Trends in ternary petrologic variation diagrams—fact or fantasy?

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Abstract

For more than 75 years petrologists (among others) have made use of triangular variation diagrams to illustrate compositional variability among members of a predefined igneous rock suite and to draw genetic information from the spatial positioning of the points on the diagram. When ternary percentages are formed, the summary univariate and bivariate statistics of the ternary percentages will usually differ from their counterparts in the parent data array. Such changes are due entirely to the effects of percentage formation. For example, reversals in the rank order of variances often occur, with the result that the variable with the smallest variance in the initial array may have the largest variance in the ternary array. Such changes may be understood by examining the row sum variable (the sum of the values of the initial variables selected to create the ternary array) and the correlation between the row sum variable and each of the initial variables (the part–whole correlation). The correlation coefficients between the three ternary variables are likely to differ considerably from their initial values. The net effect is that any observed ternary trends must be considered to result from a complicated set of interactions including: (1) the sampling strategy used to assemble the initial data set; (2) the summary statistics in the initial data set which themselves are subject to modification by percentage formation; (3) the part–whole correlations in the initial data set; (4) restrictions on the variances of a closed ternary array; (5) modifications of all univariate and bivariate statistics accompanying ternary percentage formation; (6) petrogenetic controls. Unless a rational means of separating these effects from each other can be found it would appear to be unprofitable to attempt to base genetic statements on ternary variations.

"It is frequently supposed that curves drawn in ternary diagrams reveal fundamental relations between the variables..." (Chayes, 1961, p. 160)

Introduction

For more than 100 years petrologists have debated how to most effectively portray the chemistry of igneous rocks for classification purposes and for revealing underlying petrogenetic processes. Particularly revealing are Iddings’ comments (1903, p. 9) concerning the necessity for reliance on graphical devices:

“The intricate variations in the amounts of numerous mineral components or of chemical components, baffle most attempts to comprehend their interrelationships by simple contemplation or by study of the numbers in which they may be expressed. Many facts and relations are overlooked which are readily observed when diagrams are used to represent numerical figures. Moreover, visual memory is sufficiently developed in most persons to enable them to carry in mind simple geometrical forms, where it does not permit them to recollect manifold assemblages of oft-repeated numbers. Mental impressions of simple diagrams, therefore, are more definite and lasting and enable the student to store up a much greater amount of quantitative data than he could otherwise acquire.”

Most of Iddings’ comments were directed towards classification problems and strategies, but it seems obvious that his basic philosophy has been adopted by many whose primary concern lies in elucidating petrogenetic relations.

It is hard to disagree with Iddings’ desire to uncomplicate a complicated situation, but it is incumbent upon the user to ascertain whether the ma-
The manipulations required to prepare the graphical device have in any way modified the relations among the selected variables. For example, Chayes (1971, p. 71) noted that many of the data manipulation schemes commonly resorted to by petrologists result in distortion of such magnitude that many of the trends are more a measure of numerical consequence than petrogenetic reality.

Of particular interest (to the author and most petrologists it would seem) are the ternary variation diagrams such as CaO–Na₂O–K₂O (CNK) and total iron–MgO–(Na₂O + K₂O) (FMA). Iddings (1903) credits Becke (1897) with being the first to represent the compositions of igneous rocks by recalculating Ca, Na, and K to 100% and plotting this information on an equilateral triangle in which the zero point was at the center of the diagram. Reid (1902) appears to have been the first petrologist to use the modern triangular diagram in which each side of the triangle is divided into 100 parts.

Since 1902 many petrologic presentations have made use of either the CNK or the FMA (or both) types of variation diagrams, and it appears that many of the users have inferred that the principal factor governing the configuration of the observed trends is related to some process of crystal fractionation.

Wright (1974, p. 236–237) argued against the use of FMA diagrams for deducing petrogenetic information for the following reasons:

1. For most igneous rock series the amounts of the oxides combined to form the FMA diagrams comprise considerably less than 50% (by weight) of the samples.
2. Trends which appear to be significant can be created by mixing together samples which obviously have no genetic relationships.
3. Normalization to 100% of sums that are not the same distorts the plots with the result that trend orientations do not quantitatively express specific mineral controls.

