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(Principal Investigator: E. H. Timothy Whitten)

NORTHWESTERN UNIVERSITY REPORT NUMBER 23

ENIGMAS IN ASSESSING THE COMPOSITION OF A ROCK UNIT:
A CASE HISTORY BASED ON THE MALSBURG GRANITE, S. W. GERMANY

by

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Statistical evaluation of the composition, physical properties,
and surface configuration of terrestrial test sites
and their correlation with remotely-sensed data

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PREFACE

The paper contained in this report was prepared as an invited contribution to be presented at the Section of Mathematical Methods in the Earth Sciences of the "Mining Příbram in Science and Technics, 1970" to be held in Příbram, Czechoslovakia in October 1970. Although the Malsburg Granite of Germany is used by way of illustration the subject matter is general and applicable to sampling any lithic unit at the lithosphere-atmosphere interface. It has direct and particular bearing on the subject-matter of the present NASA research grant. The main thrust of the research grant has been exploration of the interface between remote sensing methods and ground truth. Over the past five years repeated efforts have been made to convince potential remote-sensor users of the problems involved in establishing ground truth by traditional methods. It is hoped that this detailed analysis of a data set for a single lithic unit may serve to convince the remote-sensing community of the importance of the geological and statistical sampling problems - problems which have been essentially ignored, despite our repeated attempts to place emphasis upon them. This seems to be a fitting final scientific report under this grant to emphasize some of the more important conclusions of the continuing Northwestern team's effort.

ABSTRACT

In a continuing attempt to evaluate how the three-dimensional composition and variability of rock units can be assessed correctly, this paper focuses on critical sampling problems involved. The compositional variability and zonation of the Malsburg Granite (S. W. Germany) has already received considerable attention on the basis of large numbers of modes (Rein, 1961), alkali analyses (Mehnert and Willgallis, 1961), and analyses of 8 elements (Hahn-Weinheimer and Ackermann, 1967). New analyses for 10 major oxides are presented for 37 localities used by the previous workers. The autocorrelation of residuals from polynomial trend surfaces based on 110 alkali analyses (Whitten, 1962) can now be explained, in part, by many factors other than significant local geological variability. The unique assemblage of independent sets of analyses permits evaluation of the sampling problems, and the different methods of assessing the three-dimensional variability of the granite mass. Previously-published zonal maps are tested with discriminant analysis. It is concluded that Q-mode factor analysis maps provide the best available method of mapping zones in a granite; this results, in part, from the simultaneous use of numerous variables.

INTRODUCTION

The general availability of computers has permitted a number of quantitative and mathematical techniques to be applied to many aspects of economic geology and to the petrological and petrographical study of individual rock complexes. This is a significant advance for geology if, as has been suggested (Griffiths, 1962, p. 565), "Progress in scientific investigation in any specialized field is generally measured by the degree to which the subject is pervaded by mathematics." However, the value of this technology depends upon the quality and significance of the data used for the mathematical analyses.

Provided that the three-dimensional distribution of mineralogical and chemical components is known, it should be realistic to develop conceptual petrogenetic models for lithic units. When attempting to define the best mathematical model for a particular earth-science problem, it is becoming standard practice to approximate the available quantitative and qualitative data with the best current model and then to examine critically both the fit and the anomalous departures of the observed data from the model estimates. In deterministic situations the anomalies are likely to be minor. In geological contexts, however, the deviations commonly account for large and significant proportions of the total observed variability. If the data are wholly adequate and appropriate to the problem, but the model is inadequate, successive modifications should achieve progressively more efficient models; at each iteration, critical reappraisal of anomalous samples can be expected to give considerable insight into the nature and significance of minor geological features that are largely masked by the regional patterns of variability.

Unfortunately, the general availability of numerous computer-based techniques for manipulating and analyzing data has tended to distract attention from the nature and meaning of the original data. When an array of numerical values has been obtained, it is not unusual to associate with it a subjective feeling of

accuracy and correctness (especially after it has been processed and transformed into a new tabular or map format), that may be wholly unwarranted. Frequently, it is difficult or impossible to evaluate the geological significance of available data, although the geologist is commonly tempted to extrapolate and/or interpolate on the basis of available numerical values. In doing this, statistical techniques are frequently used after collection of data in an essentially arbitrary manner; at best, this tends to be inefficient and, at worst, it is completely ineffective (cf., Griffiths, 1962, p. 567).

Analytical data are developed for specimens collected from a sampled population but, in almost all geological situations, such observations do not permit statistical inferences to be made about the target population (Whitten, 1961). The numerous current statistical techniques can be used to analyze a data set fully and confidence levels can be associated with statements about the data. It may also be possible to make meaningful geological statements about the target population of interest on the basis of the sampled-population data, but such statements must rely on geological interpretation, rather than on statistical inference. Despite this inherent limitation, it has become common practice to erect petrogenetic and/or economic hypotheses on the basis of a limited data set in the course of routine petrographic studies. The raw quantitative data for granitic complexes, for example, are relatively difficult and/or expensive to obtain. Despite the availability of the so-called rapid methods of chemical analysis and the demonstration that abundant very accurate and precise data can be obtained (e.g., Baird, et al., 1967, Chappell, 1966, Rhodes, 1970), for economic reasons most geologists are still obliged to rely on a limited number of analytical results.

In a few petrographic studies, very detailed sampling and analytical programs have permitted realistic models to be erected for the target population. In most cases, however, very limited information is available about the levels of variance

of each of the several hundred variables that could be measured. Because different variables in a particular lithic unit tend to have dissimilar levels of variance, different sampling plans may be needed to establish (to the same degree of confidence) the variability pattern of each variable. Hence, it becomes very difficult, if not impossible, to determine whether the apparent pattern (established on the basis of available data for a lithic unit) and/or any anomalies with respect to a particular model, reflect errors or sampling and/or analytical inadequacies. Apparent anomalies could indicate an inadequate model requiring modification, or that the analytical data for the sampled population are an inadequate source of information about the target population of interest.

An example is appropriate. In constructing a trend-surface map for, say, modal quartz percentage in 50 granite samples, the sum of squares reduction (possibly tested with a F test) and a confidence band may indicate a very 'good' surface for describing the data set. Despite the apparently-excellent statistical tests, the surface could be a wholly misleading descriptor of the target population; such a situation could arise if each mode were based on a single, small thin section of samples collected from a granite mass seen to be heterogeneous in outcrop, where the geologist has defined the target population as all of the 3 m.² unit areas that comprise the mapped surface area of the granite. Statistical manipulation cannot transform inappropriate data into a true image of the target population. Where the same samples have been used for measuring different variables, the significance of the values for each variable will, in general, be dissimilar because in samples of a given size the variance of each variable tends to be different. Commonly, inadequate data are difficult to evaluate and acknowledge.

In most geological studies replicate sets of both samples and analytical data are not available. However, continuing study of the Malsburg Granite in the southern Black Forest, SW. Germany, has provided several sets of

independently-derived data. Each set could, in common usage, be the basis of petrographic description and of petrogenetic models. Without in any way implying criticism of the results already published, it is intended to draw attention to the dissimilarity of these "apparently-adequate" sets of data and to the inherent difficulty of using any one of them as a basis for testing petrogenetic models. Such a discussion of the sampling and/or analytical problems inherent in all, or some, of the sets of analyses could be discouraging. However, more positive conclusions should be drawn. First, petrologists must use extreme caution in basing conclusions on numerical data for which full information on (a) the statistical bases of the sampling plan and (b) the levels of variance for each variable, are not available. Second, statistically-adequate sampling procedures are a prerequisite to scientific study of rock units. In this paper, it is intended to draw attention to some of the problems that arise when this type of information is not available. It is hoped that this will serve as a challenge to petrographers to develop and incorporate adequate sampling methods in the study of rock units when it is desired to obtain the answer rather than an answer.

Finally, it is concluded that maps based in multivariate Q-mode factor analysis can portray the spatial variability of a granite more realistically than maps showing the regional and local variability of individual variables. Although having a general resemblance to the published models for the Malsburg Granite, the Q-mode maps show significant differences that will be important in any petrogenetic study of the complex.

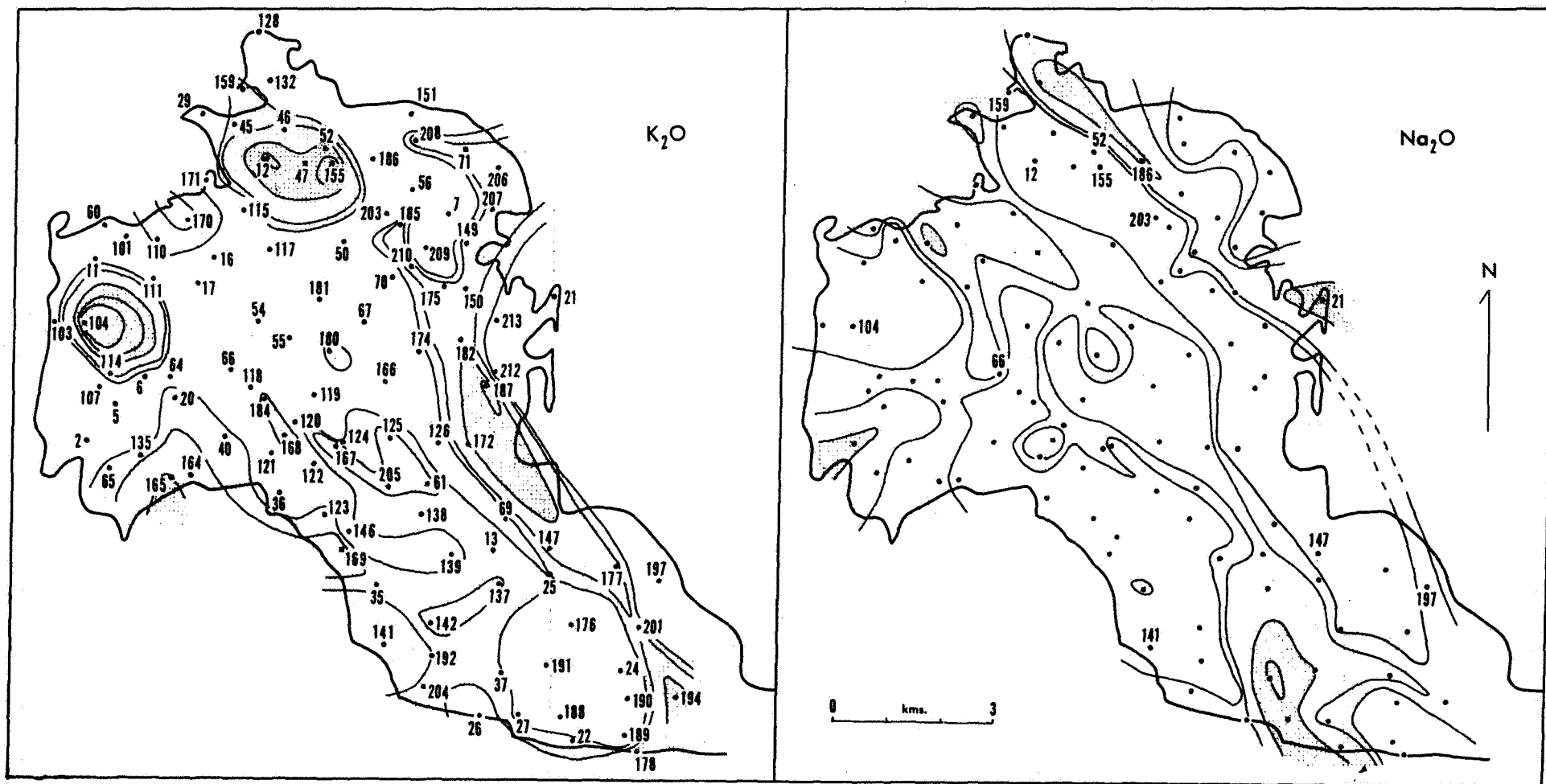
AVAILABLE DATA FOR THE MALSBURG GRANITE

The petrography and petrogenesis of the Malsburg Granite has received considerable attention in the past (e.g., Schröder, 1929; Mehnert and Willgallis, 1957; Zimmerle, 1958; Mehnert, 1963). Mehnert (1960) and Mehnert and Willgallis (1961) published K_2O and Na_2O weight percentage values and geographical grid

locations for 120 samples of the granite and Whitten (1962; 1963) used polynomial trend-surface analysis to evaluate the three-dimensional spatial variability of these valuable data. Leible (1959) had earlier published thorium and uranium analyses for 16 localities and thorium plus uranium radiation values for these and for 47 additional sites. An excellent series of detailed modal variation maps based on micrometric analyses was given by Rein (1955, 1961); most of his specimens were collected from the same localities as those used by Mehnert and Willgallis (1961).

Hahn-Weinheimer and Ackermann (1963) used X-ray fluorescence analyses to estimate the local heterogeneity of K and Ti weight percentages, and of Zr, P, Sr, Ba, and Rb p.p.m. in the Malsburg Granite. On the basis of samples from 90 of Mehnert and Willgallis' (1961) and Rein's (1961) localities, Hahn-Weinheimer and Ackermann (1967) prepared maps of equal concentration of these same elements and for Na weight percentage (determined by neutron activation analysis).

The polynomial regression model (Whitten, 1962) revealed marked autocorrelation of the deviations (Fig. 1). The linear bands of positive and negative deviations raised the question of whether distinct local geological features occur in the granite and account for the departures of the observed alkali values from the computed model; the patterns are reminiscent of the palimpsestic ghost stratigraphy described in the "older granite" of Donegal (Whitten, 1960). However, when the maps for the Malsburg Granite were published, no attempt had been made to re-examine the anomalous sample localities in the field. The present research was originally aimed at determining the significance of these deviation patterns. In 1962, the present author collected specimens from many of the localities defined by Mehnert and Willgallis (1961) and Rein (1961); emphasis was placed on localities that define the deviations shown in Figure 1. The ten major oxides and specific gravity were determined for samples from 37 of these localities; the analyses (Table 1) have not been published previously.



1. Manual contours for positive deviations from the degree 3 polynomial trend surfaces computed for 110 K_2O and Na_2O weight percentage analyses of Malsburg Granite samples published by Mehnert and Willgallis (1961); the sample numbers are those used by Rein (1961), Mehnert and Willgallis (1961), and throughout this paper. Contours at 0, 0.1, 0.3, and 0.5 per cent.

