Computers & Geosciences 89 (2016) 32–43

Contents lists available at ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

Case study

# Precursors predicted by artificial neural networks for mass balance calculations: Quantifying hydrothermal alteration in volcanic rocks

Sylvain Trépanier [a,b], Lucie Mathieu [a], Réal Daigneault [c,*], Stéphane Faure [a]

[a] CONSOREM – Mineral Exploration Research Consortium, 555 Boulevard de l'Université, Chicoutimi, Canada, G7H 2B1
[b] Redevance Aurifères Osisko Ltd., Exploration Osisko Baie James – 300 rue Saint-Paul (Office 200), Québec, Québec, Canada G1K 7R1
[c] Centre d'études sur les Ressources Minérales (CERM) – Université du Québec à Chicoutimi, 555 Boulevard de l'Université, Chicoutimi, Canada, G7H 2B1

ARTICLE INFO

*Article history:*
Received 2 February 2015
Received in revised form
9 January 2016
Accepted 11 January 2016
Available online 12 January 2016

*Keywords:*
Hydrothermal alteration
Immobile elements
Mineral exploration
Neural networks
Multi-layer perceptron
Mass balance calculations

ABSTRACT

This study proposes an artificial neural networks-based method for predicting the unaltered (precursor) chemical compositions of hydrothermally altered volcanic rock. The method aims at predicting precursor's major components contents ($SiO_2$, $FeO^T$, MgO, CaO, $Na_2O$, and $K_2O$). The prediction is based on ratios of elements generally immobile during alteration processes; i.e. Zr, $TiO_2$, $Al_2O_3$, Y, Nb, Th, and Cr, which are provided as inputs to the neural networks. Multi-layer perceptron neural networks were trained on a large dataset of least-altered volcanic rock samples that document a wide range of volcanic rock types, tectonic settings and ages. The precursors thus predicted are then used to perform mass balance calculations. Various statistics were calculated to validate the predictions of precursors' major components, which indicate that, overall, the predictions are precise and accurate. For example, rank-based correlation coefficients were calculated to compare predicted and analysed values from a least-altered test dataset that had not been used to train the networks. Coefficients over 0.87 were obtained for all components, except for $Na_2O$ (0.77), indicating that predictions for alkali might be less performant. Also, predictions are performant for most volcanic rock compositions, except for ultra-K rocks. The proposed method provides an easy and rapid solution to the often difficult task of determining appropriate volcanic precursor compositions to rocks modified by hydrothermal alteration. It is intended for large volcanic rock databases and is most useful, for example, to mineral exploration performed in complex or poorly known volcanic settings. The method is implemented as a simple C++ console program.



## 1. Introduction

Grassroots, or regional mineral exploration, necessitates the use of powerful and simple methods to interpret large amounts of chemical data. The interpretation and quantification of hydrothermal alterations in volcanic terrains, for instance, is particularly important as many economic substances are accumulated by the circulation of hydrothermal fluids in areas with magmatic activity, and because altered rocks are one of the main vectors used to explore for such mineralisations.

Geochemical studies of hydrothermally altered rocks aim at determining the amount of elements gained and lost during alteration of an initially fresh rock (i.e. the precursor), by performing mass balance calculations while assuming that one or more elements is immobile during alteration (see Gresens (1967)). Gresens' (1967) approach has been extensively and successfully used (MacLean and Kranidiotis, 1987; Shriver and MacLean, 1993; Cadieux et al., 2006; to name a few).

A major question that arises when using such mass balance equations concerns the choice of an appropriate precursor for the studied altered sample. Precursor's compositions are usually obtained by analysing "fresh" samples (i.e. samples that lack alteration minerals) that have been geologically related to the altered sample using detailed knowledge of the local geology (e.g. Grant, 1986, 2005). Such approaches are possible only for detailed deposit-scale studies, if fresh rocks exist and if our level of knowledge of the area render their identification possible. Even so, usually nothing proves that the fresh sample is an exact match for the precursor to the altered sample, and these difficulties can make mass balance calculations un-reliable.

At a more regional scale, on the other hand, these difficulties can be in-surmountable. Thus, orebody targeting using chemical datasets more often rely on alteration indexes (ratio of major elements), which values are sensitive to the precursor's compositions and could provide miss-leading indications on the intensity of alteration (see discussion in Trépanier et al. (2015)).

* Corresponding author.
*E-mail address:* real_daigneault@uqac.ca (R. Daigneault).

http://dx.doi.org/10.1016/j.cageo.2016.01.003
0098-3004/

Mass balance calculations would be more reliable if a suitable precursor composition to an altered rock could be determined directly from the chemical characteristics of the altered sample, thus providing a precursor adapted to this sample.

This paper proposes a method for estimating the composition in $SiO_2$, CaO, MgO, $FeO^T$, $K_2O$, and $Na_2O$ of fresh precursors to altered volcanic rocks, using ratios of commonly analysed least mobile elements (i.e. Zr, $TiO_2$, $Al_2O_3$, Y, Nb, Th, and Cr) and a regression method (i.e. artificial neural network). The method is provided as supplemental material, as a simple C++ program that calculates precursor compositions (this study) prior performing mass balance calculations (using published methods).

## 2. Methodology

### 2.1. Description of the method

In this contribution, a method to predict fresh precursors from the chemical composition (i.e. immobile elements content) of altered volcanic rocks is presented. Predictions are performed for magmatic rocks only because relatively simple relationships, which are controlled by magmatic processes, exist between the trace and major elements content of such rocks. For example, Zr and Si are both incompatible elements that tend to increase during fractional crystallisation, making Zr a proxy for Si (see Winchester and Floyd (1977)).

