BAYESIAN GEOCHEMICAL DISCRIMINATION OF MAFIC VOLCANIC ROCKS

JEFFREY SHRAGGE* and CAMERON A. SNOW**

ABSTRACT. Determining the original tectonic setting of volcanic rocks via their geochemical signature has been a long-standing goal for petrologists. However, current visually based methods for geochemical discrimination afford only limited success. We develop a probabilistic method for geochemical discrimination based upon statistics generated from geochemical databases and Bayesian analysis. This method incorporates elemental covariance, accounts for data measurement and theoretical uncertainty, and is not restricted in dimensionality of analysis, which is inherent in visual systems of discrimination. Furthermore, the method provides a direct way to discern statistical outliers whose inclusion would otherwise lead to lower discrimination accuracy. Tests of the approach yielded successful classification rates for single analyses of over 90 percent for volcanic arc basalts, mid-ocean ridge basalts, and ocean island basalts.

INTRODUCTION

Fully understanding the geologic history of complex areas such as active margins often requires determining the original tectonic setting of volcanic rocks. However, these rocks are often set in an ambiguous context due to subsequent rearrangement by tectonic processes and, in most cases, geological inference alone is insufficient to discriminate between possible plate-tectonic settings. Therefore, we must rely on an examination of a sample's intrinsic properties, such as its major and trace element abundances.

Geochemical discrimination techniques have been used for decades to distinguish between the original plate-tectonic setting of volcanic rocks, such as those from island arcs, mid-ocean ridges, and ocean-island hotspots. One standard approach is to use discrimination diagrams (Pearce and Cann, 1973; Pearce, 1974; Pearce and Norry, 1979; Wood, 1980; Pearce, 1982; Shervais, 1982; Mullen, 1983; Pearce, 1987), which are geochemistry plots that allow users to visually discriminate between tectonic settings based on where data plot relative to predetermined domains constructed from *a priori* data. A significant drawback of this approach is its marginal accuracy stemming from a dependence on visualization, a low dimensionality of analysis, and discrimination domains that do not reflect probabilities. Recent work has shown that these diagrams rarely classify samples with greater than 60 percent confidence (Snow, 2006). Presumably, geochemical discrimination accuracy can be improved if these constraints are either reduced or eliminated. In particular, significant advances are possible if the reliance on visualization is discarded in favor of incorporating more element analyses, if elemental covariances are integrated as additional constraints, and if a probabilistic analysis accounting for existing uncertainties is introduced.

The goal of this paper is to establish a multi-dimensional geochemical discrimination technique based on Bayesian probability theory. (The Bayesian probability formulation is presented in Appendix A.) Central to this method is the generation of probability density functions (PDFs) from *a priori* datasets that quantify the likelihood of a sample forming in a specified tectonic setting given a particular chemical composition. We then use Bayesian analysis that compares the composition of a new

*Department of Geophysics, Stanford University, 397 Panama Mall, Mitchell Building 360, Stanford, California 94305-2215; jeff@sep.stanford.edu

**Department of Geological and Environmental Sciences, Stanford University, 450 Serra Mall, Braun Hall, Building 320, Stanford, California 94305-2115; casnow@pangea.Stanford.EDU

sample taken from an unknown setting to the *a priori* PDFs to generate a probabilistic *a posteriori* estimate of the original plate-tectonic setting. Furthermore, because the PDFs are well-approximated by multi-dimensional Gaussian functions, we introduce elemental covariance in a meaningful way to provide additional constraints, resulting in a more robust geochemical discrimination analysis. Our approach is related to that of Pearce (1987); however, we focus solely on geochemistry to avoid the difficulties of assigning quantitative values to more qualitative data.

We begin this paper with a general discussion of inverse problems to provide motivation for establishing a probabilistic geochemical discrimination method. We develop a geochemical operator that generates a theoretical dataset of element concentrations for each tectonic setting, and demonstrate that it, along with elemental covariance measurements, can quantify a probabilistic theory of elemental abundances in volcanic rocks. We then incorporate *a priori* information on data and model components into the analysis, and show how combining this information with a PDF describing the discrimination theory forms a joint model-data probability space. Subsequently, from this space we generate *a posteriori* estimates of the probability that the sample was formed in a given tectonic setting. We conclude the paper by evaluating the efficacy of the Bayesian discrimination technique to properly classify volcanic rocks through blind testing of geochemical data acquired from areas of known tectonic setting. In the following sections, we often use the terms MORB, VAB and OIB, which refer to basalts erupted at mid-ocean ridges, island arcs, and ocean-island hotspots, respectively. In addition, both alkalic and tholeiitic compositions were used. We make these clarifications to emphasize that the terms have tectonic implications, and we are not referring to chemical properties.

GEOCHEMICAL DISCRIMINATION AS AN INVERSE PROBLEM

Solutions to many geological problems are approximated through forward modeling. This process entails parameterizing the model and observable data components of a system, developing a theoretical relation between the two, and generating modeled data that can be matched to observed data. These steps are iteratively repeated using different values for model components until modeled data optimally match observed data. Mathematically, this is equivalent to applying a theory operator, $\mathbf{G}$, to a set of model components, $\mathbf{m}$, to generate a modeled dataset, $\mathbf{d}$, that optimally matches observed data, $\mathbf{d}^{\text{obs}}$:

$$\mathbf{G}\mathbf{m} = \mathbf{d} \quad \text{where} \quad \mathbf{d} - \mathbf{d}^{\text{obs}} \approx 0, \quad (1)$$

where ≈ 0 reads ‘is minimized’. A list of the nomenclature used in this paper is presented in Appendix B.

Geochemical discrimination, however, is more often posed as an inverse problem, where collected data are plotted on diagrams constructed from *a priori* data (for example, Pearce and Cann, 1973). The primary difference between the forward and inverse approaches is the latter reconstructs model components directly from observed data rather than vice-versa. Mathematically, this requires solving,

$$\mathbf{m} = \mathbf{G}^{-1}\mathbf{d}^{\text{obs}} \quad \text{where} \quad \mathbf{G}\mathbf{m} - \mathbf{d}^{\text{obs}} \approx 0. \quad (2)$$

Although inverse problems are intuitively appealing, finding their solution is often difficult. For example, problems can arise because of too many contradictory or too few constraints, incomplete or erroneous datasets, and incomplete or inaccurate theory. These factors combine to make a direct calculation of $\mathbf{G}^{-1}$ impossible.

