EXPLORE
Newsletter for the
Association of Applied Geochemists
www.appliedgeochemists.org

NUMBER 201 December 2023

Inverting the missing SiO_2 and LOI contents in the North American Soil Geochemical Landscapes datasets

Patrice de Caritat
Geoscience Australia, GPO Box 378, Canberra, ACT 2601, Australia (Patrice.deCaritat@gmail.com)

Eric C. Grunsky
Department of Earth & Environmental Sciences, University of Waterloo, Waterloo, ON N2L 3G1, Canada

David B. Smith
International Union of Geological Sciences Commission on Global Geochemical Baselines, Wheat Ridge, CO 80033, USA

INTRODUCTION

Rock, sediment and soil chemical and mineralogical compositions are fundamental to the discipline of geochemistry, as they affect or even control their bulk properties. Many geological materials on Earth contain silicates, phyllosilicates, and, perhaps less commonly, carbonates (e.g. Finkl 1981; Schaetzl and Anderson 2007; Deer et al. 2013). These mineral groups impact the materials' geochemical compositions in terms of SiO_2, H_2O and CO_2 concentrations (among others).

X-ray fluorescence (XRF) is a traditional analytical method used to obtain total concentration analyses, which are agnostic of the mineral host, element speciation or oxidation state. Major elements (> 0.1 weight percent (wt%) abundance) are typically reported as a suite of oxides (i.e. Al_2O_3, CaO). This suite of oxides is either directly obtained from XRF or converted from elemental data such as acquired by Inductively Coupled Plasma-Atomic Emission Spectroscopy (ICP-AES) or -Mass Spectrometry (ICP-MS) methods. The latter ICP methods do not report SiO_2, H_2O or CO_2 because of the sample digestion requirement.

The gravimetric determination of loss-on-ignition (LOI), obtained by heating the sample to a set temperature and measuring the mass loss relative to the starting sample (at standardized temperature, pressure and humidity), often complements the XRF or ICP analyses. LOI has several components, including adsorbed water (H_2O; e.g. interlayer water in clay minerals), combined H_2O (e.g. hydrated minerals and labile hydroxyl-compounds), carbon dioxide (CO_2; e.g. from carbonates and organic matter), and volatile elements (e.g. Hg).

One advantage of reporting the major components of a geological sample as oxides is that their sum, when complemented by LOI and trace elements (TEs), should add up to 100 wt%. Any discrepancy represents components not analyzed for and/or uncertainty. Having a complete sample analysis, or at least as complete as practically possible, is important to give confidence that the sample is well characterized, which implies that the composition is closed or full and not a subcomposition (i.e. no component is unaccounted for). This has implications in subsequent data analytics, including in the development and application of Compositional Data Analysis (CoDA) methods (e.g. Chayes 1960; Aitchison 1986; Scealy et al. 2015).

Another benefit of a complete sample analysis is the direct relationship between the geochemical and mineralogical compositions, via the knowledge (or modeling) of the minerals' stoichiometric compositions. Deriving the most plausible mineralogy from geochemistry is a non-unique inversion problem known as 'normative analysis' (e.g. Caritat et al. 1994; Aldis et al. 2023). It is a useful way to ensure that chemistry and mineralogy of a sample are consistent with one another.

THE NORTH AMERICAN SOIL GEOCHEMICAL LANDSCAPES PROJECT

The North American Soil Geochemical Landscapes (NASGL) project is a recent continental-scale geochemical survey of the conterminous United States of America (Smith et al. 2013, 2014, 2019; see Smith 2022 for a project review). Soils were sampled from three levels (0–5 cm depth, A horizon and C horizon) at 4857 sites, and their <2 mm fractions were analyzed for 45 major and trace element concentrations by methods yielding 'total or near-total' elemental content (mostly ICP-AES or ICP-MS after a four-acid — hydrochloric, nitric, hydrofluoric, and perchloric acids — digestion of the milled samples at 125° to 150°C; see Smith et al. 2013 for more detail). The chemical elements reported were Ag, Al, As, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cs, Cu, Fe, Ga, Hg, In, K, La, Li, Mg, Mn, Mo, Na, Nb, Ni, P, Pb, Rb, S, Sb, Sc, Se, Sn, Sr, Te, Th, Ti, Tl, U, V, W, Y, and Zn. Note that neither Si nor LOI were included in the contracted analytical package. As ICP-based analytical techniques cannot quantify O and H present (in fact, abundant) in most if not all geological samples, the sum of all its analytes (Al, …, Zn) falls well short of the ideal, complete composition of one million parts per million (ppm). Indeed in the NASGL C horizon dataset, used herein to illustrate our method, the sum of all ICP analytes ranges from 1134 to 390,740 (average 144,869) ppm.

The NASGL project also analyzed and quantified mineralogy in those samples. The minerals quantified were quartz, K-feldspars, plagioclases, (total feldspars), 14 Å clays (i.e. smectite), 10 Å clays (i.e. illite), kaolinite, (total clays), gibbsite,

continued on page 5

EXPLORE

Newsletter No. 201 December 2023

Editor:
Beth McClenaghan (bethmcclenaghan@sympatico.ca)

Business Manager:
Steve Cook, explorenewsletter@gmail.com
Back Issues: AAG Website (www.appliedgeochemists.org)

EXPLORE is published quarterly by the Association of Applied Geochemists, P.O. Box 26099, 72 Robertson Road, Ottawa, ON Canada K2H 9RO

EXPLORE is a trademark of the Association of Applied Geochemists.

Layout of **EXPLORE** is by Elizabeth Ambrose (Ambrose-and-Associates@ rogers.com).

EXPLORE Newsletter Advertising Rates (effective Jan. 2023)

ANNUAL CORPORATE SPONSORSHIP		**USD**	**CAD**
Full year		$2,500	$3,275

Includes: Company logo on the front cover
20% off advertising rates

ADVERTISING RATES PER ISSUE (QUARTERLY)		**USD**	**CAD**
Full page	241h x 190w mm (9.5h x 7.5w in)	$1,350	$1,775
Half page	241h x 89w mm (9.5h x 3.5w in) or 124h x 190w mm (4⅞h x 7.5w in)	$750	$980
1/3 page	241h x 51w mm (9.5h x 2w in) or 178h x 89w mm (7h x 3.5w in)	$600	$785
1/4 page	124h x 89w mm (4⅞h x 3.5w in) or 241h x 41w mm (9.5h x 1⅝w in)	$425	$555
1/8 page	60h x 89w mm (2⅜h x 3.5w in)	$75	$100

Please direct advertising inquiries to
Steve Cook (explorenewsletter@gmail.com)

Note from the Editor

Welcome to the fourth and final EXPLORE issue of 2023. This issue features an article describing inverting missing SiO_2 and LOI contents in soil, for the North American soil geochemical landscapes datasets. It was written by Patrice de Caritat, Eric Grunsky, and David Smith.

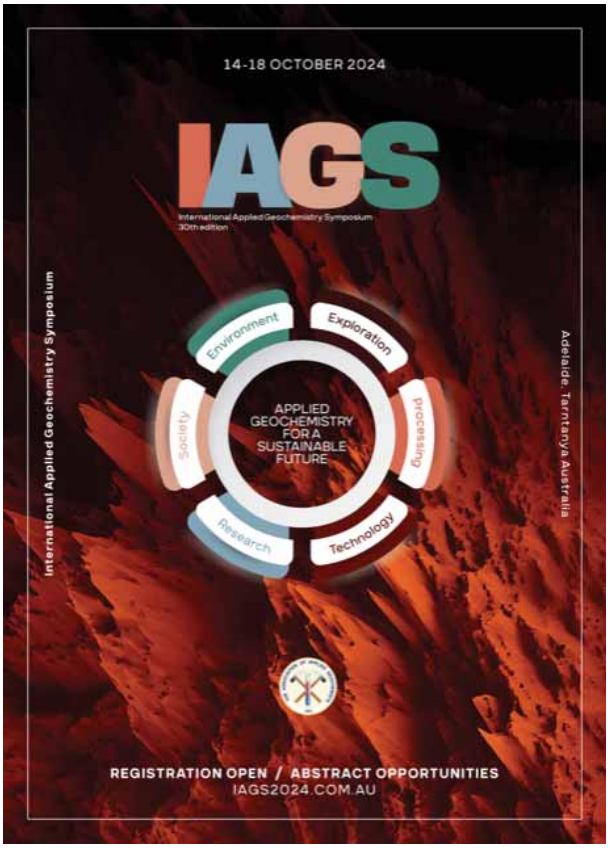
EXPLORE thanks all those who contributed to the writing and/or editing of the 4 issues in 2023 including Alfredo Lopez Alfegeme, Elizabeth Ambrose, Steve Amor, Dennis Arne, Al Arsenault, Chris Beckett-Brown, Patrice de Caritat, John Carranza, Dave Cole, Steve Cook, Theo Davies, Rory Eakin, Bob Garrett, Eric Grunsky, Grant Hagedorn, Anicia Henne, Fang Huang, James Kidder, David Leng, Nicolas Meriaud, Paul Morris, Ryan Noble, Jessey Rice, Stephen Sheppard, David Smith, Cliff Stanley, Alex Voinot, and Morgan Williams. We also thank Vivian Heggie for her dedication and graphic design expertise — she did the page layout of EXPLORE for 30 years and retired this past June. Vivian passed away a few weeks ago.

Beth McClenaghan
Editor

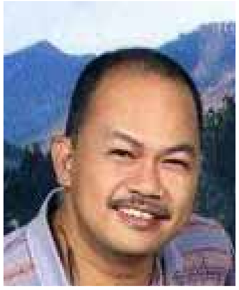
Steve Cook,
Business Manager

TABLE OF CONTENTS

ADVERTISERS



President's Message



This is my valedictory message to you, as my 2 year term as President of AAG ends on the last day of this year 2023. During my term, I have greatly benefited from the help of many people that contributed to the running of the AAG and I would like to take this opportunity to thank them. Thanks to the Executive — Yulia Uvarova (Vice President), Gwendy Hall (Treasurer) and Dave Smith (Secretary) — for running things smoothly, to Al Arsenault (Business Manager) for the day-to-day administrative operations, to our Councillors for serving with commitment both in regional and term positions, and particularly to those who are committee chairs/members. Thanks to Beth McClenaghan and Steve Cook for managing our EXPLORE newsletter. A very big thank you to Scott Wood, Editor in Chief of GEEA, for his efforts that resulted in GEEA's impact factor rising from 1.437 for 2020 to 2.266 for 2021 and to 2.4 for 2022. For the other contributors that I've forgotten to mention here, I apologize in advance but I thank you for your contributions.