Similar statements can be made concerning the CNK or any other conceivable ternary variation diagram. If one wishes to define total variability as the sum of the variances of the measured oxide components (Chayes, 1964), the FMA and CNK components generally account for considerably less than 25% of the total variability of the rock suite being investigated (Butler, 1975), and one gets the feeling that a considerable quantity of potentially useful information is being ignored.

Barker (1978) agreed in principle with Wright’s objections to the continued use of the FMA diagrams but argued that “the significance of trends on alkali–iron–magnesium diagrams can be better understood by examining the relations between compositions of rocks and their constituent minerals when projected on the AFM plane.”

An expected change in all of the univariate statistics of the selected variables and in any of the pairwise measures of association is the most insidious consequence of forming ternary percentages. Not only do the observed trends lead to non-quantitative expressions of mineralogical control (Wright, 1974), but it is conceivable that an attempt to extract information of a qualitative nature (Barker, 1978) will fail to isolate mineralogical/fractionation effects from the numerical consequences of ternary percentage formation.

The purpose of this note is to review the effects of percentage formation on the properties of ternary variables and to assess the probability of determining the underlying causes of the trends commonly observed in FMA and CNK variation diagrams.

Preparation of the ternary diagram and the part–whole correlation

The general topic of the effects of percentage formation on the properties of ternary variables has been reviewed admirably by Chayes (1971, p. 36–43) and will be referred to only with respect to the ternary case. When we decide which variables (single or in some combination) will be used to define the ternary subset, the original values (which constitute the initial data set) are recalculated to 100% (in order to keep the notation as simple as possible, unprimed letters will be used to refer to the initial variables and primed letters to the ternary percentages):

\[ A'_i = 100(A_i/T_i) \]  

T, is the sum of the values of A, B, and C in the ith row of the data matrix:

\[ T_i = A_i + B_i + C_i \]  

It is useful to focus attention on the summary statistics of the three initial variables and the row sum (T) in order to understand and appreciate the effect of percentage formation in controlling ternary trends. The importance of the row sum statistic cannot be overemphasized, although it is unlikely that the investigator would bother to compute its summary sta-
If the initial variables (A, B, and C) are uncorrelated (in which case the Pearson product moment correlation coefficient \(r\) equals zero), there will be a positive correlation between any one of the initial variables and T (this type of correlation will be referred to as the part–whole correlation as, for example, A is part of T—equation la):

\[
r_{AT} = \frac{s_A}{s_T}
\]

where \(s\) is the standard deviation of the variable identified by the subscript. Similar equations can be written for variables B and C by appropriately switching the subscripts. If the initial variables are correlated \((r \neq 0.0)\) the part–whole correlation between A and T is given by:

\[
r_{AT} = \frac{(s_A + s_B r_{AB} + s_C r_{AC})}{s_T}
\]

From equation (2a) it is clear that the part–whole correlation may be positive or negative if the initial variables are correlated, and that the sign of the part–whole correlation is controlled by the signs and magnitudes of the correlations between the initial variables. Any data set in which the sum of the values of the variables is a constant for all of the samples is considered to be a closed data set. The standard deviation of the row sum variable \(s_T\) in a set of closed data is equal to zero, and the part–whole correlation (equations 2 and 2a) is undefined. Wright's (1974) third objection to the use of the FMA variation diagrams stems from the fact that the initial values of F, M, and A do not constitute a closed data set by themselves.

I have examined the properties of many ternary arrays from a variety of published sets of chemical information (Butler, 1975), and the set of 114 chemical analyses of igneous rocks from the Big Bend National Park area of west Texas (Maxwell et al., 1967) has been selected to illustrate the effects of ternary percentage formation on the properties of the individual variables and to analyze the trends that are frequently observed in the CNK and FMA types of variation diagrams. Summary statistics for the CNK and FMA subsets are given in Tables 1 and 2 respectively.

