American Mineralogist, Volume 74, pages 273–276, 1989

SOFTWARE NOTICE

PEARCE.PLOT: Interactive graphics-supported software for testing petrologic hypotheses with Pearce element-ratio diagrams

C. R. Stanley, J. K. Russell* Department of Geological Sciences, The University of British Columbia, Vancouver, British Columbia V6T 2B4, Canada

PEARCE ELEMENT RATIOS

Commonly, in magmatic systems undergoing differentiation, there are elements whose absolute amounts are affected by the differentiation process and other elements that are not affected by the process, i.e., conserved elements (Nicholls, 1988). When one or more conserved elements exist in a system, it is viable to analyze the compositional data with Pearce element-ratio diagrams (Pearce, 1968). Pearce recognized that if there is at least one conserved element, then a simple transformation of the compositional data will reveal the exact relationships between the nonconserved constituents. Ratios that have conserved elements in their denominators depict the true relationships between the elements used in the numerators. If we know the actual variations between these extensive variables, then it is possible to determine the differentiation process. Pearce element ratios facilitate the recognition of rocks that are comagmatic, the identification of the minerals involved in the differentiation process, as well as the estimation of the modal proportions and compositions of the phases involved (Russell and Nicholls, 1988).

Pearce element ratios are calculated from the element numbers (e_i), where

$$e_i = W_i A_i / M_i \tag{1}$$

and W_i, A_i, and M_i are the weight percent, number of cations per oxide formula, and molecular weight of the oxide i. The corresponding Pearce element ratio is

$$R_i = e_i / e_z. \tag{2}$$

The z subscript refers to the requisite conserved element. Nicholls (1988) formally stated that proper Pearce element ratios are those in which the contribution of the denominator to the variance of the ratio is *very much smaller* than the contribution of the numerator.

The purpose of this notice is to introduce an interactive computer program, PEARCE.PLOT, that facilitates rapid and rigorous evaluation of Pearce element-ratio diagrams. The program has been developed to test petrologic hypotheses using major- and minor-element chemistry. Program PEARCE.PLOT provides a means to reject specific hypotheses on the basis of the following findings: the data imply that the rocks are not cogenetic, the data do not have a high correlation, the observed trends do not have slopes consistent with those expected from theory, or the trend has a zero intercept (indicating that the denominator may not be conserved; Nicholls, 1988). Although the examples presented below concern igneous differentiation, the theory, methodology, and computer program can easily be adapted to many other applications (e.g., Soret diffusion, distribution coefficients, mass-transfer reactions, etc.).

PEARCE.PLOT

The computer program PEARCE.PLOT is written in Turbo-Pascal and uses the graphics toolbox provided by Borland International (Stanley and Russell, 1988). The program runs on any IBM-compatible personal computer with at least 256 k memory and CGA, EGA, or Hercules graphics capability. Calculations and graphical results are designed to be printed on an Epson-compatible printer. The program has a flexible data-input format that does not require a specific input order for the compositional data in the raw data file. Furthermore, the program handles estimates of error on raw data by propagating the analytical uncertainties through the Pearce element-ratio calculation. These uncertainties are critical in evaluating several types of petrologic hypotheses, such as whether a group of analyses could be derived from a single magma. The major attibutes of the program lie in its interactive and flexible nature that allows easy selection of the various numerators and the denominator for the ratios plotted on the X and Y axes of the Pearce element-ratio diagram. These aspects of the program, plus the graphical nature of the output, facilitate a thorough analysis of compositional variations in process-related data and offer a tremendous advantage in testing specific petrologic hypotheses with available whole-rock chemistry.

The interactive part of the program begins by prompting the user for the name of the denominator element. The program calculates all of the simple Pearce element ratios and propagates the estimated analytical uncertainties of the oxides through the ratio calculations. To generate a plot, the operator enters the coefficients of numerator elements desired for the X and Y axes. All Pearce element-ratio diagrams have options for error representation, labeling of data points, and fitting straight lines to the data. On each plot the data points can be left unlabeled or labeled on the screen. Error bars based on the appropriate analytical uncertainties can also be plotted in the figure as the average error for the data set or the propagated error calculated for each datum.

Finally, there is an option to fit a straight line to the data set. The available options consist of (1) major-axis linear regression, (2) reduced major-axis linear regression, (3) average-error linear regression, and (4) a line with a specified slope can be placed through an arbitrary chosen data point. The third option may only be chosen when errors have been assigned to the oxide analyses. The advantage of option 2 over option 1 is that the fitted line is scale invariant. After generating the image, the plot can be sent to the printer and another plot can be generated.

