

Igpet software for modeling igneous processes: examples of application using the open educational version

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Abstract We provide here an open version of *Igpet* software, called *t-Igpet* to emphasize its application for teaching and research in forward modeling of igneous geochemistry. There are three programs, a norm utility, a petrologic mixing program using least squares and *Igpet*, a graphics program that includes many forms of numerical modeling. *Igpet* is a multi-faceted tool that provides the following basic capabilities: igneous rock identification using the IUGS (International Union of Geological Sciences) classification and several supplementary diagrams; tectonic discrimination diagrams; pseudo-quaternary projections; least squares fitting of lines, polynomials and hyperbolae; magma mixing using two endmembers, histograms, x-y plots, ternary plots and spider-diagrams. The advanced capabilities of *Igpet* are multi-element mixing and magma evolution modeling. Mixing models are particularly useful for understanding the isotopic variations in rock suites that evolved by mixing different sources. The important melting models include, batch melting, fractional melting and aggregated fractional melting. Crystallization models include equilibrium and fractional crystallization and AFC (assimilation and fractional crystallization). These, reports and proposals concerning igneous petrology are improved by numerical modeling. For reviewed publications some elements of

modeling are practically a requirement. Our intention in providing this software is to facilitate improved communication and lower entry barriers to research, especially for students.

Keywords Geochemical modeling · Igneous petrology · Magmagenesis · Partialmelting

Introduction

For initial evaluations of igneous rock suites, *Igpet* provides over 200 diagrams that rapidly display data in discrimination diagrams for defining rock type and suggesting tectonic associations. The tectonic discrimination diagrams are not absolute and should be used with reference to the original publications and must be evaluated based on field relations, petrographic descriptions, and petrological evaluation. The next steps in evaluating a rock suite include developing and testing hypotheses on the source(s) of the igneous suite, the melting process and subsequent evolutionary processes including, assimilation, mixing and fractional crystallization. *Igpet* facilitates numerical testing of these processes and can rapidly rule out flawed hypotheses and improve plausible ones. A first step in modeling can be the mix and model tools available in X-Y plots but the most powerful tools are simultaneous calculations of several elements and isotope ratios.

Igpet's forward modeling uses equations developed or summarized by Albarede (1995). The multi-element modeling strategy grew out of “spider” diagrams. These diagrams comprise 20 or more elements with varying behavior, including large ionic radius lithophile elements (LILE), high field strength elements (HFSE) and rare earth elements (REE). Sr, Nd, Pb and Hf are typically included and therefore their isotopic ratios also have to be considered. The power of this multi-element approach arises from simultaneously subjecting

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twenty or more elements and their isotopic ratios to the same modeling steps. An apparent fit on a log-based spider-diagram requires closer examination in X-Y plots. By switching between log and linear scales, the range of ‘successful’ models can be restricted and tested for internal consistency.

The main tools in *Igpet* are forward models of trace element and isotopic variations. They are useful for eliminating hypotheses and refining the range of allowable hypotheses. However, for a complete examination of igneous processes there should be internal consistency between the trace element and isotopic results from *Igpet* and major element evolutionary paths from models based on thermodynamic parameterizations of experimental data such as *MELTS* (Ghiorso et al. 2002), *Petrolog3* (Danyushevsky and Plechov 2011), *PRIMACALC2* (Kimura and Ariskin 2014) and *PRIMELT3 MEGA.XLSM* (Herzberg and Asimow 2015).

Description of software, algorithms and educational resources

Software

We provide a teaching version of *Igpet* compiled for both *Windows*, using *Visual Basic 6*, and *MacIntosh*, using *XoJo*, a programming language developed for *MacIntosh OS X* systems. The *t-Igpet* student modules differ from the professional version only in the graphics output, which is a bitmap image rather than a vector diagram. The software includes three applications and six folders (Table 1) of supporting text files that hold fundamental data, preferences, and the parameters for about 200 published diagrams, mostly for tectonic discrimination and rock nomenclature. A PC folder contains files of published crystal-liquid partition coefficients, which are vital to the multi-element geochemical modeling focused on here. To obtain *t-Igpet*, download the Mac or Windows zip files from: <https://sites.google.com/site/tsigpetteaching/>. The most important algorithms are available in text files written in *XoJo* code; *Spimix.txt* for source mixing and *Spimod.txt* and for modeling the origin and evolution of magma. Also available

are a manual and a workbook aimed at undergraduates and first-year graduate students.