In the early part of my tenure, we saw the 'split' of the African continent into northern and southern regions, as proposed by Theo Davies, who was then Regional Councillor for Africa. The boundary was decided mainly so that the two regions do not differ much in area and so that no parts of any country fall into two regions (*see* EXPLORE 195, June 2022). So, for the first time, we have two Regional Councillors in Africa, Theo Davies for southern Africa and Silas Sunday Dada for northern Africa. It is interesting to note that, prior to the split, there were only 10 AAG members in the whole of Africa, five each from these two regions. It may take time before the splitting of Africa into the two regions would impact on the number of AAG membership in this part of the world; hopefully, it will grow.

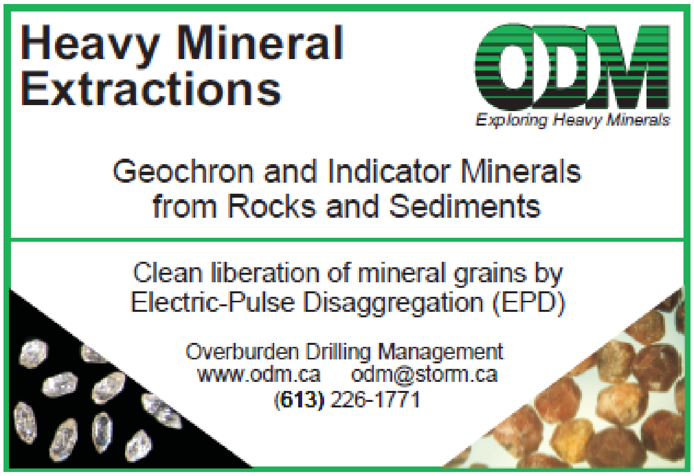
The 29th IAGS (International Applied Geochemical Symposium), which was originally scheduled November 8–13, 2020 but postponed twice due the COVID-19 pandemic, was finally held on October 23–28, 2022, in the "Garden City" of Viña del Mar, Chile. On behalf of the AAG, I thank again the Local Organizing Committee (LOC) of 29th IAGS, led by Brian Townley, for their patience and resilience to see to it that this event happened and succeeded. With its theme "Facing the Challenges of Today Using Applied Geochemistry", the 29th IAGS convened 9 different sessions, each addressing either a broad or narrow spectrum of particular challenges to which geochemistry can be applied. Many of these challenges are not new but require new paradigms or new approaches, and these were demonstrated in three keynote lectures, 77 oral presentations and 23 poster presentations. The 29th IAGS attracted at least 200 participants, including those who participated in workshops and field trips, from 20 different countries. During this event, I was pleased to award the 2019 AAG Gold Medal to Benedetto De Vivo, the 2020 AAG Gold Medal to Qiuming Cheng, and the 2020 Cameron–Hall Copper Medal to David Cooke.

This year, the AAG gave Australia the honour to host the 30th IAGS in 2024. Its LOC, led by Anna Petts of the Geological Survey of South Australia, recently distributed the 1st circular of this event, which will take place in Adelaide in 14–18 October 2024 and with the theme "Geochemistry for a Sustainable Future". The LOC is pleased to announce that the International Association for Mathematical Geosciences (IAMG) are partnering with the IAGS and AAG to convene a session on 'Big Data Analytics and Machine Learning Algorithms in Geochemistry', which will be convened by Renguang Zuo and myself. I look forward to meeting many of you at the 30th IAGS.

Overall, it was a pleasure to serve the AAG as its President in the past two years. My only regret is that the project I proposed, and approved by Council, to publish an Encyclopedia of Exploration Geochemistry within Springer's Encyclopedia of Earth Sciences Series has not lifted off until now because our editorial team is not complete yet. It is difficult to find experts who have both the expertise and the time to contribute to this project. We will, in the last Council meeting this year, consider whether to pursue this project or undertake a Wikipedia project instead.

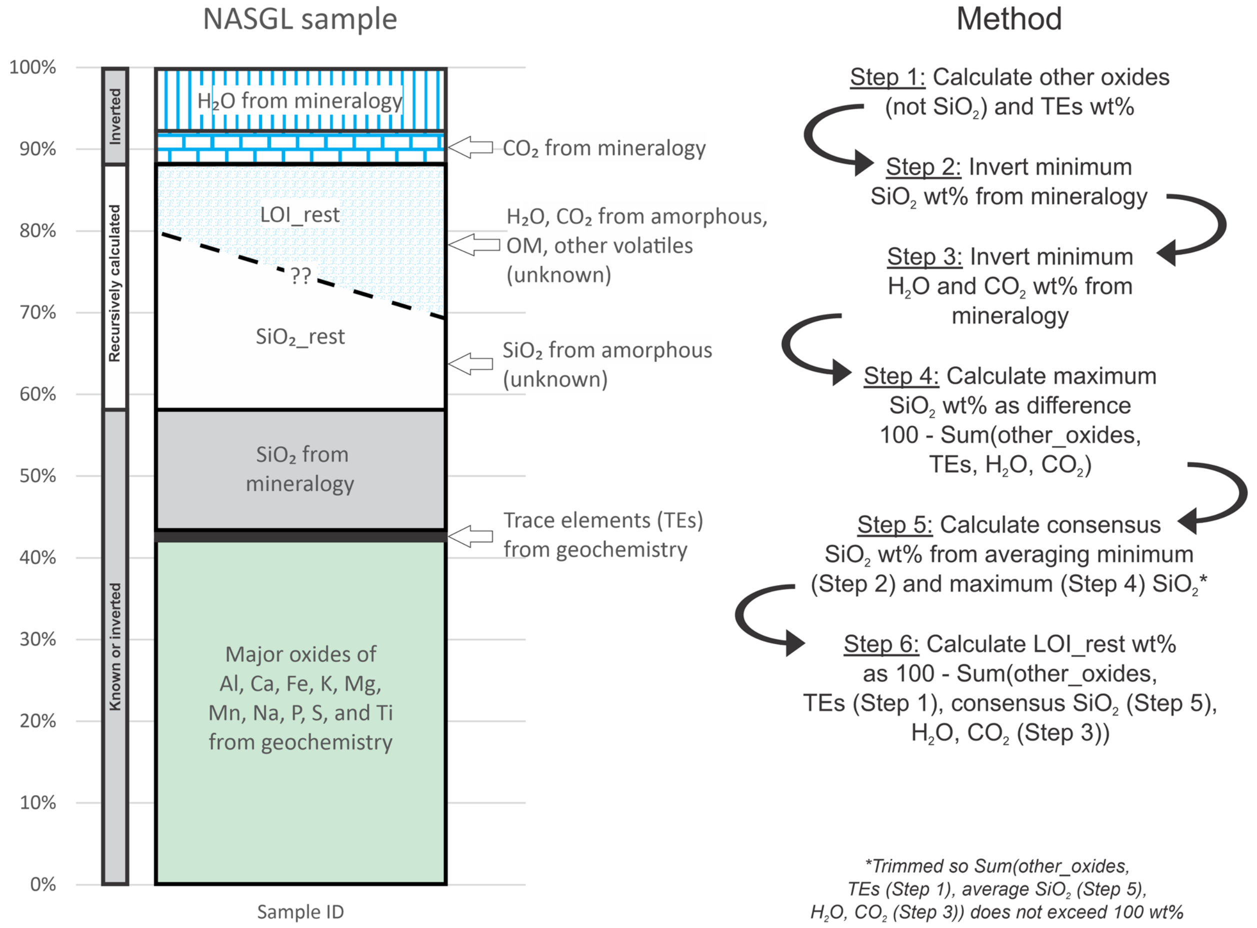
Finally, Yulia Uvarova will take over as AAG's President in 2024 and 2025, Renguang Zuo has agreed to replace Yulia as Vice-President. I in turn will replace Dennis Arne as Chair of the AAG's Awards and Medals committee. I appreciate that these individuals take on leadership roles within the AAG. I welcome our new and returning Councillors, and wish Yulia the very best as she takes the helm of the AAG for the next two years.

John Carranza
President



Inverting the missing SiO_2 and LOI contents ...

continued from page 1



Step 1: Calculate other oxides (not SiO_2) and TEs wt%

Step 2: Invert minimum SiO_2 wt% from mineralogy

Step 3: Invert minimum H_2O and CO_2 wt% from mineralogy

Step 4: Calculate maximum SiO_2 wt% as difference 100 - Sum(other_oxides, TEs, H_2O, CO_2)

Step 5: Calculate consensus SiO_2 wt% from averaging minimum (Step 2) and maximum (Step 4) SiO_2*

Step 6: Calculate LOI_rest wt% as 100 - Sum(other_oxides, TEs (Step 1), consensus SiO_2 (Step 5), H_2O, CO_2 (Step 3))

**Trimmed so Sum(other_oxides, TEs (Step 1), average SiO_2 (Step 5), H_2O, CO_2 (Step 3)) does not exceed 100 wt%*

Fig 1. Conceptual diagram of an incomplete soil analysis and workflow of the SiO_2 and LOI recursive inversion estimation methodology developed herein using geochemistry and mineralogy.

calcite, dolomite, aragonite, (total carbonates), analcime, heulandite, (total zeolites), gypsum, talc, hornblende, serpentine, hematite, goethite, pyroxene, pyrite, other, and amorphous (phases in parenthesis are summations of other minerals). The amorphous phase typically consists of material that is poorly diffracting; this will generally include clay minerals, various forms of micro-quartz, Fe-, Mn- and Al-oxyhydroxides, organic matter, volcanic glass, etc. (e.g. Tan et al. 1970; Smith et al. 2018; Tsukimura et al. 2021). Minerals were identified by X-Ray Diffraction (XRD) and quantified using a Rietveld refinement method (Smith et al. 2013). Unlike the geochemical data, the XRD data are 'complete' in the sense that they do add up to 100 wt% (range 99.6 to 100.2, average 100.03, wt% for the C horizon). The present contribution develops and tests a method for estimating the missing, yet crucial, Si/SiO_2 and LOI concentrations.

INVERTING SiO_2 AND LOI FROM GEOCHEMISTRY AND MINERALOGY

As the NASGL project did not use XRF analysis, we first need to convert the 10 reported major elements (Al, Ca, Fe, K, Mg, Mn, Na, P, S, and Ti) into oxides and unify units to wt%. These oxides are hereafter referred to as 'other_oxides' to emphasize that they do not include SiO_2. The proposed method for estimating the missing SiO_2, which draws upon both the geochemical and the mineralogical analyses of the NASGL samples, is described below and the workflow is illustrated in Figure 1. A worked example is provided as a Microsoft Excel spreadsheet (https://doi.org/10.5281/zenodo.8191288).

