# Part V Practical Modelling

In previous chapters, we have seen numerous formulae describing the compositional evolution of a magma undergoing different petrogenetic processes. From a purely mathematical point of view, these equations are relatively simple. However, in any igneous system, there are many unknowns, and several of them must be set or estimated using geological constraints before attempting to (numerically) solve the modelling equations.

It is important to bear in mind that a geochemical model can only test specific hypotheses—i.e., the geologist has to decide on the question to ask, while being aware that the only answer that the model can provide is "yes" (from a geochemical point of view, this mechanism can account for the observed data) or "no" (it is unable to reproduce the dataset). Modelling does not provide answers to "open" questions; thus we can ask, for instance:

- Is it possible to generate this dacite from that basalt, by fractional crystallization of a cumulate made up of amphibole and plagioclase? If so, what is the modal composition of that cumulate?
- Could this granite be derived by partial melting of that sediment? What was the maximum degree of melting allowed by such a source?
- Could assimilation of lower continental crust by ascending basalt yield an andesitic magma of the given composition?
- Could the compositional range observed in this igneous suite be the result of fractionation from a common parent?

Often, a negative answer is actually more useful, as it definitely rules out an assumption. In contrast, a positive answer just indicates that the proposed process is not impossible—it does not demonstrate that it actually happened!

Although there is no universal recipe, a set of tricks can be used. Frequently, there is no pure mathematical solution, and assumptions have to be made. These typically relate to the composition of the primitive magma, or the fractionating mineral phases. Often, a composite approach combining calculations and educated guesses must be employed. In general, the following steps will be implemented:

- After having demonstrated the existence of a differentiation series (e.g. plotting trends in binary plots), identify and further constrain the process(es) that could have shaped the composition of the suite. This can be done on the basis of:
  - Previous knowledge (literature), analogy with similar occurrences elsewhere, relevant experiments or personal experience.
  - Geological evidence in general, e.g. field relations or petrology.
  - Geochemical evidence, such as interpretation of variation diagrams or isotopic constraints. At this point, one may also apply semi-quantitative tests (e.g. mixing test, determination of compatibility of elements—Chap. 21) that would help in determining what processes were possible or not, and so start constraining them.
- Build a full model, which in turn implies:
  - Choose the process to be modelled: mixing, melting, crystallization…
  - Decide on key variants thereof: modal or non-modal, fractional or batch…
  - Set the key input parameters: composition of the primitive liquid, fractionating phases and their chemistry, partition coefficients…
  - Perform the actual calculations.
- Test the model, i.e. compare the computed result with real data (including all the other available information, such as that coming from geology and petrology). Most often, this leads to refining the existing model.
- Reiterate until the model fits the data satisfactorily.

As a word of caution, one cannot stress strongly enough that it is unsafe to rely on the purely mathematical "best fit". It is indeed possible that it does not make geological sense, whereas a slightly worse fit (from a numerical perspective) may be more realistic. For instance, modelling can predict the crystallization of an Ol + Qtz cumulate. Such a result is geologically meaningless. On the other hand, an Opx-bearing one is more plausible, even if the numerical fit is worse.