TESTING PETROLOGIC HYPOTHESES

The interpretation that magmatic differentiation processes have occurred in a suite of volcanic rocks implies that the analyses represent samples of a single magmatic lineage. Pearce element ratios can be used to test this premise by constructing element

---

* The PEARCE.PLOT source and object code can be obtained at cost [$8.00 (U.S.) or $10.00 (Canadian)] from the University of British Columbia by contacting J.K.R. [phone (604) 228-2703].

0003–004X/89/0102–0273$02.00

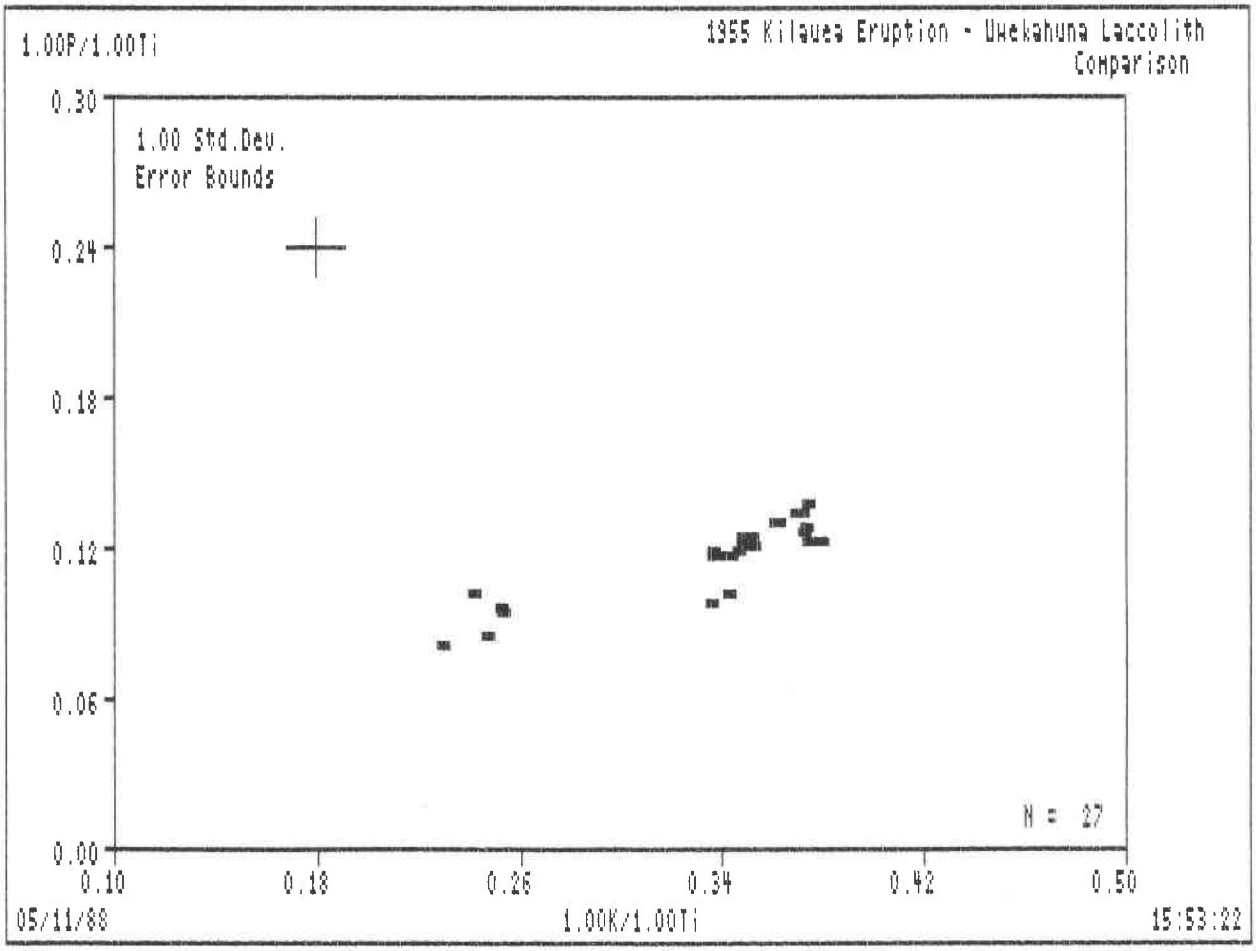

Fig. 1. Conserved element plot of P/Ti vs. K/Ti for the 1955 Kilauea lavas (right cluster) and the Uwekahuna laccolith (left cluster). The data are plotted with the calculated average 1 standard-error bars expected from analytical uncertainty. (CGA graphics screen printed on an Epson dot-matrix printer.)

