Springer Geochemistry

More information about this series at http://www.springer.com/series/13486

Vojtěch Janoušek · Jean-François Moyen
Hervé Martin · Vojtěch Erban
Colin Farrow

Geochemical Modelling of Igneous Processes – Principles And Recipes in R Language

Bringing the Power of R to a Geochemical Community

Springer

Vojtěch Janoušek
Czech Geological Survey
Prague
Czech Republic

Vojtěch Erban
Czech Geological Survey
Prague
Czech Republic

Jean-François Moyen
Université Jean-Monnet
Saint-Etienne
France

Colin Farrow
Glasgow
Scotland

Hervé Martin
Université Blaise-Pascal
Clermont-Ferrand
France

Springer Geochemistry
ISBN 978-3-662-46791-6 ISBN 978-3-662-46792-3 (eBook)
DOI 10.1007/978-3-662-46792-3

Library of Congress Control Number: 2015937379

Springer Heidelberg New York Dordrecht London

Printed on acid-free paper

Springer-Verlag GmbH Berlin Heidelberg is part of Springer Science+Business Media (www.springer.com)

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"`.

Acknowledgements

We would like to thank several people without whom this book would have hardly originated. First of all Robert Gentleman and Ross Ihaka, as well as members of the R Development Core Group, for their ideas and sterling efforts in developing the R language. In particular, Friedrich Leisch (Technische Universität, Vienna) provided valuable consultations on the development of R packages.

This book builds on hand-outs used for workshops given in Prague and Helsinki (2011), Stellenbosch, South Africa (2012) and Hyderabad, India (2013) by VJ and JFM. The authors are indebted to many people without whom these events would not materialize, especially Tapani Ramö (Helsinki), Gary Stevens (Stellenbosch) and Santosh Kumar (Nainital, India). VJ is grateful to Graeme Rogers, once supervisor of his PhD. thesis, who has taught him to ask the basic petrogenetic questions, *why and how much*, Francis Albarède for his excellent book and a motivating course of geochemical modelling and Milan Novák (Brno, Czech Republic) with František V. Holub (Prague), who requested, in 2000, a practical course on interpretation of geochemical data in R that is running ever since.

GCDkit originated during a post-doctoral stay of VJ at University of Salzburg (FWF Project 15133–GEO to F. Finger). The work was, over the years, supported by several projects from the Czech Grant Agency (GAČR), Czech Geological Survey (3314, 336200) and Ministry of Education of the Czech Republic (LK11202 to K. Schulmann). The scientific exchanges were facilitated by the French–Czech programme Mobility 7AMB13FR026.

Régis Doucelance (Clermont-Ferrand, France) brought to our attention a great reverse mixing hyperbola example from Martinique, and other papers on mantle geochemistry that escaped our attention. Nice photos were contributed by Gerhard Wörner (Göttingen, Germany), Christian Nicollet (Clermont-Ferrand), Ewa Słaby (Warsaw, Poland) and S. Hidalgo (Quito, Ecuador). Didier Laporte (Clermont-Ferrand) supplied an original version of his figure on wetting angles (Fig. 24.1). Leon Bagas (Crawley, Australia) provided dataset for the anomaly plot.

Oscar Laurent (Liège, Belgium) and Arnaud Villaros (Orléans, France)—in addition to always being pleasant company—are responsible for many good ideas and suggestions, which eventually helped to develop the existing code. We are also grateful to the many students and *GCDkit* users, whose requests, in the course of time, led to more software development, clever ideas and debugging.

We are thankful to people from Springer, Annett Buettner, Ulrike Stricker and Chris Bendall, for their hard work and patience with which they have guided us through the dire straits of preparing and publishing this monograph. The Czech brewing industry was a source of inspiration during late-night coding sessions.

In Prague, St. Etienne, Clermont-Ferrand and Glasgow, Christmas 2014

Vojtěch Janoušek *(vojtech.janousek@geology.cz)*
Jean-Francoiş Moyen *(jean.francois.moyen@univ-st-etienne.fr)*
Hervé Martin *(h.martin@opgc.univ-bpclermont.fr)*
Vojtěch Erban *(vojtech.erban@geology.cz)*
Colin Farrow *(colinfarrow537@gmail.com)*

Typographic Conventions

Most important are the warning boxes indicating potential pitfalls:

'Warning'

Pointers and additional information opening new prospects (not dealt with in this text) are labelled as:

'Next step'

The *GCDkit* implementation of the given problem is outlined in:

'*GCDkit* box'

The text is supplemented by a large number of solved exercises, graphically introduced like this:

Exercise 1.2: Fractional crystallization

An associated data file is marked by  , and the beginning of a solution to the exercise by  .

