A new approach to modelling differentiation (with particular focus on granitic magmatism): Equilibrated Major Element Assimilation with Fractional Crystallisation (EME-AFC)

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The Challenge
Modelling AFC differentiation from basaltic to silicic magma; particularly to derive granite.

The Problems
1) Current AFC models (MELTs, Rhyolite-MELTS, Magma Chamber Simulator, alphaMELTS) cannot model hydrous magmatic systems involving substantial hornblende or biotite fractionation. Given evidence for “cryptic amphibole fractionation”, this applies to most/all arc magmas.

2) Trace element partition coefficients are notoriously variable.

3) Modelling different elemental and isotopic systems produce different conclusions, so ideally all systems should be modelled simultaneously.

The Solution
A new method (Equilibrated Major Element Assimilation with Fractional Crystallisation, EME-AFC), using two-component major element partition coefficients and simultaneously modelling of major and trace elements, radiogenic isotopes, and stable isotopes.

**EME-AFC: Major Elements**

Equilibrium major element compositions of rock-building minerals can be calculated from experimentally derived, two-component partition coefficients \((K_D)\). Minor elements are calculated from their empirical relationship to the majors *(below)*.

Unlike trace element partition coefficients, major element \(K_D\) values are far less variable *(right)*.

### Two-Component Partition Coefficients

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>SD</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>Plagioclase ((Al^{\text{Plag}} x Si^{\text{Liq}}) / (Si^{\text{Plag}} x Al^{\text{Liq}}))</td>
<td>2.46</td>
<td>0.51</td>
<td>36</td>
</tr>
<tr>
<td>Plagioclase ((K^{\text{Plag}} x Na^{\text{Liq}}) / (Na^{\text{Plag}} x K^{\text{Liq}}))</td>
<td>0.09</td>
<td>0.04</td>
<td>36</td>
</tr>
<tr>
<td>Hornblende ((Fe^{\text{Hbl}} x Mg^{\text{Liq}}) / (Mg^{\text{Hbl}} x Fe^{\text{Liq}}))</td>
<td>0.36</td>
<td>0.07</td>
<td>28</td>
</tr>
<tr>
<td>Hornblende ((Al^{\text{Hbl}} x Si^{\text{Liq}}) / (Si^{\text{Hbl}} x Al^{\text{Liq}}))</td>
<td>1.13</td>
<td>0.27</td>
<td>28</td>
</tr>
<tr>
<td>Clinopyroxene ((Fe^{\text{Cpx}} x Mg^{\text{Liq}}) / (Mg^{\text{Cpx}} x Fe^{\text{Liq}}))</td>
<td>0.28</td>
<td>0.07</td>
<td>23</td>
</tr>
<tr>
<td>Clinopyroxene ((Al^{\text{Cpx}} x Si^{\text{Liq}}) / (Si^{\text{Cpx}} x Al^{\text{Liq}}))</td>
<td>0.27</td>
<td>0.18</td>
<td>23</td>
</tr>
<tr>
<td>Orthopyroxene ((Fe^{\text{Opx}} x Mg^{\text{Liq}}) / (Mg^{\text{Opx}} x Fe^{\text{Liq}}))</td>
<td>0.28</td>
<td>0.08</td>
<td>15</td>
</tr>
<tr>
<td>Orthopyroxene ((Al^{\text{Opx}} x Si^{\text{Liq}}) / (Si^{\text{Opx}} x Al^{\text{Liq}}))</td>
<td>0.19</td>
<td>0.16</td>
<td>15</td>
</tr>
<tr>
<td>Olivine ((Fe^{\text{Ol}} x Mg^{\text{Liq}}) / (Mg^{\text{Ol}} x Fe^{\text{Liq}}))</td>
<td>0.28</td>
<td>0.03</td>
<td>14</td>
</tr>
</tbody>
</table>