Data handling

The control files for *Igpet* are tab-delimited files (.txt) that are easily edited in *Notepad* or *TextEdit*. Data files are large matrices of alphanumeric entries that are easy to maintain in *Excel* and then saved for use by *Igpet* into a txt file. *Igpet* also reads comma-separated files (.csv files), because international databases of magmatic rocks, like GEOROC (Geochemistry of Rocks of the Oceans and Continents at Max Planck Institute for Chemistry in Mainz), provide csv output.

Igpet works with only minor changes to a user’s original data. Rows are samples and columns are parameters such as oxides, latitude, country, etc. *Igpet* finds the sample column by searching for the string “samp” within the column names, so the header for the column where sample names are stored may need to be changed to include the “samp” string. Symbols are keyed by three possible columns of integers; kcode (default), lcode and jcode. Adding “samp” to a column header and a kcode column are the minimum changes required.

Igneous data include numeric data and descriptions. Therefore, *Igpet* reads and stores all data as string variables. The default setting is 13,000 rows or samples by 250 columns of oxides, elements, locations, descriptors etc. Numeric values for igneous parameters like SiO₂ are obtained, as needed, by a subroutine that uses international awareness to convert strings like 52.65 or 52,65 to double precision numeric values. Keeping the oxide, element, and other numeric values in string form prevents conversion errors if the user decides to save the data file to a new name.

The order of igneous data is not universal but there are many particular calculations that require specific oxides or elements, therefore extensive searching and aliasing takes place immediately after reading a data file. First, the column positions of the major oxides are located and stored in a vector. For isotopic calculations the column positions of the isotopic ratios are saved, as are the column positions of the concentrations of their element values (e.g. Sr, Nd, Hf and Pb). Several derived parameters can be added to the data in memory using tools in the file menu. These include CIPW (Cross, Iddings, Pirsson, Washington) normative minerals, Mg# and other common parameters such as Eu*, the expected value of Eu calculated from the values of the adjacent rare earth elements Gd and Sm.

If an entire region is the subject of a research project, the data file can be very large. A useful example is the database of mid-ocean ridge glasses (the Volcanic Glass File, maintained by the Department of Mineral Sciences at the Smithsonian Institution: <http://mineralsciences.si.edu/research/glass/vg.htm>, Melson et al. 2002), which now has more than 12,000 entries. For some purposes, all the data need to be plotted, but

Table 1 *Igpet* folders and file descriptions

Folder	Description
Controls	Six initialization files read at startup Three optional files including Spider.txt for spider-diagrams
PC	Twenty partition coefficient files
Diagrams	Definitions of 128 different diagrams grouped by type into 12 files
CMAS	Seven files with definitions of 30 CMAS projections
Min	Two files with definitions of 5 ternary plots for minerals
Data	A folder with 20 data files for use with the manual and workbook

for other cases, such as a particular rift segment, only a small subset of the data is required. Initially, *Igpets* was designed for many small data files, one for each volcano or rift segment or other type of focus region. Experience with RU_CAGeochem (Carr et al. 2014) established that it is much easier to maintain and upgrade a single large data file rather than multiple small ones. Therefore, *Igpets* has a tool that emulates the sorts of questions and limits that are found in querying databases. A SubSelect window allows multiple inclusions, exclusions and numerical ranges. The first window in SubSelect is a listbox that contains all the variable names (column headers). Select a variable with a click and the next window, also a listbox, fills with all the sample names and the values for the selected variable. If the variable is a string, like volcano name or ridge segment, then an Include or Exclude listbox can be activated and particular samples that fit the filter criteria will be either selected or excluded. If the variable is a number, like SiO₂ content, the maximum and minimum values are entered and then saved to the Limits listbox. SubSelect facilitates comparisons among related groups, such as the 40 different volcanic centers in RU_CAGeochem. An intricate plot can be devised and then examined, volcano by volcano, just by changing the name in the Include listbox. Modern laptops don't seem to be limited by memory at least for the sizes of reasonable geochemical data sets. The single file approach is much easier to maintain and speeds up many types of comparisons among different data dimensions.