Initially, two estimates for SiO_2 are calculated by inverting mineralogical information; neither is ideal, as the first is likely to give a minimum, and the second a maximum value for SiO_2. Next, a 'consensus' SiO_2 concentration is obtained recursively from the two aforementioned estimates. Finally, the LOI is calculated to obtain a closed full composition at 100 wt%. The detailed steps are described below.

Step 1: Data preparation. The geochemical and mineralogical data for soils of the conterminous United States (A and C horizon datasets) were downloaded from https://mrdata.usgs.gov/ds-801/. Samples (rows) that had either incomplete or missing geochemical or mineralogical quantification (e.g. insufficient sample material) were removed. Analytes (columns) with excessive censored values (below detection/reportable limit) were removed (e.g., Ag, Cs, Te; Grunsky et al. 2018). Concentration units were unified (ppm) and censored data were imputed using the zCompositions package (lrEM function) in the R computing environment (Palarea-Albaladejo et al. 2014). Note that the imputation step is not critical to the present estimation workflow and other ways of handling cen-

continued on page 7

Inverting the missing SiO_2 and LOI contents ...

continued from page 5

sored data may be applied. After imputation, the major elements were converted to oxides and all analytes were expressed as wt%.

Step 2: Inverting 'normative' SiO_2 due to silicate minerals. The **'normative' SiO_2** is the amount of SiO_2 each sample must contain to be consistent with its mineralogy (technically this is a reverse normative or inversion approach). This 'normative' SiO_2 calculates and sums the contributions in SiO_2 of each Si-bearing mineral (silicate), for example, **1 * quartz + 0.6476 * K-feldspar + … + AVERAGE (0.4830,0.5985,0.5549,0.5173) * pyroxene**. The multipliers are the proportions of the relevant oxide (e.g. SiO_2) in each mineral (e.g. K-feldspar above), and were sourced from https://webmineral.com. Where more than one end-member mineral exists for a group (e.g. a solid-solution), the average of the (most common) end-members is used (e.g. pyroxene above). This first estimate of SiO_2 does not consider the mineral phases 'other' and 'amorphous'. Amorphous has a median abundance of 17.5 wt% and a maximum of 95.2 wt% in the NASGL C horizon dataset. It is likely to contain forms of microcrystalline silica, such as opal-A; e.g., Achilles et al. 2018), and therefore the 'normative' SiO_2 calculated here could, and most likely does, underestimate the real SiO_2 concentration.

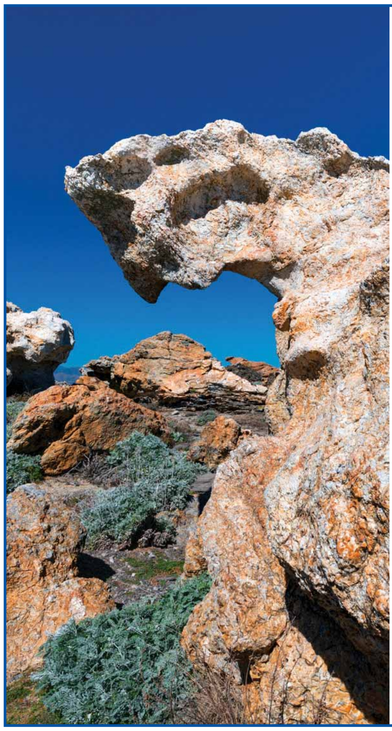
Step 3: Inverting LOI due to hydrate and carbonate minerals. The **'normative' H_2O** and **'normative' CO_2** components of LOI in each sample were calculated to be consistent with the mineralogy (e.g. amounts of gypsum and calcite). This is done in a similar way as described above, but applied to all O- and H-bearing (hydrate) minerals and all C-bearing (carbonate) minerals, respectively. As for SiO_2, the 'normative' H_2O and CO_2 contents of the amorphous phase are not known and likely important (e.g. Achilles et al. 2018). Thus this method could, and most likely does, underestimate the real LOI concentration.

Step 4: Calculating a second estimate for SiO_2. A second SiO_2 estimate is calculated by the difference **100 wt% - Sum(other_oxides, TEs, 'normative' H_2O, 'normative' CO_2)**. It could, and most likely does, overestimate the real SiO_2 concentration because LOI is almost certainly underestimated (see above). Note that in some instances, the first estimate of SiO_2 is larger than the second, which we interpret to result either from uncertainty in the mineralogical quantification (amounts of silicate, hydrate and carbonate minerals are not consistent with the geochemistry), or from an overestimation of 'normative' H_2O ('normative' CO_2 being well constrained by carbonate minerals).

Step 5: Recursively estimating a 'consensus' SiO_2. A **'consensus' SiO_2** is then calculated recursively by first taking the average of the above two SiO_2 estimates. For some samples, this SiO_2 estimate results in the **Sum(all_oxides, TEs, 'normative' H_2O, 'normative' CO_2)**, where all_oxides include the 'consensus' SiO_2 determined at Step 4, to exceed 100 wt%; in these cases, the SiO_2 estimate is trimmed so that this sum is 100 wt%.

Step 6: Calculating total LOI. Finally, the **LOI_rest**, that is volatiles others than the 'normative' H_2O and 'nor-

continued on page 9




EVIDENT

Inverting the missing SiO_2 and LOI contents ...

continued from page 7

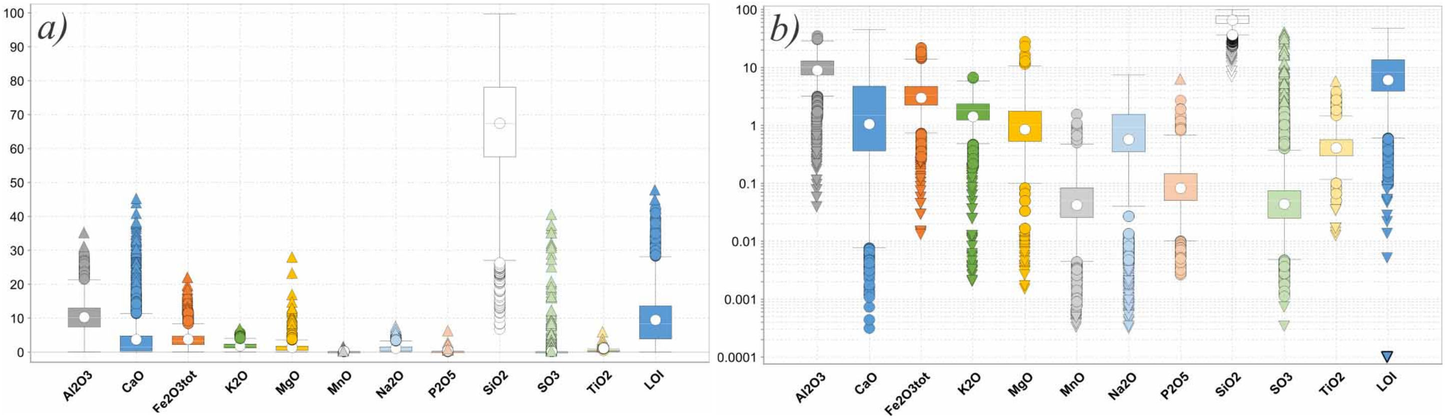


Fig. 2. Tukey boxplots for the major oxides (wt%) in the C horizon samples from the NASGL project (source: Smith et al. 2013), including SiO_2 and LOI estimated by the method described herein, with a linear (a) and log ordinate scale (b). Each box spans the 25th to 75th percentile (a.k.a. the inter-quartile range, IQR), the median is represented by a white/grey line inside the box, the mean by a white dot, the whiskers by T-shaped bars extending 1.5 x IQR away from the box, the inner outliers (up to 3 x IQR away from the box) by circles, and the outer outliers (more than 3 x IQR away from the box) by triangles.

mative' CO_2 calculated at Step 3 above, are calculated as the difference 1**00 wt% - Sum(all_oxides, TEs, 'normative' H_2O, 'normative' CO_2)**. This LOI_rest is likely to comprise H_2O and CO_2 in the amorphous phase as well as any other volatiles not specifically accounted for above. From here, total LOI or LOI_{tot} is calculated as **Sum('normative' H_2O, 'normative' CO_2, LOI_rest)**. Note that in a few cases where LOI_{tot} is zero it is replaced by 0.0001 wt% to allow log-transformation.

RESULTS AND DISCUSSION

Distributions of the SiO_2 and LOI estimates

The resultant final estimates for SiO_2 in the C horizon samples from the NASGL project have a distribution as represented in the Tukey boxplots (Tukey 1977) of Figure 2, which seem reasonable compared to the distribution of the other oxides. SiO_2 is clearly the most abundant major oxide in the NASGL soils, as is both expected and consistent with other regions (e.g. Australia, see Caritat and Cooper 2011a). The distribution of LOI is also illustrated in Figure 2. Table 1 summarizes the statistics of the estimated SiO_2 and LOI concentrations derived herein for both the A and C horizons.

Application to Selected NASGL Samples

Figure 3 shows the major oxide, including the SiO_2 estimated as described above, TEs, 'normative' H_2O, 'normative' CO_2, and LOI_rest of five selected samples from the NASGL C horizon dataset. Those samples were deliberately chosen to span the range of soil compositions in the dataset: sample from Site 7327 (California) is an Al-rich sample, 972 (Texas) is Ca-rich, 444 (Maryland) is Fe-rich, 12779 (Colorado) is K-rich, and 3808 (Florida) is Si-rich. Without the estimates for SiO_2 and LOI (and its components), only between 0.2 (3808) and 54 wt% (972) of those samples would be geochemically characterized; the rest would be unknown. This unknown 'gap' is shown by the present estimation technique to com-

Table 1. Summary statistics (count, minimum, median, average, maximum and standard deviation, in wt%) for the SiO_2 and LOI estimates in the A and C horizon samples from the NASGL project.

