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Geochemical Modeling of Fractional Magma Crystallization

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Geochemical Modeling of Fractional Magma Crystallization

Abstract

Modern day geologists use many different modeling programs such as Geospatial Information Systems in addition to R (programming language) for a wide array of applications such as: projecting collected data for mapping, visualization, and trend prediction. Computational power for these modeling programs is derived from Calculus, Probability, and Statistics. The purpose of this paper is to provide a site-specific geochemical analysis of an igneous rock formation composed of two specific compositions allowing for the predictions of rock formation derived from the resultant geochemical model.

Keywords

geology, math-balance equation, matrix operations, magma differentiation, fractional crystallization, syenite, shonkinite

Problem Statement

Identify what degree of crystallization from a known composition of primitive magma determines the differentiation and formation of syenite from the primitive magma rather than shonkinite formation from the primitive magma.

Motivation

The Earth is a complicated system that is a result of billions of years of complex physical processes that have led to its current formation. The pioneer of modern day geology, scientist James Hutton, considered the present to be the key to the past, with geologic processes driven by the same forces as those we can see at work today (Braterman). Many of these processes, such as, plate tectonics, petrology, hydrology, and geochemistry are well investigated. However, there is still a vast number of unknowns still yet to be discovered in these fields of study. Understanding how the Earth's formation occurred provides the ability to continue the expansion of knowledge. This understanding and knowledge allowing the global community to make informed decisions based on science. Mankind is still limited in its capabilities to examine and analyze the compositions of the subsurface (Chin, et al.). The world is such a large expanse that the physical examination and analyzation of the continental crust is mostly incomplete. This is due simply to the fact that there aren't enough scientists in the world to do a complete analyzation of the Earth's crust. Therefore, geologists are little by little adding data from their research of these unknowns to the scientific databases. The continued research and data collection allows for individuals in science, industry, engineering, and construction to guide their conclusions based on professionally recorded information.

The following geochemical model is a continuation of this process. A research team from the University of South Florida has provided a geochemical analysis of two specific rocks formations from an outcrop in San Rafael, Utah. The two rock types are shonkinite and syenite which form during an igneous process called fractional crystallization. The two rock types are found one on top of the other in the outcrop suggesting, they crystalize from the same primitive melt. The shonkinite, a more mafic rock, is found beneath the overlying syenite. This process of fractional crystallization is well understood. However, the specific degree of crystallization at which each rock is formed hasn't been examined for every specific rock type. This provides an opportunity to provide a geochemical model to explain these site-specific phenomena and understand the formation of the Earth's crust in further detail.

Mathematical Description and Solution

A key supposition in geochemical modeling is that it is a closed system with respects to thermodynamics. This means that the system only exchanges heat within itself and not with its surroundings. However, this is arguable when involving cases of a continually changing magma composition due to the fractionation are occurring. Even so, it is beneficial in that it allows for a mass-balance approach to modeling the crystallization process (Janoušek, et al., p. 69). The mass-balance equation will serve as the foundation for all the following calculations. However, matrix operations will be integrated during the calculation of the mass-balance equation to quantify an unknown variable C_s. The operations performed are to be repeated in a progression of steps which represent a specific fraction of crystallization of the primitive magma. Primitive melt compositional data was provided by Dr. Aurelie Germa from a rock outcrop in San Rafael, Utah (see appendix). The order of operations to be performed is as follows:

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1. Gather elemental data from the compositional analysis of parental rock (primitive melt).

2. Set up mass-balance equation and identify the unknown variables.

3. Set up matrix operations to calculate the desired unknown variable.

4. Substitute the results of the matrix operations in mass-balance equation and solve for the remaining unknown variable.