In the main text, **R code and its output** are set in a non-proportional font, the latter additionally in italics. Plain R code has a simple prompt, the *GCDkit*-specific one is marked as such:

```
> summary(x[,"Sr"])
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.    NA's
  278.0   392.5   430.0   443.0   537.5   599.0     2.0

GCDkit-> loadData("sazava.data")
GCDkit-> results <- CIPW(WR)
```

Broken, continuing lines of code have a plus sign as a prompt and are indented:

```
GCDkit-> plot(WR[,"SiO2"),
+             pch="*",col="khaki")
```

In Part VI and Appendix A, commented chunks of R code, often just outlined and not complete, are displayed as "code boxes":

We create Harker plots (Fig. 25.3) using *Plot|Multiple plots…*, i.e. the command:

```
GCDkit-> multiple("SiO2","Al2O3,Fe2O3,MgO,CaO,Na2O,K2O")
```

Names for R objects and file names, occurring in the text, are also set in a non-proportional font:
… factor `silica` from the previous exercise …

Comments in the code start with the hash mark ("#"):

```
# Fig. 4.2.1
```

Names of mathematical variables and **Menu items** are type set in italics, e.g. *Misc|Stop current computation*, indicating an item '*Stop current computation*' of the '*Misc*' menu.

Equations in the text are numbered sequentially, starting with the chapter number:

$$C_L = \frac{C_0}{D + F(1-D)} \tag{5.1}$$

The same applies to figures, tables, or exercises. Otherwise, the first number of figures or tables is that of the relevant Appendix; the second refers to a sequence there in (Fig. A1.2; Table A3.5).

Matrices are named with a bold italics letter topped by a double bar. When presented in full, they are enclosed in brackets:

$$\overline{\overline{\boldsymbol{C}}} = \begin{pmatrix} C_{Pl}^{SiO_2} & C_{Opx}^{SiO_2} & \cdots & C_{n}^{SiO_2} \\ C_{Pl}^{TiO_2} & C_{Opx}^{TiO_2} & \cdots & C_{n}^{TiO_2} \\ \vdots & \vdots & \ddots & \vdots \\ C_{Pl}^{P_2O_5} & C_{Opx}^{P_2O_5} & \cdots & C_{n}^{P_2O_5} \end{pmatrix}$$

Vectors are written in a similar way, but their symbol has a single arrow:

$$\overrightarrow{\boldsymbol{m}} = \begin{pmatrix} m_{Pl} \\ m_{Opx} \\ \vdots \\ m_{n} \end{pmatrix}$$

Equation systems are linked together by a single curly brace to their left:

$$\begin{cases} C_S^{SiO_2} = \sum_{i=1}^{n} (m_i C_i^{SiO_2}) \\ C_S^{TiO_2} = \sum_{i=1}^{n} (m_i C_i^{TiO_2}) \\ \cdots \\ C_S^{P_2O_5} = \sum_{i=1}^{n} (m_i C_i^{P_2O_5}) \end{cases}$$

Variables and Symbols

This book uses, as much as possible, a consistent set of symbols to represent variables of geochemical interest both in the text and in the accompanying R code. The following is a summary of the main symbols used. Often, a series of similar variables exists for a range of elements, minerals or portions of a system: this is indicated by subscripts and superscripts.

General

Symbol	Meaning and definition	R symbol
W	Mass (weight) of a whole system, or a portion thereof (indicated by subscript, see separate table below)	*Not used*[3]
w^{α}	The mass of an element α in a portion of the system (see subscript)	*Not used*
F	Melt fraction: $F = W_L / W_0$	`ff`
F_C	Degree of crystallization: $F_C = 1 - F = W_S / W_0$	`fc`
C, C^{α}	Concentration of element α in a system or portion thereof (subscript): $C^{\alpha} = w^{\alpha} / W$	`c0`, `cs`, `cl`…
c_i^{α}	Concentration of element α in mineral i	`mins`
T	Temperature, normally in K but some equations use °C	`tt`

[3] Some equations discussed in the text are not implemented in the R code.