Variable	Count	Min	Med	Ave	Max	SD
SiO_2-A horizon	4800	7.25	72.02	72.07	99.8	13.96
SiO_2-C horizon	4669	6.78	67.37	67.44	99.63	15.18
LOI-A horizon	4800	0.0001	8.2	8.99	44.87	6.57
LOI-C horizon	4669	0.0001	8.36	9.48	47.57	7.02

continued on page 10

Inverting the missing SiO_2 and LOI contents ...

continued from page 9

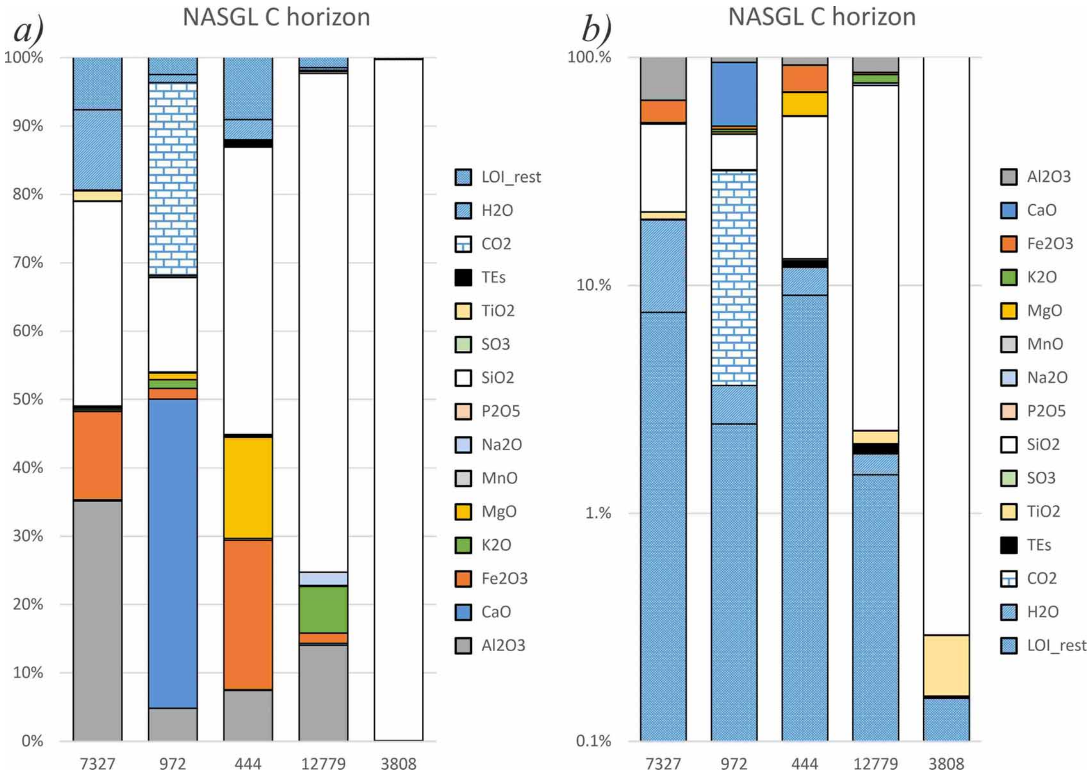


Fig. 3. Bar graphs showing the composition of five selected C horizon samples from the NASGL project (source: Smith et al. 2013) in terms of major oxides (wt%), including SiO_2 (white) and LOI (white with blue patterns) estimated by the method described herein, and trace elements (TEs). Components are shown in conventional order with a linear scale (a) and on a log scale in reverse order to emphasize the less abundant components (b).

prise widely varying proportions of SiO_2 (from silicates), H_2O (mainly from silicates), CO_2 (from carbonates), and other volatile phases (from the amorphous phase and possibly other volatile components). It is thus important to provide estimates for each sample that honor the known mineralogical characteristics rather than apply a one-size-fits-all estimation of these parameters.

Application to Selected NASGL Samples

Figure 3 shows the major oxide, including the SiO_2 estimated as described above, TEs, 'normative' H_2O, 'normative' CO_2, and LOI_rest of five selected samples from the NASGL C horizon dataset. Those samples were deliberately chosen to span the range of soil compositions in the dataset: sample from Site 7327 (California) is an Al-rich sample, 972 (Texas) is Ca-rich, 444 (Maryland) is Fe-rich, 12779 (Colorado) is K-rich, and 3808 (Florida) is Si-rich. Without the estimates for SiO_2 and LOI (and its components), only between 0.2 (3808) and 54 wt% (972) of those samples would be geochemically characterized; the rest would be unknown. This unknown 'gap' is shown by the present estimation technique to comprise widely varying proportions of SiO_2 (from silicates), H_2O (mainly from silicates), CO_2 (from carbonates), and other volatile phases (from the amorphous phase and possibly other volatile components). It is thus important to provide estimates for each sample that honor the known mineralogical characteristics rather than apply a one-size-fits-all estimation of these parameters.

For instance, sample 7327 contains significant clay minerals (40.5 wt% kaolinite) and thus has not only elevated Al_2O_3, but also elevated SiO_2 and LOI (H_2O) concentrations. Sample 972 contains significant carbonates (64.1 wt% calcite) as reflected not only by the elevated CaO, but also CO_2 concentrations. Sample 444 comprises significant amorphous

continued on page 11

Inverting the missing SiO_2 and LOI contents ...

continued from page 10

material (41 wt%) as well as notable clay (24.2 wt% of combined 14 Å clay and kaolinite), pyroxene, talc and hematite contents, imparting significant Fe_2O_{3tot}, MgO, moderate SiO_2 and relatively low LOI concentrations. Sample 12779 contains 60 wt% combined K-feldspar and plagioclase and some 10 Å clay, translating into a SiO_2-, Al_2O_3- and K_2O-rich geochemical makeup. Finally, sample 3808 contains 98.5 wt% quartz and 1.5 wt% K-feldspar, giving a geochemical composition overwhelmed by SiO_2 (estimated at 99.6 wt%); it probably also contains trace amounts of anatase or other Ti-bearing phase(s), undetected by the XRD method applied, to account for (some of) the 0.13 wt% TiO_2 reported geochemically.

Spatial Distributions of the SiO_2 in NASGL C Horizon

A map of the distributions of estimated SiO_2 concentrations in the NASGL C horizon is shown in Figure 4. The data are classified into ten quantile (decile) classes and coloured as per the mapping convention of Smith et al. (2014, 2019). The distribution shows strong similarities with the backdrop quartz distribution maps in the C horizon (Figure 141 in Smith et al. 2014), reflecting a dominant mineralogical control on the SiO_2 concentrations.

Validation and Uncertainty

Validation of the proposed method to estimate the missing SiO_2 and LOI data was performed in two different ways. The first was to apply the recursive inversion workflow to a dataset from Australia (Caritat et al. 2023) that includes both XRF (including SiO_2) and XRD data, and compare measured vs predicted SiO_2 concentrations (which gave $R^2 = 0.91$). The second was to iden-

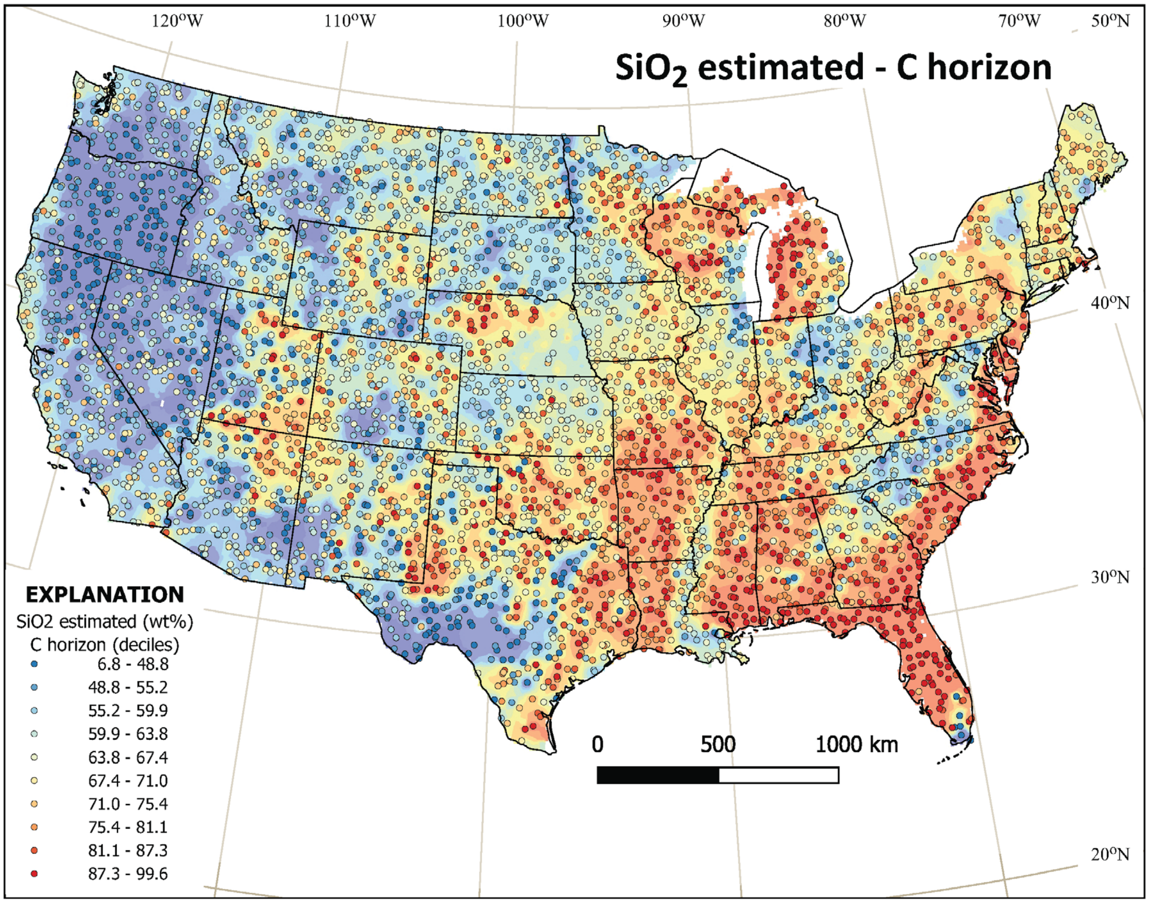


Fig. 4. Spatial distribution of the SiO_2 concentrations estimated herein for the C horizon of the NASGL samples across the USA. The symbols are classified and colored as per Smith et al. (2014), and overlain on the quartz distribution interpolated map (Figure 141 in Smith et al. 2014).

continued on page 12

Inverting the missing SiO_2 and LOI contents ...