Table 1.--New chemical analyses and norms for the Malsburg Granite (plus alkali values from Mehnert and Willgallis and modes from Rein for the same localities).

Locality*	Inner Central					Outer Central																Border with Partial Porphyroblast Development																											
	61C ³	66B ¹	125 ¹	137 ³	166 ²	2 ¹	R2	7 ³	R7	50 ¹	R50	50D ¹	R50D	55 ¹	56 ¹	R56	56D ¹	R56D	118 ¹	147 ²	184B ²	186A ²	201 ⁴	R201	21 ³	71 ³	141 ³	164 ⁴	R164	164B ³	R164D	165 ²	R165	172 ⁴	R172	177 ⁴	195 ⁴	R195	195D ⁴	R195D	197 ²	203A ²	210 ⁴	R210	212 ⁴				
Sp. Gr.	2.646	2.654	2.634	2.624	2.654	2.631		2.652		2.607				2.660	2.621				2.643	2.635	2.643	2.640	2.608		2.682	2.631	2.596	2.625					2.633		2.539		2.625	2.609				2.714	2.627	2.635		2.573			
SiO ₂	69.44	66.54	66.63	67.45	66.09	68.02		63.90		68.19		66.33		65.89	66.10		64.98		67.61	65.24	67.21	64.56	66.74		61.38	65.04	67.09	65.88				66.87		67.03		65.06		68.40	72.36		72.40		58.10	64.36	64.94		65.42		
Al ₂ O ₃	16.14	14.60	15.57	14.46	16.24	14.65		15.69		15.18		15.06		16.22	15.16		15.23		13.41	15.86	14.73	15.69	15.63		17.40	16.22	15.32	14.76				15.75		16.52		17.16		15.35	14.64		14.51		17.51	15.31	15.76		15.22		
Fe ₂ O ₃	0.98	2.59	1.40	2.16	0.79	2.04		1.80		1.49		2.42		1.50	0.87		1.61		1.98	1.94	2.21	1.32	1.10		1.70	1.20	2.15	2.93				1.35		0.83		2.20		1.65	1.05		1.07		1.95	2.62	1.51		2.56		
FeO	1.06	1.40	1.79	1.52	1.75	1.45		1.67		1.44	1.38	1.00	0.93	1.60	2.37	2.38	1.27	1.22	1.62	1.42	1.17	2.04	1.92		2.25	1.92	1.12	0.64	0.61		1.60	1.61	1.71		1.12		0.61	0.64	0.67	0.63	0.60	3.01	0.90	1.84		1.27			
MgO	1.35	2.58	2.13	1.99	1.90	1.80		2.35		1.89		2.13		1.21	1.98		1.78		2.00	2.19	1.82	1.88	2.23		2.86	3.60	1.94	1.86				2.04		2.00		2.06		1.36	0.99		0.94		4.12	2.28	2.64		1.88		
CaO	1.06	3.39	2.18	2.08	2.51	1.42	1.48	2.51	2.54	1.06		1.40		1.41	2.43		2.30		2.82	2.41	2.12	2.41	1.73		2.98	1.96	1.79	1.05				1.16	1.25	2.03		1.32		1.87	0.88	0.86	0.89		3.23	1.06	1.47		1.63		
Na ₂ O	3.98	3.89	4.15	3.91	3.73	4.32		4.34		3.67		3.60		3.81	4.03		4.23		3.88	4.00	4.01	2.86	3.56	3.61	4.79	3.60	3.72	3.78				3.65	3.72	3.74	3.84	3.84	3.88	3.61	3.91		3.83	3.88	3.69	3.79	3.85	3.80	3.77		
K ₂ O	4.44	3.99	4.20	4.47	4.19	4.39		3.77		4.56		4.78		4.05	4.25		4.12		4.08	3.98	4.58	5.26	4.49	4.49	3.79	4.67	4.51	5.01				4.80	4.75	4.46	4.45	4.29	4.30	4.70	4.59		4.53	4.52	4.34	4.43	4.33	4.35	4.31		
TiO ₂	0.24	0.36	0.38	0.36	0.46	0.34		0.47		0.37		0.37		0.46	0.37		0.38		0.39	0.44	0.30	0.42	0.42		0.58	0.39	0.43	0.42				0.42		0.42		0.49		0.32	0.20		0.17		0.84	0.47	0.47		0.48		
P ₂ O ₅	0.16	0.20	0.21	0.19	0.29	0.19		0.26		0.20		0.19		0.22	0.19		0.20		0.22	0.24	0.19	0.24	0.22		0.32	0.21	0.21	0.22				0.24		0.23		0.32		0.22	0.11		0.11		0.38	0.22	0.23		0.25		
Total	98.85	99.54	98.64	98.59	97.95	98.62		96.76		98.05		97.28		96.37	97.75		96.10		98.01	97.72	98.34	96.68	98.04		98.05	98.81	98.28	96.55				97.88		98.97		97.86		98.09	99.37		99.08		97.17	95.44	97.04		96.79		
Ignition Loss	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.		n.d.		2.32		3.05		n.d.	2.34		4.24		n.d.	n.d.	2.03	n.d.	n.d.		n.d.	n.d.	n.d.	3.80			2.49		n.d.		n.d.		n.d.		1.56		1.53		n.d.	n.d.	n.d.		n.d.		
Norms																																																	
Qz	25.13	19.16	18.48	20.61	20.15	20.71		15.71		24.50		21.46		23.60	17.41		17.42		21.88	18.86	19.77	19.61	21.56		8.46	16.39	22.06	20.32				21.91		20.72		21.31		24.00	29.00		29.79		6.89	20.31	18.92		21.41		
Or	26.24	23.58	24.82	26.42	24.76	25.94		22.28		26.95		28.25		23.93	25.12		24.35		24.11	23.52	27.07	31.08	26.53		22.40	27.60	26.65	29.61				28.37		26.32		25.35		27.77	27.12		26.77		25.66	26.18	25.59		25.47		
Pl	37.89	43.51	44.56	41.79	42.12	42.36		47.48		35.01		36.17		37.80	44.82		45.90		39.96	44.23	42.60	34.59	37.27		53.22	38.81	38.99	35.76				35.07		40.21		36.95		38.39	36.73		36.10		44.76	35.89	38.37		38.35		
Anorthite %	11.12	24.35	21.19	20.83	25.07	13.70		22.65		11.29		15.77		14.70	23.93		22.01		17.83	23.48	20.34	30.03	19.17		23.85	21.52	19.26	10.55				11.94		21.31		12.06		20.42	9.93		10.24		30.25	10.65	15.09		16.83		
Di + Hy	4.10	8.18	6.81	5.52	6.53	4.90		6.66		5.51		5.30		3.95	7.99		4.81		7.94	5.73	4.78	6.64	7.48		8.89	10.86	4.83	4.63				6.21		6.74		5.13		3.39	2.47		2.34		12.79	5.68	7.93		4.68		
Ap	0.37	0.47	0.49	0.44	0.68	0.44		0.61		0.47		0.44		0.51	0.44		0.47		0.51	0.56	0.44	0.56	0.51		0.75	0.49	0.49	0.51				0.56		0.54		0.75		0.51	0.26		0.26		0.89	0.51	0.54		0.58		
Mt + Il	1.88	4.15	2.75	3.81	2.02	3.61		3.50		2.86		2.85		3.04	1.96		3.05		3.61	3.65	3.47	2.71	2.39		3.56	2.48	3.18	1.65				2.76		2.00		3.12		1.65	1.86		1.86		4.43	2.43	3.08		3.61		
Mehnert & Willgallis' alkalis																																																	
Na ₂ O	3.93	4.07	4.17	4.11	4.12	3.98		4.00		3.72				4.10	3.89				3.55	3.59	3.87	3.93	3.58		4.13	3.66	2.95	3.79													3.72		3.55	3.74		3.56			
K ₂ O	4.75	4.70	4.83	4.79	4.47	4.72		4.34		4.72				4.35	4.22				4.37	4.71	4.73	4.40	4.68		3.86	4.74	4.06	4.72													3.67		4.00	4.92		4.49			
Rein's Modes																																																	
Quartz	24.00	22.60	21.90	21.00	24.00	22.00		21.00		23.50				22.20	24.00				22.20	21.90	21.10	22.70	22.20		14.00	25.30	22.70	25.00						25.10		25.00						27.00	30.10		11.70	22.50	20.00		n.d.
K-fs.	29.00	30.50	29.20	32.80	26.10	23.00		24.00		28.10				27.00	24.70				26.50	16.60	27.70	29.00	23.00		16.00	23.40	25.40	24.00						19.20		24.10						31.40	31.50		14.40	23.60	24.00		n.d.
Plagioclase	36.00	35.80	37.50	33.60	38.80	43.00		40.00		36.50				38.70	38.00				39.00	47.50	38.10	35.60	40.10		49.60	38.00	40.70	41.00						45.60		40.20						34.50	30.90		50.00	40.80	42.00		n.d.
Biotite	9.60	10.50	10.80	12.00	10.70	11.00		12.20		10.70				9.80	10.60				11.80	11.30	12.00	12.60	13.00		15.50	11.90	10.80	9.60						9.80		9.50						7.00	7.40		16.60	11.50	10.80		n.d.
Hornblende	1.30	0.50	0.48	0.50	0.20	0.85		2.50		1.00				2.20	2.50				0.40	2.50	0.98	0.08	1.60		4.70	1.20	0.30	0.36						0.23		1.07				0.00	0.00		7.00	1.40	3.00		n.d.		
Apatite	0.07	0.06	0.09	0.08	0.10	0.12		0.17		0.12				0.08	0.11				0.09	0.11	0.10	0.08	0.08		0.14	0.13	0.04	0.04						0.06		0.10				0.05	0.05		0.15	0.12	0.11		n.d.		
Zircon	0.02	0.01	0.02	0.02	0.02	0.01		0.02		0.03				0.02	0.03				0.02	0.02	0.01	0.02	0.02		0.02	0.03	0.01	0.01						0.01		0.02				0.01	0.01		0.03	0.02	0.02		n.d.		

*In locality number prefix R implies replicate analysis of certain oxides by same analyst; suffix D implies complete sample analyzed under coded number unknown to analytical laboratory.

¹Analyst: Kazuo Masuzawa; ²Analyst: Shirou Imai; ³Analyst: Tadashi Asari; ⁴Analyst: Hiroshi Asari

K-feldspar-blastic Border																		
222 ⁴	R222	222D ⁴	R222D	12A ¹	R12A	52 ³	103 ³	104A ³	155 ²	R155	159A ²	185 ⁴	R185	187 ⁴	R187	194 ²	194D ²	R194D
2.665				2.650		2.625	2.648	2.625	2.631		2.645	2.622		2.621		2.588		
64.21		62.80		65.63		66.34	66.09	69.03	65.08		66.64	65.40		66.22		65.38	65.49	
15.93		15.76		15.95		15.62	15.12	15.29	15.41		16.41	15.96		15.27		15.94	15.98	
1.98		2.42		1.27		1.43	1.90	1.27	2.10		0.84	2.03		2.30		2.70	2.65	
2.12	2.10	1.74	1.70	1.94		1.62	1.13	1.22	2.00		2.09	1.38		1.30		0.77	0.77	
2.57		2.82		2.02		1.73	2.17	1.06	2.13		1.90	1.78		2.08		1.84	1.88	
2.36	2.40	2.43		2.14	2.20	2.30	2.79	1.65	2.22		2.15	1.57		1.36		0.97	0.95	0.93
4.18		4.13	4.15	3.89		4.54	3.63	3.46	3.49	3.46	3.50	3.47	3.48	3.82	3.87	3.59	3.60	3.62
4.24		3.89	3.92	4.85		4.83	4.97	4.86	4.93	4.83	4.31	4.89	4.98	5.08	5.11	4.57	4.54	4.55
0.58		0.61		0.41		0.25	0.38	0.26	0.54		0.21	0.48		0.42		0.47	0.44	
0.28		0.27		0.20		0.16	0.21	0.18	0.25		0.35	0.26		0.27		0.30	0.28	
98.45		96.87		98.30		98.82	98.39	98.28	98.15		98.40	97.22		98.12		96.53	96.58	
2.09		2.88		n.d.		n.d.	n.d.	n.d.	n.d.		n.d.	n.d.		n.d.		n.d.	n.d.	
14.98		15.16		16.57		14.28	17.81	25.35	18.21		22.06	21.19		19.31		23.03	23.53	
25.06		22.99		28.66		28.54	29.37	28.72	29.13		25.47	28.90		30.02		27.01	26.83	
45.25		45.24		42.23		46.39	41.00	36.29	38.91		37.99	35.45		37.31		33.23	33.35	
21.83		22.75		22.05		17.20	25.08	19.32	24.11		22.05	17.18		13.36		8.58	8.65	
7.70		7.21		6.87		6.68	6.32	3.40	6.35		7.53	4.50		5.18		4.58	4.68	
0.65		0.63		0.47		0.37	0.49	0.42	0.58		0.82	0.61		0.63		0.70	0.65	
3.97		4.67		2.62		2.54	3.26	2.33	4.07		1.62	3.85		3.77		2.01	2.05	
n.d.				3.18		3.54	3.53	2.80	2.94		3.36	3.46		3.52		3.53		
n.d.				5.42		5.23	5.02	6.17	5.78		5.00	4.90		5.04		5.04		
19.30				23.00		23.50	21.50	22.50	22.90		22.40	24.30		13.30		21.50		
19.10				27.00		33.50	28.20	28.00	28.00		33.60	23.80		22.60		25.50		
45.60				35.00		32.50	39.70	39.40	38.00		29.70	38.40		51.80		39.00		
13.50				13.00		10.40	9.70	9.20	10.30		13.20	13.30		10.70		11.50		
2.30				1.80		0.00	0.84	0.64	0.70		0.92	0.01		1.47		2.40		
0.14				0.09		0.07	0.05	0.05	0.08		0.09	0.12		0.09		0.06		
0.03				0.03		0.02	0.01	0.01	0.02		0.03	0.02		0.02		0.01		

Available analytical data for the Malsburg Granite is unique. Because the granite outcrops in an area of considerable relief, significant advantages stem from considering the three-dimensional, in addition to the geographical, variability. Modal analyses (Rein), three independent sets of partial chemical analyses (Mehnert and Willgallis, Hahn-Weinheimer and Ackermann, and Whitten), and norms and specific gravity values (Whitten) are all available for the same 37 grid locations. These data permit interesting comparisons to be made. As with data in most published petrographic studies, there is little alternative to giving equal significance and authenticity to each analytical value, unless the actual sample sites can be visited by the reader. The Malsburg Granite sample sites are probably not unique in having distinct dissimilarities (as described in a later section).

