

## PETROMODELER (Petrological Modeler): a Microsoft® Excel® spreadsheet program for modelling melting, mixing, crystallization and assimilation processes in magmatic systems

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**Abstract:** PETROMODELER (Petrologic Modeler) is a Microsoft® Excel® spreadsheet program which numerically and graphically models magmatic processes including melting, crystallization, assimilation and mixing by using trace elements and isotopic ratios. Melting models include (a) batch, (b) dynamic (continuous) and (c) fractional melting for (1) instantaneous and (2) cumulate melts, (3) residual solid and (4) total residue. These models can also be used to treat modal and non-modal melting. Crystallization processes modelled in the program include: (1) perfect equilibrium and (2) perfect fractional crystallization (PEC and PFC), (3) equilibrium crystallization-imperfect fractional crystallization (EC-IFC), (4) zoned crystallization-imperfect fractional crystallization (ZC-IFC), and (5) combined assimilation and fractional crystallization (AFC). Mixing between two end-member compositions can also be modelled by the program. The main advantages of the program are that; (1) crystallization and mixing processes can be performed on a starting composition which may be chosen from; (a) any melting model result, or (b) any sample composition entered into the “samples” tables, (2) the results of any model can be exported as a graphic file (GIF) and as tables, (3) changes in any parameters are simultaneously updated onto all diagrams and tables. PETROMODELER also calculates other useful parameters, such as normative mineralogy, Mg#, Eu/Eu\*, εSr and εNd, σ(DM) (depleted mantle Nd model ages) of a given sample. Some classification diagrams for volcanic rocks are also included in the program. Conversion of element abundances on the basis of wt% and ppm can also be performed.

**Key Words:** Geochemical modelling, magmatic petrology, trace elements, melting, crystallization, magma mixing

### 1. Introduction

Geochemical compositions of magmatic rocks result from several petrological processes which are developed during: (1) primary processes, such as partial melting of the source rocks, (2) secondary processes, such as crystal separation, wall-rock assimilation, combined crystal separation and wall-rock assimilation, and mixing of two different magmas. These processes can be numerically modelled using major and trace element contents and isotopic ratios of magmatic rocks. Quantitative models for these processes have been formulated by several workers (see Schilling & Winchester 1967; Anderson & Greenland 1969; Shaw 1970; Langmuir *et al.* 1977; DePaolo 1981; McKenzie 1985; O'Hara 1993; Ozawa & Shimizu 1995; Shaw 2000; Ozawa 2001; Zou 1998, 2007; Nishimura 2009). Using these formulas generally requires fast computer systems as they are often complex and include many parameters. Several types of computer software have been employed in order to perform the numerical models of petrological processes (Keskin 2002, Petrelli *et al.* 2005; Ersoy & Helvacı 2010), but they largely deal with either certain melting processes or FC/AFC processes. Among the different computer

modelling approaches, spreadsheet programs have some advantages, as they are easier and faster to use during data conversion, storing, and evaluation.

In this study, I present a Microsoft® Excel® spreadsheet program that can be used for nearly all of the petrological processes outlined above, and includes trace and major elements and isotopes. The program has also some useful features, allowing the user to classify magmatic rocks and to quickly calculate useful parameters, such as normative mineralogical compositions.

### 2. Overview of magmatic processes

Magmatic rocks are formed through melting, crystallization, contamination and mixing processes over a range of depths in the asthenosphere and lithosphere. These different processes may develop in several ways, and may accompany one another. The term “melting” refers to melt production from a source rock due to increasing temperature, decreasing pressure, addition of volatile components, or by a combination of these processes. Melting of a source rock develops gradually (partial melting) and can be quantitatively indicated by

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the percentage melting. The chemical composition of the melt produced by partial melting is controlled by: (1) the chemical and (2) mineralogical composition of the source rock, and (3) the degree of partial melting. The partial melts may subsequently undergo crystallization processes in magma chambers emplaced at different lithospheric levels, as their temperature decreases. During the cooling of a magma body, some minerals begin to crystallize and may separate from the liquid body. This process also changes the initial major and trace element composition of the magma. Both melting and crystallization processes may be developed under equilibrium or disequilibrium conditions, depending on whether or not the liquid remains in connection with the solid phase. The crystallization processes may also be accompanied by wall-rock assimilation (contamination), giving rise to further changes in the magma composition. Furthermore, different magma bodies may mix to yield a new magma composition intermediate between two initial magmas. In this section, I briefly summarized the main magmatic processes that can be numerically modeled using the PETROMODELER program to describe trace element and isotope compositions.

**2.1. Melting processes**

There are three main models based on chemical equilibrium between the remaining solid (the restite) and melt that is produced: (a) batch melting, (b) fractional melting, and (c) dynamic melting (Figures 1 and 2). These processes can develop as open- or closed-systems, depending on whether or not material exchange occurs with the surrounding rocks. The reader is referred to Schilling & Winchester (1967), Shaw (1970), Langimur *et al.* (1977), McKenzie (1985), Ozawa & Shimizu (1995), Ozawa (2001) and Zou (1998, 2007) for further reading on dynamics and quantitative modelling of melting process. PETROMODELER numerically models trace

element compositions on the basis of their bulk partition coefficients and initial abundances; isotopic ratios are not changed during closed-system melting models. Differentiation of major elements by melting is not modelled by PETROMODELER.