continued from page 11

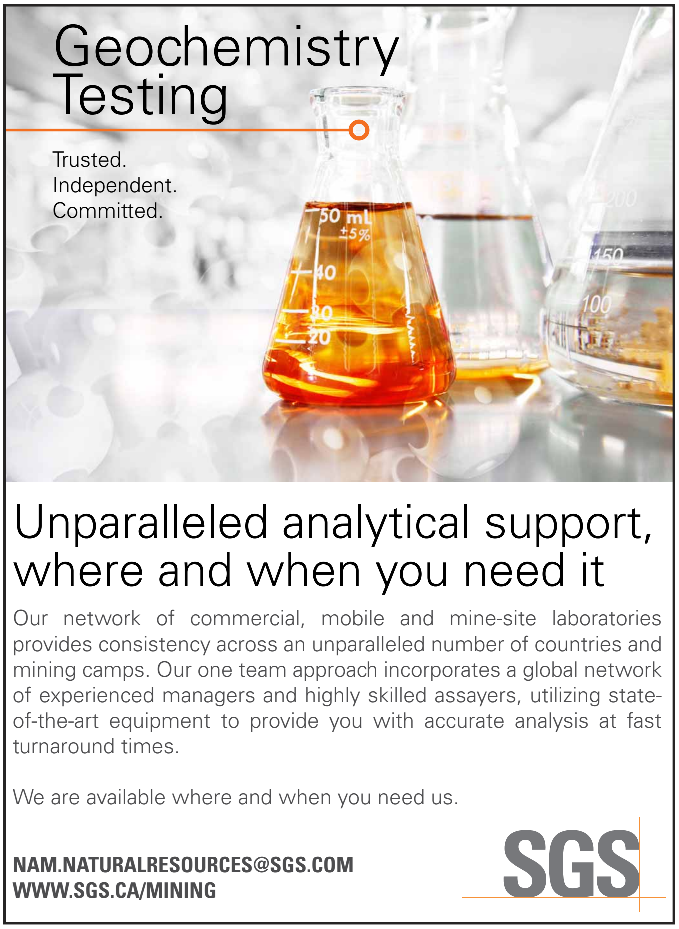
tify the closest NASGL samples to the 400 sample previously published Shacklette and Boerngen (1984) from the USA regolith geochemistry dataset (https://mrdata.usgs.gov/ussoils/) with measured SiO_2, and compare (1) the pairs of geographically 'adjacent' SiO_2 values (which gave $R^2 = 0.79$), and (2) the cumulative distribution functions of both SiO_2 values (measured by Shacklette and Boerngen and estimated from NASGL) by applying a Kolmogorov-Smirnov (K-S) test of distribution similarity (Kolmogorov 1933). All the validations indicated that the estimation method developed herein provides acceptable estimates. A further validation in the future could include analyzing certified reference soil samples.

Uncertainty of the inverted concentrations was propagated from the uncertainty in the mineralogical data using the root-sum-squares (RSS) method following Ellison et al. (1997) and Taylor (2005). The resulting uncertainty on the SiO_2 estimates was found to be 14.1 wt%. In comparison, the uncertainty of the XRF-based SiO_2 quantification in the National Geochemical Survey of Australia is estimated at 7.3 wt% (three times the RSD of 0.04 x 61.06 wt% quoted in table 1 of Caritat and Cooper 2011b).

For brevity of this contribution, the reader is referred to the fuller version of this paper published in *Geochemistry: Exploration, Environment, Analysis* with a preprint available at https://doi.org/10.31223/X5C665 for details of the validation and uncertainty of the SiO_2 estimates.

FUTURE WORK

In a complementary approach in progress, we are developing a machine learning approach using linear regression and random forest algorithms to estimate SiO_2 where it is missing, based on geochemical information, mineralogical information, and both geochemical and mineralogical information. This method will be tested on various datasets, including the NASGL and SA-Qld-NT datasets, to ensure its universal applicability and will be reported separately (Grunsky et al. *in prep.*)



DATASETS

A worked example for the five selected samples of Figure 3 is available as a Microsoft Excel spreadsheet (NALG_Ch_oxides_with_estimated_SiO2_LOI_worked example.xlsx) at https://doi.org/10.5281/zenodo.8191288. The new datasets including sample identification, coordinates, converted major oxide concentrations, and the concentration estimates for SiO_2 and LOI in wt% for the A and C horizon datasets from the North American Soil Geochemical Landscapes (NASGL) project are available as comma-separated value files (NALG_Ah_oxides_with_estimated_SiO2_LOI.csv and NALG_Ch_oxides_with_estimated_SiO2_LOI.csv) at https://doi.org/10.5281/zenodo.8191288.

CONCLUSIONS

We provide a novel method for estimating the concentrations of silica (SiO_2 wt%) and loss-on-ignition (LOI wt%) in the North American Soil Geochemical Landscapes (NASGL) project datasets. These datasets include comprehensive elemental and mineralogical compositions, determined mostly by four-acid digestion Inductively Coupled Plasma (ICP) Atomic Emission Spectroscopy (AES) or Mass Spectrometry (MS), depending on the element, and Rietveld refinement X-Ray Diffraction (XRD), respectively. Unfortunately, neither Si/SiO_2 nor LOI are quantified, both of which are significant components of most soils. Our estimation method combines the precision of the ICP determinations with the completeness of the XRD data. As the NASGL samples contain up to 95 wt% amorphous material of unknown geochemical or mineralogical composition, it is not

continued on page 13

Inverting the missing SiO_2 and LOI contents ...

continued from page 12

possible to directly calculate SiO_2 or LOI contents from mineralogy alone. However, a recursive inversion approach, i.e., calculating geochemistry from mineralogy, can be invoked to calculate minimum SiO_2, H_2O and CO_2 concentrations. Thus, we inverted an estimate for SiO_2 by adding up the SiO_2 contributions from all Si-bearing minerals (silicates). This 'normative' SiO_2 represents a minimum estimation of the total SiO_2 in each sample. Similarly, we inverted estimates for H_2O by adding up the H_2O contributions from all O-H-bearing minerals (hydrates), and for CO_2 by adding up the CO_2 contributions from all C-bearing minerals (carbonates). Combining the latter two components gives a minimum estimate for LOI. Thus, **100 wt% - (all major oxides from ICP + TEs from ICP + 'normative' H_2O + 'normative' CO_2)**, yields a maximum estimate of the total SiO_2 in each sample. The final or 'consensus' SiO_2 estimate is then calculated as the average between the two aforementioned estimates, trimmed as necessary to yield a total composition (**all major oxides from ICP + estimated SiO_2 + TEs from ICP + 'normative' H_2O + 'normative' CO_2**) of no more than 100 wt%. For most samples, the above sum falls below 100 wt% and the difference is taken to represent LOI not otherwise accounted for in the quantified hydrate and carbonate minerals. The source of this LOI contribution likely includes H_2O and CO_2 in the amorphous phase as well as other volatile components present in soil. We examine the statistical distributions of the SiO_2 and LOI estimates and validate the technique against a separate dataset from Australia where XRF, ICP and XRD data on the same samples exist. The correlation between predicted and observed SiO_2 is deemed strong ($R^2 = 0.91$). Further, we compared the estimated NASGL C horizon SiO_2 estimates with an independent dataset covering the conterminous USA, the 'Shacklette and Boerngen' dataset. The distributions of these two datasets are shown by a Kolmogorov-Smirnov test to be statistically identical. Spatially we demonstrate that the closest NAGSL sites and 'Shacklette and Boerngen' sites have highly correlated SiO_2 concentrations ($R^2 = 0.79$). Together, these validation assessments give us the confidence to recommend the approach of combining geochemical and mineralogical datasets to estimate missing SiO_2 and LOI in datasets elsewhere. However, as each situation is different, any estimation results ideally should be ground-truthed.

The full paper of this article is published in Geochemistry: Exploration, Environment, Analysis and is available at https://doi.org/10.1144/geochem2023-039.

ACKNOWLEDGMENTS

We appreciate comments on a draft version of this manuscript by Laurel G. Woodruff (United States Geological Survey) as well as internal reviews by Philip Main and Tara Webster (Geoscience Australia). EXPLORE reviewer Alexandre Voinot and editor Beth McClenaghan are thanked for their comments. PdC publishes with permission from the Chief Executive Officer, Geoscience Australia.

REFERENCES

Achilles, C.N., Downs, G.W., Downs, R.T., Morris, R.V., Rampe, E.B., Ming, D.W., Chipera, S.J., Blake, D.F., Vaniman, D.T., Bristow, T.F., Yen, A.S., Morrison, S.M., Treiman, A.H., Craig, P.I., Hazen, R.M., Tu, V.M. and Castle, N. 2018. Amorphous phase characterization through X-ray diffraction profile modeling: implications for amorphous phases in Gale Crater rocks and soils. 49th Lunar and Planetary Science Conference, LPI Contribution 2083, 2661. https://www.hou.usra.edu/meetings/lpsc2018/pdf/2661.pdf

Aitchison, J., 1986. The Statistical Analysis of Compositional Data. Chapman and Hall, London, 416 p. ISBN 9781930665781.

Aldis, M., Posch, M. and Aherne, J. 2023. Normative mineralogy of 1170 soil profiles across Canada. Minerals, 13, 544. https://doi.org/10.3390/min13040544

Caritat, P. de and Cooper, M. 2011a. National Geochemical Survey of Australia: The Geochemical Atlas of Australia. Geoscience Australia, Record, 2011/20, 557 p. http://dx.doi.org/10.11636/Record.2011.020

Caritat, P. de and Cooper, M. 2011b. National Geochemical Survey of Australia: Data Quality Assessment. Geoscience Australia, Record, 2011/021, 478 p. https://pid.geoscience.gov.au/dataset/ga/71971

Caritat, P. de, Bloch, J. and Hutcheon, I. 1994. LPNORM: a linear programming normative analysis code. Computers & Geosciences, 20, 313–347. https://doi.org/10.1016/0098-3004(94)90045-0

continued on page 14

Inverting the missing SiO_2 and LOI contents ...

continued from page 13

Caritat, P. de, Petts, A. and Kelaart, C. 2023. Contribution towards a regolith mineralogy map of the Australian continent: A study in South Australia, Queensland and the Northern Territory. Geoscience Australia, Record, 2023/15. https://dx.doi.org/10.26186/147990

Chayes, F., 1960. On correlation between variables of constant sum. Journal of Geophysical Research, 65, 4185–4193. https://doi.org/10.1029/JZ065i012p04185

Deer, W.A., Howie, R.A. and Zussman, J. 2013. An Introduction to the Rock-Forming Minerals, 3rd edition. Mineralogical Society of Great Britain and Ireland, 498 p. ISBN 9780903056274.