NEW CHEMICAL ANALYSES

The Malsburg Granite is poorly exposed; much of the outcrop area is open pastoral or arable land and part is forested. The geographic coordinates published by Mehnert and Willgallis (1961, Table 16) and Rein (1961, Table 11) make it relatively easy to locate almost all of their outcrops; through the courtesy of Drs. Rein and Ackermann, 1:25,000 topographical maps showing the actual sample localities were also available.

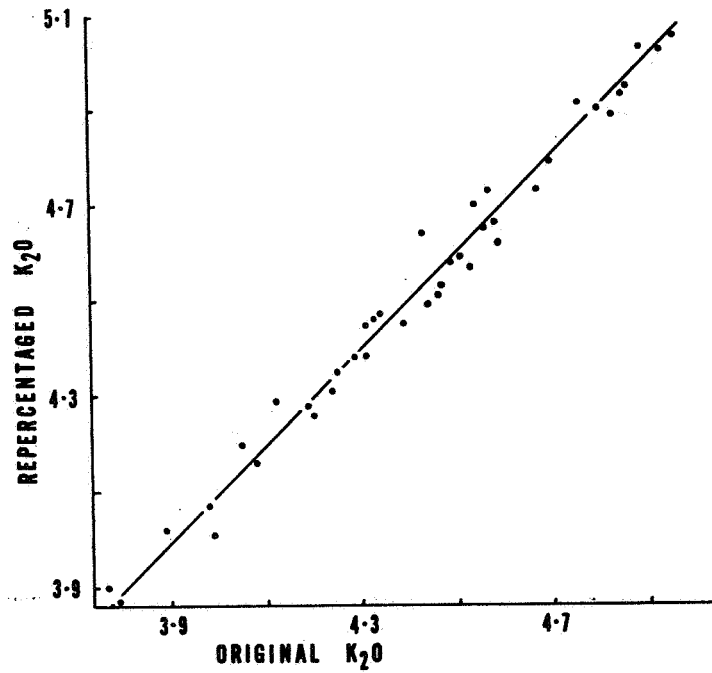
The field work and sampling in 1962 were primarily directed towards establishing the significance of the deviations (Fig. 1) from the polynomial trend surfaces computed (Whitten, 1962) for Mehnert and Willgallis' (1961) K_2O and Na_2O data. That is, specific search was made in the field for any features that could partially explain the autocorrelations reflected by the deviation maps (Fig. 1). In view of the traditional problems associated with quantitative analyses of K_2O and Na_2O , significant deviations might be anticipated to arise from analytical errors. High variance at the outcrop or sample-size level or even clerical errors might explain some of the anomalies. However, in 1962, the strong autocorrelation of deviations was thought to favor an underlying, geological control of the local anomalies.

At many outcrops the granite is very deeply weathered. Care was taken to extract the freshest available material with crow-bar and hammer. Samples were not collected from any locality without carefully determining whether the granite was in situ. At several of the localities associated with very large deviations in Figure 1, it proved impossible to find any outcrop and/or in situ material.

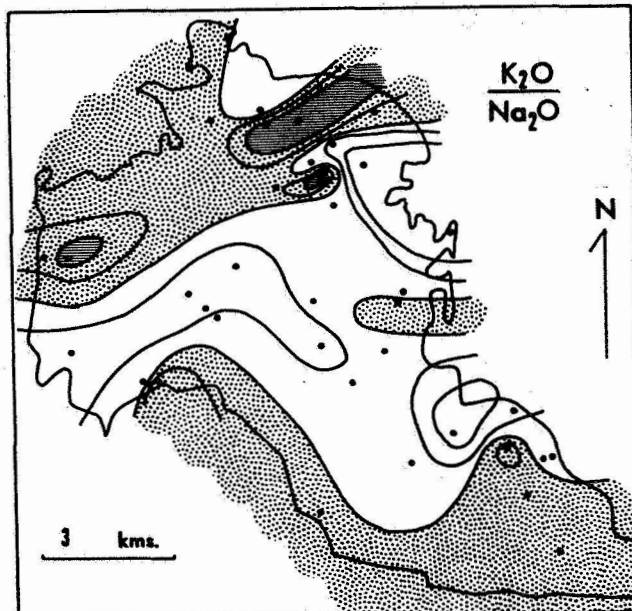
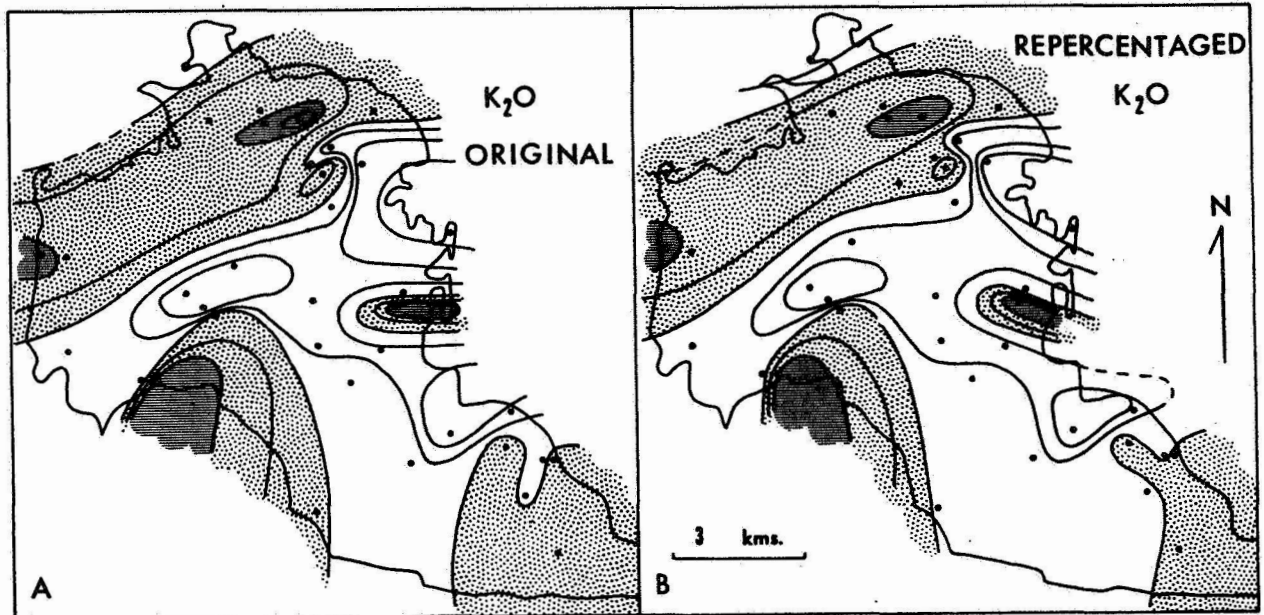
Selected samples were powdered at Northwestern University and the new chemical analyses were completed in 1965 by Japan Analytical Chemistry Research Institute (Executive Director: Dr. Tamiya Asari). SiO_2 , Al_2O_3 , CaO , MgO , and P_2O_5 were determined by gravimetric, Fe_2O_3 and FeO by volumetric, TiO_2 by photometric, and Na_2O and K_2O by flame-photometric methods. Hidden duplicates of six of the 37 samples were also analyzed at the same time. As an added check on reproducibility, FeO was reanalyzed for 10 samples (and ignition loss determined for these samples), 8 samples were reanalyzed for CaO , and 11 for both Na_2O and K_2O . The complete analytical results are shown in Table 1; four different analysts from Dr. Asari's laboratory were responsible for this work. Dr. Asari (personal communication) assumed that few analytical errors should be involved with SiO_2 , MgO , CaO , Na_2O , K_2O and TiO_2 , although he suggested that errors might be anticipated with Al_2O_3 , Fe_2O_3 - FeO , and P_2O_5 (which are calculated by differences). Additional evidence for the confidence levels to be associated with these chemical analyses is not available.

Ignition loss reported for these analyses ranges up to about 4 per cent. It is not recorded whether the partial analyses published previously (Mehnert and Willgallis, 1961, and Hahn-Weinheimer and Ackermann, 1967) have been adjusted for ignition losses. Figure 2 shows the original K_2O weight percentages from Table 1 contrasted with the values recalculated to eliminate ignition loss. Figure 3 shows that maps for these two sets of values are not materially different (except that the repercentaged values are approximately 0.1 per cent larger). The ignition-loss problem is eliminated by the use of oxide ratios, although ratios of

2. Whitten K_2O weight percentages (from Table 1) and K_2O values recalculated to eliminate ignition loss; where ignition loss was not determined, it was assumed that the loss would account for the difference between the analysis total and 100 per cent.



3. Manually-contoured maps of the Malsburg Granite for the original 37 K_2O percentages (from Table 1) and for K_2O recalculated to eliminate ignition loss. A: Contours at 3.9 and each 0.2 per cent increment; above 4.5 stippled and above 4.9 ruled. B: Contours at 4.0 and each 0.2 per cent increment; above 4.6 stippled and above 5.0 ruled.



4. Manually-contoured map of the Malsburg Granite for $K_2O:Na_2O$ ratio (derived from Table 1 for 37 samples). Contours at 1.0 and each 0.1 per cent increment; above 1.2 stippled and above 1.4 ruled.

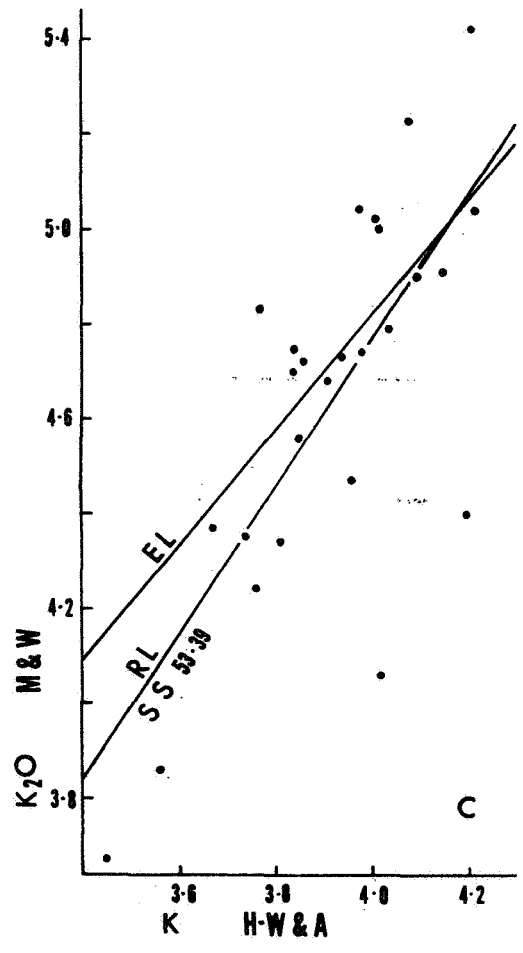
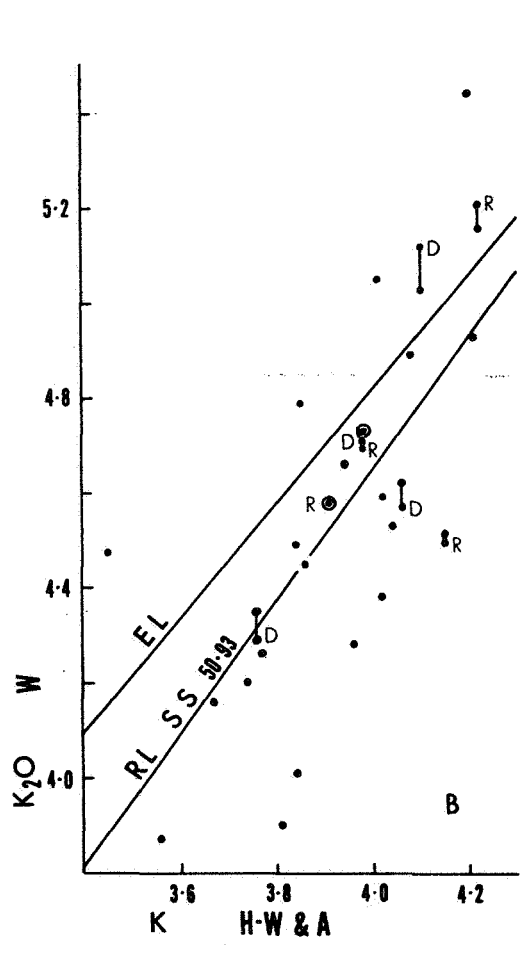
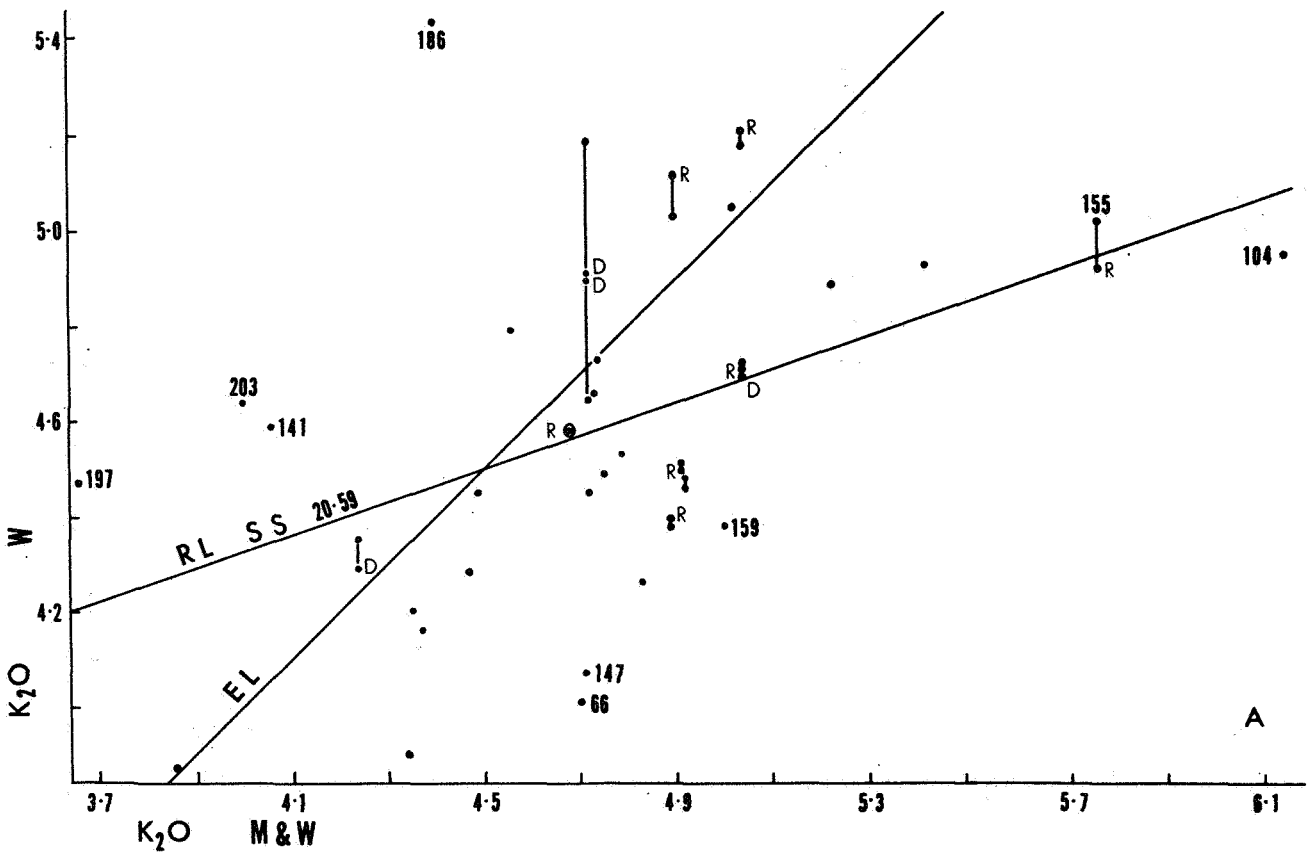
5. Comparisons of the independent K_2O and K analyses made by Whitten (W), Mehnert and Willgallis (M & W), and Hahn-Weinheimer and Ackermann (H-W & A) for samples collected from the same localities of the Malsburg Granite. EL = expected line along which analyses should lie. RL = linear regression line for actual values (not including replicate (R) and duplicate (D) analyses shown in scatter diagrams and Table 1) with percentages of total sums of squares (SS) associated with each line. Samples falling well away from EL in Figure 5A are identified by number.