**2.1.1. Batch (equilibrium) melting**

The batch melting (or equilibrium melting) model is the simplest process and assumes that the melt remains in chemical equilibrium with the solid during melting (Figure 1) (Schilling & Winchester 1967; Shaw 1970; Zou 1998). Any melting model (batch model and the others hereafter) may develop as “modal” or “non-modal”. During “modal melting”, the proportion of minerals that undergo melting is the same as that in the source. In “non-modal (eutectic) melting” models, the mineral proportions in the melt are different from that of the source as some minerals melt preferentially. Modal melting normally does not happen in nature.

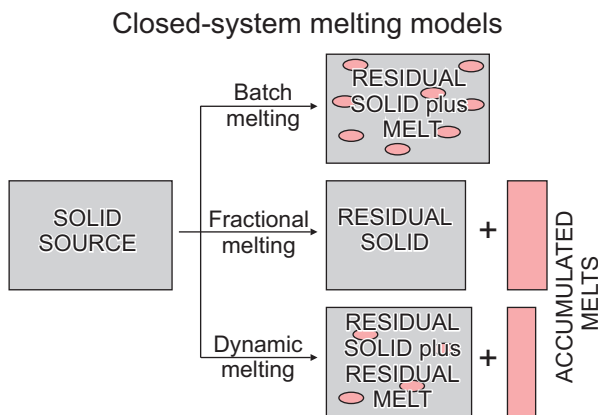
The trace element compositions of instantaneous (or accumulated) melt ( $C_I^m$  or  $C_L^m$ , respectively) produced by modal batch melting are given by;

$$C_I^m = C_L^m = \frac{C_0^m}{D_0 + F(1 - D_0)} \tag{1}$$

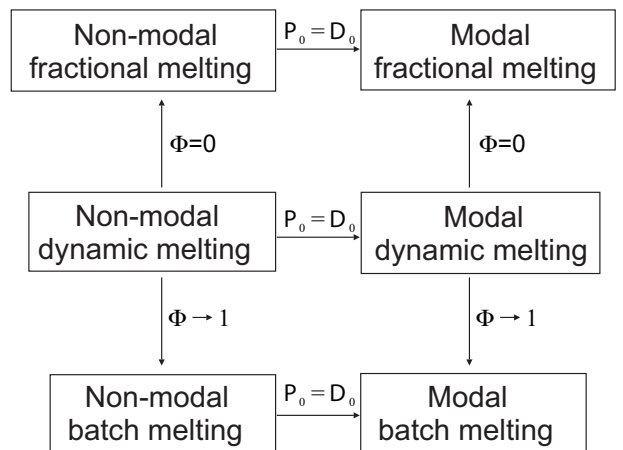
where,  $C_0^m$  is the concentration of the trace element in the source rock (starting composition),  $D_0$  is the bulk partition coefficient of the trace element,  $F$  is the fraction of liquid produced during melting. Bulk partition coefficients are calculated from;

$$D_0 = \sum D_j^i \times W_j \tag{2}$$

where,  $D$  is the partition coefficient of  $i$ th element in  $j$ th mineral, and  $W$  is the proportion of  $j$ th mineral in the source.



**Figure 1.** Cartoon showing closed-system melting models (after Zou 1998).



**Figure 2.** Cartoon showing relationships between different melting models (after Zou 1998).

During non-modal partial melting, the bulk partition coefficients of many trace elements change, as some minerals (such as garnet and clinopyroxene in mantle lherzolite) are consumed preferentially. The trace element compositions of any instantaneous or accumulated melts produced by the non-modal batch melting model ( $C_I^m$  or  $C_L^m$ , respectively) are given by;

$$C_I^m = C_L^m = \frac{C_0^m}{D_0 + F(1 - P_0)} \quad (3)$$

where,  $P_0$  is the bulk partition coefficient of the trace element of the minerals entering the melt. The other parameters are the same as previously described.  $P_0$  is calculated from;

$$P_0 = \sum D_j^i \times P_j \quad (4)$$

where,  $P$  is the weight fraction of the  $j$ th mineral entering the melt phase.

The trace element compositions in the residual solid (or total residue) ( $C_S^m$  or  $C_R^m$ ) during modal and non-modal batch melting are, in turn, expressed by;

$$C_S^m = C_R^m = \frac{D_0 C_0^m}{D_0 + F(1 - D_0)} \quad (5)$$

$$C_S^m = C_R^m = \frac{D_0 - FP_0}{1 - F} \frac{C_0^m}{D_0 + F(1 - P_0)} \quad (6)$$

When  $P_0 = D_0$ , the non-modal melting equation is equivalent to modal melting. Relationships between different melting models are summarized in Figure 2.