Ellison, S., Wegscheider, W. and Williams, A. 1997. Measurement uncertainty. Analytical Chemistry, 69, 607A–613A. https://doi.org/10.1021/ac971793j

Finkl, C.W., 1981. Soil mineralogy. *In:* Mineralogy, Encyclopedia of Earth Science. Springer, Boston, MA. https://doi.org/10.1007/0-387-30720-6_133

Grunsky, E.C., Drew, L.J. and Smith, D.B. 2018. Analysis of the United States portion of the North American Soil Geochemical Landscapes Project – A compositional framework approach. *In:* Daya Sagar, B., Cheng, Q. & Agterberg, F. (eds), Handbook on Mathematical Geosciences, Springer, Cham, 313–346. ISBN 9783319789996. https://doi.org/10.1007/978-3-319-78999-6_17

Kolmogorov, A.N. 1933. Sulla determinazione empirica di una legge di distribuzione. Giornale dell'Istituto Italiano degli Attuari, 4, 83–91.

Palarea-Albaladejo, J., Martín-Fernández, J.A. and Buccianti, A. 2014. Compositional methods for estimating elemental concentrations below the limit of detection in practice using R. Journal of Geochemical Exploration, 141, 71–77. https://doi.org/10.1016/j.gexplo.2013.09.003

Scealy, J.L., Caritat, P. de, Grunsky, E.C., Tsagris, M.T. and Welsh, A.H. 2015. Robust principal component analysis for power transformed compositional data. Journal of the American Statistical Association, 110, 136–148. https://doi.org/10.1080/01621459.2014.990563

Schaetzl, R. and Anderson, S. 2007. Soils – Genesis and Geomorphology, 1st edition reprinted with corrections. Cambridge University Press, Cambridge, 817 p. ISBN 9780521812016.

Shacklette, H.T. and Boerngen, J.G. 1984. Element Concentrations in Soils and Other Surficial Materials of the Conterminous United States: An Account of the Concentrations of 50 Chemical Elements in Samples of Soils and Other Regoliths. United States Geological Survey, Professional Paper, 1270, 105 p. https://pubs.usgs.gov/pp/1270/

Smith, D.B. 2022. Geochemical and mineralogical soil survey of the conterminous USA: a project retrospective. Geochemistry: Exploration, Environment, Analysis, 22, geochem2022-031. https://doi.org/10.1144/geochem2022-031

Smith, D.B., Cannon, W.F., Woodruff, L.G. and Ellefsen, K.J., 2014. Geochemical and Mineralogical Maps for Soils of the Conterminous United States. United States Geological Survey, Open-File Report, 2014-1082, 386 p. https://doi.org/10.3133/ofr20141082

Smith, D.B., Cannon, W.F., Woodruff, L.G., Solano, Federico, Kilburn, J.E. and Fey, D.L. 2013. Geochemical and Mineralogical Data for Soils of the Conterminous United States. United States Geological Survey, Data Series, 801, 19 p. http://pubs.usgs.gov/ds/801

Smith, D.B., Solano, F., Woodruff, L.G., Cannon, W.F. and Ellefsen, K.J. 2019. Geochemical and Mineralogical Maps, with Interpretation, for Soils of the Conterminous United States. United States Geological Survey, Scientific Investigations Report, 2017-5118. https://pubs.usgs.gov/sir/2017/5118/index.html

Smith, R.J., Horgan, B., Rampe, E. and Dehouck, E. 2018. The composition of amorphous phases in soils and sediments on Earth and Mars. 49th Lunar and Planetary Science Conference, LPI Contribution 2083, 1779. https://www.hou.usra.edu/meetings/lpsc2018/pdf/1779.pdf

Tan, K.H., Perkins, H.F. and McCreery, R.A. 1970. The nature and composition of amorphous material and free oxides in some temperate regions and tropical soils. Communications in Soil Science and Plant Analysis, 1, 227–238. https://doi.org/10.1080/00103627009366262

Taylor, J.A. 2005. Uncertainty Analysis. ES 223: Rigid Body Dynamics-Fall 2004. Arkansas State University, Jonesboro, AR. Online Lecture Notes. http://myweb.astate.edu/sharan/PMC/LectureNotes/2006/Paper%20on%20Uncertainty%20Analysis.pdf

Tsukimura, K., Miyoshi, Y., Takagi, T., Suzuki, M. and Wada, S. 2021. Amorphous nanoparticles in clays, soils and marine sediments analyzed with a small angle X-ray scattering (SAXS) method. Scientific Reports, 11, 6997. https://doi.org/10.1038/s41598-021-86573-9

Tukey, J.W. 1977. Exploratory Data Analysis. Addison-Wesley Publishing Company, Reading, MA, 688 p. ISBN 9780201076165.

ARTICLES IN PAST ISSUES OF EXPLORE

5 years ago EXPLORE 181 (December 2019)
New base metal mineral potential in southern Northwest Territories, Canada

10 years ago EXPLORE 161 (December 2013)
Evaluating the diffusive gradients in thin films technique for the detection of multi-element anomalies in soils

20 years ago EXPLORE 122 (January 2004)
Thermally speciated mercury in mineral exploration

30 years ago EXPLORE 82 (January 1994)
The use of silica sand cleaners in pulverizing mills to reduce cross contamination

https://www.appliedgeochemists.org/explore-newsletter/explore-issues

Collecting water samples with drones

The Geological Survey of Canada's (GSC) Targeted Geoscience Initiative (TGI) is conducting critical minerals exploration methods development. A team of researchers from GSC-Ottawa, led by James Kidder, is evaluating the viability and practicality of collecting lake and stream water samples using drones. The water samples are typically analyzed geochemically to aid in the assessment of mineral potential. Two types of drones were used to collect water samples at surface and at 2 m depth with point source filtering. The field-testing area for the drones was the Sharbot Lake-Long Lake region, 120 km southwest of Ottawa. The hope is that these innovative water sampling methods can be used in more remote regions across Canada's north to sample surface water for mineral resource exploration.

GSC drone sampling crew. L to R: Alain Grenier, Brad Harvey, Beth McClenaghan, Chris Beckett-Brown (Ontario Geological Survey), James Kidder.

Aurelia x6 Standard drone (far left) and SwellPro waterproof SplashDrone (left) with water bottle attachment that were used to collect water samples from the surface of a lake.

Presentation of the 2019 Cameron-Hall Copper Medal to Ally Brown

The Cameron-Hall Copper Medal (Photo by S. Cook)

The recent revival of the Vancouver Geochemical Working Group (VGWG) presentations on December 5, 2023 after a COVID pandemic hiatus provided an opportunity for a long-overdue medal presentation. Alexandra (Ally) Brown was presented with the AAG's 2019 Cameron-Hall Copper Medal for her paper, co-authored with Thomas Bissig and the late Peter Winterburn, entitled "Identification of the expression of earthquake induced surface flooding by groundwater using detailed regolith mapping at the buried Atlántida Deposit, northern Chile".

The Cameron-Hall Copper Medal is awarded to the lead author of the most outstanding scientific publication each year in the AAG's journal *Geochemistry: Exploration, Environment, Analysis*. The medal citation reads, in part, "This paper describes an innovative approach to identifying the passage of saline fluids through faults associated with buried porphyry skarn copper-gold mineralization in the Atacama region of Chile through surface mapping of saline soils developed on transported gravels."

The 2019 Cameron-Hall Copper Medal is in fact the very first instance of this award and was announced in EXPLORE 188 (September 2020). Ally's paper can be accessed in Geochemistry: Exploration, Environment, Analysis, 19(4), 474–486, at https://doi.org/10.1144/geochem2018-064

Ally Brown (right) was presented with the AAG's 2019 Cameron-Hall Copper Medal by Steve Cook (left) recently in Vancouver, Canada (Photo by Chelsea Sutcliffe).

30th International Applied Geochemistry Symposium (IAGS)

The Local Organising Committee (LOC), the Association of Applied Geochemists (AAG) welcome you to the 30th International Applied Geochemistry Symposium, IAGS 2024, Adelaide/Tartanya, Australia. This conference has the theme "Geochemistry for a Sustainable Future". Join us and contribute to sharing advances in approaches and technologies for exploration, processing and the environment for social benefit. Scientific sessions will include an emphasis on critical minerals. The IAGS LOC is pleased to announce that the International Association for Mathematical Geosciences (IAMG) are partnering with IAGS and AAG to host sessions on 'Big Data Analytics and Machine Learning Algorithms in Geochemistry'.

Aim of the IAGS 2024

The 30th IAGS will celebrate the central role of applied geochemistry in providing a sustainable future, as per the conference theme. At this conference the key sub themes will highlight the critical need for applying geochemical solutions across environmental, exploration and mining, and social solutions. These key sub themes are Exploration, Environment, Processing, Technology, Research, and Society

Why Adelaide?

A visit to Adelaide and the state of South Australia offers delegates easy access to the best of what Australia has to offer: beautiful beaches, unique Australian wildlife, world-renowned wine regions, premium culinary experiences, access to the outback, and a chance to learn about and engage with Australian Aboriginal culture.

South Australia has a strong geo-scientific community, including the Geological Survey of South Australia within the Department for Energy and Mining, resources exploration industry base, universities and research organisations including CSIRO. Currently, significant work is taking place to gain UNESCO World Heritage status for South Australia's Flinders Ranges due to its extraordinary Ediacaran fossils and geological landscape.

Adelaide is serviced by the world's best international airlines including Qantas, Virgin, Qatar Airways, Singapore Airlines, Malaysia Airlines, China Southern Airlines. It is also easily accessible from all Australian airports by all major domestic airlines. Approximate flight time from Melbourne is 1.5 hours, from Sydney is 2 hours, and from Brisbane is 3 hours

From Melbourne, the drive to Adelaide is approximately 8–9 hours, or take the scenic route along the Great Ocean Road into South Australia. From Sydney, the trip is about 16–17 hours drive time. Accommodation options, specifically for conference delegates, will be available on the IAGS website in due course. **Emirates has announced it will fly into Adelaide starting July 2024.

Dates to remember

IAGS2024 will formally commence on Monday 14th October and run through Friday, 18th October for the Scientific Program at the Adelaide Convention Centre. Wednesday 16th October will not have scheduled Scientific Program events to make room for tours and workshops.

Wednesday December 6, 2023	**Abstracts Open**
Wednesday December 6, 2023	**Registration Opens**
Wednesday March 13, 2024	**Abstracts Close**
Monday April 8, 2024	**Program Announced including Workshops & Field Trips**
Friday August 2, 2024	**Early Bird Registrations Close / Full Price Opens**
Monday October 14, 2024	**Symposium Begins**

Proposed list of scientific sessions (TBC)

The final sub-themes of the scientific sessions of the conference, including the special sessions and the Chairpersons, will be announced with the second circular later in 2023 and also on the website.

Workshops

The IAGS 2024 LOC see conference workshops as a key part of the IAGS 2024 offering and experience. Workshops will likely be held pre-conference. Workshop pricing will be at standardized day-rates with discounts for students and members of some professional organisations.