### Effect of percentage formation on the mean of ternary variables

A series of approximations can be derived which allow estimating the properties of ternary variables from the properties of the initial variables (Chayes, 1971; Butler, 1978). Chayes' first-order approximation for the mean of a percentage is given by:

\[
\bar{A}' = 100(\bar{A}/T)
\]

That is, the mean of a ternary variable is approximated by 100 times the ratio of the mean of the initial variable to the mean of the row sum variable (T). The ratio of the ternary mean to the initial mean \((R_m)\) is given by:

\[
R_m = \frac{\bar{A}'}{\bar{A}} = 100(\bar{A}/T)/\bar{A} = 100/T
\]

Obviously, the ratio \(R_m\) will be the same for all three variables. From Tables 1 and 2, however, it is clear that the ratio of the means is not constant for all three variables. A second-order approximation for the mean of ternary variables (Butler, 1978) is given by:

\[
\bar{A}' = 100(\bar{A}/T)(1 - r_{AT} C_A C_T + C_T^2)
\]
Table 2. Summary statistics for 114 west Texas analyses: total iron–MgO–(Na2O + K2O)

<table>
<thead>
<tr>
<th></th>
<th>MgO</th>
<th>Alkali</th>
<th>Alkali</th>
<th>Iron</th>
<th>Row Sum</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mean</strong></td>
<td>11.00</td>
<td>2.39</td>
<td>51.81</td>
<td>8.23</td>
<td>37.19</td>
</tr>
<tr>
<td><strong>S.D.</strong></td>
<td>12.34</td>
<td>3.10</td>
<td>21.94</td>
<td>2.35</td>
<td>12.46</td>
</tr>
<tr>
<td><strong>CV</strong></td>
<td>1.12</td>
<td>1.23</td>
<td>0.42</td>
<td>0.28</td>
<td>0.34</td>
</tr>
<tr>
<td><strong>Variance</strong></td>
<td>18.24</td>
<td>1.15</td>
<td>57.67</td>
<td>0.66</td>
<td>10.60</td>
</tr>
<tr>
<td><strong>Skewness</strong></td>
<td>1.32</td>
<td>1.71</td>
<td>-0.17</td>
<td>-0.32</td>
<td>-0.30</td>
</tr>
</tbody>
</table>

The variance of a ternary variable can be approximated from the properties of the initial variables by (Chayes, 1971; Butler, 1978):  

\[ s_{\alpha}^2 = 10^4 \left( \frac{\text{A}}{\text{T}} \right)^2 (C_A + C_T^2 - 2r_{\text{AT}} C_A C_T) \]  
(4)

The ratio of the ternary variances of variables A and B is given by:  

\[ \frac{s_{\alpha}^2}{s_{\beta}^2} = \left( \frac{s_{\alpha}^2}{s_{\beta}^2} \right) (C_A + C_T^2 - 2r_{\text{AT}} C_A C_T) \]  
(4a)

which was written in a form which emphasizes the relationship between the initial variances and the ternary variances. The behavior of MgO and total alkalis (Table 2) illustrates a situation of frequent occurrence. The variable with the smallest variance in the initial data set (total alkalis) has the largest variance in the ternary subset. Although there is a large number of variables in equation 4a, several generalizations can be made concerning reversals in variance rank order:

(1) Reversals in rank order of variance are favored when the variable with the largest initial variance has the largest initial coefficient of variation (other quantities being equal).

(2) Reversals in rank order of variance are favored when the variable with the largest initial variance has a positive part–whole correlation and the variable with the smallest initial variance has a negative part–whole correlation (other quantities being equal).

In all the FMA diagrams examined by the author (identified in Butler, 1975), the behavior exhibited by the initial and ternary variables is very similar. F, M, and A account for a very small percentage of the total initial variance (usually less than 10%), and total alkalis have the smallest variance in the initial set and the largest in the ternary subset.