### 2.1.2. Fractional melting

The fractional melting, another end-member of the melting models, assumes that the melt is removed from the residual source as soon it is formed. In the fractional melting model, only the last drop of liquid is in equilibrium with the final portion of restite, and there is no residual melt (Figure 1) (Gast, 1968; Schilling & Winchester 1967; Shaw 1970; Zou 1998). The concentration of any trace element in the melt can be calculated for two types of melt: instantaneous and accumulated. The concentration of any trace element in the instantaneous ( $C_I^m$ ) and accumulated ( $C_L^m$ ) melts during modal fractional melting is, in turn, expressed by:

$$C_I^m = \frac{C_0^m}{D_0} (1 - F)^{(1/D_0)-1} \quad (7)$$

$$C_L^m = \frac{C_0^m}{F} \left[ 1 - (1 - F)^{1/D_0} \right] \quad (8)$$

The trace element composition of the residual solid (which equivalent to total residue) during modal fractional melting is expressed by:

$$C_S^m = C_R^m = C_0^m (1 - F)^{(1/D_0)-1} \quad (9)$$

The trace element composition of the instantaneous melt, accumulated melt and the residual material during non-modal fractional melting are, in turn, expressed by:

$$C_I^m = \frac{C_0^m}{D_0} \left[ 1 - \frac{FP_0}{D_0} \right]^{(1/P_0)-1} \quad (10)$$

$$C_L^m = \frac{C_0^m}{F} \left[ 1 - \left( 1 - \frac{FP_0}{D_0} \right)^{1/P_0} \right] \quad (11)$$

$$C_S^m = C_R^m = \left[ \frac{D_0 - FP_0}{1 - F} \right] \frac{C_0^m}{D_0} \left[ 1 - \frac{FP_0}{D_0} \right]^{(1/P_0)-1}$$

### 2.1.3. Dynamic (continuous or critical) melting

Dynamic melting involves the retention of a critical fraction of melt in the restite. The amount of this fraction depends on the critical mass porosity of the source rock. Therefore, this model is intermediate between the two end-member models of batch and fractional melting (Figure 1). The advantage of this model is that it may explain the fractionation of some strongly incompatible elements (Langmuir *et al.* 1977; Wood 1979; Maaløe 1982; McKenzie 1985; Zou 1998). In this model, no melt extraction occurs (as in batch melting) when the mass porosity of the restite (melt mass fraction,  $\psi$ ) is less than the critical mass porosity of the residue (the critical value for separation,  $\Phi$ ).

The trace element compositions of the instantaneous and accumulated melts produced by modal dynamic melting are, in turn, expressed by:

$$C_I^m = \frac{C_0^m}{\Phi + (1 - \Phi)D_0} (1 - X)^{[1/\{\Phi + D_0(1 - \Phi)\}]} \quad (13)$$

$$C_L^m = \frac{C_0^m}{X} \left[ 1 - (1 - X)^{1/\{\Phi + D_0(1 - \Phi)\}} \right] \quad (14)$$

where,

$$X = \frac{F - \Phi}{1 - \Phi} \quad (15)$$

The equations for trace element compositions in the instantaneous and accumulated melts produced by non-modal dynamic melting are, in turn:

$$C_I^m = \frac{C_0^m}{D_0 + \Phi(1 - P_0)} \times \left( 1 - \frac{X[P_0 + \Phi(1 - P_0)]}{D_0 + \Phi(1 - P_0)} \right)^{[1/\{\Phi + P_0(1 - \Phi)\}] - 1} \quad (16)$$

$$C_L^m = \frac{C_0^m}{X} \left\{ 1 - \left[ 1 - \frac{X[P_0 + \Phi(1 - P_0)]}{D_0 + \Phi(1 - P_0)} \right]^{1/[\Phi + (1 - \Phi)P_0]} \right\} \quad (17)$$

The concentration of any element in the residual solid ( $C_S^m$ ) and total residue ( $C_R^m$ ) is similar for batch and fractional melting models. However, these differ for the dynamic melting models; the concentration in the total residue is related to the concentration in the residual solid and the concentration in the residual melt. The concentration in the residual melt during melting is equivalent to that of instantaneous melt.

The trace element composition of the residual solid during modal dynamic melting is expressed by:

$$C_S^m = D_0 \times C_I^m = \frac{D_0 C_0^m}{\Phi + (1 - \Phi)D_0} (1 - X)^{[1/\{\Phi + D_0(1 - \Phi)\}] - 1} \quad (18)$$

The concentration in the total residue is related through:

$$C_R^m = \Phi C_I^m + (1 - \Phi)C_S^m \quad (19)$$

Therefore, the trace element composition of the total residue during modal dynamic melting is expressed by:

$$\begin{aligned} C_R^m &= \Phi C_I^m + (1 - \Phi)C_S^m \\ &= \Phi \left\{ \frac{C_0^m}{\Phi + (1 - \Phi)D_0} (1 - X)^{[1/\{\Phi + D_0(1 - \Phi)\}] - 1} \right\} \\ &+ (1 - \Phi) \left\{ \frac{D_0 C_0^m}{\Phi + (1 - \Phi)D_0} (1 - X)^{[1/\{\Phi + D_0(1 - \Phi)\}] - 1} \right\} \\ &= C_0^m (1 - X)^{[1/\{\Phi + D_0(1 - \Phi)\}] - 1} \end{aligned}$$

The trace element compositions of the residual solid ( $C_S^m$ ) during non-modal dynamic melting are expressed by;

$$C_S^m = D \times C_I^m \quad (21)$$

where  $D$  is the bulk partition coefficient during partial melting, which is different from the initial bulk partition coefficient in the source ( $D_0$ ).  $D$  is expressed by:

$$D = \frac{D_0 - FP_0}{1 - P} = \frac{D_0 - (P_0[X + \Phi(1 - X)])}{(1 - X)(1 - \Phi)} \quad (22)$$