Mineral proportions in various portions of a system (always summing up to 1)

Symbol	Meaning and definition	R symbol
m_i	… in the whole solid (cumulate or restite)	`m`
q_i	… in the peritectic assemblage	*Not used*
p_i	… in the reactants (non-modal melting)	*Not used*
$m_{0,i}$	… in the original solid (non-modal melting)	*Not used*

Mixing

Symbol	Meaning and definition	R symbol
$f_1, f_2 ... f_m$	Fraction of end-members 1, 2, …m involved in mixing	`f1`, `f2`.. or `f[1]`, `f[2]`…
a, b, u, v	Various elements for which mixing is modelled (Sect. 11.3)	*Not used*
A, B, C, D	Parameters of a mixing hyperbola (Sect. 11.3)	`AA`, `BB`, `CC`, `DD`

Element partitioning

Symbol	Meaning and definition	R symbol
$K_{D\alpha}^{min/L}$	Partition coefficient of element α between mineral (min) *i* and liquid: $K_{D\alpha}^{min/L} = \frac{c_{min}^{\alpha}}{C_L^{\alpha}}$ Often just K_D in text, when its meaning (element/mineral) is clear from the context	`kd`, or commonly `kd[j,i]` or `kd[elt,min]` assuming `elt` and `min` have been defined before…
D_α	Bulk distribution (solid/liquid) of element α $D_\alpha = \frac{C_S^{\alpha}}{C_L^{\alpha}} = \sum_i^n m_i K_{D\alpha}^{i/L}$ Often just *D* in text when the meaning is unambiguous	`dd` `dd[elt]` `dd[j]`
$D_{0\alpha}$	"Bulk distribution coefficient" for the initial melting assemblage (non-modal melting): $D_{0\alpha} = \sum_{i=1}^{n} m_{0i} K_{D\alpha}^{i/L}$ (or just D_0 when unambiguous)	*Not used*
$D_{P\alpha}$	"Bulk distribution coefficient" for the reactants (non-modal melting): $D_{P\alpha} = \sum_{i=1}^{n} p_i K_{D\alpha}^{i/L}$ (or just D_P when unambiguous)	*Not used*

AFC

Symbol	Meaning and definition	R symbol
$\dot{W}_A$	Rate of assimilation	*Not used*
$\dot{W}_C$	Rate of fractional crystallization	*Not used*
r	Rate of assimilation to fractionation: $r = \frac{\dot{W}_A}{\dot{W}_C}$	`r`
r_C	Critical value of r for AFC, above which assimilation is dominant	`rc`
z	Convenience parameter: $z = \frac{r + D - 1}{r - 1}$	`z`
S	Slope of a mixing array in a diagram $1/c$ vs. I employed in reverse AFC modelling	*Not used*
C_0, I_0	Element concentration and isotopic ratio in pristine melt	`c0, i0`
C_A, I_A	Element concentration and isotopic ratio in assimilant	`ca, ia`
C_L, I_L	Element concentration and isotopic ratio in liquid	*Not used*

Radiogenic isotopes

Symbol	Meaning and definition	R symbol
Ab	Isotopic abundance, e.g. $Ab_{^{87}Rb}$	*Not used*
AW	Atomic weight, e.g., AW_{Rb}	*Not used*
I	Ratio of daughter and stable, unradiogenic isotopes of the same element (e.g., $^{87}Sr/^{86}Sr$, $^{143}Nd/^{144}Nd$), measured	`I`
I^X, I^Y	Two such isotopic ratios for two distinct isotopic systems, e.g., Sr and Nd	*Not used*
R	Ratio of parental isotope/stable, unradiogenic isotope of the daughter element (e.g., $^{87}Rb/^{86}Sr$, $^{147}Sm/^{144}Nd$)	`R`
λ	Decay constant	`lambda`
I_i I_1, I_2, I_M	Initial isotopic ratio (subscripts *1, 2, M* indicate isotopic ratios in mixing)	`i1, i2, im`
X, Y	Isotopic systems if two involved in plotting	e.g., `cx1, iy1`
b	Slope of an isochron	*Not used*
α	Parameter controlling the shape of a mixing hyperbola	`alpha`
q	Curvature of a mixing hyperbola	`q`
x_0, y_0	Asymptotes of a mixing hyperbola	`x0, y0`