Even when reversals in rank order of the variances do not occur, changes in the ratio of the variances almost always occur when ternary percentages are formed (Tables 1 and 2). It seems intuitively reasonable to expect that the trend and scatter appearing on any form of ternary variation diagram in part reflect the variances of the variables. Given the fact that major reversals of variance can occur simply as the result of ternary percentage formation, it should be just as reasonable to expect that at least part of any trend may be artificial.
Effect of ternary percentage formation on the skewness of ternary variables

The skewness of a variable is a measure of the asymmetry of its distribution. Pearson (1926) noted that a ratio formed from two symmetrically distributed variables (zero skewness) will have an asymmetrical distribution (non-zero skewness). The sign of the skewness of such a ratio (for example, A/T) will be given by the sign of L (Merrill, 1928):

\[ L_A = C_T - r_{AT}C_A \]  

As the initial variables in a set of chemical analyses commonly have non-zero values of skewness, \( L_A \) does not give the sign of the skewness but does indicate the direction of change of skewness following ternary percentage formation. For example, MgO (Table 2) has a skewness of 1.71 in the initial data set, and the computed \( L_{MgO} \) of −0.85 indicates that percentage formation should and does decrease the skewness to 1.32. In general, it does not make sense to worry about a genetic interpretation of skewness of a percentage, as its sign and magnitude may be numerical rather than petrologic in origin (Butler, 1978).

Effects of percentage formation on the total variance of a closed array and on the correlation between a pair of variables

Chayes (1961, 1962) showed that no closed standard deviation can be as large as the sum of the standard deviations of the remainder of the variables. The situation where one standard deviation equals the sum of the other two (in the case of ternary percentages) can occur only when that variable is perfectly negatively correlated with the other variables and the other variables are perfectly positively correlated with each other:

\[ s_A = s_B + s_C \text{ if, and only if,} \]
\[ r'_{AB} = r'_{AC} = -1.0 \text{ and } r'_{BC} = 1.0 \]

A plot of the ternary variables which obey these relations will define a straight line in an equilateral triangle. The line heads away from the apex of the triangle at which the variable with the largest standard deviation is plotted. As the quantity \( s_B + s_C \) begins to exceed \( s_A \), the straight line is replaced by a linear trend and the three correlations depart from an absolute value of 1.0. The CNK diagram for the west Texas data set, given in Figure 1, is typical of other CNK plots examined by the author. The trend begins near the CaO apex and extends to the Na₂O-K₂O limiting binary.

Qualitatively it appears that the linear trend expressed in Figure 1 evolves into a simple curvilinear trend as the quantity \( s_B + s_C \) departs from \( s_A \) and \( r_{AB}, r_{AC} \) and \( r_{BC} \) approach 0.0. The FMA variation diagram for the west Texas data set, given in Figure 2, appears to be typical of curvilinear ternary plots. The trend is initiated near the apex where the variable with the largest standard deviation is plotted (total alkalis for Fig. 2), and the inflection point is nearest the apex where the remaining variable with the largest mean is plotted (total iron).

One normally considers the correlation coefficient...
to be a measure of the strength of the linear pair-wise association between a pair of variables. However, Chayes (1971) showed that the correlation between a pair of ternary variables can be expressed as a function of the variances of the three ternary variables:

$$r_{BC} = \frac{\left(\bar{s}_A^2 - (\bar{s}_B^2 + \bar{s}_C^2)/2\bar{s}_A\right)}{s_A^2}$$ (7)

where similar expressions can be given for $r_{AC}$ and $r_{AB}$ by appropriately switching subscripts. From equation 7 it is clear that ternary variables pose a difficult problem in interpretation. The correlation between a pair of ternary variables (for example, B' and C') is positive if, and only if, the sum of the variances of B' and C' is less than the variance of ternary variable A'. If all three initial variables are positively correlated, only one pair of the ternary variables will be positively correlated and, commonly, all three pairs will be negatively correlated. In the CNK and FMA diagrams examined there are no reversals in the sign of the correlation coefficients, but there certainly is a change in their magnitudes (see Tables 1 and 2). For example, the correlation coefficient between initial values of MgO and total iron (Table 2) is 0.760 and that between the two ternary variables is 0.566. If the other two correlations (between MgO and total alkalis, and between total iron and total alkalis) were to remain constant and if the correlation between MgO and total iron were to approach 1.0, the trend would approach linear behavior, whereas if the value were to approach 0.0 the trend would become curvilinear with an even more pronounced curvature (compared to Fig. 2).

In summarizing the difficulties inherent in working with ternary variables, Chayes (1961, p. 161) stated “many of the alleged ternary trends are probably best regarded as complicated and camouflaged statements of variance relations largely controlled by the criteria set up in the sampling plan.” Recalling that ternary percentage formation can result in major changes in variance and in the rank order of the three variances, Chayes’ reference to “camouflaged statements of variance relations” must be taken seriously. Perhaps, however, it would be more appropriate to say that the ternary trends are best thought of as reflections of the part-whole correlations present in the parent data set.