Geochemical discrimination is an over-determined inverse problem characterized by precise, though sometimes incomplete, data (for example, not all elements are usable due to secondary alteration), and poor resolution of the scales of physical

Fig. 1. Schematic illustrating the methodology of, and required inputs for, the Bayesian geochemical discrimination analysis. Left-most chart represents initial (unbiased) probability of a sample's tectonic origin. Center shows the necessary inputs that are used in discrimination calculations. Right-most chart shows the probabilities of a given sample having a particular setting after Bayesian analysis. This scenario depicts a sample that is most likely VAB in origin, and least likely OIB.

processes (for example, degree of partial melting and/or fractionation). These factors combine to make the results of geochemical discrimination analysis less certain. Because intrinsic uncertainty exists, in this paper we argue that the language of geochemical discrimination should be couched in the language of probability. Importantly, many of the aforementioned problems are either accounted for, or overcome, using a probabilistic inverse problem framework. Therefore, we approach the challenges of geochemical discrimination by applying Bayesian probability calculus (Bayes, 1763) in the manner advocated by Tarantola (1987).

Figure 1 illustrates our Bayesian geochemical discrimination approach. The discrimination process begins with an initial probability estimate that an unknown sample is formed at either an island arc, mid-ocean ridge, or ocean-island hotspot. For example, the left-hand side of figure 1 illustrates a situation where all settings have an equal probability. We then use statistics from geochemical databases (that is, elemental covariances) with analytic measurement uncertainties (which can be adjusted according to the method of analysis), to generate a probabilistic geochemical theory for each tectonic setting that specifies the likelihood of formation given its elemental abundances. Data from the unknown setting are input to the discrimination algorithm and then compared with data calculated from the statistical theory (as illustrated in the center of fig. 1). The algorithm then outputs a probabilistic estimate quantifying the likelihood that the sample formed in a given tectonic setting. For example, the right-hand side of figure 1 shows the sample most (least) likely formed an island-arc (ocean-island hotspot) setting.

PROBABILISTIC GEOCHEMICAL DISCRIMINATION

Physical theories are inexact and therefore have associated uncertainties; however, these are usually difficult to estimate because uncertainties in theory are often of the same order of magnitude as those of the measured data. In geochemical discrimination, however, data measurements are far more accurate than our physical modeling of geologic processes. Accordingly, we must describe irresolvable geologic processes with a statistical theory, and translate the observed variance of elemental abundances

in volcanic rocks into theoretical uncertainty. This is achievable in a robust fashion using the Bayesian framework developed in the sections below.

Parameterizing Model and Data Space

The first step in developing a Bayesian geochemical discrimination method is parameterizing model and data space. We represent the model space of all possible plate-tectonic settings with vector $\mathbf{m}$ of size M where,

$$\mathbf{m} = \begin{bmatrix} m_1 \\ m_2 \\ m_3 \end{bmatrix} = \begin{bmatrix} \text{island arc} \\ \text{mid - ocean ridge} \\ \text{ocean - island hotspot} \end{bmatrix}. \quad (3)$$

Note that a model component can only assume a binary value (that is, where true=1 and false=0), and only one component of model space can be true in any single analysis. This restriction arises because the existence of two or more simultaneous true values does not make sense: the sample had to form in one and only one tectonic setting.

The data used for geochemical discrimination are the elemental abundances of a particular sample. We write these as a list of N elements to form data vector $\mathbf{d}$,

$$\mathbf{d} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_{N-1} \\ d_N \end{bmatrix} = \begin{bmatrix} \log(\text{Ni}/\text{Ni}_{\text{ref}}) \\ \log(\text{Sr}/\text{Sr}_{\text{ref}}) \\ \log(\text{Zr}/\text{Zr}_{\text{ref}}) \\ \vdots \\ \log(\text{Pb}/\text{Pb}_{\text{ref}}) \\ \log(\text{Ta}/\text{Ta}_{\text{ref}}) \end{bmatrix}, \quad (4)$$

where $\log$ refers to natural logarithm, and the variables with subscript $_{\text{ref}}$ are mean N-MORB values (Sun and McDonough, 1989) that are used to generate a non-dimensional vector space. The data vector is a particular realization from a continuous distribution defined on the interval $[-\infty, \infty]$, where $P(d_j = X)$ represents the probability that datum, d_j , has the value X .

Developing a Geochemical Operator

The next step is generating a geochemical operator, $\mathbf{G}$, that links model and data spaces, $\mathbf{m}$ and $\mathbf{d}$. Specifying $\mathbf{G}$ is possible due to the existence of extensive geochemical databases from regions of known tectonic setting. Thus, we develop $\mathbf{G}$ from the statistics of the known historical data, $\mathbf{h}$. A sample in a database is identified by the values of the three indices on h_{jip} : j relating the particular element, i describing the plate-tectonic setting, and p giving the measurement redundancy for a particular i and j . For example, if $j = 1$ refers to Ni and $i = 3$ refers to OIB, then $h_{jip} = h_{135}$ refers to the fifth Ni measurement in the OIB database.

We develop a geochemical operator by assuming that the action of operator, G_{ji} , on model parameter, m_i , yields the expected value (that is, mean concentration) of the j^{th} element in the i^{th} tectonic setting. Hence, we compute the matrix elements of geochemical operator, $\mathbf{G}$, by calculating the mean of the P database measurements for a particular i and j ,

$$G_{ji} = \frac{1}{P} \sum_{p=1}^P h_{jip}. \quad (5)$$

Quantifying Theoretical Uncertainty

Even though we have quantified our geochemical operator, $\mathbf{G}$, we have not yet measured how accurately it represents the true geochemical theory, θ . For example, if all Ni measurements collected in an OIB database have the same value, then we would be extraordinarily certain about our statistical geochemical theory of OIB Ni abundance. Conversely, the greater and more random the variance in Ni abundances found in an OIB database, the less certain we are. Hence, properly representing this uncertainty requires ascribing a probabilistic representation of the true statistical geochemical theory. Similar to the model and data spaces, we must formulate a probability measure over θ , $P(\theta(\mathbf{d}|\mathbf{m}))$, relating the probability that data, $\mathbf{d}$, from theory, θ , is correct given the veracity of model components, $\mathbf{m}$.