User interface

Igpets's interface evolved to display the user's data as easily as possible to encourage exploration of the data. The interface prevents most invalid choices. As *Igpets* opens, the only active control is the File menu. As soon as the user selects a file, many other menu items and control buttons activate. The Plot menu is likely the user's next choice. XY plots are the most common type in igneous petrology. Assuming XY is selected, a Variable window presents buttons from which to select an X variable and then a Y variable, and so only two clicks are needed. As soon as Y is selected the plot is made. The scaling of the plot is automatic to allow rapid turnover of plots, for quick views of "what if" scenarios. The automatic scaling is a hazard if samples are all very similar. In that case a small range in X or Y will fill the screen and primarily reveal the random noise inherent in geochemical analysis. This is a real weakness, but one that is overcome with experience. Through trial and error, all of the plot routines were optimized for minimum input with the goal of creating rapid response from just a mouse click or two. These rather trivial design choices make exploration easier and lead to a wider breadth of exploration.

The parameters for more than 200 commonly used diagrams are available in *Igpets* as text files. The equations for the axes or ternary end-members are stored as text statements

(e.g. K₂O + Na₂O) that are solved with a recursive equation parser. These diagrams greatly facilitate the preliminary evaluation of a rock suite by rapidly making the necessary evaluations of rock nomenclature and tectonic setting.

Igpets provides multiple methods for identifying each sample. For a small data set a Name button writes the sample name adjacent to each sample. For large datasets an Identify button can be turned on or off. When on, a click on the diagram will cause the nearest sample to be highlighted and named. If one seeks a particular sample, there is a Pick button that brings up a list box holding all the sample names to pick from. The strong emphasis on identifying particular samples had two origins: the first is a preference for subdividing data into meaningful groups rather than assuming all data are from a single magmatic unit. The three different symbol codes (kcode, jcode, lcode) allow coarse, medium and fine-grained subdivisions of the data and near immediate switching between these options. This is useful because what might seem like a clear geochemical discrimination of groups in one plane may fail completely when looking at the data in a different dimension. The second motivation for identifying particular samples is the need to identify end-members for geochemical modeling. All these possibilities make *Igpets* easy to use and allow customizing the datafile before attempting modeling.

Modeling algorithms

Albarede (1995) comprehensively compiled and clearly derived many models of melting and crystallization. DePaolo (1981) derived equations for coupled assimilation and fractional crystallization (AFC) and Langmuir et al. (1977) derived the equation for magma mixing. Converting these equations to algorithms allowed the multi-element forward modeling in *Igpets*. The models are accessed in spider plots with a button labeled, Model. After choosing a model from one of choices in Table 2, a window opens (SpiMod) for selecting the parameters needed for the model chosen. For most models a partition coefficient file is needed. *Igpets* includes files for several published compilations of partition coefficients. These files can be easily modified by the user. All the elements in the partition coefficient file selected will be modeled even if they are not displayed in the spider-diagram. If partition coefficients are not needed (e.g. mixing) the elements modeled are those in the spider-diagram.

Sources can be designed by mixing components in a window (SpiMix) opened by the Mix button. Up to five components can be mixed and each element in the data file is included. For example, equation 15b from DePaolo (1981) allows calculation of the isotopic ratios of the mix. This allows a specific mantle to be calculated by adding end-member mantle components, e.g. 95 DM (depleted mantle) and 5 EMI (enriched mantle I).