closed-system data (percentages) introduce additional statistical problems. The geological significance of oxide ratios is not always obvious but, in this case, the K_2O/Na_2O ratio (Fig. 4) has a somewhat similar map pattern to that for K_2O weight percentage (Fig. 3).

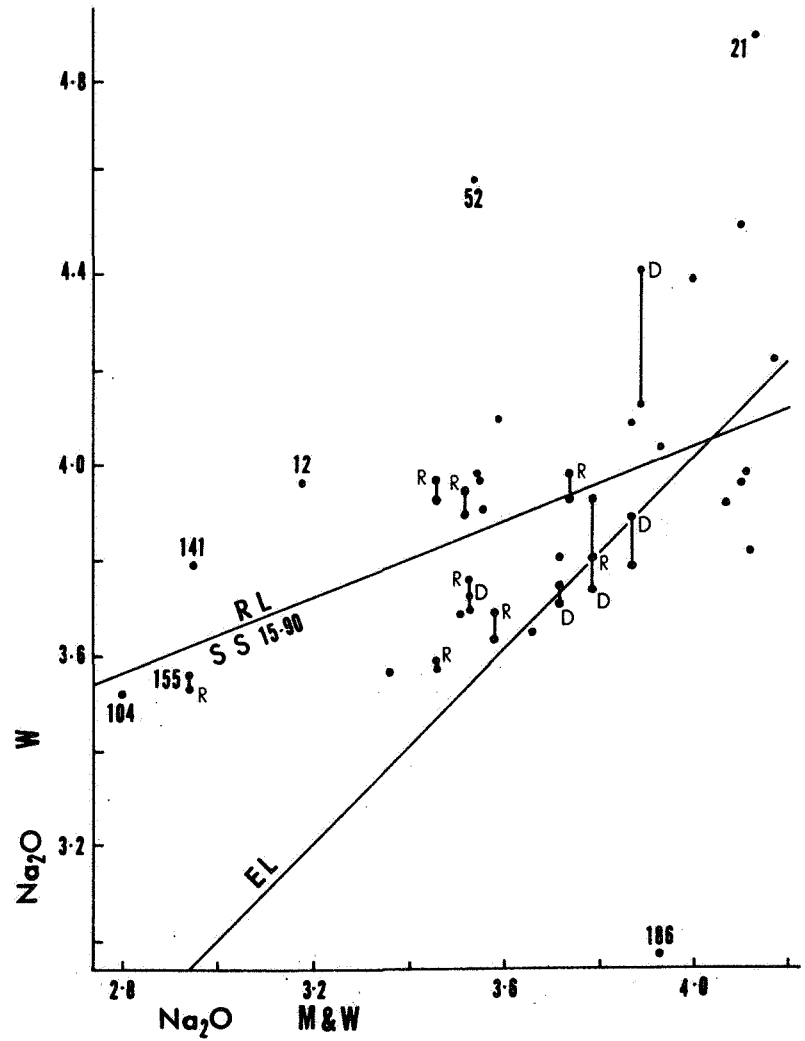
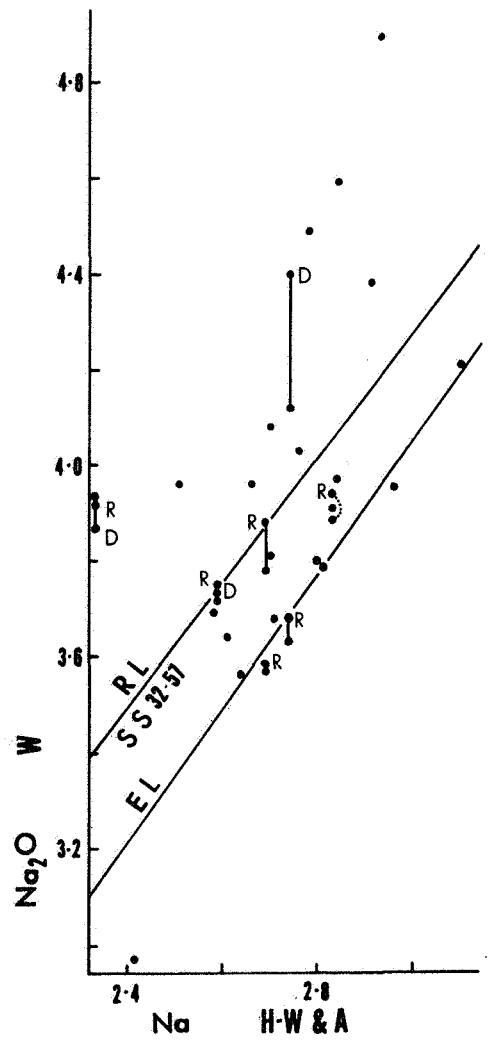
THE THREE INDEPENDENT SETS OF CHEMICAL ANALYSES

Hahn-Weinheimer and Ackermann (1967, p. 2217) considered that, on the whole, their results for Na and K are in agreement with the flame photometric determinations of Mehnert and Willgallis (1961). However, the linear correlation coefficient for K_2O and K of these workers is 0.73 and only 0.45 for Na_2O and Na (on the basis of 26 common sites included in Table 1). The correlation coefficient for K_2O values for the 35 samples common to Mehnert and Willgallis (1961) and Table 1 is only 0.45; for the corresponding Na_2O values, the coefficient is 0.39. The relatively small magnitude of these correlation coefficients (Table 2) suggests that the three sets of chemical analyses should be scrutinized more thoroughly. Whitten's K_2O values (Table 1) and those of Mehnert and Willgallis (1961) are plotted against Hahn-Weinheimer and Ackermann's (1967) K values in Figures 5B and 5C; the K_2O analyses of Mehnert and Willgallis (1961) and Whitten (Table 1) are compared in Figure 5A. Figure 6 shows similar diagrams for Na_2O and Na percentages. The TiO_2 percentages from Table 1 and Hahn-Weinheimer and Ackermann's (1967) Ti values are compared in Figure 7. Each of these graphs shows considerable scatter which may reflect

- (a) analytical or clerical errors within either or both sets of analyses - either random errors, consistent bias in one or more analytical technique, or variability within the limits of precision of the analytical methods,
- (b) local variability within the sample sites designated by the geographic coordinates, or
- (c) sampling differences or errors in the field - assignment of incorrect coordinates or collection of specimens from the wrong locality, from erratic



6. Comparisons of the independent Na_2O and Na analyses made by Whitten (W), Mehnert and Willgallis (M & W), and Hahn-Weinheimer and Ackermann (H-W & A) for samples from the same localities of the Malsburg Granite. EL = expected line along which analyses should lie. RL = regression line for actual values (not including replicate (R) and duplicate (D) analyses shown in scatter diagrams and Table 1) with percentages of total sums of squares (SS) associated with each line. Samples falling well away from EL in Figure 6B are identified by number.



7. Independent TiO_2 analyses by Whitten (W) and Ti analyses by Hahn-Weinheimer and Ackermann (H-W & A) for samples collected from the same localities of the Malsburg Granite. EL = expected line along which analyses should lie. RL = regression line for actual values (excluding replicate (R) and duplicate (D) analyses shown in scatter diagram and Table 1) with percentage of total sum of squares (SS) associated with the line.

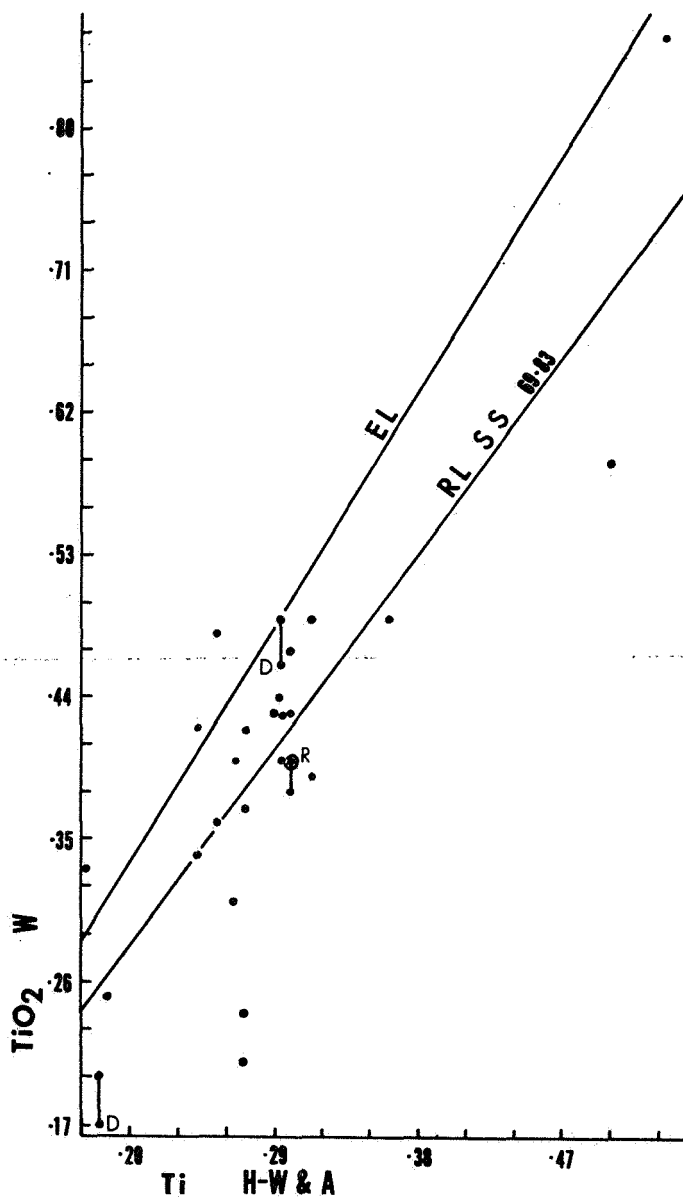


Table 2. - Linear correlation coefficients based on the sample localities common to all three sets of chemical analyses.

Source of analyses	K ₂ O/K	Na ₂ O/Na	TiO ₂ /Ti
Mehnert and Willgallis and Hahn-Weinheimer and Ackermann	0.73	0.45	.*
Mehnert and Willgallis and Whitten	0.45	0.40	.*
Hahn-Weinheimer and Ackermann and Whitten	0.71	0.57	0.84

*Mehnert and Willgallis did not give TiO₂ analyses.

Table 3. - Coefficients of variation for experimental error and local heterogeneity in outcrops estimated by Hahn-Weinheimer and Ackermann (1963, 1967).

Element	Experimental error	Locality 20 (N=13)	Locality 66 (N=10)	Locality 69 (N=10)	Locality 128 (N=9)*
K	0.37	2.61	2.72	3.79	4.58
Na	0.70	3.11	3.09	2.62	3.27
Ca	0.49	21.35	14.35	10.60	17.10
Ti	0.58	7.77	4.67	3.13	2.86

*N = number of samples individually analyzed for that locality.

material, or from material too weathered or too decomposed to represent the fresh parent rock.

In preliminary tests, Hahn-Weinheimer and Ackermann (1963, 1967) found that their X-ray fluorescence analyses have small errors and mean deviations in comparison with the variances of groups of samples from localities 20, 66, 69, and 128 (see Figure 1). The coefficients of variation* deduced by these authors are

*The coefficient of variation is the standard deviation divided by the mean and then expressed as a percentage.

shown in Table 3. Local heterogeneity was estimated on the basis of 9 to 13 samples of 5 to 10 kg each collected at 10 to 15 m intervals in each outcrop. Intuitively, the variances deduced for Ca weight percentage appear to be surprisingly large. Hahn-Weinheimer and Ackermann implied that the values in Table 3 indicate the confidence level to be associated with their complete array of Malsburg Granite analyses.