As discussed in the preceding example, measuring theoretical uncertainty requires examining dataset (co)variance. We denote an element of covariance matrix, ${}^T\mathbf{C}_i^{jk}$, where subscript i relates the tectonic setting, double superscript jk represents two elements, and prescript T refers to theory. We compute the covariance operator through,

$${}^T\mathbf{C}_i^{jk} = \frac{1}{P-1} \sum_{p=1}^P [G_{ji} - h_{jip}][G_{ki} - h_{kip}], \quad (6)$$

where, for the i^{th} tectonic setting, the covariance matrix diagonals (where $j = k$) represent the dataset element variances, and the off-diagonals (where $j \neq k$) quantify how elements co-vary. Covariance values can be transformed into a normalized measure of correlation, ρ_i^{jk} , through,

$$\rho_i^{jk} = \frac{{}^T\mathbf{C}_i^{jk}}{\sqrt{{}^T\mathbf{C}_i^{jj}} \sqrt{{}^T\mathbf{C}_i^{kk}}} \text{ where } -1 \leq \rho_i^{jk} \leq 1. \quad (7)$$

Theoretical covariance matrix ${}^T\mathbf{C}$, and correlation matrix ρ , are directly related to the state of information in the system, and can be used to specify a PDF quantifying the certainty that geochemical operator $\mathbf{G}$ accurately represents the true theory. The covariance measure is particularly important because it dictates the shape of the theory PDF. Figure 2 illustrates how different covariance (here correlation) values can focus a 2-D Gaussian PDF. The two PDFs in the upper panels of figure 2 have the same variances; however, the PDF in the upper left panel has zero x-y correlation ($\rho^{xy} = 0$), whereas the PDF in upper right panel has a strong x-y correlation ($\rho^{xy} = 0.9$). Note that the probability density cross-sections along lines $X = 5$ and $Y = 5$ in the lower right panel are significantly more concentrated than those in the left panel, indicating enhanced spatial resolution.

Fully specifying the theoretical PDF, though, requires making further assumptions about its shape. In this paper we use a Gaussian hypothesis, which imposes the following key assumptions:

1. individual element PDFs are adequately described by Gaussian functions;
2. the shape of the PDF representing abundances of elements j and k is adequately represented by a 2-D Gaussian function with ellipticity defined by covariance function, ${}^T\mathbf{C}_i^{jk}$;
3. the global theory of geochemical discrimination is adequately represented by a N-dimensional Gaussian function defined by covariance function, ${}^T\mathbf{C}$.

The Gaussian hypothesis allows us to represent a probabilistic geochemical discrimination theory with the following N-dimensional Gaussian PDF (Tarantola, 1987),

Fig. 2. Examples of 2-D Gaussian probability density functions with x- and y-covariance values of $C^{xx} = 2$ and $C^{yy} = 4$. Top left: Gaussian function where x and y are completely uncorrelated ($\rho^{xy} = 0$); top right: Gaussian function where x and y are highly correlated ($\rho^{xy} = 0.9$); bottom left: x- and y- cross-section through the center of the Gaussian function in the top left; and bottom right: as in bottom left, but through Gaussian function in top right panel. Note the greater concentration of probability density in right-hand panels.

$$\theta(\mathbf{d}|\mathbf{m}) = \frac{\exp[-\frac{1}{2}(\mathbf{Gm} - \mathbf{d})^{\dagger} \mathbf{C}^{-1}(\mathbf{Gm} - \mathbf{d})]}{[(2\pi)^N \det(\mathbf{C})]^{1/2}}, \quad (8)$$

where $\mathbf{d}$ is the true data vector, and $\mathbf{Gm}$ is a vector containing the expected trace element abundances, superscripts $\dagger$ and -1 represent matrix transpose and inverse, respectively, and $\det(\mathbf{C})$ is the determinant of covariance matrix, $\mathbf{C}$.

There are a number of notable points regarding the expression given in equation (8). First, the dimensions of matrices $(\mathbf{Gm} - \mathbf{d})^{\dagger}$, and $\mathbf{C}^{-1}$, $(\mathbf{Gm} - \mathbf{d})$ are $1 \times N$, $N \times N$ and $N \times 1$, respectively. Multiplication of these three matrices yields a single number as the argument of the exponential function. Second, because the inverse of covariance matrix, $\mathbf{C}^{-1}$, is used to define the PDF, elements with greater (lesser) covariances tend to broaden (narrow) the probability distribution. Third, this approach is applicable to any finite dimensionality; for example, any commonly analyzed trace element or isotope, or ratios thereof, can be used as constraints in this geochemical discrimination approach.

For completeness, we also define a state of information of the theory over a joint data and model space, $\theta(\mathbf{d}, \mathbf{m})$, through (See Appendix A),

$$\theta(\mathbf{d}, \mathbf{m}) = \theta(\mathbf{d}|\mathbf{m})\mu(\mathbf{m}). \quad (9)$$

Function $\mu(\mathbf{m})$ is a reference state of information on model parameters $\mathbf{m}$, used to normalize the density function; however, a value is not assigned to $\mu(\mathbf{m})$ insofar as it is eliminated by other PDFs in equation (12).

INCORPORATING A PRIORI UNCERTAINTY

In many inverse problems, it is desirable to incorporate known information into the analysis. One source of information is the statistical uncertainty associated with analytical techniques. A second type of information is where a particular model space component is infeasible. This section discusses how to incorporate this information into the analysis.

Data Measurement Uncertainty

Incorporating data measurement uncertainty requires estimating the relationship between measured, $\mathbf{d}^{\text{obs}}$, and true, $\mathbf{d}$, data values. For example, where measurements are exact we may equate the two: $\mathbf{d}^{\text{obs}} = \mathbf{d}$. However, especially for elements with extremely low abundance (that is, near detection limits), properly specifying this relationship is extremely important. For example, the abundance of Ta in volcanic rocks for all settings can be near detection limits for XRF analysis. Therefore, incorporating the appropriate level of uncertainty in Ta measurements is essential if we are not to ascribe a physical meaning to the measurement noise.

We assume that the analytical measurement uncertainty, $p_D(\mathbf{d})$, is well-represented by a Gaussian PDF. We also assume the measurement uncertainty of an element is uncorrelated with all others. Hence, we describe the analytical data measurement uncertainty with the following PDF,

$$\frac{p_D(\mathbf{d})}{\mu_D(\mathbf{d})} = \frac{\exp[-\frac{1}{2}(\mathbf{d} - \mathbf{d}^{\text{obs}})^t \mathbf{d} \mathbf{C}^{-1} (\mathbf{d} - \mathbf{d}^{\text{obs}})]}{[(2\pi)^N \det(\mathbf{d} \mathbf{C})]^{1/2}}, \quad (10)$$

where $\mu_D(\mathbf{d})$ is a reference state of information, and the diagonal elements of covariance function $\mathbf{d} \mathbf{C}_i$ contain appropriate variance estimates of analytic measurement uncertainty.

