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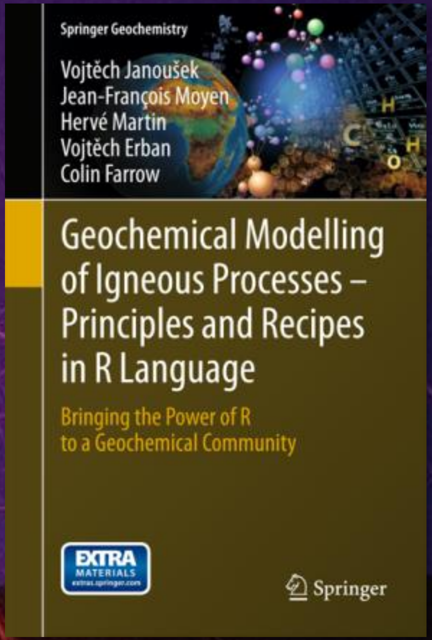
Dealing with mixtures: interpretation of major-element data from igneous rocks



Major vs. trace elements, units of measurement

	ZV14	ZV85	ZV10
Major element oxides (wt %)			
SiO_2	48.91	45.26	45.26
TiO_2	0.45	0.33	0.29
Al_2O_3	9.24	6.74	6.07
Fe_2O_3	2.62	2.13	1.68
FeO	8.90	8.66	8.70
MnO	0.18	0.17	0.17
MgO	15.32	22.98	26.21
CaO	9.01	6.94	6.41
Na_2O	1.15	0.88	0.78
K_2O	0.08	0.05	0.04
P_2O_5	0.03	0.02	0.02
S	0.04	0.05	0.05
H_2O+	3.27	3.41	2.20
H_2O-	0.72	0.57	0.28
CO_2	0.46	0.84	1.04
Total	100.38	99.03	99.20

	ZV14	ZV85	ZV10
Selected trace elements (ppm)			
Ni	470	1110	1460
Cr	2080	2770	2330
V	187	140	118
Y	10	6	6
Zr	21	16	14
Rb	3.38	1.24	1.38
Sr	53.3	32.6	31.2
Ba	32	12	10
Nd	2.62	1.84	2.31
Sm	0.96	0.68	0.85
Radiogenic isotope ratios			
εNd	+2.4	+2.4	+2.5
$^{87}Sr/^{86}Sr$	0.7056	0.70511	0.70501
Stable isotope ratios (‰)			
$\delta^{18}O$	+7.3	+7.0	+6.8

