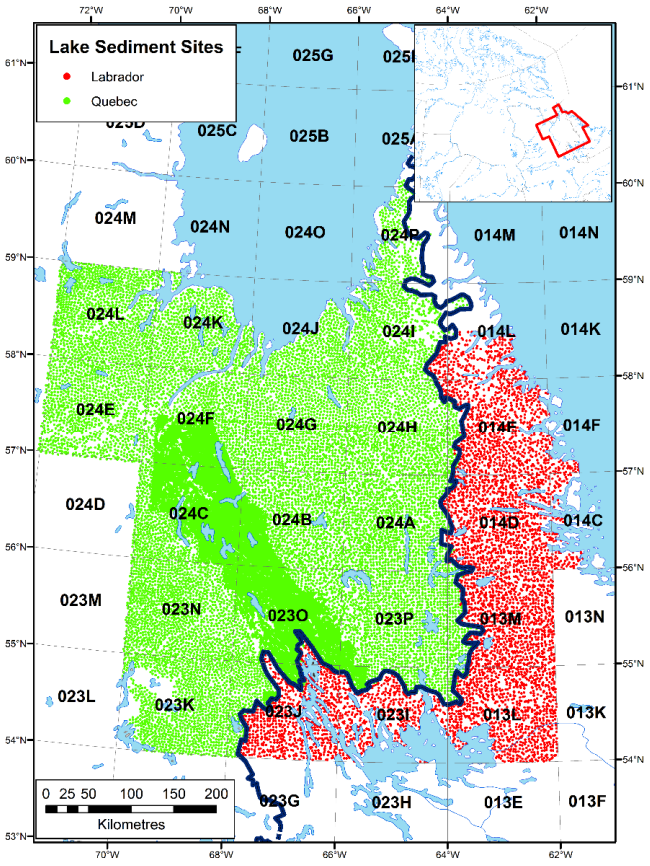

Figure 1. Lake sediments collected from sites in Québec and Labrador between 1973 and 1997 and re-analyzed using ICP-MS for 53 elements. Note higher sample density over Québec section of Labrador Trough. For statistical calculation and data presentation in these areas, the Québec data were sub-sampled to yield a data set with the same average sample density as the other parts of Québec and adjacent Labrador.

Sample Collection for Québec and Labrador Samples

Lake-sediment samples were collected from a helicopter equipped with floats, held stably on the surface of the water. Samples were selected so as to maintain an even distribution with a density of one sample per 12 to 14 km^2 across most survey areas of Labrador or Quebec, resulting in a range of lake areas and depths. A bottom-valve, hollow-pipe sampler (Fig. 2) was used to collect approximately one kilogram of wet lake sediment. Ideally, the entire length of the weighted sampler penetrated the lake bottom sediments to a

depth below the sediment-water interface so that the upper layers of *gyttja* were forced out of the vent located towards the tail of the sampler, reducing the possibility of contamination of the sample by recent (Anthropocene) sources.

Figure 2 About 1 kg of wet lake sediment (*gyttja*) is collected by dropping the sampler (pictured) from a platform attached to the float of the helicopter (photograph by M.W. McCurdy, NRCan photo 2021-198).

Sample Preparation for Québec and Labrador Samples

Partially dried samples were shipped to sample-preparation facilities, where they were unpacked and dried at temperatures below 45° C. After drying, samples were disaggregated and sieved through an 80-mesh (177 µm) screen (Maurice and Labbé, 2009; Girard et al, 2004). Typically, one kilogram (wet) of *gyttja*, the preferred collection material, yielded about 50 g of material for analysis.

ANALYTICAL PROCEDURES

Inductively Coupled Plasma Mass Spectrometry

Québec and Labrador samples were analysed at Bureau Veritas Commodities Canada Limited (formerly Acme Analytical Laboratories, Ltd.), Vancouver, using a proprietary *aqua regia* digestion and Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) package. For the 53 elements listed in Table 2, a 0.5 gram sample was leached with a modified *aqua regia* solution (HCl:HNO3, 1:1) and elemental concentrations determined by ICP-MS.

Table 2. Elements in lake sediments determined by Inductively Coupled Plasma –Mass Spectroscopy (ICP-MS). Loss-on-ignition (LOI) was determined by heating a one-gram sample for one hour at 500° C and weighing the cooled residue.

	Detection Limit	Units of Measurement	Element	Detection Limit	Units of Measurement
Ag	2	ppb	**Na**	0.001	%
Al	0.01	pct	**Nb**	0.02	ppm
As	0.1	ppm	**Ni**	0.1	ppm
Au	0.2	ppb	**P**	0.001	%
B	20	ppm	**Pb**	0.01	ppm
Ba	0.5	ppm	**Pd**	10	ppb
Be	0.1	ppm	**Pt**	2	ppb
Bi	0.02	ppm	**Rb**	0.1	ppm
Ca	0.01	pct	**Re**	1	ppb
Cd	0.01	ppm	**S**	0.02	%
Ce	0.1	ppm	**Sb**	0.02	ppm
Co	0.1	ppm	**Sc**	0.1	ppm
Cr	0.5	ppm	**Se**	0.1	ppm
Cs	0.02	ppm	**Sn**	0.1	ppm
Cu	0.01	ppm	**Sr**	0.5	ppm
Fe	0.01	pct	**Ta**	0.05	ppm
Ga	0.1	ppm	**Te**	0.02	ppm
Ge	0.1	ppm	**Th**	0.1	ppm
Hf	0.02	ppm	**Ti**	0.001	%
Hg	5	ppb	**Tl**	0.02	ppm
In	0.02	ppm	**U**	0.1	ppm
K	0.01	pct	**V**	2	ppm
La	0.5	ppm	**W**	0.1	ppm
Li	0.1	ppm	**Y**	0.01	ppm
Mg	0.01	pct	**Zn**	0.1	ppm
Mn	1	ppm	**Zr**	0.1	ppm
Mo	0.01	ppm	**LOI**	0.1	%