5. Repeated process for each desired percent of crystallization: 5.0%, 25.0%, 50.0%, 75.0%, and 95.0%.

6. Plot magmatic series data and contrast the data trend with the known compositional data of syenite.

The mass-balance equation for a closed system relies on the law of conservation of mass. As it relates to fractional crystallization, the mass-balance equation is simplified into the following form:

$$C_o^{\alpha} = FC_L^{\alpha} + (1 - F)C_s^{\alpha} \ . \qquad \text{(I)}$$

Equation (I) allows us to calculate the concentration (C) of any given element (α) where the subscripts O, L, and S are used to represent the primitive melt, the differentiated melt (see appendix), and the cumulate (see appendix) and where F represents the degree, or fraction, of crystallization (Janoušek, et al., p. 70). A rock is composed of minerals each with a composition that contains multiple elements or oxides. A multiple mineral cumulate can be cast into a matrix to allow for easier computation. The general formula for a cumulate containing any number of minerals is as follows:

$$C_s{}^{\alpha} = \sum_{k=1}^{n} (m_k c_k^{\alpha}), \qquad \text{(II)}$$

where m_k is the mass fraction of mineral k in the cumulate ($0 < m_k < 1$, all summing up to 1, i.e. $\sum_{k=1}^{n} m_k = 1$) and c_k^{α} is the concentration of each element α in mineral k (Janoušek, et al., p. 71). In this study's case the decisive rock forming minerals are olivine (*Ol*), clino-pyroxene (*Cpx*), and potassium feldspar (*Ks*). The major elements of value in determining mineral and therefore rock formation for the study are SiO_2, *FeO,* and Al_2O_3. For sake of clarity the oxides will be noted by their cations *Si*, *Fe*, and *Al*. This cumulate (formula (II)) can be further described by the following system of equations which will result in a vector $\overrightarrow{C_s^{\alpha}}$:

$$\left\{\begin{array}{l} C_s^{Si} = \sum_{k=1}^{n}\left(m_k c_k^{Si}\right) = m_{Ol}c_{Ol}^{Si} + m_{Cpx}c_{Cpx}^{Si} + m_{Ks}c_{Ks}^{Si} \\ C_s^{Fe} = \sum_{k=1}^{n}\left(m_k c_k^{Fe}\right) = m_{Ol}c_{Ol}^{Fe} + m_{Cpx}c_{Cpx}^{Fe} + m_{\ Ks}c_{Ks}^{Fe} \\ C_c^{Al} = \sum_{k=1}^{n}\left(m_k c_k^{Al}\right) = m_{Ol}\,c_{Ol}^{Al} + m_{Cpx}c_{Cpx}^{Al} + m_{Ks}c_{Ks}^{Al} \end{array}\right\}. \qquad \text{(III)}$$

System (III) may be condensed by expressing the compositions as a vector in the defined space:

$$\overrightarrow{C_s} = \begin{bmatrix} C_s^{Si} \\ C_s^{Fe} \\ C_s^{Al} \end{bmatrix}. \qquad (1)$$

Furthermore, to aid in a computer friendly version for calculation purposes, this vector and the previous system of equations (III) may be recast into a more compact form:

$$\overrightarrow{C_s} = \overline{\overline{C_c}}\; x\; \vec{m}, \qquad (1.1)$$

where $\overline{\overline{C_c}}$ represents the relevant compositions of all the individual cumulate minerals that has been recast into a matrix with *p* elements in rows and *n* minerals in columns. Therefore:

$$\overline{\overline{C_c}} = \begin{bmatrix} c_{Ol}^{Si} & c_{Cpx}^{Si} & c_{Ks}^{Si} \\ c_{Ol}^{Fe} & c_{Cpx}^{Fe} & c_{Ks}^{Fe} \\ c_{Ol}^{Al} & c_{Cpx}^{Al} & c_{Ks}^{Al} \end{bmatrix}. \qquad (1.2)$$

which further defines a vector $\vec{m}$ with *n* mineral mass fractions:

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$$\vec{m} = \begin{bmatrix} m_{Ol} \\ m_{Cpx} \\ m_{Ks} \end{bmatrix}. \qquad (1.3)$$