Model Space Uncertainty

Incorporating *a priori* information on a plate-tectonic setting requires specifying an additional probability function. In most cases, *a priori* biased results are undesirable, and we want to use a non-informative PDF, where all M model components have equal likelihood,

$$p_M(\mathbf{m}) = \frac{1}{M}. \quad (11)$$

However, we include this function to allow for situations where eliminating a model space component is justified.

Multiplying p_D and p_M creates a joint probability density space, $p(\mathbf{d}, \mathbf{m}) = p_D(\mathbf{d}) p_M(\mathbf{m})$, representing the *a priori* state of information. In the next section, we show how new data and the probabilistic geochemical theory, θ , combine to refine distribution $p(\mathbf{d}, \mathbf{m})$ to generate an *a posteriori* estimate of the likelihood a sample formed in a given tectonic setting.

GENERATING A POSTERIORI PROBABILITIES

So far we have generated PDFs representing *a priori* data and model space, and the geochemical discrimination theory. Combining these probability measures creates

PDF $\sigma(\mathbf{d}, \mathbf{m})$ that represents the *a posteriori* state of information on joint model and data space (Tarantola, 1987),

$$\sigma(\mathbf{d}, \mathbf{m}) = \frac{p(\mathbf{d}, \mathbf{m})\theta(\mathbf{d}, \mathbf{m})}{\mu(\mathbf{d}, \mathbf{m})}, \quad (12)$$

where $\mu(\mathbf{d}, \mathbf{m})$ again represents a reference state of information.

Computing an *a posteriori* estimate of the model space components, $\mathbf{m}$, requires integrating function $\sigma(\mathbf{d}, \mathbf{m})$ with respect to true data values, $\mathbf{d}$, through,

$$\begin{aligned} \sigma(\mathbf{m}) &= \int_{-\infty}^{\infty} \mathbf{d} \mathbf{d} \theta(\mathbf{d}, \mathbf{m}), \\ &= \int_{-\infty}^{\infty} \mathbf{d} \mathbf{d} \frac{p(\mathbf{d}, \mathbf{m})\theta(\mathbf{d}, \mathbf{m})}{\mu(\mathbf{d}, \mathbf{m})}, \\ &= p_M(\mathbf{m}) \int_{-\infty}^{\infty} \mathbf{d} \mathbf{d} \frac{p_D(\mathbf{d})\theta(\mathbf{d}|\mathbf{m})}{\mu_D(\mathbf{m})}. \end{aligned} \quad (13)$$

Note that integrating with respect to data vector, $\mathbf{d}$, allows us to relate observed data $\mathbf{d}^{obs}$ in equation (10) directly to estimates described by $\mathbf{Gm}$ in equation (8). Moreover, because the PDFs are assumed to be Gaussian, the integral in equation (13) is simply a convolution of two Gaussian functions. This integration can be performed analytically to yield another Gaussian PDF,

$$\sigma_M(\mathbf{m}) \propto p_M(\mathbf{m}) \exp\left[-\frac{1}{2}(\mathbf{Gm} - \mathbf{d}^{obs})^{\dagger} \mathbf{C}^{-1}(\mathbf{Gm} - \mathbf{d}^{obs})\right], \quad (14)$$

where the resulting covariance matrix, ${}^D\mathbf{C}$, is the sum of the covariance matrices representing the theory and analytical measurement uncertainties,

$${}^D\mathbf{C} = {}^d\mathbf{C} + {}^T\mathbf{C}. \quad (15)$$

Because model space $\mathbf{m}$ is finite dimensional, the PDF in equation (14) is normalized by the sum of all possible outcomes,

$$\sigma_M(\mathbf{m}) = \frac{p_M(\mathbf{m}) \exp\left[-\frac{1}{2}(\mathbf{Gm} - \mathbf{d}^{obs})^{\dagger} \mathbf{C}^{-1}(\mathbf{Gm} - \mathbf{d}^{obs})\right]}{\sum_{\alpha=1}^M p_M(m_{\alpha}) \sum_{j,k=1}^N \exp\left[-\frac{1}{2}(\mathbf{G}_{j\alpha} m_{\alpha} - \mathbf{d}_j^{obs})({}^D\mathbf{C}^{-1})_{\alpha}^{jk}(\mathbf{G}_{k\alpha} m_{\alpha} - \mathbf{d}_k^{obs})\right]}, \quad (16)$$

where M is the number of candidate tectonic settings. The explicit solution for, say, the third model component, $m_3 = \text{OIB}$, may be found by setting the model vector $\mathbf{m} = m_3$ in equation (16) to yield,

$$\sigma_M(m_3) = \frac{p_M(m_3) \sum_{j,k=1}^N \exp\left[-\frac{1}{2}(\mathbf{G}_{j3} m_3 - \mathbf{d}_j^{obs})({}^D\mathbf{C}^{-1})_3^{jk}(\mathbf{G}_{k3} m_3 - \mathbf{d}_k^{obs})\right]}{\sum_{\alpha=1}^M p_M(m_{\alpha}) \sum_{j,k=1}^N \exp\left[-\frac{1}{2}(\mathbf{G}_{j\alpha} m_{\alpha} - \mathbf{d}_j^{obs})({}^D\mathbf{C}^{-1})_{\alpha}^{jk}(\mathbf{G}_{k\alpha} m_{\alpha} - \mathbf{d}_k^{obs})\right]}. \quad (17)$$

The magnitude of the normalization constant in the denominator of equation (16) measures the degree to which a sample is an outlier of the geochemical database. It also may be used as a filter to reject data whose abundances fall too far away from the statistical mean. We introduce an outlier cutoff value, Γ , that can be used to eliminate

data points having insufficient information content (as defined by the user) to be useful for geochemical discrimination,

$$\Gamma = \sum_{\alpha=1}^M p_M(m_\alpha) \sum_{j,k=1}^N \exp \left[-\frac{1}{2} (G_{j\alpha} m_\alpha - d_j^{\text{obs}})^{\dagger} (D C^{-1})_{\alpha}^{jk} (G_{k\alpha} m_\alpha - d_k^{\text{obs}}) \right]. \quad (18)$$