Database

The data considered in this study consist of analyses of lake sediments collected on 1:250 000 map sheets 23K, 23N, 23P, 24B, 24C, 24E, 24F, 24G, 24H, 24J, 24K and 24L (entirely in northeastern Québec); 14C and 14F (entirely in Labrador) and 13L, 13 M, 14D, 14E, 14L, 23I, 23J, 23O, 24A, 24H, 24I and 24P (straddling the border between the two provinces) of Canada's National Topographic System (NTS; https://www.nrcan.gc.ca/earth-sciences/geography/topographic-information/maps/national-topographic-system-maps/9767). Each sheet is 1° of latitude high and 2° of longitude wide, with an approximate area, in the region of study, of 14 000 km^2.

The total number of Québec samples collected within these map areas is 24 261, while the Labrador subset comprises 5 511 samples. The samples were collected in a series of helicopter-supported campaigns between 1979 and 1997. Although a sample density of 6–8 samples per 100 km^2 was maintained over most of the study area in both Labrador and Québec, the sample density over the Québec portion of the Labrador Trough, south of 57°30' N, was four times as high (Amor 2015). To create a dataset of more evenly spaced samples, a subset of 25% of the samples from this latter region was randomly selected for the current study. Sub-selection was done independently within each NTS 1: 50 000 map sheet (with an approximate area of 875 km^2), to avoid regions of over- or under-selection, or 'clumping', but the resulting coverage is still somewhat uneven compared to the remainder of the study area. This resulted in a reduction in the total number of Québec analyses from 24 261 to 16 167. Maps showing the sample density, before and after this adjustment, are presented by Amor (2015). The raw Labrador data have already been released as two GSC open file reports (McCurdy 2016; McCurdy et al. 2016) and the raw Québec data can also be downloaded from https://sigeom.mines.gouv.qc.ca .

Amalgamating Lake-Sediment Data

The application of the same methods of digestion and analysis to both the Québec and Labrador samples greatly facilitates the merging of data, even though the samples were collected and analyzed at different times, and as part of two separately administered programs. To verify the degree of correspondence, analyses of samples from the Québec dataset, collected close to the border between the two provinces, were paired with their 'nearest neighbours' on the Labrador side. In all cases, the paired samples were separated by a distance of 2 km or less. Paired t-tests (R-Project, 2021), following $\log_{10}$ transformations, were applied to subsets of the data divided into a high- and low-Loss-on-Ignition (LOI) subset using a threshold of 18.4%, as well as to both subsets combined. This led to the conclusion that if attention was restricted to sample pairs separated by distances of 2 km or less, there was no significant difference that would suggest a 'background shift' between determinations of Al, Ba, Cd, Co, Cr, Cu, Fe, Hg, K, La, Li, Mg, Mo, Ni, Pb, Rb, S, Sr, Th, Ti, U or V in the Labrador and Québec datasets at the 95% confidence level. In the case of Be, Ca, Ce, Cs, Ga, Mn, Nb, P, Sc, Se, Sn, Tl, V, Zn and Zr, at least one (but not all three) of the paired t-tests showed no significant differences. Only Ag showed significant differences in all three tests. More than 10% of the analyses of As, Au, Ge, Hf, In, Re, Sb, Te and W were less than the lower detection limit in all six datasets and are not amenable to statistical calculations of this kind; nevertheless, map plots of some of these elements are instructive. For detailed descriptions of the reasons for subsetting high and low LOI samples and the methods used to harmonize data, see Amor (2015), Amor et al., 2016) and Amor et al., (2019).

Results of the paired t-tests described above suggest that there is very little need for levelling of the two datasets. Therefore, the datasets can be combined without a serious discontinuity appearing at the provincial border (e.g., Amor 2015). One exception to this generalization is Ag; therefore the data from Labrador for this element have been levelled using regression equations derived for nearest-neighbour pairs, separated into high-LOI (>18.4%) and low-LOI groups.

In the dataset from Québec, an internal levelling issue was apparent for certain elements, with samples from a later survey showing significantly higher values of the Cd and Zn, and lower values of Hg, than in samples from adjacent, earlier surveys. This resulted in a linear discontinuity along the boundary between the areas of coverage. A nearest-neighbour regression exercise was also carried out on these data, with levelling functions derived from individual sample pairs for Cd and Hg, and paired quantiles for Zn. A more detailed description of the methods used to level data can be found in Amor et al. (2016).

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Sources for Data

Natural Resources Canada, Geological Survey of Canada, Ottawa, ON

http://geoscan.nrcan.gc.ca/

Bureau de la connaissance géoscientifique du Québec, Val-d'Or, QC

http://sigeom.mines.gouv.qc.ca/