The three regression lines for Hahn-Weinheimer and Ackermann's and Whitten's values (Figs. 5B, 6A, and 7) show some consistent differences which suggest that constant analytical differences occur in addition to sporadic noise; these diagrams show that these samples (which were separately collected from the same grid locations) have surprisingly little local variability. By comparison, the correlations of the alkali analyses derived by Mehnert and Willgallis and by Whitten are significantly weaker (Figs. 5A and 6B). Seven specimens (localities 12, 21, 52, 104, 141, 155, and 186) on the Na_2O weight percentage diagram (Fig. 6B) lie well off the theoretical expected line (EL on Fig. 6B). Field relationships suggest that localities 12, 21, 52, and 186 should not present collecting difficulties. Localities 141 and 155 are poor, weathered outcrops from which fresh rock can only be obtained after considerable labor; the geographic

coordinates for 104 define the middle of an exposureless meadow which makes the origin of the previously-analyzed sample uncertain. The K_2O graph is less satisfactory in that nine samples lie well away from the expected line (EL on Fig. 5A), but several of these outcrops could have caused collection difficulties, viz: localities 66, 159, 186, and 197 should not have presented difficulty, except that rock at 66 and 159 is visibly heterogeneous; localities 141, 155, and 203 have poor, weathered outcrops (141 and 155 referred to previously); 147 is a poor locality essentially comprising boulders and it is uncertain whether any material is genuinely in situ; 104 was referred to above (published coordinates define exposureless meadow).

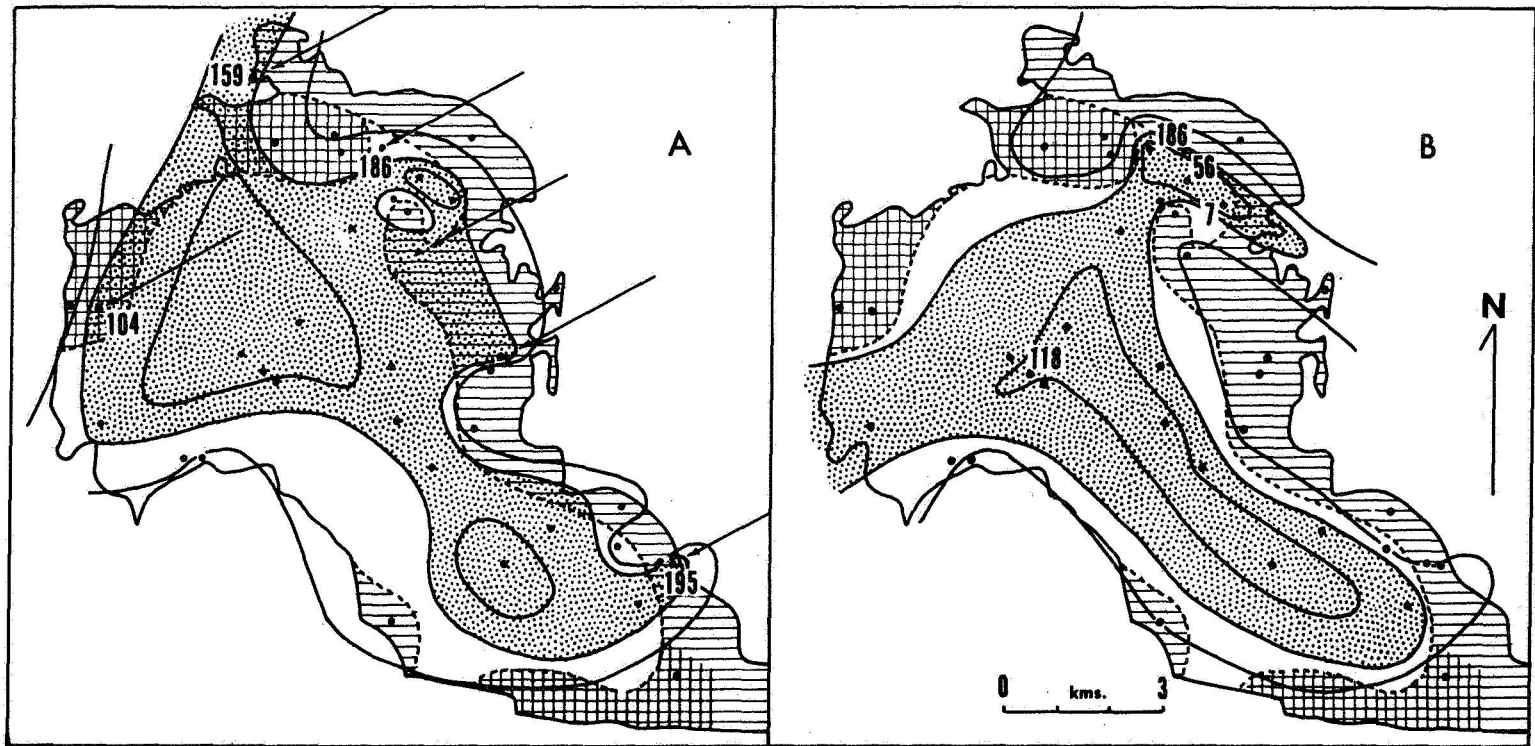
Such considerations suggest that field sampling problems may account for some of the scattered distribution of points in Figures 5A and 6B. However, from these graphs it is not possible to identify the actual source of trouble as being positively due to sampling, analytical, clerical, or other error in either set of results.

Figures 5A and 6B have considerable importance in interpreting the deviation maps for K_2O and Na_2O percentages (Fig. 1). The more anomalous localities in terms of Figures 5A and 6B are shown in Figure 1 and they define most of the very large deviation maxima. In other words, most of the major maxima in Figure 1 are defined by data that are suspect.

DISCRIMINATION OF ZONES WITHIN THE MALSBURG GRANITE

Rein (1961) showed that for his sampled population of the Malsburg Granite regional modal variability is much greater than the local modal variability - a conclusion subsequently supported by Hahn-Weinheimer and Ackermann (1963) on the basis of their chemical analyses of seven elements for four localities. Rein (1961) demonstrated a distinct zonal pattern for modal quartz, potash feldspar, plagioclase, biotite, hornblende, apatite, and zircon with the periphery of the granite being relatively more basic and the center more leucocratic. On the basis

8. Maps of discriminant functions (for 37 samples) superimposed on Mehnert and Willgallis' (1961) zones for the Malsburg Granite. No pattern - Class A central granite: Horizontal ruling - Class B border granite with partial K-feldspar porphyroblast development: Horizontal and vertical ruling - Class B K-feldspar-blastic border granite. A. Discriminant function for subset 2 (of Table 6); manual contours for the discriminant function are (i) within stippled area - mean value of function for specimens allocated to Class A (ii) boundary of stippled area is the discriminant value, and (iii) outside the stippled area - mean value of function for specimens allocated to Class B. The six samples misclassified by this function are indicated by arrows. Four samples most commonly misclassified (see text) are identified by number.
- B. Discriminant function for subset 8 (of Table 6); manual contours have same significance as in Fig. 8A. All samples are correctly classified. Four samples identified as transitional in character by Mehnert (see text) are identified by number.



of their own field experience and the subjectively-contoured mineralogical maps of Rein (1961), Mehnert and Willgallis (1961, Plates 21 and 22) constructed a single qualitative petrographical map of the Malsburg Granite; the mapped lines are incorporated in Figure 8. In their synthesis these lines are arbitrary so that, depending upon which minerals they considered to be the most significant, the authors could have drawn somewhat dissimilar boundaries. Mehnert and Willgallis placed much importance on potash feldspar porphyroblasts in defining their boundaries, although quantitative information about the characteristics of these porphyroblasts has not been published; in some places, the lines were shown as "uncertain."* On these bases, Mehnert (personal communication) recognized the

*Hahn-Weinheimer and Ackermann (1967) used precise mathematical operational definitions to delimit zones of equal concentration for each individual element but they did not develop a system for mapping the variability of all eight of their variables simultaneously.

following zones:

1. Inner central granite
 - i Typical
 - ii Transitional to the outer central granite
2. Outer central granite
 - i Typical
 - ii Transitional to the Inner Central Granite
 - iii Transitional to the Border Granite
3. Border granite with partial K-feldspar porphyroblast development
 - i Typical
 - ii Transitional to the K-feldspar-blastic granite

4. K-feldspar-blastic border granite

i Typical

ii Transitional to the outer central granite

Without questioning or debating the propriety of these zones, it is instructive to examine whether the available measured attributes permit these petrographically recognized and defined groups to be discriminated in a quantitative manner. For this purpose two classes are considered: Class A representing the central granite (zones 1 and 2 of Mehnert) and Class B the border granite (zones 3 and 4 of Mehnert). It must be recognized that the analyzed samples were collected by different people from designated geographic localities; in consequence, the same specimens were not analyzed for each set of variables and local variability factors must unavoidably be included in, and partially confuse, the discriminants.

A computer program that can calculate sequential linear discriminant functions (Whitten, 1970A) with up to 25 independent variables was employed to calculate several hundred discriminant functions with various combinations and subsets of the following variables:

- a. Elevation and specific gravity.
- b. 10 oxides (Whitten, Table 1) - because Fe_2O_3 , FeO , and MgO seem not to have good reproducibility, these oxides and the alkalis were treated separately for some discriminant functions.
- c. 8 element analyses published by Hahn-Weinheimer and Ackermann (1967).
- d. Normative values (calculated from the chemical analyses of Whitten, Table 1).
- e. Modal values published by Rein (1961).
- f. K_2O and Na_2O values from Mehnert and Willgallis (1961).

Table 4 shows some of the subsets of variables for which discriminant functions were calculated and the efficiency with which these functions separate the samples into the two classes A and B. For these calculations only the 37

Table 4. - Sets of data used to calculate discriminant functions and efficiencies achieved.

Number of Variables	Variables used								Number of Samples		Efficiency per cent
	Elevation	Specific Gravity	Whitten oxides			Whitten norms excluding Mgt	Rein modes	Mehnert Na ₂ O K ₂ O	Misclassified	Used	
			SiO ₂ , Al ₂ O ₃ CaO, TiO ₂ P ₂ O ₅	Fe ₂ O ₃ FeO MgO	Na ₂ O K ₂ O						
12	x	x	x	x	x				7	37	81.1
11		x	x	x	x				6	37	83.8
8		x	x						6	37	83.8
25	x	x	x	x		x	x	x	0	34	100.0
25	x	x	x	x	x	x	x		0	36	100.0
15	x	x				x	x		3	36	91.7
7		x				x			5	34	85.3
8		x					x		13	36	63.9
2								x	7	35	80.0
2					x				15	37	59.5
19	x	x	x	x	x		x		1	36	97.2
14						x*	x		1	36	97.2
8	Hahn-Weinheimer and Ackermann's eight elements								5**	26	80.8
2	Whitten's TiO ₂ and K ₂ O only								6	37	83.8
12	x	x	x	x	x				**	37	**
14						x	x		**	36	**

* includes Mgt; ** analyzed or also analyzed sequentially - see Table 5.

Table 5. - Examples of 'best' subsets of variables for the Malsburg Granite selected by sequential discriminant function analysis.

Data Set	Whitten's 10 oxides plus elevation and specific gravity N = 37*		Hahn-Weinheimer and Ackermann's 8 elements N = 26*			
	Variables included in subset	Number Misclassified	Efficiency	Variables	Number Misclassified	Efficiency
All 12		7	81.08	All 8	5	80.77
			<u>'Best' Pairs</u>			
K ₂ O + TiO ₂		6	83.78	P + Rb	5	80.77
K ₂ O + P ₂ O ₅		8	78.38	Ba + Rb	5	80.77
			<u>'Best' Individual</u>			
Specific gravity		13	64.86	Ba	9	65.38

*N is number of samples in whole set.

Table 7. - Correlation coefficients based on 36 of the sample locations listed in Table 1.

Variables		<u>r</u>	Variables		<u>r</u>
Normative value (Whitten)	Modal percentage (Rein)		Oxide percentage (Whitten)	Modal percentage (Rein)	
quartz	quartz	0.68	SiO ₂	quartz	0.69
orthoclase	potash feldspar	0.31	CaO	plagioclase	0.16
plagioclase	plagioclase	0.29	CaO	hornblende	0.29
apatite	apatite	0.45	Na ₂ O	plagioclase	0.24
			K ₂ O	potash feldspar	0.31
			K ₂ O	biotite	-0.23

Table 6. - Malsburg Granite sample sites misclassified by linear discriminant functions using different data subsets; misclassified samples marked x

Data Subset	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	
Sample																								
2						x						x	x	x	x	x								
7 T																								
12A						x								x	x	x								
21				x	x	x					x	x	x							x				
50	x		x	x		x																		
52														x	x	x		x					x	x
55																x								
56 T						x													x					
61C																								
66B																								
71															x	x		x			x	x	x	
103						x								x				x						x
104A	x	x	x															x						
118 T																				x				
125																								
137						x																x	x	x
141					x						x											x		
147														x	x	x		x	x					
155														x	x	x		x	x					
159A	x	x		x		x						x	x	x	x	x		x						
164																								x
165						x												x		x				
166					x			x		x				x		x							x	
172												x	x											
177													x	x	x			x	x				x	
184	x											x	x		x							x		
185																	x		x					
186 T		x	x	x	x						x	x	x					x				x	x	
187																								
194														x		x								x
195	x	x	x	x	x				x		x	x	x	x	x	x		x						
197						x																		
201				x		x						x	x	x	x				x	x				
203A			x		x					x	x													
210	x	x	x		x	x					x	x	x											
212	x	x			x																			
222						x			x															
Total misclassified	7	6	6	6	8	13	0	0	3	1	7	9	10	12	12	12	5	13	7	1	5	5	5	
Total samples	37	37	37	37	37	37	34	36	36	36	36	36	36	36	36	36	34	36	35	36	26	26	26	
Efficiency per cent	81	84	84	84	78	65	100	100	92	97	81	75	72	67	67	67	85	64	80	97	81	81	81	

Identification of data subsets:

- 1 - all Whitten oxides + specific gravity + elevation
- 2 - all Whitten oxides + specific gravity
- 3 - all Whitten oxides except (FeO + Fe₂O₃ + MgO) + specific gravity
- 4 - Whitten K₂O & TiO₂ only
- 5 - Whitten K₂O + P₂O₅ only
- 6 - Whitten specific gravity only
- 7 - Whitten oxides except alkalis + Mehnert and Willgallis alkalis + Whitten norms except Mgt + Rein modes + specific gravity + elevation
- 8 - as 7 but Whitten alkalis in place of Mehnert and Willgallis alkalis
- 9 - all norms except Mgt + Rein modes + specific gravity + elevation
- 10 - all norms + Rein modes
- 11 - normative orthoclase and apatite only; 11,12, & 13 'best' three pairs from all norms and all modes
- 12 - normative orthoclase and modal plagioclase only
- 13 - normative orthoclase and modal K-feldspar only
- 14 - modal quartz and plagioclase; 14, 15, and 16 'best' three pairs from all modes
- 15 - modal K-feldspar and zircon
- 16 - modal plagioclase and biotite
- 17 - all norms except Mgt + specific gravity
- 18 - all modes + specific gravity
- 19 - Mehnert and Willgallis alkalis only
- 20 - as 8 without norms
- 21 - all eight Hahn-Weinheimer and Ackermann analyses
- 22 - P and Rb; 22 and 23 'best' two pairs from all variables in 21
- 23 - Ba and Rb

^T samples identified by Mehnert as being transitional between Classes A and B

localities listed in Table 1 were included so that less than 37 sample sites were used when data from Hahn-Weinheimer and Ackermann, Mehnert and Willgallis and/or Rein were included (these authors did not give analyses for all of the 37 locations in Table 1).