Additional subscripts/superscripts for isotopic ratios

SA	Sample
DM	Depleted Mantle
CC	Average Crust
CHUR	Chondritic Uniform Reservoir
0	Present-day
i	Initial
t	At the time *t*

Parts of a system (subscript)

Subscript	Meaning	Process
0	Source	[zero] solid source in the case of melting, primitive magma for crystallization
L	Liquid	melt for melting or differentiated liquid for crystallization
L.inst	Instantaneous liquid	fractional melting
L.bulk	Bulk (aggregated) liquid	fractional melting
S	Solid	restite for melting, cumulate for crystallization
S.inst	Instantaneous solid	fractional crystallization
S.bulk	Bulk (aggregated) solid	fractional crystallization
M	Mixture	mixing
P	Reactants	non-modal melting
C	Crystallized phases	AFC
A	Assimilant	AFC
Q	Peritectic assemblage	Melting or crystallization (with slightly different meanings)

Additional sub- and superscripts

Object	**Symbol**	**Numbering**
Minerals	A, B…	*i = 1* to *n*
Chemical elements (components)	α, β…	*j = 1* to *p*
End-members in a mixing	1, 2…	*k = 1* to *m*
Step of a stepwise process	t	*Not used*

It is not always possible to use the same conventions for printed text and R variables. For instance, mixed case variables (both upper and lower case) are dangerous in R, because it is case sensitive. Therefore, we use lower case in (most) R variable names. Furthermore, many single-letter symbols are reserved words: for instance `c`, `D` and `t` refer to common R functions (see Appendix A), whereas `T` and `F` are shorthand notations for logical `TRUE` and `FALSE`. For this reason, the commonly used *F* (melt fraction) and *D* (bulk distribution coefficient) are represented by `ff` and `dd` in our R code. Note also that the suffix used to indicate the source/parental magma is the number 0, not the letter O!

List of Abbreviations

AFC	Assimilation and Fractional Crystallization
ASCII	American Standard Code for Information Interchange
BSE	Back-Scattered Electrons, Mad Cows Disease
CBPC	Central Bohemian Plutonic Complex
CHUR	Chondritic Uniform Reservoir
CL	Cathodoluminescence
DM	Depleted Mantle
ESC	Essential Structural Component
FAQ	Frequently Asked Questions
fO_2	oxygen fugacity
Ga	10^9 years
GUI	Graphical User Interface
HFSE	High-Field Strength Element(s)
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
INAA	Instrumental Neutron Activation Analysis
ICP-OES	Inductively Coupled Plasma Optical Emission Spectrometry
ka	10^3 years
LA ICP-MS	Laser-Ablation Inductively Coupled Plasma Mass Spectrometry
LILE	Large Ion Lithophile Element(s)
Ma	10^6 years
MORB	Mid-Ocean Ridge Basalt
MME	Mafic Microgranular Enclave
NB	Nota Bene
ppm	Parts Per Million
REE	Rare Earth Elements; LREE, MREE, HREE: light, medium, heavy REE
SIMS	Secondary Ion Mass Spectrometry
TIMS	Thermal Ionization Mass Spectrometry
TTG	Tonalite–Trondhjemite–Granodiorite association
XRF	X-Ray Fluorescence Spectrometry

Abbreviations of Mineral Names

Symbols for mineral names mostly follow Kretz (1983):

Ab	Albite
All	Allanite
Amp	Amphibole
An	Anorthite
Ap	Apatite
Bt	Biotite
Cpx	Clinopyroxene
Crd	Cordierite
Di	Diopside
En	Enstatite
Fo	Forsterite
Grt	Garnet
Hbl	Hornblende
Ilm	Ilmenite
Kfs	Potassium feldspar
Mnz	Monazite
Ms	Muscovite
Mt	Magnetite
Ol	Olivine
Opx	Orthopyroxene
Phl	Phlogopite
Pl	Plagioclase
Qtz	Quartz
Rt	Rutile
Sil	Sillimanite
Spl	Spinel
Zrn	Zircon

Reference

Kretz R (1983) Symbols for rock-forming minerals. Amer Miner 68:277-279.

Contents

Part II Modelling Major Elements

Part III Modelling Trace Elements

Part IV Radiogenic Isotopes

Part V Practical Modelling

Appendix A R Syntax in a Nutshell

Appendix B Introduction to *GCDkit*

Appendix C Solving Systems of Linear Algebraic Equations in R