In some cases we may want to analyze multiple data samples taken from region of unknown geologic history. For these cases, we can either choose to perform P independent discrimination tests using equation (16), or perform a batch analysis combining all measurements. The former approach treats each unknown sample as an independent test, whereas the latter approach involves solving a modified version of equation (16) that includes a summation over all samples in the batch,

$$\sigma_M(\mathbf{m}) = \frac{p_M(\mathbf{m}) \sum_{j,k=1}^N \exp \left[-\frac{1}{2} (\mathbf{G} \mathbf{m} - \sum_{p=1}^P \mathbf{d}_p^{\text{obs}})^{\dagger} D C^{-1} (\mathbf{G} \mathbf{m} - \sum_{p=1}^P \mathbf{d}_p^{\text{obs}}) \right]}{\sum_{\alpha=1}^M p_M(m_\alpha) \sum_{j,k=1}^N \exp \left[-\frac{1}{2} (G_{j\alpha} m_\alpha - \sum_{p=1}^P d_{pj}^{\text{obs}})^{\dagger} (D C^{-1})_{\alpha}^{jk} (G_{k\alpha} m_\alpha - \sum_{p=1}^P d_{pk}^{\text{obs}}) \right]}, \quad (19)$$

Here, summation $\sum_{p=1}^P \mathbf{d}_p^{\text{obs}}$ forces the observed data values toward the expected mean facilitating improved discrimination. However, if the samples in the batch represent more than one tectonic setting, then the batch processing approach violates the initial assumption that all samples are from one tectonic setting rendering the results invalid.

MODEL TESTING AND RESULTS

In this section, we evaluate the efficacy of the developed geochemical discrimination method using samples from existing databases in blind tests of using equations (16) and (19). We describe the data sources and usage, outline our approach to optimizing parameters, and present the results of the geochemical discrimination tests.

Data Sources

The geochemical data used for the analysis described in this paper were compiled from two open-access geochemical databases GEOROC (<http://georoc.mpch-mainz.gwdg.de/georoc/>) and PetDB (<http://www.petdb.org/>). The structure and content of these databases are thoroughly examined by Lehnert and others (2000), and will not be discussed further in this paper. This study used data from twenty-three arc systems (> 10,000 VAB analyses), eighteen mid-ocean ridges (> 3,000 MORB analyses), and forty-four ocean islands (> 6,000 OIB analyses). We note that the varying number of analyses for each tectonic setting is unimportant as long as a statistically significant number of samples are present for defining the statistical mean for each element and covariance values between each pair of elements. We compiled forty-two major and trace elements for each end-member tectonic setting. Isotopes were not utilized for this study.

The assembled data set were filtered to eliminate samples with weight % SiO_2 greater than 60 percent and less than 40 percent. Data were then randomly subdivided into two batches, where 50 percent were used for generating the required statistics and the remaining 50 percent were reserved for independent tests. We constructed the covariance tables required in equations (16) and (19) according to equation (6) using samples from the first half data set that fell within 10 standard deviations of the elemental abundance means.

Optimizing Parameters

The developed geochemical discrimination technique introduced several degrees of freedom that can be tuned to produce a more robust discrimination result. For example, one may determine how many and which elements and tectonic settings to use, and the values for analytic measurement uncertainties and outlier cutoff. The choice of these input parameters significantly affects the outcome of the discrimination tests, and therefore parameter optimization is necessary. Unfortunately, an exhaustive examination of parameter space is infeasible owing to the sheer magnitude of possible element and parameter combinations. Hence, we used the following *ad hoc* method of parameter optimization.

Because the discrimination method is N-dimensional, we could use all elements for which databases exist. However, this produces less than optimal results for a number of reasons. First, many elements have broad and overlapping compositional distributions for all three tectonic environments. This leads to a situation where the distributions are too statistically similar to afford resolution of the model space components. Second, many elemental distributions are too non-Gaussian in shape (for example, not logarithmically distributed) to validate the aforementioned key assumptions. Finally, some elements that seem to be the most useful for discrimination (that is, the most statistically independent) are highly mobile in metamorphic fluids (for example, Na and K). Susceptibility to secondary alteration makes them unsuitable for discriminating because of the extreme difficulty in separating the signature of the original melt from that of the subsequent alteration processes.

Based on the above constraints, we selected seven elements that have significantly different distribution statistics for each tectonic setting, have roughly Gaussian-shaped distributions, and are relatively immobile: Ni, Sr, Zr, Nb, Ti, Pb, and Ta. The distributions of each of these elements (labeled as Disb.), as well as our Gaussian representations of the distribution (labeled as Gauss.), are illustrated in figure 3. For testing purposes, we only retained samples with measurements of all seven elements. Although this limited the number of analyses, it minimized over-reliance on individual elements thereby generating more consistent and standardized results.

We employed an analytic uncertainty parameter that effectively doubled the variances for each of the used elements. Although realistic values are probably lower for many elements, we argue that a higher value is warranted to account for the imperfect Gaussian shape of the PDFs shown in figure 3. In general, increasing this value decreases model space resolution and lowers the certainty of classification estimates, but it better accounts for non-Gaussian statistical outliers. Conversely, decreasing this value affords greater statistical significance to the data, but makes the method less robust to outlying samples.

Results

Tests of the geochemical discrimination technique were conducted with the seven aforementioned elements and data uncertainty factor for all permutations of outlier cutoff values of $\Gamma = 0, 0.01$, and 0.10 and batches of one, two, and three samples. Data points excluded during covariance calculations were included in the testing. We also randomly selected the samples analyzed in batch mode to minimize the possibility of including measurements from only one locale. We classified a discrimination result as successful where a sample known to be from tectonic setting X was classified by the algorithm as having formed in setting X with the greatest probability.

Testing results are presented in table C-1 of Appendix C. Figure 4 shows the discrimination results for an outlier cutoff value of $\Gamma = 0$ for single batches processing. Figure 5 shows the discrimination results again for an outlier cutoff value of $\Gamma = 0$, but for batch processing of three samples. The elemental abundance means used in the

Fig. 3. PDFs showing log-normalized element concentrations used in the present analysis: Ni, Sr, Zr, Nb, Ti, Pb, and Ta. Panels with caption Disb. represent the distribution generated from the geochemical databases. Panels with caption Gauss. represent our best Gaussian fit to the distributions. Solid lines represent VAB, dot-dash lines represent MORB, and heavy dotted lines represent OIB. Note that generated distributions have been broadened to account for both the non-Gaussian shape of the distribution and analytical uncertainty in data measurement.