ratios from conserved constituents (Nicholls, 1988). Ratios formed from conserved elements should be identical for all cogenetic rocks. For example, a basic understanding of crystallization processes in basalts leads us to expect that the elements K, Ti, and P are not involved in the early crystallization of such magmas. If true, ratios such as P/Ti and K/Ti should be single-valued for all related basalt lavas. Figure 1 is a conserved-element plot P/Ti vs. K/Ti for two groups of basalts from Kilauea volcano, Hawaii. Five analyses from Uwekahuna laccolith (Murata and Richter, 1961) define the cluster to the left, whereas lavas from the 1955 eruption of Kilauea (Wright and Fiske, 1971) plot as a group on the right of the figure. Ideally, if all basalts were derived from a single magma, the data should plot as a point. Practically, for cogenetic rocks we expect the variance in the conserved-element ratios for the data to be less than or equal to the variance arising from analytical error. From Figure 1 it is apparent that (1) the two groups of basalts are significantly different and must be derived from different magmas and (2) the scatter in the two data sets is smaller than the 2 standard-error bars due to analytical error. Consequently, we cannot reject the hypothesis that the two data sets represent two distinct magma series.

The same chemical data are presented in Figure 2 on a Pearce element-ratio diagram with the axes $Y = 0.5(\mathrm{Mg} + \mathrm{Fe})/\mathrm{Ti}$ and $X = \mathrm{Si}/\mathrm{Ti}$. On this diagram, all ferromagnesian silicates that crystallize from basalts have a unique slope. Consequently, this figure can model the effects of olivine, Ca-poor pyroxene, augite, and plagioclase or Fe-Ti oxide crystallization and separation. The Uwekahuna data are plotted, and a line with a slope of 1.0 is forced through the most Mg-rich analysis. All rocks that can be related to this composition by the sorting of olivine alone will lie on the line. It is clear in Figure 2 that we cannot reject the hypothesis that the Uwekahuna rocks are related by fractionation of olivine. Conversely, the 1955 data describe a linear trend with a best-fit slope of 0.25, which is consistent with fractionation of augite alone or a combination of minerals. The latter explanation is more reasonable given that the lavas were described as porphyritic with plagioclase, augite, and olivine (micro-) phenocrysts (Wright and Fiske, 1971). Further analysis in other Pearce element-ratio diagrams can ascertain which of the