#### Calculations used for major element modelling of plagioclase

<table>
<thead>
<tr>
<th>Composition</th>
<th>(K_D) equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al-Si Kd</td>
<td>(K_D = (Al^{\text{Plag}} x Si^{\text{Liq}}) / (Si^{\text{Plag}} x Al^{\text{Liq}}))</td>
</tr>
<tr>
<td>K-Na Kd</td>
<td>(K_D = (K^{\text{Plag}} x Na^{\text{Liq}}) / (Na^{\text{Plag}} x K^{\text{Liq}}))</td>
</tr>
<tr>
<td>Fe</td>
<td>(a \times (Fe + Al))</td>
</tr>
<tr>
<td>Mg</td>
<td>(b \times (Mg + Mn + Ca))</td>
</tr>
<tr>
<td>Mn</td>
<td>(c \times (Mg + Mn + Ca))</td>
</tr>
</tbody>
</table>

**EME-AFC methodology for plagioclase.**

\(K_D\) equations derive two-component major element partition coefficients from experimental data

‘\(a\)’, ‘\(b\)’, and ‘\(c\)’ for the minor elements are calculated from mean mineral chemistry of the rocks being modelled
EME-AFC: Major Elements

The equilibrium mineral compositions are calculated and fractionated from the magma by mass balance for successive increments of fractionation, “F”. Assimilation is modelled at each increment by binary mixing for the major elements according to a user-determined rate of assimilation, “r” (the mass assimilated / mass crystallised). The instantaneous and bulk cumulate composition is also calculated.

EME-AFC modelling of the Mt Kinabalu granite, Borneo

Analysed and modelled mineral chemistries of the Mt Kinabalu granite, Borneo
EME-AFC: Trace Elements and Radiogenic Isotopes

Trace element and isotopic compositions are calculated at each increment using the AFC equations of DePaolo (1981).
EME-AFC: Oxygen Isotopes

Oxygen isotope fractionation between coexisting phases varies with temperature. Experimental melt SiO$_2$ correlates strongly with temperature (below), allowing oxygen isotope AFC modelling at each increment (bottom right).

\[ T = -19 \times \text{SiO}_2 + 2050 \pm 62^\circ\text{C} \ (1\text{SD}) \]
\[ R^2 = 0.75 \]

- Villiger et al. (2004)
- Krawczynski et al. (2012)
- Villiger et al. (2005)
- Alonso-Perez et al. (2009)
- Nandedkar et al. (2014)
EME-AFC Excel Spreadsheet

EME-AFC can be applied using a spreadsheet-based model (with instructions).

Inputs:
- Primary melt composition
- Target magma composition
- Assimilant composition
- Mineral separate data (optional, but ideally)

Variables:
- Rate of assimilation
- Fractionating assemblage
- Partition coefficients

Outputs:
- Elemental and isotopic composition of magma and cumulates
- Bulk cumulate mineralogy
- Sum of the squares, to evaluate model agreement
- Bivariate and spidergram plots

https://github.com/Alex-Burton-Johnson/EME-AFC-Modelling
EME-AFC allows modelling of magmatic differentiation even in hydrous systems

- Explore the effects of inputs and variables of the magmatic system of interest

- EME-AFC can be freely applied using a spreadsheet-based model, latest version available: https://github.com/Alex-Burton-Johnson/EME-AFC-Modelling


<- Introduces EME-AFC and applies it to Mt Kinabalu in Borneo (J. Pet. Editors choice, July 2019, Open access)

<- Further example using EME-AFC
Case Study 1: The Mt Kinabalu granitic pluton, Borneo

Whole rock isotopes indicated a continental signature, but compiled experimental melts of all rock types, melt degrees, and water contents cannot reproduce the pluton’s chemistry (*below*).

EME-AFC allowed the derivation of Mt Kinabalu from basaltic AFC to be tested with different primary melts and assimilants. The primary melt was a low-degree, K-rich, extensional mantle melt, that assimilated the sedimentary country rock.

Case Study 2: The Segama Valley granitoids, Borneo

The granitoids were proposed to be windows or partial melts of continental crust beneath Borneo. EME-AFC showed how they could be derived from primary mantle melts without a continental crustal contribution, and how garnet fractionation was variable.