

Preface

*Because I have known the torment of thirst,
I would build a well where others may drink.*

—Ernest Thompson Seton

The goal of generations of igneous geochemists is to use mineralogical and chemical laws in an attempt to explain the geological processes they are investigating. This scientific approach is both simple and rigorous. Initially it consists of highlighting magmatic differentiation trends and determining the possible underlying petrogenetic mechanism(s). Then, the major elements are used to establish the nature and the modal composition of the fractionating mineral assemblage responsible for the differentiation trends; its temporal evolution is also addressed. Finally all these data are fed into models calculating the behaviour of trace elements (and possibly isotopes), in order to account for the chemistry of the investigated igneous rocks and evolution of the parental magma.

Such methodology is very powerful; not only because it is consistent with field geological data but also it is based on several independent methods. Indeed, major elements, trace elements and isotopes are governed by different principles. Thus any model predicting the coherent behaviour of these three independent parts of the dataset would possess a high internal consistency, making the modelled scenario robust.

Everyone, needing to interpret whole-rock geochemical data from igneous rocks, faces the same problem. Regardless of whether he/she has to calculate some simple indexes, more complex norms, plot a diagram for a paper or model effects of some petrogenetic process, he will end up using a computer. He would be certainly delighted to find that several programs exist designed specifically for this purpose. At first glance, most look useful with a plethora of built-in functions, but after a second look, he realizes that they are essentially black boxes, in which he soon loses track of exactly what is happening with his precious data. Worse still, there could be something missing or not quite appropriate to the required task. The code is difficult or impossible to alter (many geochemical programs are commercial). And even when the required diagram is plotted correctly, it may need to be altered extensively before reaching publication quality.

Indeed, graphical and numerical methods remain the alpha and omega of modern igneous geochemistry. The problem is how to implement the necessary diagrams or formulae so that the code can be understood and used by an ordinary

geochemist. We strongly believe that this knowledge can be mediated in the form of simple numerical recipes in a high-level programming language that includes built-in mathematical and statistical functionality, matrix manipulation tools and be capable of generating publication-quality graphics. There are currently available several potentially suitable environments, but only one of them—the R language (www.r-project.org)—has the advantage of being freely available for all the main platforms (MS Windows, Mac OS and various dialects of Linux). Moreover, there already exists an R package *GCDkit* (www.gcdkit.org)¹, containing most of the required geochemical calculation procedures and graphics. Furthermore, the underlying code can be easily viewed, modified or extended.

In the realm of geochemical modelling, there does not exist any prescribed scenario. In fact, the modelling strategy not only depends on the geological problem, but also on the nature of the available data: hence the approach must be adapted and optimized to each individual case. The purpose of this book is to show, using many concrete examples, how a researcher can proceed in developing a realistic model tailored to his questions. It is in this investigative adventure that the authors of this book invite you. Let's embark on a scientific journey in the intimacy of petrogenetic modelling!

Book structure—how to read?

This textbook gives a detailed overview of modelling approaches to petrogenesis of igneous rocks using whole-rock geochemical data. The theoretical chapters are followed by their implementation using R/*GCDkit*, and by numerous exercises, mostly based on real-life problems.

The text is divided into six parts, and three appendices. **Part I** gives a short but comprehensive introduction to R (with, or without *GCDkit*), the implementation of simple geochemical computations, calculation of norms, statistical evaluation of complex data sets, and plotting the most common diagrams. In all cases, the geological and geochemical backgrounds are briefly discussed. Moreover, a refresher on radiogenic isotope data interpretation is presented. For newbies, the fundamentals and syntax of the R language are explained in **Appendix A**, and an introduction to the *GCDkit* system is given in **Appendix B**.

The core of the book (**parts II–IV**) is dedicated to modelling of the main processes in igneous petrogenesis using various types of geochemical data. These include major elements (treated by the concept of mass balance), trace elements (modelling based on solid/liquid partitioning or saturation concepts) and radiogenic isotopic data (either constraining open-system processes such as mixing and assimilation or giving direct information on the source). The principles of forward and reverse numerical techniques are presented and explained, as is the underlying mathematical apparatus; the R code necessary for their implementation is also given. The specific problem of solving sets of linear algebraic equations is outlined in **Appendix C**.

¹ Natively for Windows, but can be run on other platforms with a suitable emulator environment.

Part V provides a practical guide on how to formulate and run a sensible petrogenetic model simulating natural systems. It stresses the fundamental significance of additional information coming, e.g., from field relations, petrology or physics. Above all, the importance of critical thinking is underlined.

The text is supplemented by numerous solved **exercises**. It is crowned by two worked **real-world problems (Part VI)** that illustrate the complex approach to petrogenetic modelling based on the techniques described in this book.

On the other hand, intentionally omitted are most of the more sophisticated statistical methods as these have been dealt with by other, more competent authors. This is also the case for detailed mathematical derivations of laws governing geochemical variations in complex petrogenetic scenarios.

The book is intended for senior undergraduate and postgraduate courses, as well as all potential users of *R/GCDkit* interested in the implementation of graphical, statistical and numerical methods. The prerequisite is a sound knowledge of secondary school maths as well as of basic principles of solid-rock geochemistry.

Electronic supplementary material

Errata, code to the exercises and data sets from this book are available on: <http://book.gcdkit.org>. Moreover, this web site also contains the scripts used to produce many of the figures. However, in the latter case the code is not always simple and easy to comprehend by a beginner. It is supplied purely for the sake of curiosity, and in order to stimulate the interested reader. They are unlikely to work without at least some adaptations. If reading an electronic version of this book, the exercises, dataset icons and relevant figures are clickable.



Most of the exercises in this book are designed to run in an interactive mode. To adopt them for batch use, the contents of any variable should be displayed using the functions `print` or `cat` (see Appendix A, Sect. 3.1).

The code supplied, obviously, will run only if the current R directory is that in which the data file(s) reside. The best is probably to save all the needed files in a directory of your choice and, before starting, set the working directory either from the GUI (*File|Change dir...*), or with a command such as:

```
GCDkit->Rbook.dir<-"C:/user/my_name/Documents/Rbook"2
GCDkit->setwd(Rbook.dir)
```



This text is based on version 2.13 of R for Windows, 4.0 of *GCDkit*. It concentrates on MS Windows implementation of the R language. Plain R will run on other systems, including Linux and Mac OS, but the current *GCDkit* will require a suitable emulation environment, e.g. Wine on Linux. The code, relying on *GCDkit* functions, will be displayed with the namesake prompt, `GCDkit->`.

² Backslash is an escape character in R, so it would need to be preceded by another one, i.e.:

```
"C:\\user\\my_name\\Documents\\Rbook".
```

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Geochemical Modelling of Igneous Processes –

Principles And Recipes in R Language

Bringing the Power of R to a Geochemical Community

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