Table 2 Models available in Spider plots

Model	Equation coded from
batch melting	Albarede (1995)
fractional melting	“
aggregated fractional melt melting	“
continuous melting	“
rayleigh fractional crystallization	“
equilibrium crystallization	“
AFC	DePaolo (1981)
Mixing	Albarede (1995)
Recharge	“
REE inverse model-C ₀ D ₀ P ₁	Feigenson et al. (2003)

Examples of multi-element models

Multi-element fractional crystallization modeling at Klyuchevskoy, Kamchatka

Modeling fractional crystallization requires samples representing parental magma and several derivative magmas, as well as observed mineralogy and appropriate partition coefficients. *Igpet* can model steps along the magma evolution pathway but does not allow for continuous changes in

cumulate mineralogy or partition coefficients. Nevertheless, satisfactory models are often possible because of the relative simplicity of the system. At Klyuchevskoy volcano MgO-rich lavas with primarily clinopyroxene phenocrysts evolve via decompression-crystallization during ascent to the surface (Ozerov et al. 1997; Almeev et al. 2013). Consistent with this model, the mafic lavas from Almeev et al. (2013) are bracketed by four fractional crystallization models based on one cumulate of 100 % clinopyroxene and another with 10 % olivine and 90 % clinopyroxene (Fig. 1). The two most mafic samples are the starting compositions and the partition coefficients are from Laubier et al. (2014). With the exception of Sc, all eighteen of the elements and oxides with partition coefficients are reasonably fit by fractional crystallization. The models seek to match the lower bound of the data arrays, which are generally concave upward as shown by the Nb and Ce diagrams in Fig. 1. Mixing is indicated for some samples that plot above the main data array, as is indicated in the MgO versus K₂O diagram. *Igpet* models all the elements simultaneously and then allows rapid evaluation by just changing the element chosen for the Y parameter. The results obtained with *Igpet* using trace elements can be explored further by the *MELTS* family of algorithms (e.g., Ghiorso et al. 2002) or *Petrolog3* (Danyushevsky and Plechov 2011) in search for internal consistency with the major element data.