Table 4 shows that use of all of the variables* permits 100 per cent

*Except that either Mehnert and Willgallis' or Whitten's alkali values only were included.

efficiency in discriminating the two classes. Specific gravity plus Rein's modal values used together achieve only 63.9 per cent efficiency. A combination of the norms and modes (with elevation and specific gravity), however, causes only 3 of the 36 sites to be misclassified. Use of Whitten's chemical analyses alone or of the norms alone is less efficient than use of the combination of norms and modes. Surprisingly, Mehnert and Willgallis' (1961) alkali values alone (80 per cent efficiency) are almost as efficient as Whitten's ten oxides (coupled with elevation and specific gravity) used together (81 per cent efficiency). The discriminant function calculated for the eight elements analyzed by Hahn-Weinheimer and Ackermann (1967) only misclassifies 5 of 26 samples (81 per cent efficiency).

The discriminant function can be visualized more clearly when represented in map form. As an example, the locations of correctly and incorrectly classified sample locations in subset 2 (Table 6) are shown in Figure 8A. In Figure 8B one of the discriminant functions that is 100 per cent efficient (subset 8) is mapped to show the relative distance of each sample from the linear partition.

Effectiveness of discriminant functions can be considered differently. In many cases, the same (or even better) efficiency is achieved by use of only a small subset of the available variables (cf., Chayes and Velde, 1965). Table 5

illustrates some representative results produced by sequentially calculating the discriminant function for each subset of one variable, each possible subset of two variables, etc., in a total data array. For the available Malsburg Granite data, a single variable is commonly a very inefficient basis for a discriminant function but, in several cases, occasional pairs of variables are as efficient as, say, 8 or 14 variables used together. However, the "best" subsets selected in this manner are not always those that would be selected intuitively or on the basis of subjective geological experience (see Table 5).

It can be assumed that Rein's (1961) modes are good representations of the samples concerned but, as Table 4 shows, they are poor bases for discrimination between Mehnert and Willgallis' two mapped zones (Classes A and B).

It is possible that, in terms of their operational definitions, Mehnert and Willgallis misclassified some of the sample localities and, as a result, drew the boundary between the central and border granite zones incorrectly. In Table 6, the samples that were misclassified by a selection of the discriminant functions are listed; samples that appear repeatedly in this Table should be re-examined in terms of both Mehnert and Willgallis' original classification and the accuracy of the analytical data. Localities 159, 186, and 195 (and possibly 104) should be evaluated in this way (cf., Fig. 8A). Many of the 37 localities are classified correctly by all or most of the discriminant functions. Mehnert (personal communication) considered that four (numbers 7, 56, 118, and 186) of the localities used here are outer central granite transitional to border granite (see Fig. 8B); although the discriminant functions commonly misclassify 186, all major functions correctly classified the other three localities as central granites (see Table 6). It can be seen from Table 6 that there are several other sample sites that are more liable to misclassification (on the basis of available data) and which are, in this sense, truly transitional between Classes A and B. Of course, although Mehnert and Willgallis primarily based their maps on Rein's modes and their

alkali values, they were probably subjectively and qualitatively influenced (appropriately) by additional factors recognized (but not quantified) during their field work.

At this time, discrimination cannot be efficiently made on the basis of characteristics that could be estimated quantitatively in the field. The chemical and normative variables that permit efficient discrimination of the Classes can only be measured in the laboratory. Such results may prove not to be unusual. For example, Chayes (1964) and Chayes and Velde (1965) discovered that TiO_2 percentage is the only major oxide that efficiently discriminates between ocean-island and circumoceanic basalts. In such circumstances, in order that unequivocal quantitative discrimination may be made in the field during a mapping project, additional different criteria (e.g., textural characteristics, number and size of porphyroblasts, etc.) must be measured and mapped. If there is any basis for Mehnert's petrologically-significant model for the Malsburg Granite, there must be variables that could be measured in the field and be used as a basis for objective definition of his zones. In an economic situation, discovery of the few variables that can efficiently discriminate between commercially significant and unprofitable rock masses could greatly reduce the costs of exploration (cf., Whitten, 1966a).

PREDICTION MODELS FOR THE VARIABILITY OF THE MALSBURG GRANITE

Predictor models have many uses for testing petrogenetic and search models for individual granitic bodies. Predictions, made on the basis of samples gathered from a single lithic unit, can be made without reference to the spatial locations of the specimens. Commonly, more useful models result from including the spatial coordinates; three types are considered here: (i) models without mapped results, (ii) trend-surface maps for single dependent variables, and (iii) Q-mode factor-analysis maps based on simultaneous use of numerous measured variables.

Prediction models without mapped results

Some attributes are measured more precisely, accurately, and/or cheaply than others. As mentioned already, the variance of each variable in samples of a specified size and collected from one rock unit is, in general, different. Because of the large variance of some variables (and/or the difficulties of measurement), direct estimates of their distribution within rock units are difficult. Table 7 shows that simple linear correlation of many pairs of variables is not likely to be useful for prediction purposes. However, it might be anticipated that such attributes could be predicted on the basis of more-easily-assayed variables.

Vistelius (1962) demonstrated that the P_2O_5 content of some Tien Shan granitic rocks can be predicted with a simple linear model using modal quartz, potash feldspar, plagioclase, and mafic mineral percentages as independent variables. Similarly, Whitten (1966, 1968) demonstrated that sequential multiple linear regression can be used to "sort out" some of the interrelationships between chemical and specific gravity data for the Aulanko Granodiorite, Finland, and the Malsburg Granite. It seems probable that such prediction techniques could have considerable value for prospecting and evaluation in economic geology, in remotely-sensing the terrestrial surface from aircraft and satellites, and in a wide variety of petrological studies. However, at present, very little is known about the variance and interrelationships of the many hundreds of variables that can be measured for rock samples.

In the linear equation

$$\underline{Y} = \underline{a}_0 + \underline{a}_1\underline{X}_1 + \underline{a}_2\underline{X}_2 + \underline{a}_3\underline{X}_3 + \dots\dots\dots \underline{a}_{13}\underline{X}_{13}$$

let \underline{Y} be TiO_2 percentage and $\underline{X}_1, \dots, \underline{X}_{13}$ be specific gravity, nine other analyzed oxides, and the three spatial coordinates. Solving the equation by the method of least squares* and using the data for all thirteen "independent"

*The FORTRAN computer program prepared by Krumbein et al. (1964) was used for this purpose. As stated the model includes spatial coordinates and independent variables; by omitting these spatial variables a model without reference to location of the samples is involved.

variables available for the Malsburg Granite samples (Table 1), 86.97 per cent of the total variability of TiO_2 can be predicted. However, it is instructive to examine the prediction equations when only a few "independent" variables are used. Table 8 shows that

$$TiO_2 = \underline{a}_0 + \underline{a}_1 (SiO_2)$$

accounts for 75.53 per cent of the total sum of squares. Hence, for many purposes, prediction on the basis of SiO_2 alone would be adequate and inclusion of specific gravity or the other eight oxides would be redundant; that is, inclusion of a few oxides in addition to SiO_2 adds little to predictive power.

Use of the linear equation for prediction of P_2O_5 permits 75.09 per cent of the variability to be accounted for when all the other variables are used. Use of SiO_2 alone permits 56.34 per cent of the variability to be accounted for (Table 8).*

*This is a significant improvement over use of even the cubic trend surface (based on geographic coordinates and described in a subsequent section of this paper) which accounts for only 19.14 per cent of the total sum of squares (see Table 11). The three orthogonal spatial coordinates are identified as U, V, and W (expressed in kilometers) in Table 8 and the remainder of this paper. For

Table 8. - 'Best' predictions of TiO₂ and P₂O₅ percentages and specific gravity for the Harburg gneiss using sequential linear regression analysis.

Number of independent variables taken at a time	TiO ₂ percentage ¹ N = 37		P ₂ O ₅ percentage ¹ N = 37		Specific Gravity			
	Independent variables	Sum of squares reduction %*	Independent variables	Sum of squares reduction %**	N = 37 ²		N = 36 ³	
					Independent variables	Sum of squares reduction %***	Independent variables	Sum of squares reduction %****
1	SiO ₂	75.53	SiO ₂	56.34	CaO	37.76	CaO	38.97
	MgO	47.31	TiO ₂	47.23	FeO	31.89	Norm. Qtz.	34.84
	P ₂ O ₅	47.23	Al ₂ O ₃	42.32	SiO ₂	18.64	Norm. Anorth.%	33.86
2	<u>V</u> , SiO ₂	81.69	SiO ₂ , Al ₂ O ₃	62.57	FeO, CaO	43.11	CaO, Hornbl.	51.13
	<u>W</u> , SiO ₂	79.28	Al ₂ O ₃ , TiO ₂	59.90	SiO ₂ , CaO	40.24	Hornbl., Norm. anorth.%	48.80
	SiO ₂ , Fe ₂ O ₃	76.90	SiO ₂ , Na ₂ O	59.37	Fe ₂ O ₃ , CaO	40.13	CaO, Qtz.	48.31
3	<u>U</u> , <u>V</u> , SiO ₂	83.43	Al ₂ O ₃ , Fe ₂ O ₃ , FeO	65.54	SiO ₂ , Fe ₂ O ₃ , CaO	45.26	CaO, P ₂ O ₅ , Hornbl.	53.40
	<u>V</u> , SiO ₂ , Na ₂ O	82.48	SiO ₂ , Al ₂ O ₃ , Na ₂ O	65.42	FeO, CaO, Na ₂ O	44.28	Fe ₂ O ₃ , CaO, Hornbl.	52.82
	<u>V</u> , SiO ₂ , Fe ₂ O ₃	82.26	SiO ₂ , Al ₂ O ₃ , Fe ₂ O ₃	64.60	<u>U</u> , FeO, CaO	44.13	Fe ₂ O ₃ , CaO, Qtz.	52.75
	<u>V</u> , <u>W</u> , SiO ₂	82.24	SiO ₂ , Na ₂ O, K ₂ O	64.24	Fe ₂ O ₃ , CaO, TiO ₂	44.11	MgO, CaO, Hornbl.	52.25

1 Prediction based on all nine other oxides (Table 1), Specific Gravity, U, V, and W

2 Prediction based on all ten oxides (Table 1), U, V, and W

3 Prediction based on all ten Whitten's oxides, seven Rein's modes, 4 major Whitten's norms, and W

* Maximum with all 13 'independent' variables - 86.97 per cent.

** Maximum with all 13 'independent' variables - 75.09 per cent.

*** Maximum with all 13 'independent' variables - 53.47 per cent.

**** Maximum with all 22 'independent' variables - 70.61 per cent.

N = Number of samples available

convenience, the axial origin was placed just north of the granite with U increasing in a southwesterly, V in a southeasterly, and W in the upwards direction.

Intuitively, geologists have little basis for deciding whether these results for TiO_2 and P_2O_5 are reasonable and common, or whether they are markedly dissimilar to those that would be found for the majority of granitoid masses. For specific gravity, however, many geologists would anticipate significant correlations with modal mineralogy. Dawson and Whitten (1962) and Whitten (1963A, p. 111; 1966a) suggested that specific gravity might be a more efficient variable for expressing the three-dimensional composition and variability of granitic masses than the customary modal variables. This contention was based on (i) the similarity of trend surfaces for specific gravity and modal variables (e.g., in the Lacorne, LaMotte, and Preissac granitic complex, Quebec, Canada and the "older granite" of Donegal, Ireland), (ii) the fact that much larger specimens can be used for measuring specific gravity than are commonly used for modes or chemical analyses, so that the smallest levels of variance can be eliminated, and (iii) consideration of problems arising from the fact that modal data necessarily involve closed-number (percentage) arrays. Moore (1963) also demonstrated that strong correlation of specific gravity with modal quartz and feldspars for the Cartridge Pass pluton, Sierra Nevada, California, and concluded that the mineralogical zonation of the Arrow, Cartridge Pass, Lamarck, Paradise, and Spook silicic granodiorite plutons is accurately reflected by specific gravity. Peikert (1962; 1965) analyzed the three-dimensional variability of specific gravity and some modal variables in the Glen Alpine stock, Sierra Nevada, California, but did not evaluate the correlation between these

variables. However, in a similar three-dimensional study of the San Isabel Granite, Colorado, Whitten and Boyer (1964, Figs. 7 and 8) presented data that strongly suggest significant correlations between specific gravity (for powdered rock samples) and weight percentages of various heavy-mineral fractions. Whitten (1968) also showed that for the Aulanko Granodiorite, Finland, use of the ten major oxides in a linear regression equation permits 94.83 per cent of the variability of specific gravity to be predicted.