It should be noted that all concentrations required in the matrix are derived from the known and accepted experimental data by the professional geological community for the formation of the specified minerals (see appendix). The mineral mass fractions are also derived from known data (see appendix) in relation to the fraction of mineral within a rock which classifies it between one of our two known rock compositions: the more primitive shonkinite (which is formed from a lower fraction of crystallization) and shonkinite (which is formed at a higher fraction of crystallization). The data from the resultant vector of the matrix operation $\overrightarrow{C_s} = \overline{\overline{C_c}}\ x\ \vec{m}$ may then be used in the mass balance equation to find the desired unknown variable C_L^{α} noting, however, that a separate mass balance equation must be done for each specific oxide *SiO_2*, *Al_2O_3*, and *FeO*. Re-arranging the mass balance equation (I) to solve for C_L^{α} provides the following formula:

$$C_L^{\alpha} = \frac{C_o^{\alpha} - (1-F)C_s^{\alpha}}{F}. \qquad (2)$$

To calculate the model, we begin at a step zero that represents rock (shonkinite). It was calculated that the sample specimen collected was 5.0 percent crystalized. Therefore, F = 0.05 at step zero. The degree of F has been pre-selected for each subsequent step. Following each step of differentiation, the calculated C_L from the previous step becomes the new C_o of the subsequent step. This is the phenomena that allows for the modeling of a magmatic series as each portion of crystalized material is differentiated. Although, it stays a part of the system, the liquid portion of magma remaining becomes altered as the crystallization depletes some elements from the liquid portion of the magma. This in turn changes the proportion of the remaining elements in the liquid

portion of the system increasing the proportion of some. Additionally, each new step has a prior calculated mass fraction vector $\vec{m}$ which corresponds to the degree of crystallization of each step. Computing the data and projecting the magmatic series results in the following:

Step 0

$$\overrightarrow{C_s} = \begin{bmatrix} C_s^{Al} \\ C_s^{Fe} \\ C_s^{Si} \end{bmatrix} = \begin{bmatrix} 0.15 & 8.60 & 18.59 \\ 18.75 & 5.96 & 0.00 \\ 39.02 & 48.30 & 65.71 \end{bmatrix} x \begin{bmatrix} 0.09 \\ 0.42 \\ 0.15 \end{bmatrix} \approx \begin{bmatrix} 6.41 \\ 4.19 \\ 33.65 \end{bmatrix}. \qquad (1.4)$$

Substitute the primitive C_0 and values of the sampled rock (shonkinite) that has been analyzed and the calculated C_s values into the re-arranged mass balance formula with F = 0.95 (5.0 % crystallization):

$$C_L^{Al} = \frac{14.73-(1-0.95)6.41}{0.95} \approx 15.16\% , \qquad (2.1)$$

$$C_L^{Fe} = \frac{10.17-(1-0.95)4.19}{0.95} \approx 10.49\% , \qquad (2.2)$$

$$C_L^{Si} = \frac{46.52-(1-0.95)33.65}{0.95} \approx 47.20\% . \qquad (2.3)$$

Step 1

Repeat the process, however, using F = 0.75 (25.0% crystallization) and corresponding $\vec{m}$ values for that degree of crystallization. Additionally, the new C_o values are the resultant C_L values from the previous step. This is what creates the magmatic series:

$$\overrightarrow{C_s} = \begin{bmatrix} C_s^{Al} \\ C_s^{Fe} \\ C_s^{Si} \end{bmatrix} = \begin{bmatrix} 0.15 & 8.60 & 18.59 \\ 18.75 & 5.96 & 0.00 \\ 39.02 & 48.30 & 65.71 \end{bmatrix} x \begin{bmatrix} 0.07 \\ 0.38 \\ 0.25 \end{bmatrix} \approx \begin{bmatrix} 6.23 \\ 3.39 \\ 37.17 \end{bmatrix}. \qquad (1.5)$$

Therefore,

$$C_L^{Al} = \frac{15.27-(1-0.25)6.23}{0.75} \approx 18.28\% , \qquad (2.4)$$

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$$C_L^{Fe} = \frac{10.51-(1-0.25)3.39}{0.75} \approx 12.88\% , \quad (2.5)$$

$$C_L^{Si} = \frac{47.18-(1-0.25)37.17}{0.75} \approx 50.51\% . \quad (2.6)$$

Step 2

Repeat previous steps once again using the C_L values from the previous step as the new C_o values and continue the trend for the remainder of the steps. However, the value of F for the following steps remains

constant as the subsequent steps degree of crystallization will be controlled by the associated $\vec{m}$ values. The 50.0% crystallization at step 2 is as follows:

$$\overrightarrow{C_s} = \begin{bmatrix} C_s^{Al} \\ C_s^{Fe} \\ C_s^{Si} \end{bmatrix} = \begin{bmatrix} 0.15 & 8.60 & 18.59 \\ 18.75 & 5.96 & 0.00 \\ 39.02 & 48.30 & 65.71 \end{bmatrix} x \begin{bmatrix} 0.05 \\ 0.34 \\ 0.34 \end{bmatrix} \approx \begin{bmatrix} 7.96 \\ 2.97 \\ 40.31 \end{bmatrix}. \quad (1.6)$$