Fig. 4. Probability ternary plot showing the distribution of discrimination results for outlier cutoff value of $\Gamma = 0$ and single sample analyses. Panel (A) 471 known VAB samples with 91.5% correct classification; panel (B) 185 known MORB samples with 91.4% correct classification; and panel (C) 298 known OIB samples with 90.3% correct classification.

calculation of these results are given in table C-2, while the covariance functions are presented in tables C-3 through C-5. The main subroutine used for discrimination is given in Appendix D. Note that the data plotted on the ternary diagrams are probabilistic measurements, and are not discrimination diagrams.

Results of the geochemical discrimination testing show significant improvement over typical results from visually based discrimination. The tests demonstrate that VAB, OIB, and MORB are well and fairly evenly resolved, generally with a high percentage of certainty. Incorrect VAB data classifications are evenly split between MORB and OIB. However, MORB and OIB are more likely to be misclassified as OIB and MORB, respectively.

Increasing the outlier cutoff values improved the rate of successful classification for MORB and OIB; however, a more stringent cutoff value results in fewer overall classifications. Increasing the number of samples in the batch-processing mode also improved the rate of successful discrimination. This was expected since the averaging filter in equation (19) minimized the impact of an outlier in a batch as one might expect from the Central Limit Theorem. However, this test is not a completely fair one because we have randomly chosen samples from the database, whereas samples from any given site are likely to have systemic biases.

DISCUSSION

These results clearly demonstrate that the technique has an excellent ability to discriminate between samples generated in VAB, MORB, and OIB. However, we caution that this technique should not be treated as a black box algorithm, because the user can bias results by virtue of a particular parameter choice. We emphasize that resolution tests with data from known settings must be conducted before applying the

Fig. 5. Probability ternary plot showing the distribution of discrimination results for outlier cutoff value of $\Gamma = 0$ for batch processing of three samples. Panel (A) 157 known VAB sample batches with 98.1% correct classification; panel (B) 62 known MORB sample batches with 98.4% correct classification; and panel (C) 100 known OIB sample batches with 92.0% correct classification.

technique with alternative parameter settings. In addition, although the elements used in this study are generally stable during metamorphism, it is possible that they are mobile in some fluids and therefore the generated probabilities will reflect the sample's modified, not its original, chemistry. Because of this possibility, we suggest choosing a high value for the outlier cutoff parameter, Γ , which is the most robust measure of the possibility of secondary alteration. However, using higher cutoff values may again necessitate collecting and processing of additional geologic samples.

This study examined only three tectonic settings. Future work will examine whether incorporating additional environments into the model space by subdividing the existing tectonic settings into more specific categories is feasible. Also, we emphasize that the statistical approach does not elucidate specific deterministic geologic processes; rather, only the likelihood of a sample forming in a certain environment.

Finally, one of the difficulties when trying to classify an unknown sample's tectonic setting is determining when it is appropriate to use geologic inference versus less intuitive inverse statistical techniques. For example, samples with $>70\%$ SiO_2 may be correctly classified by this approach; however, geologic inference would strongly suggest that VAB and MORB are the highest and lowest likelihoods, respectively. Therefore, discrimination via an inverse approach is unnecessary.

ACKNOWLEDGMENTS

We thank Gary Ernst and Norm Sleep for reviews of the paper in the early stages of writing. The paper also benefited by reviews from two anonymous reviewers and Dr. Julie Morris.

APPENDIX A

Let $\mathbf{x}$ and $\mathbf{y}$ represent two vector parameter sets, and let $f(\mathbf{x}, \mathbf{y})$ be a normalized probability density. Two definitions are important: the *marginal probability density* for $\mathbf{y}$:

$$f_Y(\mathbf{y}) = \int_{\mathbf{x}} d\mathbf{x} f(\mathbf{x}, \mathbf{y}). \quad (\text{A-1})$$

The *conditional probability density* for $\mathbf{x}$ given $\mathbf{y} = \mathbf{y}_0$:

$$f_{X|Y}(\mathbf{x}|\mathbf{y}_0) = \frac{f(\mathbf{x}, \mathbf{y}_0)}{\int_{\mathbf{x}} d\mathbf{x} f(\mathbf{x}, \mathbf{y}_0)}. \quad (\text{A-2})$$

From these definitions, it follows that the joint probability density equals the conditional probability times the marginal probability density:

$$f(\mathbf{x}, \mathbf{y}) = f_{X|Y}(\mathbf{x}|\mathbf{y}) f_Y(\mathbf{y}), \quad (\text{A-3})$$

and *Bayes theorem*:

$$f_{X|Y}(\mathbf{x}|\mathbf{y}) = \frac{f_{X|Y}(\mathbf{x}|\mathbf{y}) f_Y(\mathbf{y})}{\int_{\mathbf{y}} d\mathbf{y} f(\mathbf{x}|\mathbf{y}) f_Y(\mathbf{y})}. \quad (\text{A-4})$$

In this paper, we frequently identify $\mathbf{y}$ with model space variables $\mathbf{m}$, and $\mathbf{x}$ with data space variables $\mathbf{d}$.

APPENDIX B

TABLE B1

Nomenclature used in the Bayesian geochemical discrimination

Parameter	Meaning
$\mathbf{m}$	Tectonic setting model vector
m_i	A particular tectonic setting
$\mathbf{d}$	True element concentration data vector
d_j	A particular element concentration
$\mathbf{G}$	Geochemical operator
G_{ji}	Element of $\mathbf{G}$
$\mathbf{G}^{-1}$	Inverse of $\mathbf{G}$
$\mathbf{d}^{obs}$	Observed element concentration data vector
$P(x)$	Probability of x being true
$P(x y)$	Probability x is correct given y
θ	PDF representing the geochemical theory
$\theta(\mathbf{d}, \mathbf{m})$	Joint theoretical PDF space
$\mathbf{h}$	Historical database of geochemical theory
h_{jip}	p^{th} sample of database for j^{th} element in i^{th} setting
${}^T\mathbf{C}$	Theoretical covariance matrix
${}^d\mathbf{C}$	Data measurement covariance matrix
${}^T C_i^{jk}$	Element of ${}^T\mathbf{C}$
${}^T C_i^{-1}$	Inverse of ${}^T\mathbf{C}$
${}^D\mathbf{C}$	Total covariance matrix
ρ_i	Theoretical correlation matrix for i^{th} setting
ρ_i^{jk}	Correlation between elements j and k in i^{th} setting
$\mu(x)$	Reference state of information on x
$\mu(\mathbf{d}, \mathbf{m})$	Joint reference PDF
$p_D(\mathbf{d})$	<i>a priori</i> PDF on data space
$p_M(\mathbf{m})$	<i>a priori</i> PDF on model space
$p(\mathbf{d}, \mathbf{m})$	PDF on joint data and model space
$\sigma(\mathbf{d}, \mathbf{m})$	<i>a posteriori</i> PDF
$\sigma(m_i)$	<i>a posteriori</i> probability on i^{th} tectonic setting

APPENDIX C

TABLE C-1

Results of the geochemical discrimination analysis for VAB, MORB, and OIB data from known tectonic setting for various values of outlier cutoff value, Γ , and number of samples used for batch processing. Values are given as probabilities where numbers in brackets refer to the number of samples examined.