Sequential linear regression analysis of the data given by Moore (1963, Tables 11, 12, 13, 24) for the Arrow, Cartridge Pass, and Spook plutons confirms that specific gravity is strongly correlated with the modal components (Table 9); these granites have mean color indices of 13.3, 9.7, and 8.4, respectively. However, Table 9 also shows that this relationship does not hold for Bullfrog pluton (mean color index 3.0). For a small set of data for the Climax Stock granodiorite, Nevada (analyses from Houser and Poole, 1959, and Izett, 1960), the linear correlation coefficients between specific gravity and each of the major-oxide and modal variables is less than 0.5 (Whitten, 1963, p. 112). This relationship is reflected by Table 10 (all variables taken one at a time and even when three modal variables are taken at a time). However, the oxides taken two or more at a time and large groups of modal variables both permit reasonable predictions of specific gravity with these data. Cain (1964) also showed on the basis of 53 samples that modes have little value in predicting specific gravity of the Newingham Granodiorite, Wisconsin.

For the Malsburg Granite samples, Table 8 shows that only 53.47 per cent of their specific gravity variation can be predicted on the basis of all ten oxides, and three spatial coordinates. Although only accounting for 37.76 per cent, it is surprising that CaO provides the best prediction on the basis of a single oxide. In an attempt to find those factors that control

Table 9. - 'Best' predictions of specific gravity on the basis of modes of plutons in the Mount Pinchot Quadrangle, California (data from Moore, 1963) using sequential linear regression analysis.

Number of modal variables taken at a time	Arrow Pluton N = 18		Bullfrog Pluton N = 27		Cartridge Pass Pluton N = 45		Spook Pluton N = 21	
	Independent variables	Sum of squares reduction %*	Independent variables	Sum of squares reduction %*	Independent variables	Sum of squares reduction %*	Independent variables	Sum of squares reduction %*
1	Plagioclase	61.28	Biotite	10.23	Hornblende	76.89	Hornblende	53.18
	K-feldspar	51.74	Color index	7.91	Color index	75.29	Color index	33.38
	Pyroxene	27.85	Nonopaque accessories	7.86	Biotite	65.24	K-feldspar	30.64
2	Plagioclase, biotite	72.35	Opaque accessories, color index	19.50	K-feldspar, hornblende	80.72	K-feldspar, hornblende	65.99
	Plagioclase, color index	68.35	Perthite, biotite	16.45	Plagioclase, hornblende	80.35	K-feldspar, color index	61.56
	Quartz, K-feldspar	68.05	Biotite, opaque accessories	14.39	Plagioclase, color index	78.65	Plagioclase, hornblende	59.55
3	Plagioclase, biotite, opaque accessories	74.18	Perthite, opaque accessories, color index	30.04	Quartz, K-feldspar, hornblende	81.53	K-feldspar, hornblende, nonopaque accessories	68.49
	Plagioclase, opaque accessories, color index	72.90	Quartz, opaque accessories, color index	27.64	Plagioclase, biotite, hornblende	81.45	K-feldspar, hornblende, color index	67.87
	Plagioclase, biotite, nonopaque accessories	72.60	Perthite, biotite, opaque accessories	23.25	K-feldspar, plagioclase, hornblende	81.26	K-feldspar, biotite, hornblende	67.73

* Maximum with all 'independent' modal variables - 78.91% for Arrow, 37.28% for Bullfrog, 82.29% for Cartridge Pass, and 71.81% for Spook Pluton.

N = Number of samples available

Table 10. - 'Best' predictions of specific gravity for the Climax Stock Granodiorite, Nevada, using sequential linear regression analysis.

Number of variables taken at a time	Data subset 1* N = 14		Data subset 2** N = 20		Data subset 3*** N = 16	
	Independent variables	Sum of squares reduction %	Independent variables	Sum of squares reduction %	Independent variables	Sum of squares reduction %
1	K ₂ O	53.48	Magnetics	20.95	Elevation	31.88
	CaO	39.23	Elevation	20.26	Magnetics	18.45
	MgO	21.28	Chlorite	14.99	Susceptibility	16.27
2	SiO ₂ , CaO	72.04	Elevation, magnetics	48.92	Elevation, magnetics	49.90
	Na ₂ O, K ₂ O	71.42	Elevation, plagioclase	28.86	Elevation, chlorite	38.81
	CaO, Na ₂ O	70.10	Elevation, biotite	28.27	Susceptibility, magnetics	32.88
3	Elevation, MgO, K ₂ O	88.41	Elevation, quartz, magnetics	52.02	Elevation, chlorite, magnetics	57.39
	Elevation, Na ₂ O, K ₂ O	87.38	Elevation, plagioclase, magnetics	51.43	Susceptibility, chlorite, magnetics	53.73
	Elevation, SiO ₂ , K ₂ O	87.29	Elevation, biotite, magnetics	50.26	Elevation, plagioclase, magnetics	51.68

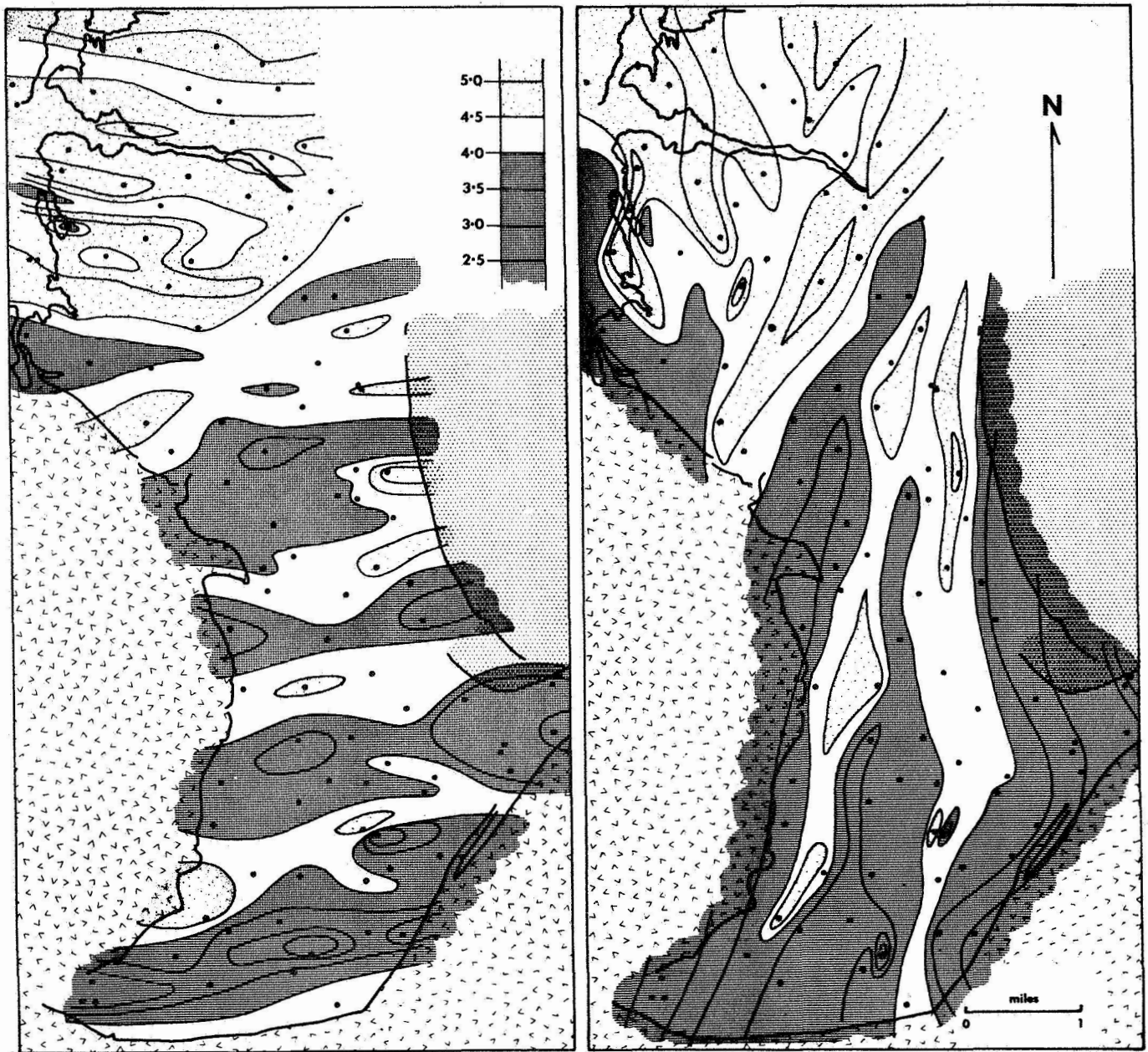
¹ Eight variables - elevation, SiO₂, Al₂O₃, total iron, MgO, CaO, Na₂O, and K₂O; maximum sum of squares with all variables 94.68 per cent.

² Seven variables - elevation, plagioclase, K-feldspar, quartz, biotite, and chlorite volume per cent, and weight per cent of magnetics; maximum sum of squares with all variables 55.80 per cent.

³ Eight variables - elevation, magnetic susceptibility, plagioclase, K-feldspar, quartz, biotite, and chlorite volume per cent, and weight per cent of magnetics; maximum sum of squares with all variables 77.19 per cent.

N - number of samples in subset

9. Variation of K_2O weight percentage in the 'older granite' of the Bunbeg-Thorr area, Donegal, Eire; based on analyses of rock from the 114 localities indicated. The two maps are different but equally-valid manually contoured representations of the same raw data. After Whitten, 1966b.



specific gravity in the Malsburg Granite, Rein's (1961) modal values and the four main normative components were included with the chemical analyses before recomputing the linear regression relationships. CaO remains the "best" single variable (Table 8) and the "best" pair of variables is CaO with modal hornblende; modal hornblende with normative anorthite percentage gives the "next-best" pair. Such relationships can be rationalized in terms of petrography although they are dissimilar to those for, say, the Aulanko Granodiorite.

These results for samples from different granite masses are perplexing. It is not known, for example, what characteristics cause specific gravity to be predictable in some granites, but not in others. Lack of predictability may result from poor chemical analyses, clerical errors, or real differences in composition between the material used for chemical or modal analysis and that used for density determination. The latter could readily occur if variances are large at the level of small samples and analyses are made for part of a larger sample weighed for specific gravity measurement. Until more is known about the factors controlling such correlations, predictions cannot be extended to specimens from the sampled population of granite complexes that have not been subjected to preliminary study (let alone be extended to most possible target populations).

Trend-surface maps for single dependent variables

It must be recognized that in computing trend components many assumptions are made about the data. Baird, et al., (1964, 1965) considered the significance of individual chemical analyses before attempting to map the chemical composition and variability of a granite pluton. It is well known that each variable has a different variance in samples of a given size and that the components of variance at different levels of sampling vary in a different complex manner for each variable. These problems which significantly affect

sampling are additional to those concerning the analytical accuracy for each selected sample. Very little is known about the levels of variance in different plutons. Baird, et al. referred to the Rattlesnake Pluton, California and it is probable that equally complex, but different, relationships occur in other plutons (cf., Rhodes, 1969).

Once a set of analyses has been acquired for the sampled population it is customary to assess their pattern of spatial variability; it is commonly implicitly (but erroneously) assumed that the pattern is that of the target population too. The variability can be assessed subjectively by drawing manual contours although, because there is no information about the behavior of the variables between the actual sample sites, an infinite number of dissimilar maps can be drawn (Whitten, 1966b). Figure 9 illustrates two possible subjective contour maps for 114 unpublished analyses of K_2O for the "older granite" of Donegal, Eire. Neither map violates the data. The method permits the geologist to incorporate appropriate subjective geological factors in the final map. Commonly, however, one of the many quantitative objective methods of depicting the spatial variability of mapped variables has been used. Polynomial trend-surface analysis permits the regional and local components of variability of a set of samples to be mapped separately; it is illustrated here. Other linear (e.g., double Fourier Series) and nonlinear trend surfaces could be used, although selection of one of these models would be more appropriate when the nature and underlying petrogenetic causes of the spatial variability are more clearly understood.

Table 11 lists the proportions of the total sums of squares associated with polynomial trend components (calculated with the computer program published by Whitten et al., 1965) for Mehnert and Willgallis' (1961) alkalis, Whitten's chemical analyses (Table 1), and Hahn-Weinheimer and Ackermann's (1967) analyses of eight elements.

Table 11. - Percentages of total sums of squares associated with polynomial trend surfaces for the Malsburg Granite.

Variables	Two geographic independent variables (<u>U</u> , <u>V</u>) only					Three spatial independent variables (<u>U</u> , <u>V</u> , <u>W</u>)	
	Degree 1 3 coefficients	Degree 2 6 coefficients	Degree 3 10 coefficients	Degree 4 15 coefficients	Degree 5 21 coefficients	Degree 2 10 coefficients	Degree 3 20 coefficients
<u>Whitten's variables (N = 37)</u>							
Specific gravity	2.85	8.33	25.78	41.89	51.45	13.65	50.25
SiO ₂ wt. per cent	15.51	20.89	23.60	25.77	32.55	29.18	58.56 U
Al ₂ O ₃	15.57	17.33	23.27	40.31	67.81	29.79	70.86
Fe ₂ O ₃	7.23	8.98	20.30	28.88	65.70	21.73	57.92 D
FeO	18.35	19.11	25.13	32.48	48.61	24.45	49.42
MgO	10.86	23.04	28.18	29.76	44.99	27.93	52.19 U
CaO	3.36	4.44	24.49	42.02	54.22	14.65	45.96 D
Na ₂ O	0.49	17.25	22.16	47.04	55.91	26.50	54.44
K ₂ O	4.71	17.54	22.94	39.76	62.50	23.15	49.09 D
TiO ₂	13.16	21.24	29.26	30.65	37.36	28.01	55.39 U
P ₂ O ₅	10.59	11.73	19.14	43.62	48.26	17.51	48.52
<u>Hahn-Weinheimer and Ackermann's variables (N = 64)</u>							
Ti wt. per cent	22.18	32.62	41.68	48.20	55.26	44.98	56.83
Zr ppm x 10 ⁻²	15.47	26.06	28.78	35.32	38.38	37.62	46.16 U
P ppm	14.45	32.51	49.58	59.83	70.47	43.13	67.69
Sr	22.43	50.14	66.07	70.16	73.77	58.89	73.30
Ba	22.56	39.60	63.81	69.56	77.50	48.94	69.74 D
Rb	3.87	32.45	35.91	37.85	45.05	40.37	50.04
K wt. per cent	1.49	39.69	44.83	52.01	59.26	45.18	53.15 D
Na wt. per cent	11.96	32.23	33.28	44.45	51.30	36.13	44.03 D
<u>Mehnert and Willgallis' variables (N = 110)</u>							
K ₂ O wt. per cent			31.91	33.28	42.22	32.45	47.43
Na ₂ O wt. per cent			27.82	34.76	53.16	30.46	45.61 D

N = number of samples; U = sum of squares for U, V, W degree 3 appreciably greater than for U, V degree 5; and D sum of squares appreciably smaller.