Therefore,

$$C_L^{Al} = \frac{18.28-(1-0.25)7.96}{0.75} \approx 21.72\% , \quad (2.7)$$

$$C_L^{Fe} = \frac{12.88-(1-0.25)2.97}{0.75} \approx 16.18\% , \quad (2.8)$$

$$C_L^{Si} = \frac{50.51-(1-0.25)40.31}{0.75} \approx 53.91\% . \quad (2.9)$$

Step 3

Continue the trend using designated $\vec{m}$ values for 75% crystallization:

$$\overrightarrow{C_s} = \begin{bmatrix} C_s^{Al} \\ C_s^{Fe} \\ C_s^{Si} \end{bmatrix} = \begin{bmatrix} 0.15 & 8.60 & 18.59 \\ 18.75 & 5.96 & 0.00 \\ 39.02 & 48.30 & 65.71 \end{bmatrix} x \begin{bmatrix} 0.03 \\ 0.30 \\ 0.44 \end{bmatrix} \approx \begin{bmatrix} 9.69 \\ 2.55 \\ 43.46 \end{bmatrix}. \quad (1.7)$$

Therefore,

$$C_L^{Al} = \frac{21.72-(1-0.25)9.69}{0.75} \approx 25.75\% , \quad (2.10)$$

$$C_L^{Fe} = \frac{16.18-(1-0.25)2.55}{0.75} \approx 20.72\% , \quad (2.11)$$

$$C_L^{Si} = \frac{53.91-(1-0.25)43.46}{0.75} \approx 57.40\% . \quad (2.12)$$

Step 4

Final step of the series with designated $\vec{m}$ values for 95% crystallization:

$$\overrightarrow{C_s} = \begin{bmatrix} C_s^{Al} \\ C_s^{Fe} \\ C_s^{Si} \end{bmatrix} = \begin{bmatrix} 0.15 & 8.60 & 18.59 \\ 18.75 & 5.96 & 0.00 \\ 39.02 & 48.30 & 65.71 \end{bmatrix} x \begin{bmatrix} 0.01 \\ 0.26 \\ 0.53 \end{bmatrix} \approx \begin{bmatrix} 11.42 \\ 2.12 \\ 46.61 \end{bmatrix}. \quad (1.8)$$

Therefore,

$$C_L^{Al} = \frac{25.73-(1-0.25)11.42}{0.75} \approx 30.50\% , \quad (2.13)$$

$$C_L^{Fe} = \frac{20.72-(1-0.25)2.12}{0.75} \approx 26.92\% , \quad (2.14)$$

$$C_L^{Si} = \frac{57.40-(1-0.25)46.61}{0.75} \approx 61.00\% . \quad (2.15)$$

Having completed the computation for the magmatic series, a projection of the data in a graphical representation will allow for further data analysis. The graphical results are presented on the subsequent pages. The data on the following table may be cast into two plot charts representing the two rock determining oxides (*FeO* and Al_2O_3) content versus the SiO_2 content at each step of the crystallization process.