Therefore,

$$C_S^m = \frac{D_0 - (P_0[X + \Phi(1 - X)])}{(1 - X)(1 - \Phi)} \times \frac{C_0^m}{D_0 + \Phi(1 - P_0)} \times \left( 1 - \frac{X[P_0 + \Phi(1 - P_0)]}{D_0 + \Phi(1 - P_0)} \right)^{[1/\{\Phi + P_0(1 - \Phi)\}] - 1} \quad (23)$$

The trace element compositions of the total residue ( $C_R^m$ ) is expressed by:

$$\begin{aligned} C_R^m &= (1 - \Phi)C_S^m + \Phi C_I^m = \\ &[1 - \Phi] \times \left[ \frac{D_0 - (P_0[X + \Phi(1 - X)])}{(1 - X)(1 - \Phi)} \times \frac{C_0^m}{D_0 + \Phi(1 - P_0)} \times \left( 1 - \frac{X[P_0 + \Phi(1 - P_0)]}{D_0 + \Phi(1 - P_0)} \right)^{[1/\{\Phi + P_0(1 - \Phi)\}] - 1} \right] \\ &+ \Phi \left[ \frac{C_0^m}{D_0 + \Phi(1 - P_0)} \times \left( 1 - \frac{X[P_0 + \Phi(1 - P_0)]}{D_0 + \Phi(1 - P_0)} \right)^{[1/\{\Phi + P_0(1 - \Phi)\}] - 1} \right] \quad (24) \end{aligned}$$

## 2.2. Crystallization and contamination processes

As the melt cools, it begins to crystallize. Each mineral phase derived from the liquid has a different crystallization temperature, also depending on other parameters, such as chemical composition and pressure. For example, at low pressures, olivine is usually the first phase to crystallize from basic (low-SiO<sub>2</sub>) melts. Crystallization processes in this study are considered to be developed in closed-systems; i.e., no material input occurs during crystallization. Only the assimilation and fractional crystallization model (AFC) acts as an open-system. PETROMODELER numerically models trace element compositions for all the crystallization models summarized below. Isotopic ratios are not changed during close-system crystallization models. Major element differentiation during crystallization processes can only be applied to perfect fractional crystallization (PFC) processes by PETROMODELER.

### 2.2.1. Perfect equilibrium crystallization (PEC)

If all the crystallized solid phases remain in the liquid, they can be assumed to stay in chemical equilibrium with

the magma. This process is known as *Perfect Equilibrium Crystallization* (PEC). The trace element composition of the liquid phase during PEC ( $C_{lc}^{PEC}$ ) is expressed by:

$$C_{lc}^{PEC} = C_0^f / [F + D_0(1 - F)] \quad (25)$$

where,  $C_0^f$  is the initial trace element composition of the magma,  $F$  is the mass fraction of the residual magma relative to the initial mass, and  $D_0$  is the bulk partition coefficient for the fractionating mineral assemblage which is calculated by Eq. (2).

### 2.2.2. Perfect fractional crystallization (PFC)

If the early formed mineral phase is continuously and perfectly removed from the initial liquid, both the major and trace element composition of the initial melt would be differentiated from the PEC model. This process is termed *Perfect Fractional Crystallization* (or Rayleigh fractionation, Rayleigh (1896)). The trace element composition of the remaining liquid phase during fractional crystallization ( $C_{lc}^{PFC}$ ) is expressed by:

$$C_{lc}^{PFC} = C_0^f F^{(D_0-1)} \quad (26)$$

Major element differentiation during PFC can also be modelled by PETROMODELER. This is based on the major element compositions of fractionated minerals, instead of their partition coefficients. The weighted major element composition of the fractionated mineral assemblage is calculated in a similar way to that shown by Eq. (2), and then subtracted from the initial major element composition ( $C_0^f$ ) on the basis of fractionation ratio ( $F$ ).

### 2.2.3. Equilibrium crystallization and imperfect fractional crystallization (EC-IFC)

The Rayleigh fractionation equation (Eq. 22; Rayleigh 1896) is only valid for perfect crystal separation from the liquid. However, this excludes crystals that are removed in infinitesimally small batches. Note that crystal-liquid separation is generally imperfect in nature (e.g., Anderson & Greenland 1969; O'Hara 1993, Nishimura 2009). IFC is particularly useful in explaining the variation of highly compatible elements in basalts and their source rock restite compositions. If it is assumed that there is perfect equilibrium between the suspended crystals in the cooling magma and imperfect separation of formed crystals, then the suspended crystals do not develop chemical zoning. In this case, trace element composition of the liquid phase during equilibrium crystallization and imperfect fractional crystallization ( $C_{lc}^{AFC}$ ) is expressed by:

$$C_{lc}^{EC-IFC} = C_0^f F \left( \frac{D_0}{1-\delta+\delta D_0} - 1 \right) \quad (27)$$

where,  $\delta$  is the mass fraction of the suspended crystals.