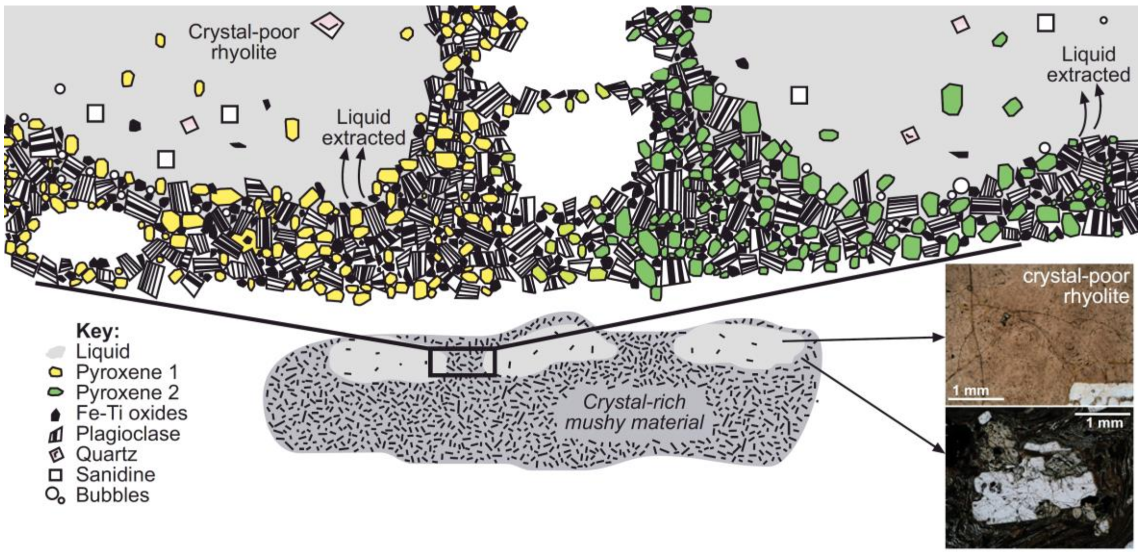
Major-elements

- **wt. % of oxides** (comes from the days of wet chemistry analysis)

Trace elements

- **ppm, ppb**, **ppt** (by weight)

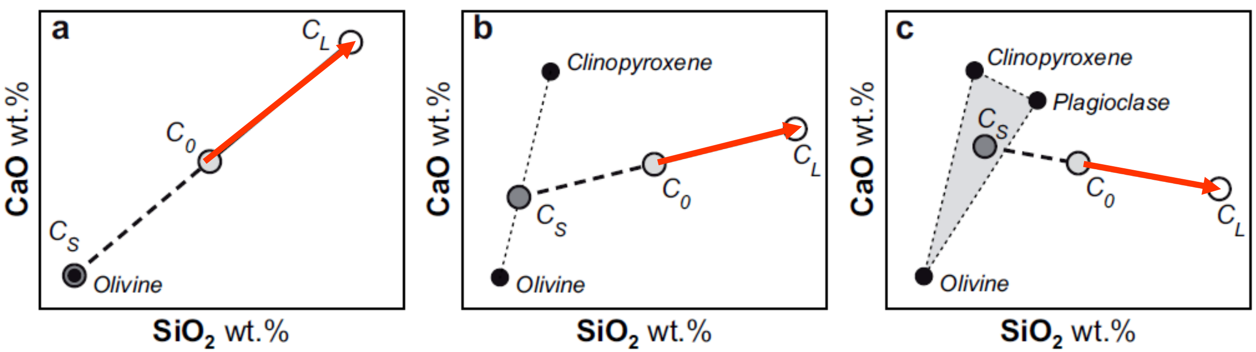
Fractional crystallization



Simplified from: ELLIS, B. S., BACHMANN, O. & WOLFF, J. A., 2014. Cumulate fragments in silicic ignimbrites: The case of the Snake River Plain. *Geology*, **42,** 431–434.

Liquid [0, L]

Solid cumulate [S]



8.5: Generalized mixing

Table contains compositions of three ideal rock-forming minerals making up a model olivine gabbro:

wt. %	SiO_2	Al_2O_3	FeOt	MgO	CaO	Na_2O
Pl	50.54	31.70	0.00	0.00	14.36	3.40
Ol	39.19	0.00	18.75	42.06	0.00	0.00
Di	55.49	0.00	0.00	18.61	25.90	0.00

`gabbro_modal.data`

- Calculate whole-rock geochemical composition of gabbro that contains 50 % Pl, 30 % Ol and 20 % Di by weight.

https://www.virtualmicroscope.org/content/olivine-gabbro-huntly

8.5: Generalized mixing

This is a simple calculation leading to a matrix multiplication of a vector with mineral proportions (*m*) by a matrix of mineral compositions (C_C) stored in the datafile.