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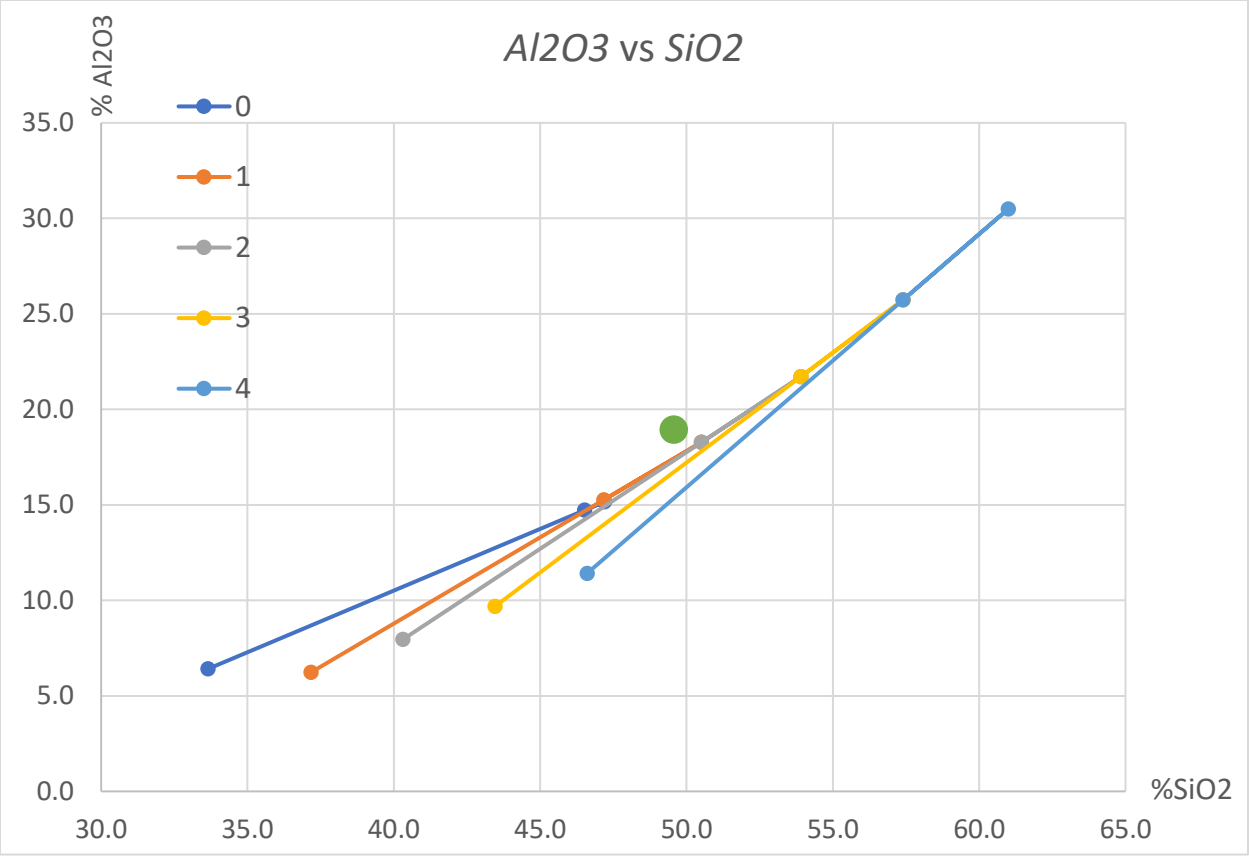
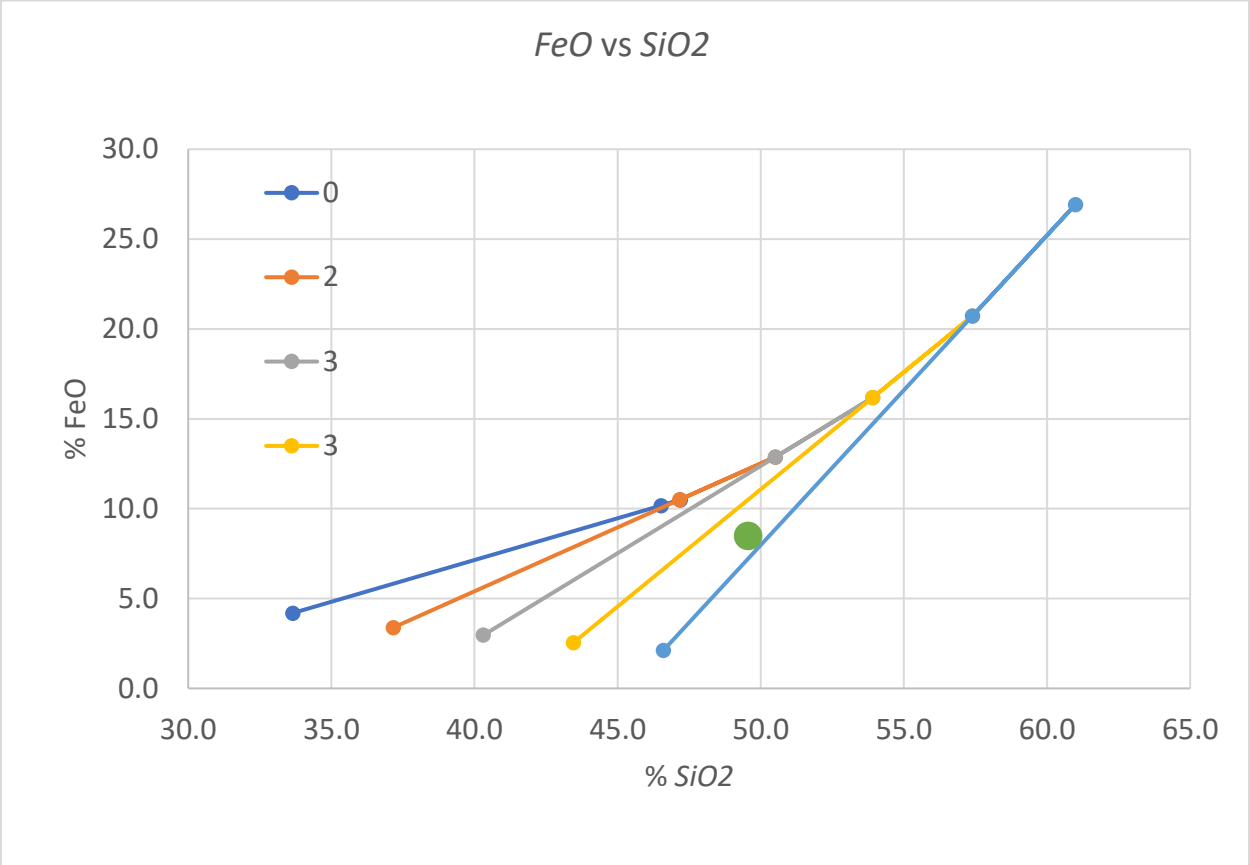