### 2.2.4. Zoned crystallization and imperfect fractional crystallization (ZC-IFC)

Natural volcanic rocks are often characterized by the presence of zoned phenocrysts in the volcanic matrix or glass, indicating that chemical equilibrium was only achieved between the crystal surface and the surrounding liquid (no perfect equilibration; e.g., Nishimura (2009)). The trace element composition of the liquid phase during zoned crystallization and imperfect fractional crystallization ( $C_{lc}^{ZC-IFC}$ ) is expressed by:

$$C_{lc}^{ZC-IFC} = C_0^f \left[ F^{\frac{1-\delta}{\delta}} + \frac{(1-\delta)^{D_0}}{1-\delta D_0} \left( F^{(D_0-1)} - F^{\frac{1-\delta}{\delta}} \right) \right] \quad (28)$$

where,  $\delta D_0 \neq 1$  and  $\delta \neq 0$ , and by:

$$C_{lc}^{ZC-IFC} = C_0^f F^{(D_0-1)} \left[ 1 + (1 - D_0) \left( 1 - \frac{1}{D_0} \right) \ln F \right] \quad (29)$$

in the case of  $\delta D_0 = 1$  (Nishimura 2009).

### 2.2.5. Combined assimilation and fractional crystallization (AFC)

During the cooling of magmas emplaced into the shallow crustal chambers, the fractional crystallization process is likely accompanied by assimilation of the surrounding wall rocks (DePaolo 1981). In this case, the trace element composition of a magma affected by AFC process ( $C_{lc}^{AFC}$ ) is expressed by:

$$C_{lc}^{AFC} = C_0^f \left[ F^{-z} + \left( \frac{r}{r-1} \right) \frac{C_a}{z C_0^f} (1 - F^{-z}) \right] \quad (30)$$

where,  $C_a$  is the concentration of an element in the assimilating material (wall rock). The “ $r$ ” value describes the relative ratio of assimilated material to crystallized material, and is expressed by:

$$r = \frac{m_a}{m_c} \quad (31)$$

where,  $m_a$  is the amount of assimilated material and  $m_c$  is the amount of crystallized material. The  $z$  value in the AFC equation is expressed by:

$$z = \frac{r + D_0 - 1}{r - 1} \quad (32)$$



Isotopic ratios are not changed during closed-system melting and crystallization processes, but assimilation processes generally do cause changes in the isotopic ratios of an initial magma. The isotopic compositions of a magma undergoing the AFC process ( $IC_{lc}^{AFC}$ ) is modelled by;

$$IC_{lc}^{AFC} = \frac{\left(\frac{r}{r-1}\right)\left(\frac{C_a}{z}\right)(1-F^{-z})IC_a + C_0^f F^{-z} IC_0}{\left(\frac{r}{r-1}\right)\left(\frac{C_a}{z}\right)(1-F^{-z}) + C_0^f F^{-z}} \quad (33)$$

where,  $IC_a$  and  $IC_0$  are the isotopic ratios in the assimilating material and in the initial magma, respectively.

### 2.3. Mixing processes

The trace element composition of a magma produced by simple mixing (e.g., Powell 1984) of two parental magmas is expressed by;

$$C_m = X(C_1 - C_2) + C_2 \quad (34)$$

where,  $C_1$ ,  $C_2$  and  $C_m$  are the concentrations of an element in magma  $a$ , in magma  $b$ , and in the mixed magma resulting from mixing of magmas  $a$  and  $b$ , respectively.  $X$  is the degree of mixing. Eq. (36) can be applied to both major and trace elements. For isotopic compositions, the equation is expressed by;

$$IC_m = IC_1\left(\frac{C_2 X}{C_m}\right) + IC_2\left(\frac{C_2(1-X)}{C_m}\right) \quad (35)$$

where,  $IC_a$ ,  $IC_b$  and  $IC_m$  are the isotopic ratios of any element in magma  $a$ , magma  $b$  and in the mixed magma resulting from mixing of magmas  $a$  and  $b$ , respectively.

## 3. Program structure

PETROMODELER is designed on several sheets on a Microsoft® Excel® file and is structurally similar to FC-AFC-FCA and mixing model developed by Ersoy & Helvacı (2010) that can be used only to model fractional crystallization (FC), combined and decoupled fractional crystallization and assimilation (AFC and FCA) and mixing processes. The sheets of PETROMODELER include data input and output sections. The input section includes two sheets: (1) parameters and (2) samples, which are designed similarly to that of the FC-AFC-FCA and mixing model.

### 3.1. Data input

#### 3.1.1. Parameters sheet

Acid, intermediate and basic partition coefficients for 14 minerals (which can be changed by the user) are entered into 3 tables. On these tables, partition coefficients should be used for trace elements (to use in fractionation and melting

models). However, mineral compositions ( $wt\%$ ) should be used for major elements (to use only in fractionation models). 10 different assimilant compositions are entered into the "Assimilants" table which can be used in AFC and mixing models. 4 different chemical compositions of rocks are entered into the "Normalizing Values" table, which are used on the normalized spider-diagram on the models sheet (see below). 12 different types of rock composition can be entered into the "Source Rocks" table, which are used in the melting models. 9 different types of source and melt mineral composition (facies) can be entered into the "Mineral Modes" table, which are used in calculation of the bulk partition coefficients for the source and melt modes (for calculation of  $D_0$  and  $P_0$ ) in the melting models. A graphic has been designed to show the variations of the mineral abundances during the course of melting. Mineral names on this table (and also on partition coefficient tables) are already entered by using the first table ("Mineral Names" table). Several isotope ratios to calculate some parameters are also entered into the last table in the parameters sheet.