The LOC is seeking expressions of interest from the geoscience community to run workshops at the IAGS 2024. If you are interested in this, please contact Ned Howard and Anna Petts by 23rd December 2023.

As part of your submission, please provide information regarding the following:

- Names of individuals who are leading/involved and the organisation/s they represent,
- General topic and outline of workshop content,
- Brief outline of how the proposed workshop aligns with the targeted workshop themes listed below,
- Duration,
- Any requirements for the workshop venue (other than standard AV equipment),
- Representatives of commercial providers will need to demonstrate inclusion of general content non-specific to technologies or services they are promoting.

continued on page 17

IAGS 2024 ...

continued from page 17

Suggested workshop topics:

- Geochemical data collection, analysis and interpretation applied to exploration, ore deposit characterization and/or remediation
- Geochemical characteristics of ore deposits, hydrothermal alteration and mineralization processes
- Isotope geochemistry and geochronology
- Environmental geochemistry and hydro-geochemistry
- Geology and geochemistry of the regolith/critical zone and transported cover
- Sample theory, sampling practices and QA/QC
- Training in commonly used geochemical and geological software
- Novel or commonly used geochemical and mineralogical technologies and their application, e.g., portable analysers, micro-analytical techniques, scanning and imaging technologies
- Pre-competitive geochemical datasets and their application to exploration
- Geometallurgy, ore deposit knowledge and characterisation
- Soil geochemistry and viticulture
- Other topics relating to applied geochemistry where justified in the EOI submission

Already confirmed workshops include: “Applied geochemistry for exploration, geology and geochemistry of the critical zone/regolith and geology” and “Geochemistry of iron oxide-copper-gold deposits”.

Successful workshop submissions will be announced and registration opened with distribution of the Second Conference Circular.

Field trips

It is not mandatory to participate in IAGS2024 to register for a Field Trip. Field Trips will be held with a minimum number of registered participants. There will be a number of field trips planned, including pre, mid and post conference. A call for expressions of interest will be made for field trips, when announced in the Second Circular.

Sponsors

The Organising Committee is seeking organisations interested in sponsoring the IAGS 2024, and invites potential Sponsors/Exhibitors to follow the link below, or to contact the committee for a prospectus. Participating as a Sponsor or Exhibitor provides your organisation with the opportunity to demonstrate your level of support and commitment to the industry and connects your organisation with your target audience.

Conference fees

The IAGS and AAG will provide membership registration for IAMG members. Students and participants from some developing countries will be able to apply for a bursary to support travel to IAGS2024. Please check the conference website regularly for application details.

	EARLY BIRD		STANDARD	
TICKET TYPE	**Member**	**Non-Member**	**Member**	**Non-Member**
All inclusive	980	1190	1190	1380
Sponsor / Exhibitor	650	650	650	650
Symposium	850	1050	1050	1250
Student	350	350	450	450
Gala Dinner	150	150	150	150

N.B. Price is in AUD and includes GST

All Inclusive registration:
Includes 4-day conference and gala dinner

Sponsor/Exhibitor registration:
4-day conference only for Sponsors/Exhibitors

Symposium registration:
4-day conference only

Student registration:
4-day conference

Gala Dinner registration:
Dinner only

Visa information

If you are planning on attending IAGS2024 from overseas, please consider the various options before going through the registration phase. Australia has some tough immigration laws, so we don’t want you to get stuck if you are considering a visit to Australia to attend the conference.

The visa that you will have to apply for depends on your passport. We have provided the following link, but please make sure you read the information thoroughly before starting the process of your visa application.

https://immi.homeaffairs.gov.au/visas/getting-a-visa/visa-finder

Good luck with this process, and make sure you are aware of the visa processing time, to make sure it’s finalized before the conference.

Latest Updates

If you would like regular information, and all the latest updates for IAGS2024, please sign up to our mailing list by clicking the following link.

https://docs.google.com/forms/d/e/1FAIpQLSeNtXrQExR8Wnn8uPc2-rGshr3pUel-jOem6yiuxYrmdaFe8w/viewform

continued on page 18

IAGS 2024 ...

continued from page 14

Local Organising Committee

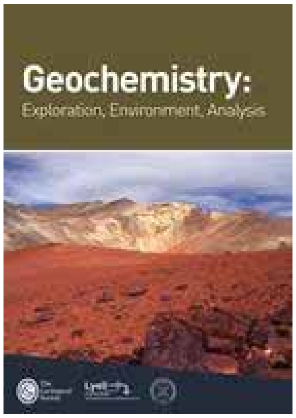
Name	Position	Affiliation
Anne Petts	Chair	Department of Energy and Mining, South Australia
Philip Main	Treasurer	Geoscience Australia
Laura Jackson	Secretary	Sustainable Mineral Institute/University of Queensland
Yulia Uvarova	Sponsoship and Trade Coordinator	CSIRO
Mark Arundell	Scientific Program Coordinator	iMEx Consulting
David Cohen	AAG Events Representative	University of New South Wales
Ned Howard	Short Course Coordinator	Evolution Mining
Adrian Fabris	Field Trips Coordinator	Department of Energy and Mining, South Australia
Travis Batch	Student Representative	UniSA
Jessika Gluchowska	Early Career Professional Representative	Rio Tinto Exploration
Erin Martin	Diversity & Inclusion Representative	WOMEESA and IGO
Jessica Walsh	Diversity & Inclusion Representative	WOMEESA and Geoscience Australia
Anthony Budd	Diversity & Inclusion Representative	Geoscience Australia
Mike Whitbread	General Committee Member	Rio Tinto Exploration
Philip Baker	General Committee Member	Rio Tinto Exploration
Mar Pirlo	General Committee Member	ALS
Stacey Priestley	General Committee Member	CSIRO
Richard Green	General Committee Member	ANU
Paul Morris	Abstract Volume Editor	AAG

More information is available on the website at https://iags2024.com.au
or
email iags2024@bie.com.au

Geochemistry: Exploration, Environment, Analysis

VOLUME 23, ISSUE 3, AUGUST 2023

Research Articles



Gold metallogeny in Iran; implications for gold exploration and conceptual modelling
F. Darabi-Golestan
https://doi.org/10.1144/geochem2023-010

Surface expression of Late Caledonian magmatic lithium concentration in the Rhynie Chert, UK
J. Parnell and J.G.T. Armstrong
https://doi.org/10.1144/geochem2023-028

Geochemical dispersion evaluation by criterion-based backward elimination at the Glojeh polymetallic Au (Ag–Cu–Pb–Zn) vein deposit, NW Iran
F. Darabi-Golestan
https://doi.org/10.1144/geochem2023-011

Estimating the silica content and loss-on-ignition in the North American Soil Geochemical Landscapes datasets: a recursive inversion approach
P. de Caritat, E.C. Grunsky and D.B Smith
https://doi.org/10.1144/geochem2023-039

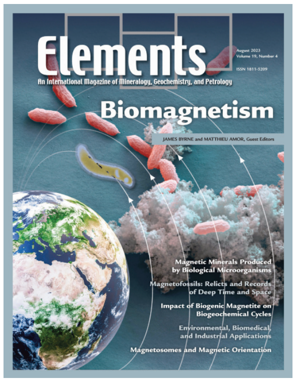
Thematic collection: Geochemical processes related to mined, milled, or natural metal deposits

Critical raw materials associated with the lateritic bauxite and red mud in West Kalimantan, Indonesia
A. Yahya Al Hakim, D. Sunjaya, A. Naftali Hawu Hede, T. Indriati and T. Hidayat
http://dx.doi.org/10.1144/geochem2022-064

Anthropogenic influence on groundwater geochemistry in Horn Creek Watershed near the Orphan Mine in Grand Canyon National Park, Arizona, United States
K.R. Beisner, C. Davidson and F. Tillman
https://doi.org/10.1144/geochem2023-007

Recently Published in Elements

August 2023, v. 19, no. 4, Biomagnetism



Many biological microogranism possess magnetic behavior owing to their formation of magnetic nanoparticles (MNP) such as magnetite (Fe_3O_4), maghemite (γ-Fe_2O_3), and greigite (Fe_3S_4). The articles in this current issue look into biomagnetism and the production of magnetic minerals by microorganisms, the relationship between biogenic MNP formation and biomagnetism, the mechanisms responsible for these minerals by bacteria, whether MNP hold clues to the evolution of life on Earth and potentially beyond, the contribution of biomagnetism to the biogeochemical cycling of iron, the potential application of MNP for industrial remediation, and the presence of MNP in multicellular prokaryotes and eukaryotic organisms.

The are no AAG news items in this Elements issue.

The last two 2023 issues of the Elements Magazine, which are about Large Igneous Provinces (Oct. 2023, v. 19 no. 5) and Geometallurgy (Dec. 2023, v. 19 no. 6), respectively, are pending production.

Reminder

AAG members can access past issues of Elements at
http://elementsmagazine.org/member-login/
using their e-mail address and AAG member ID.

John Carranza
President

Welcome New AAG Member

REGULAR MEMBERS
Regular Members are non-voting members of the Association and are actively engaged in the field of applied geochemistry at the time of their application and for at least two years prior to the date of joining.

Mr. Carl Brauhart
Consultant, Camp Oven Exploration
48 Lisle St.
Mt Claremont, WA
AUSTRALIA 6010
Membership # 452

Download the form here:
https://www.appliedgeochemists.org/

Other **Membership levels** in the Association include

STUDENT MEMBERS
Student Members are students that are enrolled in an approved course of instruction or training in a field of pure or applied science at a recognized institution. Student members pay minimal membership fees.

FELLOWS
Fellows are voting members of the Association and are actively engaged in the field of applied geochemistry. They are Regular AAG Members that are nominated to be a Fellow by a Fellow of the Association by completing the Nominating Sponsor's Form. Consider becoming a Fellow of the AAG.

PDAC MARCH 3-6 2024 THE WORLD'S PREMIER MINERAL EXPLORATION & MINING CONVENTION

EXPLORATION SHORT COURSE:
TILL GEOCHEMISTRY AND INDICATOR MINERAL METHODS FOR EXPLORATION IN GLACIATED TERRAIN

Date: Friday March 1 – Saturday March 2, 2024 (1.5 days)

Location: Prospectors and Developers Association Convention (PDAC), Toronto Canada

This short course will present overviews of till sampling and analytical methods, use of LiDAR, and the application of machine learning to till geochemical data. Several commodity case studies will be presented for lithium, gold, magmatic Ni-Cu-PGE, VMS, and porphyry Cu deposits.

https://www.pdac.ca/convention/programming/short-courses/sessions/short-courses/till-geochemistry-and-indicator-mineral-methods-for-exploration-in-glaciated-terrains-1-5-days-

CALENDAR OF EVENTS

International, national, and regional meetings of interest to colleagues working in exploration, environmental and other areas of applied geochemistry. These events also appear on the AAG web page at: www.appliedgeochemists.org.