Al2O3 vs SiO2
% Al2O3
0
1
2
3
4
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
30.0
35.0
40.0
45.0
50.0
55.0
60.0
65.0
%SiO2



Discussion

After having compiled all the required data from the magmatic series the results have provided an estimated evaluation of the geochemical behavior during crystallization of the original primitive melt (shonkinite). The data is meant to be suggestive only and is merely a model for the ideal situation in nature. However, this data allows for an estimation of the geochemical composition during any point of the magmatic fractional crystallization series. Comparing the data point of the known composition of a syenite rock formation, the graph suggests a Syenite rock formation at its nearest neighboring C_o data point. Using this data point

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and relating its associated degree of crystallization for the step of crystallization allows for an estimation of what degree of crystallization the syenite forms at. Even when comparing the two-major rock relative oxides, the nearest neighboring C_o data point for both charts is during the second step, which is the result of a 50.0% crystallization of the primitive melt.

Conclusion and Recommendations

The results of the data analysis suggest that syenite formation will start at an estimated 50.0% degree of crystallization of the primitive melt. Although the results provided by the graph for the magmatic series and the known composition of syenite match up to provide a reasonable estimation of degree of crystallization at which syenite forms, it could be clarified even further. The inclusion of all the 10 major rock forming elements in nature as well as the incorporation of all of the rock forming minerals specific to the two-rock end members would allow for a further clarified projection. Finally, the increments of degree of crystallization could also be measured and analyzed in smaller increments to provide a more detailed model. This would allow for even further accuracy of the model. In conclusion, the results of the model and analysis have provided the acceptable and useful results that can be further expanded upon.