Outlier Cutoff – Γ	Num. in Batch	VAB	MORB	OIB
0.00	1	0.915 (471)	0.914 (185)	0.903 (298)
0.00	2	0.966 (236)	0.936 (93)	0.920 (149)
0.00	3	0.981 (157)	0.984 (62)	0.920 (100)
0.01	1	0.907 (374)	0.918 (183)	0.899 (286)
0.01	2	0.963 (219)	0.936 (93)	0.917 (144)
0.01	3	0.980 (150)	0.984 (62)	0.917 (96)
0.10	1	0.871 (163)	0.992 (122)	0.937 (175)
0.10	2	0.950 (120)	0.935 (77)	0.951 (102)
0.10	3	0.978 (89)	0.981 (53)	0.947 (75)

TABLE C-2

Normalized log-space mean concentration for elements used in this study that comprise matrix **G**.

	Nb	Sr	Zr	Ti	Ta	Pb	Ni
VAB	-0.873	0.648	-0.0442	-0.446	-1.410	1.011	-0.773
MORB	-0.584	-0.150	-0.088	-0.062	-0.692	-0.547	-0.130
OIB	1.759	1.375	0.720	0.588	1.481	1.024	0.344

TABLE C-3

Covariance Matrix ${}^D\mathbf{C}$ used for VAB.

	Nb	Sr	Zr	Ti	Ta	Pb	Ni
Nb	4.659	0.688	0.895	0.329	2.494	0.872	0.091
Sr	0.688	1.751	0.271	-0.004	0.612	0.601	-0.280
Zr	0.895	0.271	1.288	0.267	1.017	0.315	0.049
Ti	0.329	-0.004	0.267	0.538	0.473	0.008	0.035
Ta	2.494	0.612	1.017	0.473	5.211	0.796	0.208
Pb	0.872	0.601	0.315	0.008	0.796	2.723	-0.318
Ni	0.091	-0.280	0.049	0.035	0.208	-0.318	3.317

TABLE C-4

Covariance Matrix ${}^D\mathbf{C}$ used for MORB.

	Nb	Sr	Zr	Ti	Ta	Pb	Ni
Nb	4.103	0.577	0.433	0.293	1.340	1.109	-0.169
Sr	0.577	0.911	0.153	0.104	0.512	0.468	-0.071
Zr	0.433	0.153	0.698	0.165	0.397	0.408	-0.127
Ti	0.293	0.104	0.165	0.482	0.322	0.219	-0.096
Ta	1.340	0.512	0.397	0.322	4.359	0.984	-0.082
Pb	1.109	0.468	0.408	0.212	0.984	2.738	0.198
Ni	-0.169	-0.071	-0.127	-0.096	-0.082	0.198	1.024

TABLE C-5
Covariance Matrix ${}^P\mathbf{C}$ used for OIB.

	Nb	Sr	Zr	Ti	Ta	Pb	Ni
Nb	1.899	0.284	0.199	0.090	0.410	0.324	-0.352
Sr	0.284	1.559	0.159	0.095	0.272	0.178	-0.328
Zr	0.199	0.159	0.930	0.097	0.246	0.186	-0.270
Ti	0.090	0.095	0.097	0.679	0.113	0.048	-0.183
Ta	0.410	2.72	0.246	0.113	1.935	0.308	-0.334
Pb	0.324	0.178	0.186	0.048	0.308	3.109	-3.04
Ni	-0.352	-0.328	-0.270	-0.183	-0.334	-0.304	8.263

APPENDIX D

This appendix contains the subroutine called to perform the discrimination test on individual samples for a user specified outlier cutoff value (that is, it will perform equations (17) and (18)). There are three output probabilities for each analysis input: $\sigma_M(m_1)$, the probability of a VAB origin; $\sigma_M(m_2)$, the probability of a MORB origin; and $\sigma_M(m_3)$, the probability of an OIB origin. In the code, these are referred to as Prob_VAB, Prob_MORB, and Prob_OIB, respectively. A fourth output is a 1xM matrix called 'reject', which will place a 1 in the column if the sample is above the outlier cutoff value (rho) or a 0 if the sample is below the outlier cutoff value (that is, and acceptable analysis). For referencing cells within a matrix X, X(M, N) refers to matrix X, row M, column N. A '%' sign refers to documentation for user reference and not actual code.

This program requires the following matrices to be input:

% 1) Data – a Mx7 matrix of the data from the unknown samples in the order Nb, Sr,

% Zr, Ti, Ta, Pb, and Ni

% 2) CM_VAB; CM_MORB; CM_OIB – The covariance matrices given in tables C-3, C-4, and C-5, respectively, in the same order as Data matrix

% 3) G_VAB; G_MORB; G_OIB – The mean elemental concentrations given in table C-2 in the same order as Data matrix

% and the following parameter:

% 4) rho – the outlier cutoff value discussed in equation (18)

% Created by Cameron A. Snow and Jeffrey C. Shragge . . .

% last modified February 14, 2006 . . .

load Data

load CM_VAB

load CM_MORB

load CM_OIB

load G_VAB

load G_MORB

load G_OIB

rho = 0.01;

% . . . the following performs necessary matrix inversions . . .