The status of the meetings was confirmedat the time of publication, but users of the listing are strongly advised to carry out their own research as to the validity of an announcement.

Please let us know of your events by sending details to:
Steve Amor, Email: steve.amor2007@gmail.com
or
Elizabeth Ambrose, Email: eambrose0048@rogers.com

2024

14–19 January	Gordon Research Conference: Geobiology: Past, Present and Future. Galveston TX USA. Website: www.grc.org/geobiology-conference/2024
15–20 January	Winter Conference on Plasma Chemistry. Tucson AZ USA. Website: icpinformation.org/winter-conference
22–25 January	Mineral Exploration Roundup 2024. Vancouver BC Canada. Website: roundup.amebc.ca
1–3 February	1st International Congress on Green Environmental Catalysis. Osaka Japan. Website: tinyurl.com/34ah4ew3
2–3 February	Atlantic Geoscience Society Annual Colloquium. Moncton NB Canada. Website: atlanticgeosciencesociety.ca/colloquium-2024
18–23 February	2024Ocean Sciences Meeting. New Orleans LA USA. Website: www.agu.org/ocean-sciences-meeting
3–6 March	Prospectors & Developers Association of Canada Annual Convention. Toronto ON Canada. Website: www.pdac.ca/convention
3–7 March	Minerals, Metals & Materials Society 2024 Annual Meeting & Exhibition. Orlando FL USA. Website: www.tms.org/AnnualMeeting/TMS2024
18–20 March	Sedimentology of plastics: state of the art and future directions. Birmingham UK. Website: tinyurl.com/ycx7d36c
18–21 March	XV Latin American Symposium on Environmental Analytical Chemistry. Ouro Preto Brazil. Website: tinyurl.com/3v76363s
14–19 April	EGU General Assembly. Vienna Austria. Website: www.egu24.eu
2–4 May 2024	10th International Conference on Geographical Information Systems Theory, Applications and Management. Angers France. Website: gistam.scitevents.org
8~9 May	International Mining Geology Conference 2024. Perth WA Australia. Website: tinyurl.com/4dp4mffx
19–22 May	GAC-MAC Annual Meeting. Brandon MB Canada. Website: gac.ca/events/gac-mac-annual-meeting
21–23 May	11th World Conference on Sampling and Blending. Muldersdrift South Africa. Website: tinyurl.com/ycx9psc8
10–12 June	SIAM Conference on Mathematics of Planet Earth (MPE24). Portland OR USA. Website: www.siam.org/conferences/cm/conference/mpe24
17–19 June	GeoConvention 2024. Calgary AB Canada. Website: geoconvention.com
23–28 June	Geochemistry of Mineral Deposits for a Low Carbon society (Gordon Research Conference). Newry ME USA. Website: tinyurl.com/bddja374
29 June –8 July	XXIV International Multidisciplinary Scientific GeoConference - Surveying, Geology and Mining, Ecology and Management (SGEM). Varna Bulgaria. Website: www.sgem.org/index.php
8–12 July	12th International Kimberlite Conference. Yellowknife NT Canada. Website: 12ikc.ca
15–18 July	11th Annual International Conference on Geology & Earth Science. Athens Greece. Website: www.atiner.gr/geology
21–26 July	International Conference on Mercury as a Global Pollutant. Cape Town South Africa. Website: tinyurl.com/mw37tdh4
28 July – 1 August	Microscopy & Microanalysis 2024, Cleveland OH USA. Website: tinyurl.com/mpwbhcw7
28 July – 2 August	Navigating the Modern Era of Organic Geochemistry (Gordon Research Conference). Holderness NH USA. Website: www.grc.org/organic-geochemistry-conference/2024
11–15 August	IWA World Water Congress & Exhibition. Toronto ON Canada. Website: worldwatercongress.org
11–18 August	ISEG: International Symposium on Environmental Geochemistry. Galway Ireland. Website: www.universityofgalway.ie/iseh-iceph
18–23 August	4th European Mineralogical Conference. Dublin Ireland. Website: emc-2024.org
18–25 August	Goldschmidt 2024. Chicago IL USA. Website: tinyurl.com/5cr87s7e
24–30 August	35th International Geographical Congress. Dublin Ireland. Website: igc2024dublin.org
25–27 August	14th International Conference on Environmental Pollution and Remediation (2024). Barcelona Spain. Website: icepr.org
25–31 August	37th International Geological Congress. Busan, Republic of Korea. Website: www.igc2024korea.org
15–19 September	Geoanalysis 2024. Wuhan China. Website: tinyurl.com/yeyj8nuh
22–25 September	GSA Connects 2024. Anaheim CA USA. Website: community.geosociety.org/gsa2024/home
27–30 September	SEG 2024 Conference in Namibia. Windhoek Namibia. Website: tinyurl.com/zsb3kkrf
6–9 October	MS&T24: Materials Science &Technology. Pittsburgh PA USA. Website: www.matscitech.org/MST/MST24
14–18 October	30th International Applied Geochemistry Symposium (IAGS). Adelaide SA Australia. Website: iags2024.com.au

EXPLORE Publication Schedule

Quarterly newsletters are published in March, June, September, December

- **Deadlines** for submission of articles or advertisements:

  March newsletter: January 15 June newsletter: April 15
  September newsletter: July 15 December newsletter: October 15

- **Manuscripts** should be double-spaced and submitted in digital format using Microsoft WORD®. Articles should be between 2000 and 3000 words. Do **not** embed figures or tables in the text file.
- **Figures and/or photos** (colour or black and white) should be submitted as separate high-resolution (2000 dpi or higher) tiff, jpeg or PDF files.
- **Tables** should be submitted as separate digital files in Microsoft® EXCEL format.
- All scientific/technical articles will be reviewed. Contributions may be edited for clarity or brevity.
- Formats for headings, abbreviations, scientific notations, references and figures must follow the Guide to Authors for *Geochemistry: Exploration, Environment, Analysis* (GEEA) that are posted on the GEEA website at:
  https://www.geolsoc.org.uk/geea-authorinfo
- An **abstract** of about 250 words must also be submitted that summarizes the content of their article. This abstract will be published in the journal ELEMENTS on the 'AAG News' page.

Submissions should be sent to the Editor of **EXPLORE**:
Beth McClenaghan
Geological Survey of Canada 601 Booth Street, Ottawa, ON, CANADA K1A 0E8
Email: bethmcclenaghan@sympatico.ca

THE ASSOCIATION OF APPLIED GEOCHEMISTS

P.O. Box 26099, 72 Robertson Road, Ottawa, Ontario K2H 9R0 CANADA • Telephone (613) 828-0199
www.appliedgeochemists.org

OFFICERS

January – December 2023

President, **John Carranza**
Department of Geology
University of the Free State
205 Nelson Mandela Drive
Park West, Bloemfontein
SOUTH AFRICA 9301
ejmcarranza@gmail.com

Secretary, **David B. Smith**
U.S. Geological Survey
Box 25046, MS 973
Denver, CO 80225, USA
TEL: (303) 236-1849
dbsmith13@gmail.com

Vice-President, **Yulia Uvarova**
CSIRO
26 Dick Perry Ave.
Kensington W.A., AUSTRALIA 6151
yulia.uvarova@csiro.au

Treasurer, **Gwendy E.M. Hall**
110 Aaron Merrick Drive
Merrickville, ON K0G 1N0 CANADA
TEL: +1-613-269-7980
gwendyhall@gmail.com

Past-President, **Dennis Arne**
Yackandandah, Vic,
AUSTRALIA 3749
Arne.dennis@gmail.com

COUNCILLORS

2022–2023
Thomas Bissig
tbissig@gmail.com
Jamil Sader
jamilsader@yahoo.com
Alexander Seyfarth
Alexander.Seyfarth@sgs.com
Cliff Stanley
Cliff.stanley@acadiau.ca
Renguang Zuo
zrguang@cug.edu.cn
Dennis Arne *(ex-officio)*
Arne.dennis@gmail.com

2023–2024
Aaron Baensch
aaron_baensch@hotmail.com
Ray Lett
Raylett@shaw.ca
Paul Morris,
xrficpms@outlook.com
Ryan Noble,
Ryan.noble@csiro.au
Pim van Geffen
Pim.VanGeffen@csaglobal.com

REGIONAL COUNCILLORS

Brazil
João Larizzatti
joao.larizzatti@cprm.gov.br

Chile
Brian Townley
btownley@ing.uchile.cl

China
Xueqiu Wang
wangxueqiu@igge.cn

Northern Europe
Pertti Sarala
pertti.sarala@oulu.fi

Southern Europe
Benedetto De Vivo
bdevivo@unina.it

Southeast Asia
Iftikar Malik
malik.iftikhar@gmail.com

Northern Africa
Silas Sunday Dada
sdada@aol.edu.ng

Southern Africa
Theo Davies
theo.clavellpr3@gmail.com

UK and Republic of Ireland
Kate Knights
kknights@hotmail.com

AAG COMMITTEES

New Membership
Paul Morris,
xrficpms@outlook.com

Awards and Medals
Dennis Arne
Arne.dennis@gmail.com
Chris Benn
Pertti Sarala
Theo Davies
Yulia Uvarova

Education
David Murphy, *chair*
davidmkmurphy@gmail.com
Erick Weiland,
erickweiland@terra-technology.com
Eric Grunsky, egrunsky@gmail.com
James Kidder,james.kidder@outlook.com
Ray Lett, raylett@shaw.ca

Symposia
David Cohen, d.cohen@unsw.edu.au

AAG COORDINATORS

AAG Student Paper Prize
David Cohen,
d.cohen@unsw.edu.au

AAG Website
Web maintenance
Elizabeth Ambrose,
eambrose0048@rogers.com

Geoscience Councils
David Cohen,
d.cohen@unsw.edu.au

GEEA
Scott Wood,
scott.wood@ndsu.edu

EXPLORE
Beth McClenaghan,
bethmcclenaghan@sympatico.ca
Steve Cook,
explorenewsletter@gmail.com

ELEMENTS
John Carranza
ejmcarranza@gmail.com

AAG Regional Councillors
Yulia Uvarova
yulia.uvarova@csiro.au

AAG BUSINESS MANAGER

Al Arseneault
P.O. Box 26099, 72 Robertson Road,
Ottawa, ON K2H 9R0 CANADA
TEL: (613) 828-0199 FAX: (613) 828-9288,
office@appliedgeochemists.org