Nomenclature

F	Fraction of liquid remaining in the system
α	Any given element
C_o^{α}	Mass percent of α in primitive melt
C_L^{α}	Mass percent of α in the differentiated melt
C_s^{α}	Mass percent of α in the cumulate
m	Mass fraction
$\underset{m}{\rightarrow}$	Vector of mass fraction
$\overline{\overline{C_c}}$	cumulate compositional matrix
Fe	Iron oxide
Si	Silicon dioxide
Al	Aluminum oxide
Ol	Mineral Olivine
Cpx	Mineral Clinopyroxene
Ks	Mineral Potassium Feldspar

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Appendix

San Rafael Site Analysis provided by Dr. Germa

Location	sample	rock type	SiO2	TiO2	Al2O3	FeOt	MnO	MgO	CaO	Na2O	K2O	P2O5
Frying	FP-1	syenite	49.5746	1.5883	18.93668	8.4736	0.1474	3.4948	7.5198	4.6179	4.7820	0.8650
Frying	FP-2	shonkinite	46.5183	1.3452	14.7271	10.17047	0.2095	10.1419	10.41104	2.4496	2.7108	1.3161
Frying	FP-05B	syenite	50.7979	1.4178	17.6918	7.0058	0.2491	1.9139	6.3310	5.0286	3.8639	0.5518

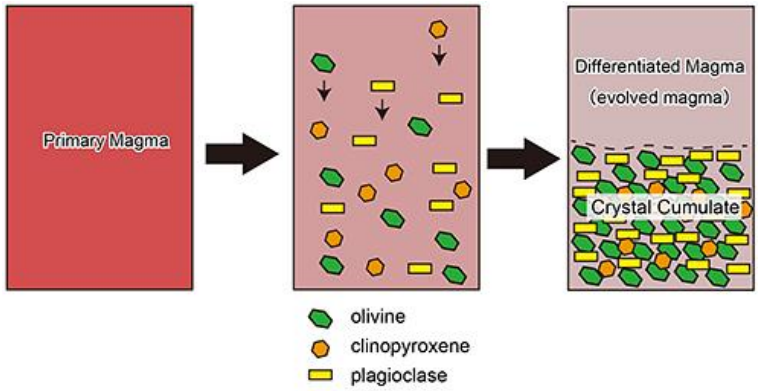
Pre-calculated mineral mass fraction of shonkinite – syenite end members

mineral fraction	Step0	Step1	Step2	Step3	Step4
Ol	0.09	0.07	0.05	0.03	0.01
Cpx	0.42	0.38	0.34	0.3	0.26
Kspar	0.15	0.245	0.34	0.435	0.53

Calculated values during model computation

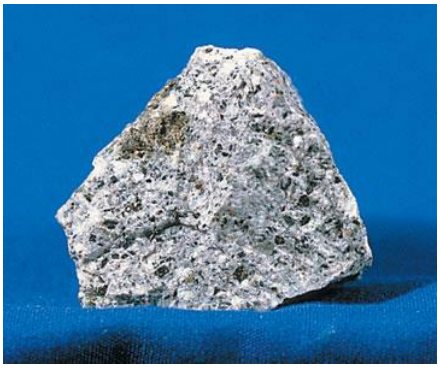
Crystallization step		%Al203	%FeO	%SiO2
0	C_o	14.7	10.2	46.5
0	C_L	15.2	10.5	47.2
0	C_S	6.4	4.2	33.7
1	C_o	15.3	10.5	47.2
1	C_L	18.3	12.9	50.5
1	C_S	6.2	3.4	37.2
2	C_o	18.3	12.9	50.5
2	C_L	21.7	16.2	53.9
2	C_S	8.0	3.0	40.3
3	C_o	21.7	16.2	53.9
3	C_L	25.7	20.7	57.4
3	C_s	9.7	2.5	43.5
4	C_o	25.7	20.7	57.4
4	C_L	30.5	26.9	61.0
4	C_s	11.4	2.1	46.6

Visual of simplified magma differentiation process



Shonkinite

Syenite



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Glossary of terms

Differentiation- an igneous process that causes the chemical composition of a magma to be altered.

Outcrop- a rock formation that had been exposed to the surface of the earth through processes such as erosion, plate tectonics, and uplift.

Cumulate- an accumulation of settled minerals in a magma chamber during fractional crystallization.

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