#### 3.1.2. Samples sheet

Ten datasets, each including 20 sample columns, can be entered into the samples sheet. The names of the datasets and the sample numbers are linked to the related sites in the other sheets. In these datasets, the major element oxides (on  $wt\%$  basis), trace elements (on  $ppm$  basis), isotopic compositions (including  $^{87}Sr/^{86}Sr$ ,  $^{143}Nd/^{144}Nd$ ,  $^{147}Sm/^{144}Nd$ ,  $^{206}Pb/^{204}Pb$ ,  $^{207}Pb/^{204}Pb$ ,  $^{208}Pb/^{204}Pb$ ,  $\delta^{18}O$ ), and ages (presented as Ma) for up to 200 samples can be entered. Some parameters, such as Mg#, Eu/Eu\*,  $\epsilon Sr$ ,  $\epsilon Nd$  and  $\sigma^{(DM)}$  (depleted mantle Nd model ages), and water-free major element contents (normalized to 100%), are automatically calculated on this sheet.

### 3.2. Data output

#### 3.2.1. Classification sheet

In this sheet, the total alkali ( $K_2O+Na_2O$ ) - silica ( $SiO_2$ ) classification diagram (LeBas *et al.* (1986), the  $K_2O$  -  $SiO_2$  diagram (LeMaitre 2002), the  $MgO$  -  $K_2O/Na_2O$  diagram which is constructed for ultrapotassic rocks based on the criteria proposed by Foley *et al.* (1987), and the  $K_2O$  -  $Na_2O$  (Peccerillo & Taylor 1976) diagram are included. The alkaline - subalkaline line is shown according to Irvine and Baragar (1971) on the TAS diagram of LeMaitre (2002). Any dataset from the samples sheet can be shown on these diagrams, by ticking the related checkboxes. The symbols for the datasets are illustrated with their names in an explanation box on the sheet. The samples can also be plotted on these diagrams on the basis of either hydrous or water-free major element contents.

#### 3.2.2. Models sheet

The main panel of the PETROMODELER, models sheet, contains four columnar sections: (a) parameters

for bivariate and spider diagrams, (b) melting model parameters, (c) crystallization and contamination model parameters (Figure 3).

In the first section, the  $x$ - and  $y$ -axes of the bivariate diagram are chosen using three combo-boxes for each axis (such as Sr vs. Ba; Sr/Ba vs.  $\text{SiO}_2$ ,  $^{87}\text{Sr}/^{86}\text{Sr}$  vs. La/Yb) (Figure 3a). The axes can also be set with *linear* or *logarithmic*-scales. Below this section, the rock groups are chosen by ticking on the related check-boxes in order to plot them on the diagrams (Figure 3b). The names of the rock groups automatically come from the samples sheet. The “Melt Composition” combo-box allows the user to select any melt composition, such as acidic, intermediate, or basic for their partition coefficient data sets already entered into the parameters sheet (Figure 3c). The “Normalizing Factor” combo-box allows the user to select any chemical compositions which will then be used as normalizing values on the spider diagram (Figure 3c). These values may be entered or changed on the parameters sheet. The names of the normalizing values in the combo-box are updated by the related table on the parameters sheet, which can be changed by the user. The name of the selected normalizing factor appears on the logarithmic  $y$ -axis of the spider diagram. Below this, three combo-boxes are used to choose any “ $F$ ” values (melt fraction) for the melting, crystallization and mixing model results (Figure 3d). The model results for the chosen value of “ $F$ ” are shown on the spider diagram. The “ $F$ ” value is also labelled on the spider-diagram (Figure 4). The values in these combo-boxes may be changed by using the related buttons on the second and third columns on the models sheet (by changing the melting degree and increment buttons).

In the second columnar section on the models sheet, the melting parameters and models are set (Figures 3e–f). First, a starting material composition is chosen from the “Starting Composition ( $C_0^m$ )” combo-box (Figure 3e). The names in this combo-box are updated from related table on the parameters sheet (source rock table), which can be changed by the user. A check-box near the combo-box is used to show the composition of the selected material on the bivariate and spider diagrams. The selected material is also labelled on both the bivariate and spider-diagrams (Figure 4). The “Melting Facies (Mineral Modes)” combo-box is used to set the mineral modes for the source and melt (Figure 3e). The names in this combo-box are entered into the “Mineral Modes” table on the parameters sheet, which can be changed by the user. In the “Melting Degree” section, two buttons are used to choose; (a) the degree of melting for the first step (the melting curve starts from this point on the bivariate diagram), and (b) the increment for melting. For example if the first button is chosen as 1% and the second as 2%, then the curve of any melting models are drawn beginning from 1% with increments of 2%, and the

points on the curve represents 1%, 3%, 5% ....19% partial melting (Figure 3e) (10 incremental points describe the melting curve on the bivariate diagram which appear in the “for melting” combo-box shown on Figure 3d).

The buttons for melting models are placed below this section (Figures 3f). By ticking the related check-boxes, the instantaneous ( $C_I$ ) or accumulated ( $C_L$ ) melt and residual solid ( $C_S$ ) and total residue ( $C_R$ ) compositions for batch, fractional and dynamic melting models (for modal and non-modal models) can be shown on the bivariate and spider diagrams. If a melting model is selected, the name of  $C_0^m$  is labelled on both the bivariate and spider diagrams (Figure 4).  $F$  is also labelled on the spider diagram. The critical mass porosity for the dynamic melting models ( $\Phi$ ) is also set by the related buttons. Major element compositions for melting models are not modelled by PETROMODELER. Isotopic ratios remain constant during closed-system melting models.