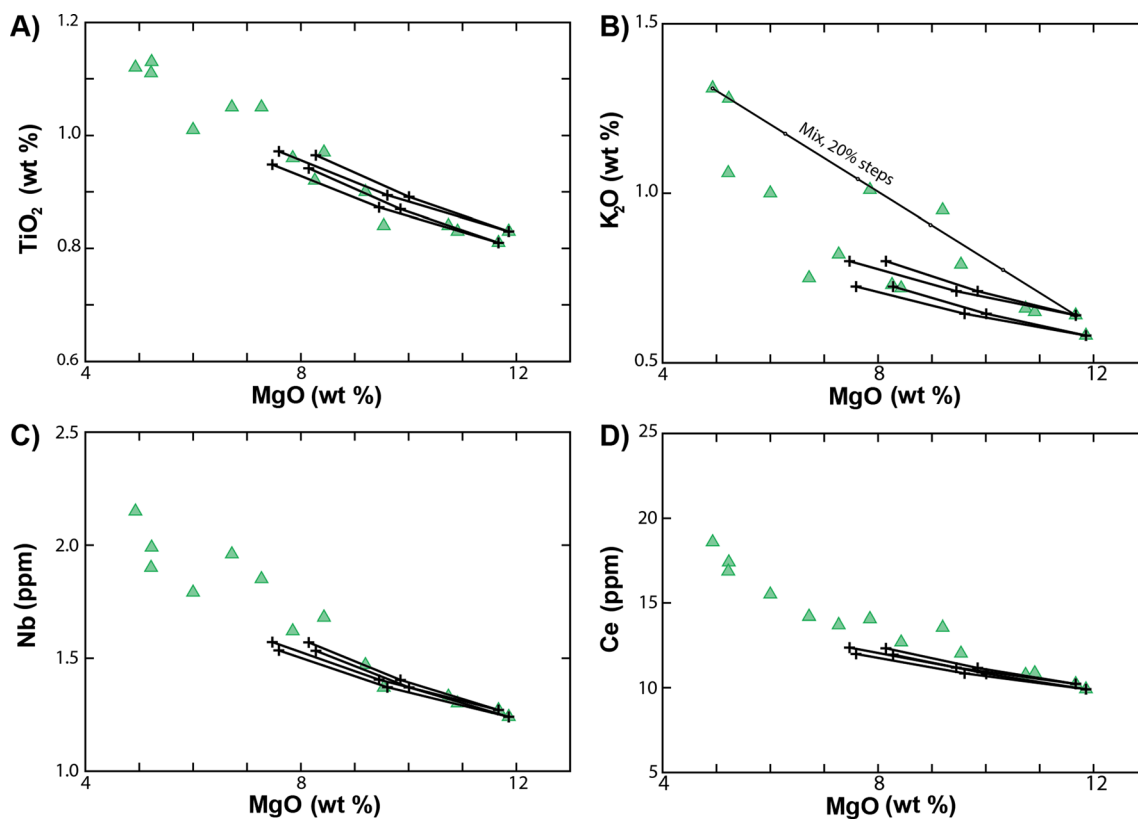


Fig. 1 Four fractional crystallization models for Klyuchevskoy mafic lavas. The two most mafic samples are parents. The two cumulate assemblages are 100 % olivine, which extends to the lowest MgO contents, and 90 % olivine and 10 % clinopyroxene

A subduction-modified mantle for explaining lavas from Cerro Negro, Nicaragua

One of the most complex problems in igneous geochemistry is determining the origin of magmas at convergent margins where fluids extracted from the subducting plate trigger melting in the mantle wedge. Potential subducting sources include; sediment, altered oceanic crust and serpentinized mantle. The upper plate provides a variable crustal column above an asthenospheric wedge of depleted mantle with possible veins of enriched mantle (Feigenson and Carr 1986; Gazel et al. 2011). In Central America the sediment on the subducting Cocos Ridge is not scraped off and consists of a lower carbonate section and an upper hemipelagic section, whose trace chemistry has a pattern of enrichments and depletions very similar to the lavas at the volcanic front (Patino et al. 2000). However, very little of the Sr in this sediment can be incorporated in the modified mantle because its Sr isotopic ratio, about 0.7080, is much higher than that of the lavas, about 0.7040. Nevertheless, Sr is strongly enriched compared to elements with similar incompatibility in mantle minerals such as Pr and Nd. Thus, a simple model of fluid from subducted sediment infiltrating and triggering melting in depleted mantle cannot satisfy the combined constraints of Sr composition and Sr isotopic ratio. Additional sources with abundant non-radiogenic Sr isotopic ratios are needed.

The components comprising the modified mantle cannot be directly sampled but local analogs can be. The sediment components (Sed) were characterized from drill core at DSDP (Deep Sea Drilling Project) Site 495 adjacent to the trench (Patino et al. 2000). A depleted mantle (DM) was derived from a sample of a basaltic seamount entering the trench offshore Nicaragua (Sadofsky et al. 2009). Altered oceanic crust (AOC) was obtained as the mean of three perturbed basaltic samples from ODP (Ocean Drilling Project) Site 1256 (Sadofsky et al. 2009). Ranero et al. (2003) found evidence of serpentinization of the Cocos Plate lithosphere entering the trench offshore Nicaragua. This mantle (Serp) is assumed the same as the DM mantle but hydrated.

Depleted mantle (DM) and Sed1, a 20 % melt of a 70 % hemipelagic and 30 % carbonate mixture, were estimated by Gazel et al. (2009). Our f_{Sed} is a 5 % melt, rather than 20 %. A 5 % melt of the altered basalts of ODP 1256 with a mineralogy of 49 % garnet, 49 % clinopyroxene, 1.5 % rutile and 0.5 % phengite yields f_{AOC} . Partition coefficients are from the eclogite compilation of Kelemen et al. (2003) and Kessel et al. (2005). A 5 % melt of DM mantle using a mineralogy of 2 % garnet, 35 % clinopyroxene, 0.1 % rutile and 62.9 % olivine yields f_{Serp} . Preliminary examination of isotopic constraints, using the binary mix tool (Fig. 2a), indicates that only about 0.1 % f_{Sed} can be added to DM to fit the isotopic range of western Nicaragua samples. Considerably more f_{Sed} can be added with f_{AOC} , up to a few percent. The