$$\overrightarrow{C_S} = \begin{pmatrix} c_S^{SiO_2} \\ c_S^{Al_2O_3} \\ \vdots \\ c_S^{Na_2O} \end{pmatrix}$$

$$\overline{\overline{\mathbf{C_c}}} = \begin{pmatrix} c_{Pl}^{SiO_2} & c_{Ol}^{SiO_2} & c_{Di}^{SiO_2} \\ c_{Pl}^{Al_2O_3} & c_{Ol}^{Al_2O_3} & c_{Di}^{Al_2O_3} \\ \vdots & \vdots & \vdots \\ c_{Pl}^{Na_2O} & c_{Ol}^{Na_2O} & c_{Di}^{Na_2O} \end{pmatrix}$$

$$\overrightarrow{\mathbf{m}} = \begin{pmatrix} m_{Pl} \\ m_{Ol} \\ m_{Di} \end{pmatrix}$$

$$\overrightarrow{\mathbf{C_S}} = \overline{\overline{\mathbf{C}_C}} \times \overrightarrow{\mathbf{m}}$$ ~ Eq. [6.14]

Matrix multiplication in R is implemented via the `%*%` operator.

8.2: Fractional crystallization (direct)

Table contains analyses of Sázava tonalite (Janoušek et al. 2004) and some of its rock-forming minerals (Janoušek et al. 2000):

wt. %	Tonalite	Pl	Bt	Amp
SiO_2	55.09	53.41	35.32	45.35
TiO_2	0.75	0	2.11	1.39
Al_2O_3	17.59	29.48	15.31	9.47
FeOt	7.73	0.09	23.56	18.57
MgO	3.52	0	9.05	9.82
CaO	8.2	11.27	0.01	11.92
Na_2O	2.83	5.05	0.1	1.08
K_2O	2.04	0.12	9.81	1.02

sazava_fc.data

- Calculate the composition of residual melt after 20% fractional crystallization of a cumulate consisting of 50 % Pl, 30 % Bt and 20 % Amp by weight.
- What is the composition of the cumulate?

8.2: Fractional crystallization (direct)

For each element *j* in the unfractionated/primitive magma (C_0), fractionated magma (C_L) and the crystallizing cumulate (C_s) can be written a mass-balance equation [Eq. 6.6]:

$$C_0^j = \left(1 - F_C\right) C_L^j + F_C C_S^j$$

Where degree of fractionation (F_c) is related to the mass fraction of melt (F) in the system:

$$F_C = (1 - F)$$

And also:

$$C_S^j = \sum_{i=1}^{n} (m_i c_i^j)$$

Eq. [6.8]

$$\overrightarrow{\boldsymbol{C_S}} = \overline{\overline{\boldsymbol{C}_C}} \times \overrightarrow{\boldsymbol{m}}$$

$$\sum_{i=1}^{n} m_i = 1$$

$$C_L^j = \frac{C_0^j - C_S^j F_c}{(1 - F_c)}$$

Eq. [8.2]

9.4: "Normative" calculations (reversed Ex. 8.5)

wt. %	gabbro	Pl	Ol	Di
SiO_2	48.125	50.54	39.19	55.49
Al_2O_3	15.85	31.7	0	0
FeO	5.625	0	18.75	0
MgO	16.34	0	42.06	18.61
CaO	12.36	14.36	0	25.9
Na_2O	1.7	3.4	0	0

`gabbro_modal2.data`

- Given the analyses of a gabbro and its mineral constituents (Table), estimate the wt. % of individual minerals using the least-square method.

9.4: "Normative" calculations (reversed Ex. 8.5)

Defining
(C_s = crystallizing cumulate, C_L = fractionated magma, C_0 = unfractionated/primitive magma, m = mass proportions of minerals in the cumulate):

$$\overrightarrow{C_S} = \begin{pmatrix} c_S^{SiO_2} \\ c_S^{Al_2O_3} \\ \vdots \\ c_S^{Na_2O} \end{pmatrix} \qquad \overline{\overline{C_C}} = \begin{pmatrix} c_{Pl}^{SiO_2} & c_{Ol}^{SiO_2} & c_{Di}^{SiO_2} \\ c_{Pl}^{Al_2O_3} & c_{Ol}^{Al_2O_3} & c_{Di}^{Al_2O_3} \\ \vdots & \vdots & \vdots \\ c_{Pl}^{Na_2O} & c_{Ol}^{Na_2O} & c_{Di}^{Na_2O} \end{pmatrix} \qquad \overrightarrow{\boldsymbol{m}} = \begin{pmatrix} m_{Pl} \\ m_{Ol} \\ m_{Di} \end{pmatrix}$$

