Graphical Interpretation of Geochemical-Petrological Data

Igpet and Mixing can display data beautifully and make a surprising variety of complicated calculations, but rarely do these tools prove anything! What these programs can most easily and reliably do is prove hypotheses incorrect. Usually, one can conclude that a hypothesis, such as fractional crystallization, is consistent with available evidence, not that it is proved. All too often this inherent limitation is forgotten and weak hypotheses are deemed proved on flimsy graphical evidence. In my experience the worst pitfall of this software package is the ease with which dumb ideas or fuzzy thinking are translated into attractive diagrams that are pasted into papers and theses without much useful thought. I am intimately familiar with some varieties of misbegotten interpretations because I have done them myself! The paragraphs below summarize some of the false paths Igpet can lead a student down.

The correct approach to solving the problem of how a suite of samples of igneous rocks might be related to each other is first to look at the hand samples and thin sections of all (or at least half) of the samples. The thin sections can immediately set the tone for the problem at hand. Assuming the samples are all from the same volcano or from a group of geographically and temporally associated vents, one can start wondering about how they are related. My preferred sample set is a long stratigraphic sequence from a caldera wall. Nature is rarely so co-operative. If the samples are aphyric, or nearly so, there is a reasonable chance you may be examining a set of separate melts, so some type of partial melting hypothesis can be considered. If a plot of MgO versus K_2O is a mess, with a large K_2O range and little or no potash increase as MgO decreases, then you should get more incompatible element data, especially REE data, in order to test various partial melting models. If, instead, there is a strong inverse relationship between potash and magnesia, then fractional crystallization becomes the hypothesis of choice.

The presence of abundant phenocrysts and, especially, the presence of disequilibrium textures and assemblages should make one worry about mixing and accumulation processes. If olivines and quartz are in the same thin section, then something is wrong! Either mixing or assimilation is being signaled. Electron microprobe analyses of minerals (olivines, plagioclase, clinopyroxene, etc) that define two distinct populations (a bimodal distribution) are fairly definitive evidence for magma mixing that has occurred too recently for the phenocryst evidence to be swept away by the thermodynamic drive toward equilibrium.

Igpet is a tool but not a textbook. There are several useful petrology and geochemistry books. The more elegant calculations in Igpet either came from Albarede's 1995 book, Introduction to Geochemical Modeling, or are reproduced there. The reference list at the end of this manual is included to be used, especially, some rather old references: e,g. O'Hara (1968 and 1976) for CMAS projections; Bryan, Finger and Chayes (1968) for petrologic mixing calculations; Chayes (1964) on the shortcomings of Harker or Fenner diagrams; Pearce (1968) for clever methods to test fractionation hypotheses using major elements; Langmuir et al, (1977) of the mixing equation; DePaolo (1981) for AFC calculations.

Another area where Igpet graphics must be complemented by careful reading is the use of the many predesigned diagrams (e.g. for CMAS projections, rock nomenclature and tectonic discrimination). Many of these diagrams have specific limitations on their use. Igpet points out

the rudiments of restrictions using the nota bene (NB) line at the top of many diagrams. However, there is no substitute for reading the original reference. Rollinson has done a terrific job in comparing and summarizing many discrimination diagrams in his 1993 book, Using geochemical data: Evaluation, presentation, interpretation.

One of the dirty tricks in Igpet is the automatic setting of the range of X and Y axes. The automatic setting is useful as a starting point but it is DUMB. Your rock suite may be very homogenous but Igpet is dumb and will stretch the X and Y range to the full amount possible. In such a case the variation that appears (a random mess) is just noise. Don't panic that your data are of poor quality, just look the range and adjust it.

Be wary of log-log plots. I almost regret including the Log_{10} function in Igpet. I am coauthor on papers that use log-log plots. The excuse for using log transformation is the huge range in source compositions for arc rocks; depleted mantle at one end and hydrous fluids highly enriched in incompatible elements at the other. It is satisfying to see the full range of the mixing line between the end-member compositions, but all the detail concerning the relationships between the actual samples becomes highly compressed. It is a common mistake in science to propose spurious functional relationships based on roughly linear data arrays in log-log space.