Irvine and Baragar (1971) argued that tholeiitic (simple linear) and calc-alkaline (curvilinear) suites could be easily distinguished by their trends on FMA variation diagrams. As noted above, however, a gradation between these two end-member trends is to be expected as a function of the variances of the variables which are a function of: (1) the sampling strategy used to construct the data array and (2) the part-whole correlation. Miyashiro (1975), in fact, argued that a complete gradation exists between the tholeiitic and calc-alkaline suites. Barker (1978) attributed the increased scatter of the typical calc-alkaline trends in an FMA variation diagram to a more pronounced fractionation of plagioclase. However, as evidenced by the previous discussion, ternary curvilinear relations are characterized by two correlations with relatively large negative values and one correlation that is usually positive but may be close to zero. Thus, one should expect greater scatter with a curvilinear trend than with a linear trend, regardless of whether plagioclase is precipitating from or dissolving into a magma; unless, of course, one could relate plagioclase behavior to the part-whole correlation in the initial data set.

Extension of the preceding arguments to the initial data set

Chayes (1971, p. 44-45) has argued that a chemical analysis is closed by observation. Errors of omission and/or commission account for the fact that a good analysis will commonly total between 98.5 and 101.5. The point is, one must recognize that the univariate and bivariate statistical properties of the parent data set contain some contribution from the closure effect.

Wright’s (1974) objection concerning normalization to 100% of sums that are not constant has been discussed previously. In the same discussion Wright suggests that petrologic relations can be best discerned by using a bivariate plot of MgO vs. all other major oxides, rather than by using SiO₂ (which leads to the familiar Harker diagram) for the mafic and ultramafic suites. All binary variation diagrams (including Harker diagrams and Wright’s MgO variation diagrams), while reasonable on petrologic grounds, fail to consider that an unknown portion of the observed correlation and scatter is the result of percentage formation. At this time it does not appear possible to satisfactorily separate the effects of percentage formation from fractionation, assimilation, or whatever petrologic model the investigator may have in mind.

Wright and Hamilton (1978) suggested using MgO variation diagrams to define chemical types of igneous rocks. Samples from an igneous unit that is stratigraphically restricted are plotted on such a vari-
ation diagram and used to define a polygonal field which may aid in characterizing the chemical type of unit and aid in identifying unknown samples. The spread of data points on such a binary diagram reflects the variances of the plotted variables and the correlation between them. As both the variance and correlation are likely to have been modified by percentage formation, the shape of the defining polygon may have a component due to the closure effect.

Summary and conclusions

The preceding discussion shows that when one forms percentages the summary univariate and bivariate statistics change. This effect may be so drastic as to change the rank order of the means, variances, and correlation coefficients so that, for example, the variable with the smallest variance in the initial data set has the largest variance in the ternary data set. This combination of changes in means, variances, and correlations manifests itself in the nature of the distribution of the sample points in an equilateral triangle. Simple linear and curvilinear trends are gradational as revealed by the following relations:

1. straight line: \( r_{AC} = r_{AB} = -1.0 \) and \( r_{BC} = +1.0 \)
2. linear trend: \( r_{AC} \) and \( r_{AB} \) are large negative; \( r_{BC} \) is large positive
3. curvilinear: \( r_{AC} \) and \( r_{AB} \) are intermediate to large negative; \( r_{BC} \) is intermediate to small positive

Therefore, the observed ternary trend must be considered to result from a complicated set of interactions including: (1) the sampling strategy used to assemble the initial data set; (2) the summary statistics in the initial data set, which themselves are subject to modification by percentage formation effects; (3) the part-whole correlations in the initial data set; (4) restrictions on the variances of a closed subset; (5) modifications of all univariate and bivariate summary statistics accompanying ternary percentage formation; (6) petrogenetic controls.

Unless a rational means of separating these effects from each other can be found, it would appear to be unprofitable to attempt to base genetic statements on ternary variations by themselves.

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