Allows a matrix formulation of:

$$\overrightarrow{\boldsymbol{C_S}} = \overline{\overline{\boldsymbol{C}_C}} \times \overrightarrow{\boldsymbol{m}}$$ ~ Eq. [6.14]

That can be solved for $\overrightarrow{\boldsymbol{m}}$ by the least-squares method.

9.4: "Normative" calculations (reversed Ex. 8.5)

In R the least-squares method is implemented by the function `lsfit` setting `intercept = FALSE`, so that the model passes through the origin.

$$\overrightarrow{\boldsymbol{C}_S^*} = \overline{\overline{\boldsymbol{C}_C}} \times \overrightarrow{\boldsymbol{m}^*}$$

The value of mean squared residuals (R^2) represents an useful measure for goodness of fit:

$$R^2 = \left| \overrightarrow{\boldsymbol{C}_S^*} - \overrightarrow{\boldsymbol{C}_S} \right|^2 = \min.$$

9.1: Fractional crystallization (reversed Ex. 8.2)

wt. %	tonalite	dif. magma	Pl	Bt	Amp
SiO_2	55.09	57.270	53.41	35.32	45.35
TiO_2	0.75	0.710	0	2.11	1.39
Al_2O_3	17.59	16.681	29.48	15.31	9.47
FeOt	7.73	6.956	0.09	23.56	18.57
MgO	3.52	3.230	0	9.05	9.82
CaO	8.2	8.245	11.27	0.01	11.92
Na_2O	2.83	2.845	5.05	0.1	1.08
K_2O	2.04	1.748	0.12	9.81	1.02

sazava_fc2.data

- Given the compositions of the parental magma (tonalite), differentiated melt and crystallizing minerals (Table), estimate (by the least-square method) the degree of fractional crystallization and mineral proportions in the cumulate.

9.1: Fractional crystallization (reversed Ex. 8.2)

Setting

(C_0 = unfractionated/primitive magma, C_L = fractionated magma, C_{Pl}, C_{Bt}, C_{Amp} = mass proportions of plagioclase, biotite, amphibole in the crystallizing cumulate, F = melt fraction left in the system, m = mass proportions of minerals in the cumulate):

$$\overrightarrow{\boldsymbol{C_0}} = \begin{pmatrix} C_0^{SiO_2} \\ C_0^{TiO_2} \\ \vdots \\ C_0^{K_2O} \end{pmatrix} \quad \overline{\overline{\boldsymbol{C}}} = \begin{pmatrix} C_L^{SiO_2} & c_{Pl}^{SiO_2} & c_{Bt}^{SiO_2} & c_{Amp}^{SiO_2} \\ C_L^{TiO_2} & c_{Pl}^{TiO_2} & c_{Bt}^{TiO_2} & c_{Amp}^{TiO_2} \\ \vdots & & \vdots & \vdots \\ C_L^{K_2O} & c_{Pl}^{K_2O} & c_{Bt}^{K_2O} & c_{Amp}^{K_2O} \end{pmatrix} \quad \overrightarrow{\boldsymbol{f}'} = \begin{pmatrix} (F) \\ (1-F)m_{Pl} \\ (1-F)m_{Bt} \\ (1-F)m_{Amp} \end{pmatrix}$$

Allows a matrix formulation:

$$\overrightarrow{\boldsymbol{C_0}} = \overline{\overline{\boldsymbol{C}}} \times \overrightarrow{\boldsymbol{f}'}$$

Eq. [6.27]

That can be solved for $\overrightarrow{\boldsymbol{f}'}$ by the least-squares method.