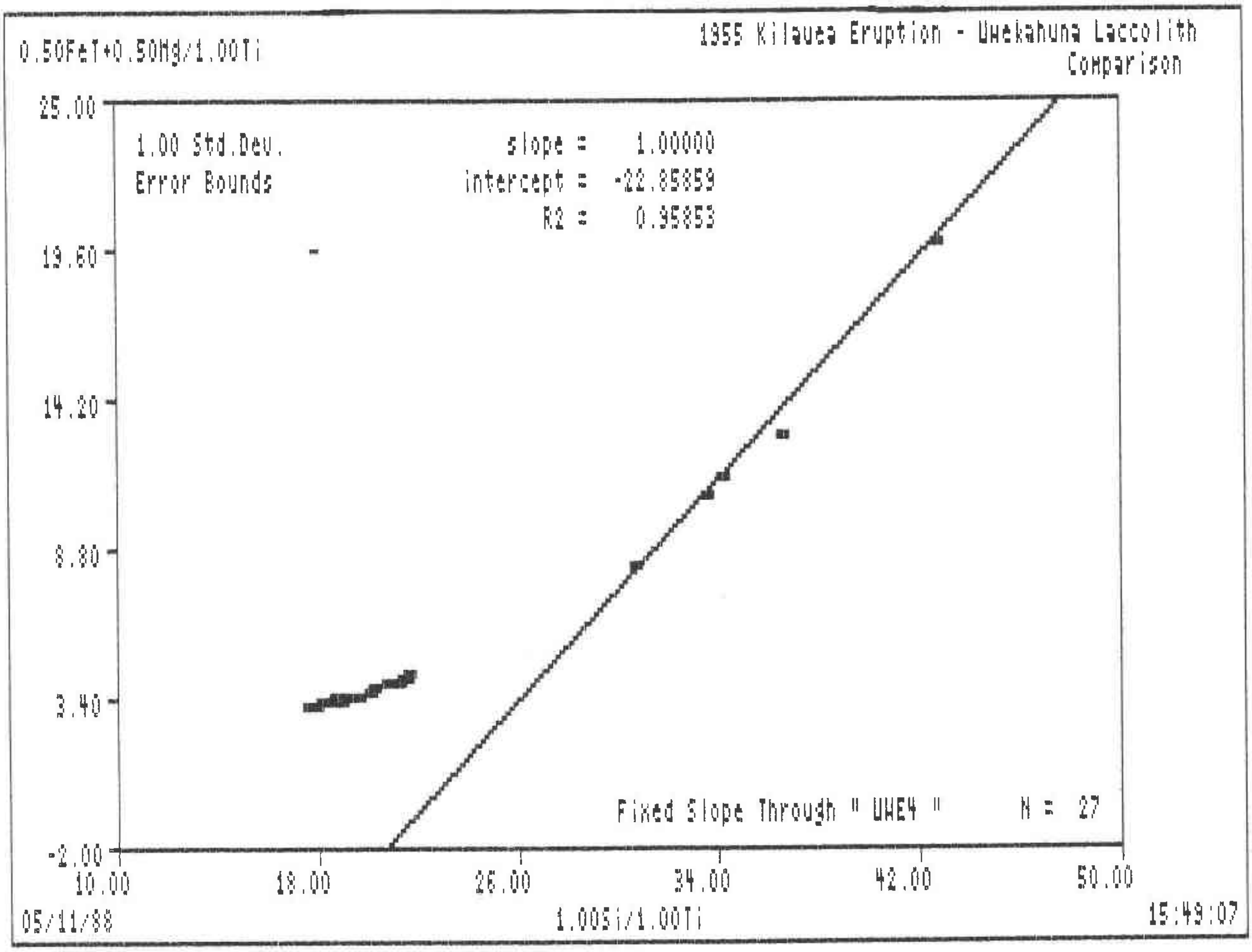

Fig. 2. The data from the 1955 Kilauea lavas and the Uwekahuna laccolith are plotted in the Pearce element-ratio diagram of Si/Ti vs. 0.5(Mg + Fe)/Ti. The trends to be expected from fractionation of plagioclase, augite, Ca-poor pyroxene, olivine, and Fe-Ti oxides have slopes 0.0, 0.25, 0.5, 1.0, and ∞, respectively. A line with a slope of 1.0 is forced through the Uwekahuna data. (CGA graphics screen printed on an Epson dot-matrix printer.)

observed minerals are actually responsible for the differentiation of the 1955 magma.

CONCLUSIONS

Program PEARCE.PLOT facilitates testing hypotheses concerning igneous differentiation processes with Pearce element ratios because (1) the program is interactive, (2) subsets of the data can be analyzed separately, (3) the analysis is done graphically, (4) analytical error can be represented in a variety of ways, and (5) straight lines can be fit to the data or straight lines with prescribed slopes can be superimposed on the data. These attributes play a crucial role in recognizing hypotheses that can be rejected. Whenever the theoretical path of the process can be envisaged, Pearce element ratios should provide a means of testing the hypothesis. Pearce element ratios could be used to extract trace-element distribution coefficients from experimental data, to determine the phase assemblage in small experimental charges where only the glass can be analyzed, to characterize the effects of diffusion, and to quantify the nature of mass-transfer reactions in hydrothermal systems or metamorphic petrology (Nicholls et al., 1988).

ACKNOWLEDGMENTS

This research was supported by the Natural Science and Engineering Research Council through operating grant A0820 (J.K.R.) and a University of British Columbia Graduate Fellowship awarded to C.R.S.

REFERENCES CITED

Murata, K.J., and Richter, D.H. (1961) Magmatic differentiation in the Uwekahuna laccolith, Kilauea caldera, Hawaii. Journal of Petrology, 2, 424–437.

Nicholls, J. (1988) The statistics of Pearce element diagrams and the Chayes closure problem. Contributions to Mineralogy and Petrology, 99, 11–24.

Nicholls, J., Stout, M.Z., and Ghent, E.D. (1988) Partly open system chemical variations in clinopyroxene amphibolite boudins, Three Valley Gap, British Columbia. Geological Association of Canada–Mineralogical Association of Canada Annual Meeting, Program with Abstracts, p. A90.

Pearce, T.H. (1968) A contribution to the theory of variation diagrams. Contributions to Mineralogy and Petrology, 19, 142–157.

Russell, J.K., and Nicholls, J. (1988) Analysis of petrologic hypotheses with Pearce element ratios. Contributions to Mineralogy and Petrology, 99, 25–35.

Stanley, C.R., and Russell, J.K. (1988) Analysis of igneous processes with Pearce element ratio diagrams. Geological Association of Canada–Mineralogical Association of Canada Annual Meeting, Program with Abstracts, p. A116.

Wright, T.L., and Fiske, R.S. (1971) Origin of differentiated and hybrid lavas of Kilauea volcano, Hawaii. Journal of Petrology, 12, 1–65.

Manuscript received February 22, 1988
Manuscript accepted September 6, 1988