Be wary of "trends" or "trend lines." I do not think that these terms have any actual meaning. Igpet calculates statistics needed to test for linear regression, including the Pearson correlation coefficient, r, and the Spearman rank order correlation coefficient, r'. You will need a competent statistics text to understand these statistics. I hope you have had a good course in applied statistics for the physical sciences. I was unlucky and suffered through a horrible course on statistics for economics and have a weak statistical background as a result. If you hear about a good stats course, take it.

Know your data and use the different symbols judiciously. Few of the volcanoes I have looked at are homogenous. Identifying subsets, defined stratigraphically or geochemically, almost always leads to increased understanding. Even among basalts from the same volcano, there are usually apples and oranges. Using the same symbol for two different magma types results in a hodgepodge that cannot be interpreted in detail. Igpet now has 36 symbols, more than enough to define subsets of any reasonably sized sample suite. The drive to subdivide and pigeonhole can be overdone and I doubt there are any hard and fast rules. I tend to overdo it and then back off and combine similar groups. At the other extreme, some geochemists never subdivide at all.

Obviously, I have turned into an opinionated grump in my advanced middle age. However, on the brighter side, I hope you will have serendipity with Igpet. Several times Igpet has allowed my students and me to discover unsuspected order in volcanic geochemistry. The ease allowed by Igpet allows lots of experimentation. Sometimes there will be too much and you will end a session of data examination lost and confused. Try again and try to stay focused on what is plausible.

The following argument, derived from Patino et at. (2000), describes an approach to looking at data. The problem was a new batch of ICP-MS data for Central American volcanic rocks and for the sediments just about to be subducted beneath Central America. In some plots of pairs of incompatible element ratios, like Ba/La versus La/Yb, there were clear systematics indicating mixing and melting relationships between the most plausible sources; the mantle and the

sediments being subducted. However most possible ratio-ratio plots of incompatible elements produced just a mess, not systematics. So why do some plots work and others fail? One problem was the complexity of the source. Most of the source was MORB-like mantle but the subducted plate contributed a basalt layer and two sediment layers, providing a minimum four sources. Plausible processes, such as partial melting or hydrothermal transport added further complications.

The first criterion we used to select useful trace element ratios was to identify the incompatible elements with the largest difference between the two sedimentary units. Arranging the elements in order of their overall hemipelagic/carbonate ratio (U, Cs, Th, K, Pb, La, Y, Ba, Sr), we saw maximum difference by comparing element ratios from opposite sides of this spectrum (e.g., Ba/Th and U/La). On the other hand, we could minimize the confusing effect of having two sediments by looking at elements near each other on the spectrum (e.g. Ba/La or U/Th).

We found that the useful ratios, the ones with apparent systematics, were defined by separation. The potential sources (mantle wedge, subducted MORB, carbonate sediments and hemipelagic sediments) occupied separate fields in ratio/ratio plots. The mantle wedge and MORB components often overlap in the ratios of highly incompatible elements. Therefore, we preferentially selected pairs of ratios where MORB + mantle, carbonate sediment and hemipelagic sediment defined a triangle. Where two components are close to each other, as the two sediments are in Ba/La versus U/Th, the field of volcanic data collapsed into an apparent binary mixing array between mantle and bulk sediment.

In general, given a plausible data set (Cs, K, Rb, U, Th, Nb, Ta, La, Gd, Yb, Zr, Hf, Pb, Sr, Ti) you can plot a huge number of combinations. The reduced list above can be further trimmed of Hf and Ta, which behave like Zr and Nb, but even so you have 13 elements from which to pick 4. I think that provides 715 possible ratio-ratio plots, most of which are useless. What you are doing is looking at 13 dimensionsal space and trying to discover volumes were there are clear systematics. This happens when some components line up and fold into each other simplifying the problem.

If you have 4 or 5 sources, you have trouble because ratio-ratio plots become very confused if there are more that 3 well separated sources. The place to start is to look at the plausible sources. Do any overlap on nearly all elements, allowing the problem to be simplified? The next step is to find at least a few ratios that are nearly the same for two or more otherwise distinct sources. This allows a simplified window, folding a couple of sources together. Finally, focus on plots that show the largest separations among source components. Having large separation is crudely like being perpendicular in the mathematical sense. So you are seeking windows within the data space where the sources are either parallel (folded into each other) or perpendicular. In these views, the systematics will be the most clear. Many other plots may be similar but suffer from smaller degrees of orthogonality and have confused and unconvincing data arrays. The plan is to find the clearest views and then model them.