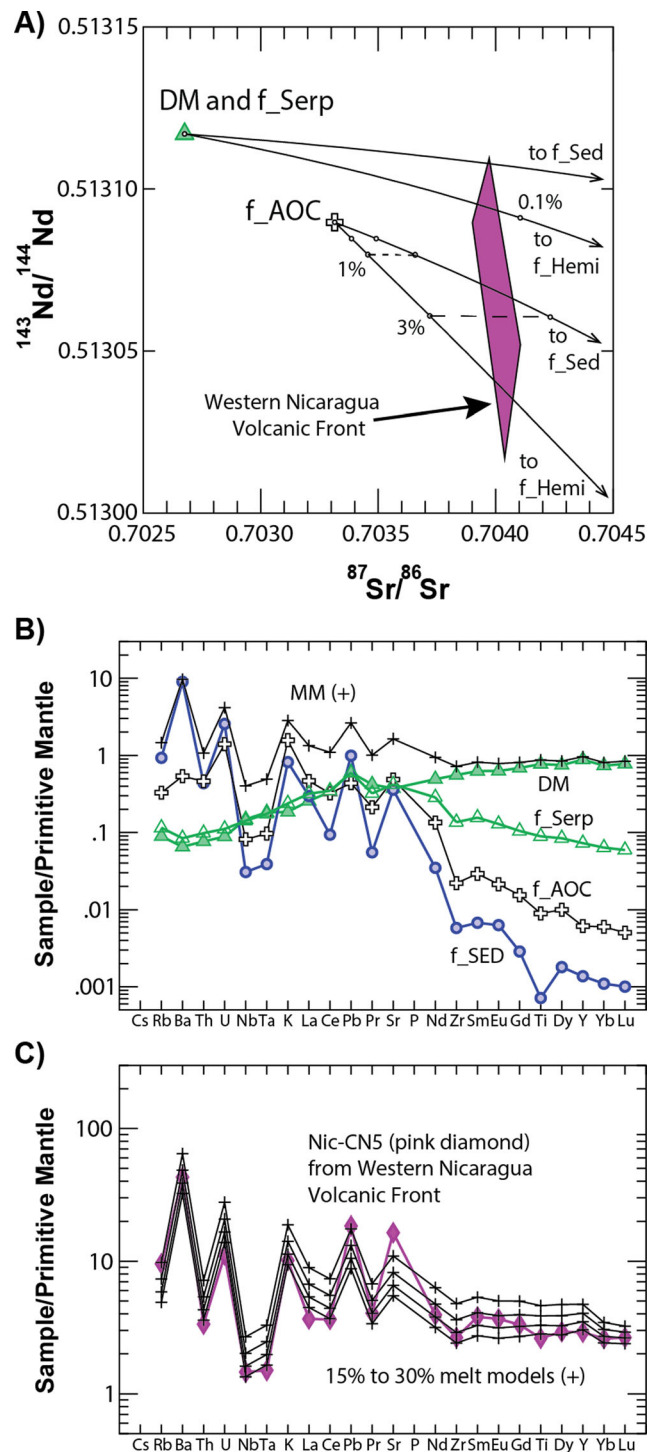


Fig. 2 Modeling Cerro Negro magmas using a modified mantle derived from local sources

lower end of the western Nicaragua array is bracketed by including a mix of f_{AOC} and a melt of just the hemipelagic component of the sediment, f_{Hemi} (Fig. 2a).

Modified mantle (MM) in Fig. 2b) is a mix of 92.9 % DM, 6 % f_{Serp} , 1 % f_{AOC} and 0.1 % f_{Sed} . This mixture results in Sr and Nd isotopes within the narrow range of lavas in

western Nicaragua. The components in Fig. 2b are weighted by their proportions in the mix. This allows examination of which components contribute most to particular elements. The salient features of MM are: the middle to heavy rare earth elements are dominated by DM. Ba is overwhelmingly from Sed, U and Pb are controlled by Sed, K is primarily from AOC, Th comes equally from Sed and AOC and Sr is primarily from AOC but includes significant amounts of all four sources.