In the third columnar section on the models sheet, the crystallization and contamination parameters and the models are set (Figures 3g–j). A starting material composition is first chosen from the “Starting Composition ( $C_0^f$ )” combo-box to crystallize or contaminate the melt.  $C_0^f$  can be chosen from; (1) any samples which are already entered into the samples sheet (by “choose from samples” button), or (2) any melting models performed in the second column on the sheet (by “choose from melting results” button) (Figures 3g). If first button is selected, then the sample numbers appear on a combo-box placed just below the first button, and any sample can be set as starting composition from this combo-box. If the second button is selected, then the user should set the melting type and melt fraction by using the four combo-boxes placed below the button. A check-box in the “starting composition ( $C_0^f$ )” label is used to show the composition of the selected material on the bivariate and spider diagrams. The name of the selected  $C_0^f$  is labelled on both the bivariate and spider-diagrams if any crystallization and contamination model is selected (Figure 4). Below the “starting composition ( $C_0^f$ )” section, the fractionating mineral assemblage is set, by giving their percentage (Figures 3h). The names of the minerals can be updated from the parameters sheet. The increment percent for the crystallization and contamination models is set by a button (Figures 3i). 10 increments are set automatically, beginning from  $F=100\%$  and the end of the crystallization is indicated below the button. For example if the first button is chosen as 1% then the curve of any fractionation models are drawn beginning from 100% with increments of 1%, and the points on the curve represents 0%, 1%, 2%, 3% .... 9% crystallization (Figure 3e). 10 incremental points describe the fractionation curves on the bivariate diagram, which also appear in the “for FC/AFC” combo-

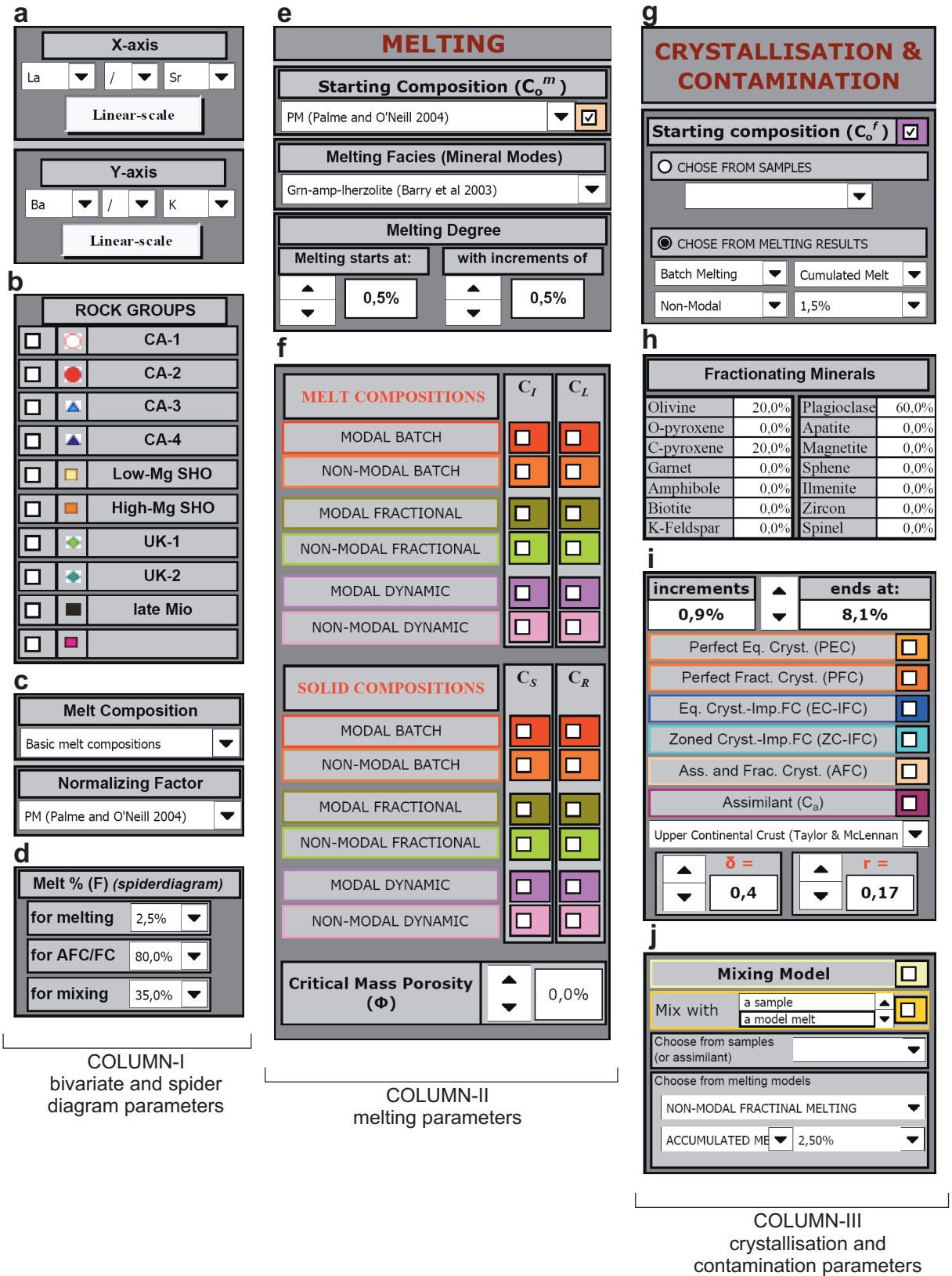


Figure 3. Partial screenshots of models sheet of PETROMODELER: (a–d) diagram parameters, (e–f) melting parameters, (g–j) crystallization and contamination parameters.