ICM_VAB = inverse(CM_VAB);

ICM_MORB = inverse(CM_MORB);

ICM_OIB = inverse(CM_OIB);

% . . . The following performs calculations for equation (17) for all rows (samples) in

% . . . matrix Data

for ii = 1 to # of samples;

for aa = 1 to 7;

for bb = 1 to 7;

P_VAB(bb) = .33333*exp(-0.5*(G_VAB(aa)-

log(Data(ii,aa)))*(ICM_VAB(aa,bb))*(G_VAB(bb)-

log(Data(ii,bb))));

```
P_MORB(bb) = .33333*exp(-0.5*(G_MORB(aa)-
log(Data(ii,aa)))*(ICM_MORB(aa,bb))*(G_MORB(bb)-
log(Data(ii,bb))));
P_OIB(bb) = .33333*exp(-0.5*(G_OIB(aa)-
log(Data(ii,aa)))*(ICM_OIB(aa,bb))*(G_OIB(bb)-
log(Data(ii,bb))));

end

sigma_VAB(ii) = sum(P_VAB);
sigma_MORB(ii) = sum(P_MORB);
sigma_OIB(ii) = sum(P_OIB);

end

PP_VAB(ii) = sum(sigma_VAB);
PP_MORB(ii) = sum(sigma_MORB);
PP_OIB(ii) = sum(sigma_OIB);

Prob_VAB(ii) = PP_VAB(ii)/(PP_VAB(ii)+PP_MORB(ii)+PP_OIB(ii));
Prob_MORB(ii) = PP_MORB(ii)/(PP_VAB(ii)+PP_MORB(ii)+PP_OIB(ii));
Prob_OIB(ii) = PP_OIB(ii)/(PP_VAB(ii)+PP_MORB(ii)+PP_OIB(ii));

% . . . This labels rows not meeting cut-off value with ones, acceptable
% . . . values with zeroes
if (PP_VAB(ii)+PP_MORB(ii)+PP_OIB(ii)) < rho
    reject(ii) = 1;
else
    reject(ii) = 0;
end
end
```

APPENDIX E

This appendix briefly goes through the process of taking a number of chemical analyses from an area and determining their tectonic origin using the geochemical discrimination method. This appendix is to serve as a practical guide for how to implement the method and as a way to double-check that the user has correctly implemented the code given above. The data used below are taken from the Hawaiian Islands database from the GEOROC website.

TABLE E-1
Geochemical data from Hawaiian Islands tholeiite for selected elements.

	Nb	Sr	Zr	Ti	Ta	Pb	Ni
Sample A	31	664	269	23620	2	1.92	38
Sample B	33	697	202	22900	2.3	1.8	64
Sample C	43	815	259	22061	3.2	2.08	8
Sample D	44	781	264	22061	3.4	2.21	9
Sample E	67	886	380	18164	4.3	3.3	4
Sample F	67	1477	182	15467	3.03	5.09	220
Sample G	70	1260	325	14807	4.5	3.3	9
Sample H	72	1013	445	13848	4.5	4.23	4
Sample I	79	649	629	16306	5.1	4.42	3
Sample J	83	740	484	12049	4.9	4.38	4
Sample K	88.4	1072	736	6864	5.7	4.85	5

The data shown in table E-1 were input as matrix ‘Data’ in the above code. The resulting output from the code is shown below in table E-2.

TABLE E-2

Probabilities output by code shown in Appendix D. Highest output probabilities are shown in bold.

	Prob_VAB	Prob_MORB	Prob_OIB	Reject
Sample A	0.3753	0.2371	0.3876	0
Sample B	0.3800	0.2360	0.3840	0
Sample C	0.3636	0.2464	0.3899	0
Sample D	0.3644	0.2452	0.3903	0
Sample E	0.3553	0.2657	0.3789	0
Sample F	0.3659	0.2792	0.3549	0
Sample G	0.3627	0.2479	0.3894	0
Sample H	0.3545	0.2670	0.3785	0
Sample I	0.3513	0.2771	0.3716	0
Sample J	0.3548	0.2674	0.3778	0
Sample K	0.3573	0.2609	0.3818	0

Inspection of the calculated probabilities reveals three important pieces of information: 1) that 10 of the 11 samples are likely of an OIB origin; 2) none of the samples are statistical outliers with $\rho = 0.01$; and 3) all of the samples had only a slightly higher probability of having an OIB origin than of having a VAB origin. The fact that most of the samples have similar values for either an OIB or VAB origin may suggest that the values are somewhat atypical for an OIB composition. However, inasmuch as 10 of the 11 were classified as OIB, one can be more confident in the discrimination test.

REFERENCES

- Bayes, T., 1763, Essay towards solving a problem in the doctrine of chances, 1958: republished in *Biometrika*, Vol. 45, p. 293–315.
- Lehnert, K., Su, Y., Langmuir, C., Sarbas, B., and Nohl, U., 2000, A global geochemical database structure for rocks: *Geochemistry, Geophysics, Geosystems*, 1, 1999GC000026.
- Mullen, E. D., 1983, MnO/TiO₂/P₂O₅: A minor element discriminant for basaltic rocks of oceanic environments and its implications for petrogenesis: *Earth and Planetary Science Letters*, v. 62, p. 53–62.
- Pearce, J. A., 1974, Statistical analysis of major element patterns in basalts: *Journal of Petrology*, v. 17, p. 15–43.
- 1982, Trace element characteristics of lavas from destructive plate boundaries, in Thorpe, R. S., editor, *Andesites*: London, John Wiley and Sons, p. 525–548.
- 1987, An expert system for the tectonic characterization of ancient volcanic rocks: *Journal of Volcanology and Geothermal Research*, v. 32, p. 51–65.
- Pearce, J. A., and Cann, J. R., 1973, Tectonic setting of basic volcanic rocks determined using trace element analyses: *Earth and Planetary Science Letters*, v. 19, p. 290–300.
- Pearce, J. A., and Norry, M. J., 1979, Petrogenetic implications of Ti, Zr, Y, and Nb variations in volcanic rocks: *Contributions to Mineralogy and Petrology*, v. 69, p. 33–47.
- Shervais, J. W., 1982, Ti-V plots and the petrogenesis of modern and ophiolitic lavas: *Earth and Planetary Science Letters*, v. 59, p. 101–118.
- Snow, C. A., 2006, A re-evaluation of tectonic discrimination diagrams and a new probabilistic approach using large geochemical databases: Moving beyond binary and ternary plots: *JGR Solid Earth*.
- Sun, S. S., and McDonough, W. G., 1989, Chemical and isotopic systematics of oceanic basalts: Implications for mantle composition and processes, in Saunders, A. D., and Norris, M. J., editors, *Magmatism in the oceanic basins*: Geological Society of London Special Publication, v. 42, p. 313–325.
- Tarantola, A., 1987, *Inverse problem theory*: Amsterdam, Elsevier, 613 p.
- Wood, D. A., 1980, The application of a Th-Hf-Ta diagram to problems of tectonomagmatic classification and to establishing the nature of crustal contamination of basaltic lavas of the British Tertiary volcanic province: *Earth and Planetary Science Letters*, v. 50, p. 11–30.