Figure 2c has 15, 20, 25 and 30 % melts of MM using aggregated fractional melting and a mantle mode of 60 % olivine, 25 % orthopyroxene, 12 % clinopyroxene, 2 % spinel and 1 % garnet. The models reproduce the overall shape of the Cerro Negro trace element geochemistry but the sizes of the positive spikes are imperfect, especially for Sr. The lack of agreement is not surprising given the wide ranges of possible variations in sources, partition coefficients, relative proportions of components and possible components and processes not included. Many similar fits are possible through variations in the proportions of source components, the degrees of melting, the choices of partition coefficients and so forth. All approaches yield low Sr contents like those in Fig. 2c which suggests the need for a further source of non-radiogenic Sr which would boost the Sr content without excessively perturbing the isotopic fit. Melt-rock reaction as the melt penetrates the lid of DM above the melt source, as envisioned by Kelemen et al. (2003), is one possible way to accomplish this.

The Arc Basalt System (ABS) of Kimura et al. (2009) is a sophisticated forward modeling spreadsheet that supports slab dehydration based on metamorphic phase equilibria using P-T paths estimated for the global set of arcs. Flux induced melting in the mantle wedge is similarly sophisticated and variable. Furthermore, a Monte Carlo engine allows random search through specified limits of numerous petrologic and tectonic input parameters. Hundreds of successful models for Cerro Negro are easily obtained with ABS (Feigenson et al. 2012), where ‘successful’ refers to user specified ranges for the modeled trace elements and isotopic ratios. The ABS models were based on the same sources as those used in Fig. 2b and care was taken to accept only models within an isotopic range similar to the field in Fig. 2a. Although ABS has greater flexibility and sophistication, all successful models had Sr contents lower than the Cerro Negro lavas. Thus, ABS reveals the same problem in fitting both Sr content and Sr isotopic ratios. The differences between ABS and *Igpet* are that ABS uses more sophisticated modeling but provides results whose path through the system is very difficult to trace. *Igpet* is much simpler and the user is in full control because there is a sequence of discrete steps. *Igpet* is an excellent method for learning about magma generation and, since it provides a result consistent with ABS, it provides confidence in the ABS results.

Additional examples in downloadable workbook

A workbook with 12 problems aimed at undergraduates and first-year graduate students is also available. It begins with a CIPW norm exercise and includes a least squares petrologic mixing problem. These exercises use utility programs, *CIPW* and *Mixing*, which are included with *Igpet*. Other problems involve nomenclature and tectonic association, introductions to CaO-MgO-Al₂O₃-SiO₂ (CMAS) projections, fractional crystallization, AFC calculations, partition coefficient variations, magma mixing in ratio/ratio plots and simple melt modeling. Real world complexity is stressed in problems involving Telica volcano in Nicaragua and the origin of temporal variations in Pleistocene maar deposits at Lake Purrumbete in southeastern Australia (Jordan et al. 2015).

Concluding remarks

Igpet provides petrologists and geochemists with a useful toolkit. The rock identification and tectonic discrimination diagrams are typically parts of undergraduate and MS theses. Forward modeling designed around spider-diagrams is an efficient way to explore magma evolution models. Multi-element mixing and modeling algorithms provide rapid methods for assessing the sources and processes that may be contributing to the magma evolution found in an igneous rock suite.

The models in *Igpet* are useful for calculating magma evolution paths. A typical approach is to first create a composite source by using the SpiMix window to make blends of possible components. Isotopic plots can then identify the range of mixes that match a rock suite’s isotopic data (e.g. Figure 2a). An isotopically satisfactory source composition can then be turned into a series of model melts by making several choices in the SpiMod window: e.g. the melt model, a partition coefficient file, the mantle and melt modes, the degrees of melting. AFC models can further trace magmatic evolution assuming a reasonable contaminant is identified and a partition coefficient file suitable for the P and T conditions where assimilation and fractional crystallization take place.

In our research groups the search for successful forward models was extensive because many different assumptions were tested. Our experience is that the speed provided by *Igpet* leads to a thorough search for possible solutions. Because the modeling is fast and efficient, a fair solution did not stop the modeling process but instead reinvigorated the search for very good solutions and provided impetus for alternative modeling procedures in the search for internal consistency.

MacIntosh or Windows versions of *t-Igpet* software and associated files can be downloaded from: <https://sites.google.com/site/tsigpetteaching/>. Data discussed in the

examples are found within the data folder of the *Igpets* packages.

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