Also, precursor predictions are performed using ratio of elements considered immobile in regard of hydrothermal processes. Ratios are used because the value of immobile elements ratios is not modified by mass or volume changes and because ratios are unlikely to be strongly fractionated by hydrothermal processes. Instead, such ratios mostly vary between volcanic rocks of different types and affinities, which originate from various sources and different conditions of partial melting, fractional crystallisation and other processes. Because ratios of immobile elements are insensitive to alteration and can reflect geodynamic settings and differentiation, they have been extensively used by discrimination diagrams (e.g. Winchester and Floyd, 1977; Barrett and MacLean, 1994), and their use is here extended to predict major elements compositions of the fresh precursors to altered volcanic rocks.

In order to relate immobile element ratios to the major elements of volcanic rocks, the typical composition of least-altered volcanic rocks is documented using a large dataset of samples of various volcanic rock types from different tectonic settings and ages (see Section 3.1; Figs. 1 and 2) and on which predictions are performed using a method able to solve regression problems. Since this prediction implies a large variety of rocks, non-linear solutions can be expected. Tests were initially performed with various methods, e.g. multiple regressions, but non produced results as good as these obtained with neural networks. For this reason, a multi-layer perceptron neural network was trained on a large dataset of least-altered volcanic rocks and used to predict precursor compositions.

### 2.2. Immobile elements ratios

Hydrothermal fluids modify the mineral assemblages (alteration) and chemical composition (metasomatism) of rocks, with various minerals and elements being more or less susceptible to be modified or displaced. Here, the immobile elements used by the proposed method are immobile in most mineralised contexts and are commonly analysed, so that the method can be applied to datasets typically used by exploration geologists.

Elements relatively immobile during hydrothermal alteration, weathering and low-grade metamorphic processes are characterized

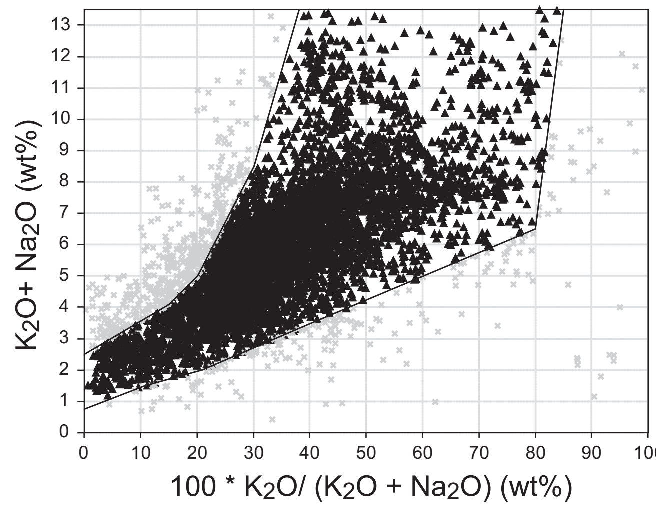


**Fig. 1.** Modified Hughes' diagram (Hughes, 1972) on which the Georoc dataset is represented. This diagram has been used to remove K–Na altered samples from the initial dataset. Black triangles highlight kept samples and grey crosses correspond to discarded samples.

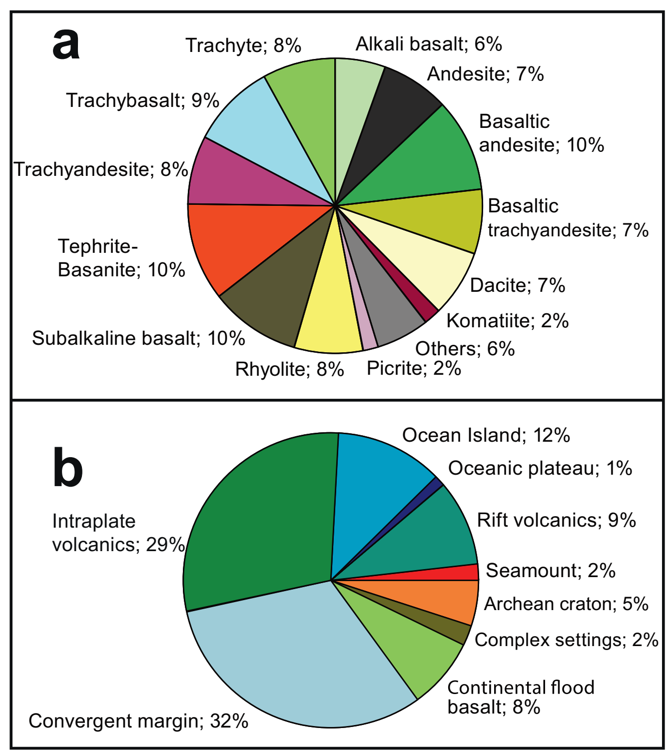


**Fig. 2.** Pie plots displaying several characteristics of the samples of the least-altered dataset ($n$=5810). The displayed characteristics are: (a) the proportions of rock types (see IUGS geochemical classification of volcanic rocks; Le Maitre et al. (1989)); and (b) the tectonic settings, as identified in the Georoc database.

by ions that are of intermediate ionic potential (0.03–0.1 $ppm^{-1}$; Pearce, 1996). From the elements considered immobile by various authors (Cann, 1970; Pearce and Norry, 1979; Hill et al., 2000; Kurtz et al., 2000; Hastie et al., 2007), seven elements were selected as inputs to the neural networks (i.e. Zr, Al, Ti, Nb, Cr, Y, and Th) because, according to Pearce (1996), these elements are sufficient to properly characterize most basalts and, presumably, most volcanic rocks. These elements have indeed been used to characterize various magmatic processes, such as: (1) the degree of differentiation (Winchester and Floyd, 1977; Pearce and Norry, 1979); (2) the alkalinity of rocks (Pearce and Cann, 1973); (3) the geodynamic context