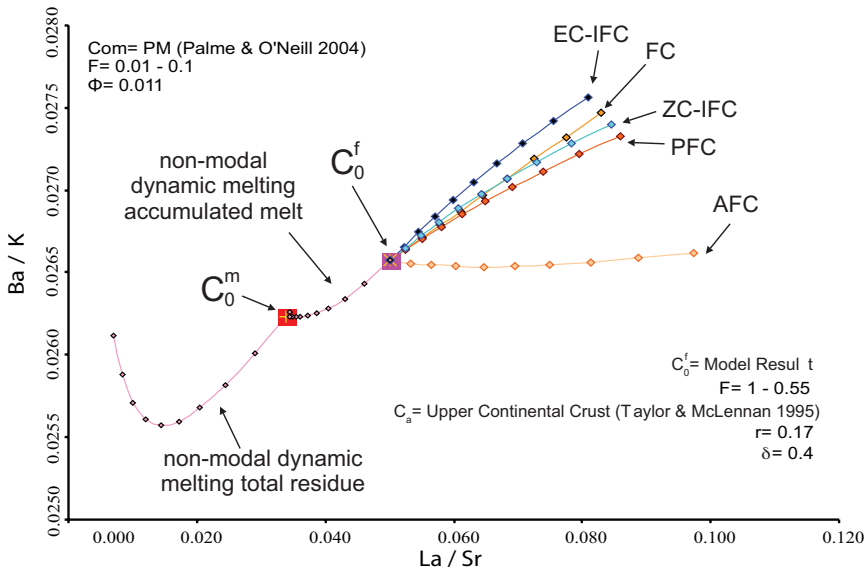


Figure 4. An example of bivariate diagram showing several differentiation trends for Ba/K vs La/Sr.

box shown on Figure 3d.  $F$  value for the spider diagram is chosen from the related combo-boxes in the first column on this sheet (Figure 3d). Any crystallization model can be selected by ticking on the related check-boxes (Figure 3i). The “ $\delta$ ” value for the EC-IFC and ZC-IFC can be set by a button (Figure 3i).

Contamination models are constructed using either the AFC or Mixing models. The assimilant material composition for the AFC model ( $C_a$ ) is chosen from a combo-box and related check-box. The names in the list of the “Assimilant” combo-box can be updated from the parameters sheet, which can be changed by the user. The “ $r$ ” value for the AFC model is set by the related button (Figure 3i). Another contamination process, mixing model can be constructed by selecting the check-box.  $C_1$  is already selected from the “starting composition ( $C_0^f$ )” section, which is used for other crystallization processes (Figure 3g).  $C_2$  is selected from the combo-box labelled as “Mix with:” (Figure 3j). In this section,  $C_2$  can be chosen from; (1) any samples which are already entered into the samples sheet (by selecting “a sample”), or (2) any melting models performed in the second column on the sheet (by selecting “a model melt”) (Figures 3g). If “a sample” is selected, then the sample numbers appear on a combo-box placed just below the first button, and any sample can be set as starting composition from this combo-box. The last item of this list is the assimilant composition ( $C_a$ ; selected from AFC section), which can also be selected as  $C_2$ . If “a model melt” is selected, several melting results appear in the related combo-boxes (Figures 3j). Hence, mixing models between two samples or between a sample and assimilant, or between a sample and a modelled melt composition can be modelled.

### 3.2.3. Converter sheet

In this sheet the normative mineralogical compositions of the samples entered into the tables in the samples sheet are calculated. The normative mineralogical compositions of a given sample are calculated on both a weight% and volume% basis. The sample can be chosen from a combo-box, for which the major element composition and group name appear on a table. In this sheet, the oxide abundances can also be converted to element abundances on basis of wt% or ppm.

### 3.3.4. Numerical output sheet

In this sheet, the numerical outputs of the selected melting or crystallization model are derived from two tables. The results and parameters of the melting model appear in the first table. Three combo-boxes are used to choose the melting model. The relevant parameters appear in the columns related to the selected melting model. A similar table is constructed for the crystallization and contamination processes.

## 4. Conclusions

PETROMODELER (*Petrologic Modeler*) is a Microsoft® Excel® spreadsheet program which numerically and graphically models magmatic processes, such as melting, crystallization and mixing by using trace elements and isotopic ratios. In the program, trace element compositions of; (a) cumulated, and (b) instantaneous partial melts, and (c) residual solid, and (d) total residue from melting of any rock type can be calculated by using batch, dynamic and fractional melting models. The composition of these model melts (or any analyses of natural samples entered into the program) can also be used as the starting

composition for; (a) perfect equilibrium crystallization, (b) perfect fractional crystallization, (c) equilibrium crystallization-imperfect fractional crystallization, (d) zoned crystallization-imperfect fractional crystallization, (e) combined assimilation and fractional crystallization, and (f) mixing models.

All these models can be graphically shown on a bivariate diagram, for which axes can be set as linear- or log-scaled, or on a logarithmic multi-element spider

diagram. The diagrams can be exported as “gif” files. The numerical outputs of these models can also be exported as tables.

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