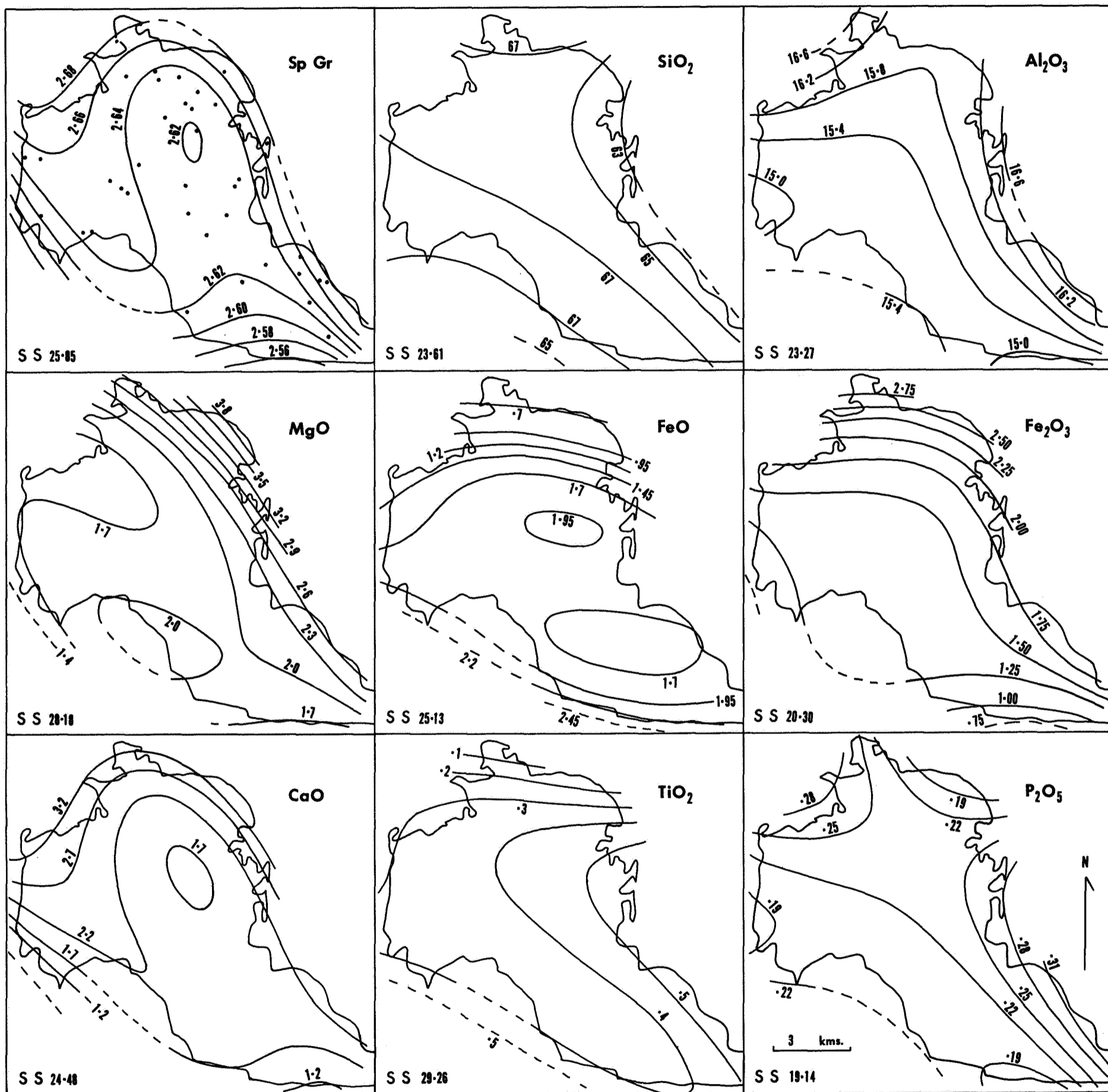
For the Malsburg Granite data, the low degree trend surfaces based on U and V only are almost all associated with small sums of squares predicted (Table 11); Sr and Ba are exceptions. This implies that, for most variables, the deviations are large by comparison with the degree one, two, and three regional gradients and that, for each variable, the variability of the samples analyzed has a complex local pattern. The regional gradients are shown in Figures 10, 11, and 12. For Whitten's chemical analyses and specific gravity only 37 sample sites are available so that surfaces of higher degree than third (with 10 coefficients) should not be calculated, no matter what proportion of the variability is accounted for. For the trace elements (Fig. 12), 64 samples were used and the degrees of freedom make it possible to use trend surfaces up to the fifth degree (which require 21 coefficients in the polynomial equation). For the alkalis, maps (Fig. 11) are presented for all three independent sets of chemical analyses; degree 3 or degree 5 surfaces are illustrated depending on the number of degrees of freedom associated with each data set. Because each group of alkali analyses would be accepted by many petrographers as an adequate representation of the pluton and serve as a basis for petrogenetic conclusions, it is instructive to compare and contrast these three pairs of maps more thoroughly.

Without very careful evaluation, such trend maps could readily give erroneous concepts about both the sampled and the target populations. Confidence levels can be associated with each trend component (see Dawson and Whitten, 1962, p. 8; Whitten, 1963; Chayes, 1970) and, when considered separately, most of the linear, quadratic, and cubic components for Whitten's chemical analysis data (Figs. 10 and 11) have no significant confidence level. The situation is demonstrated very clearly by scanning the \underline{z}^2 -arrays which can be computed by using orthogonal polynomials for the irregularly-spaced data (Whitten, 1970B);

for these data, trivial values occupy the top left corner of the z^2 -arrays in most cases. The 'best' array is that for TiO_2 , while SiO_2 , Al_2O_3 , Fe_2O_3 , FeO , MgO , K_2O , and P_2O_5 have one or two reasonably strong linear terms surrounded by trivial terms in the z^2 -array (Table 12). Such evidence confirms that the available data provide only a poor basis for evaluating the spatial variability of the sampled population (let alone the target population).

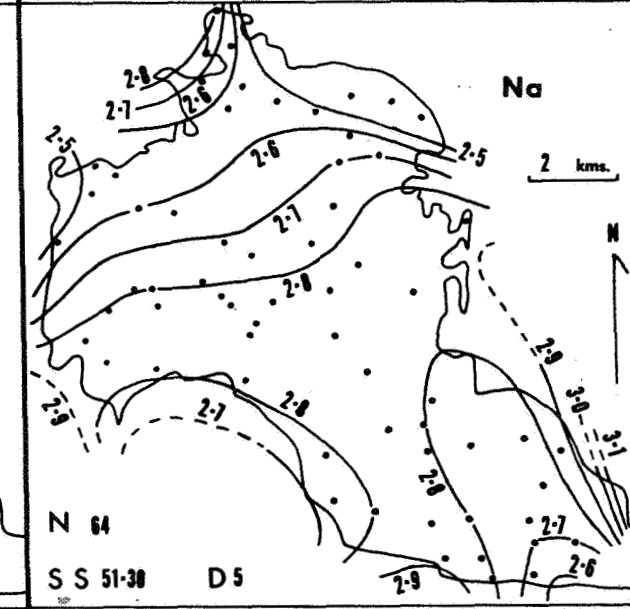
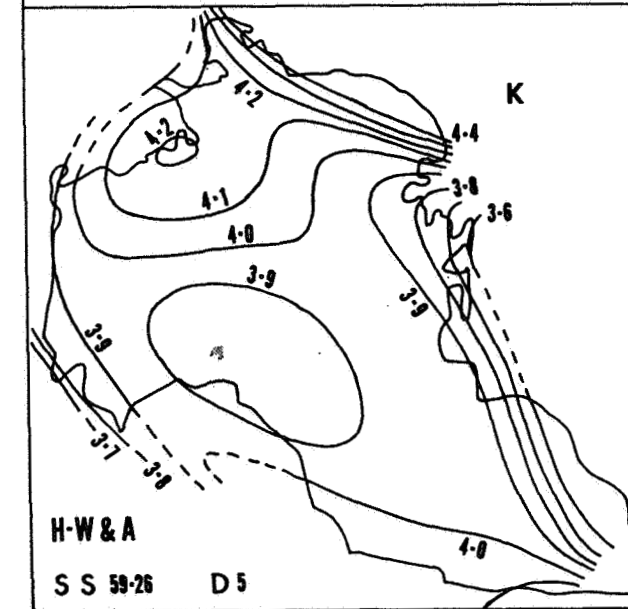
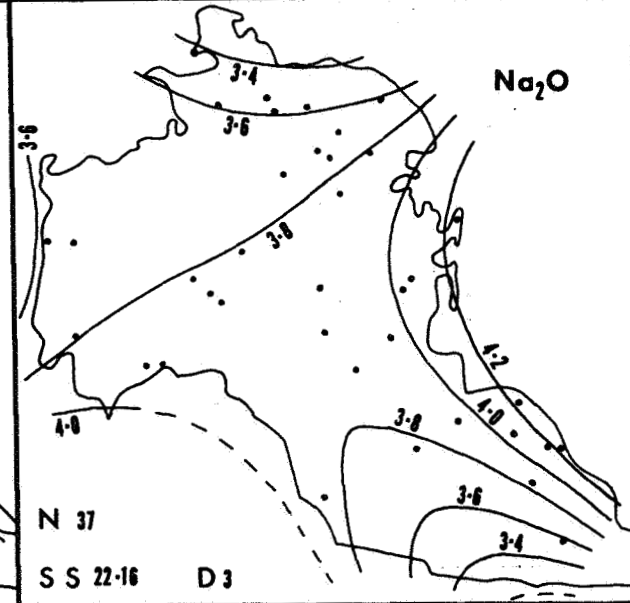
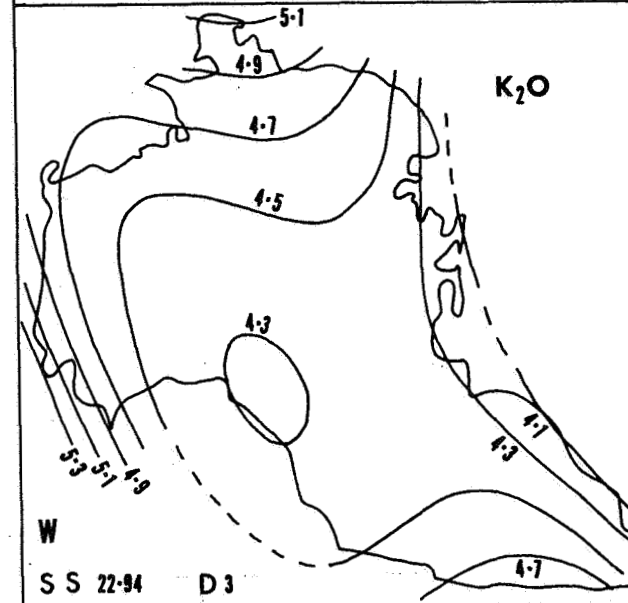
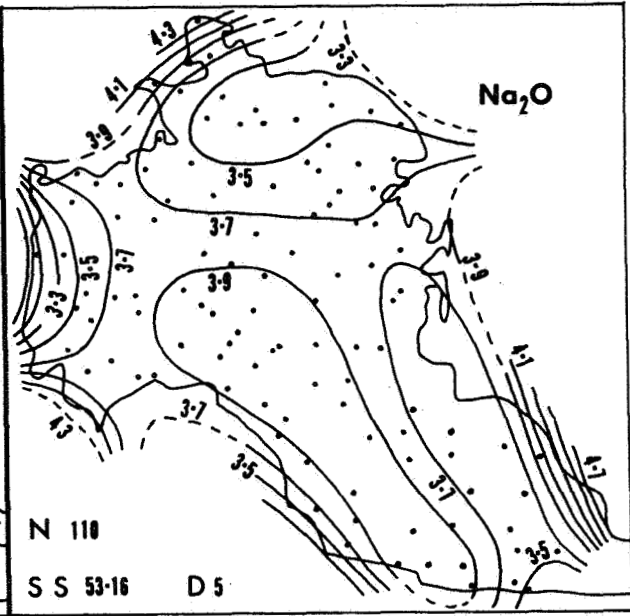
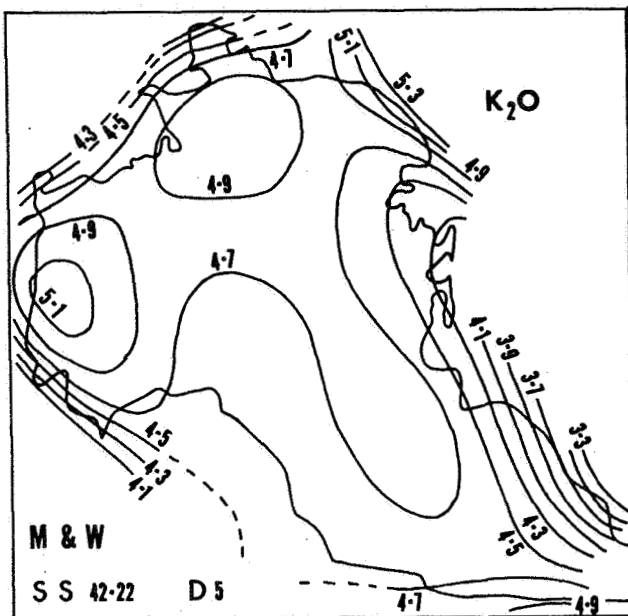
Weight percentages have been used for these maps because it is customary to use this unit in petrology although, in mapping spatial variability within a rock unit, the more appropriate units are weights per unit volume. Density is known for the 37 analyzed samples, so the oxides can be expressed in gm/100 cc.; although no longer percentages, the restraints of closed-number tables still apply to such data, which yield slightly different trend components and different correlation coefficients.

Because the samples were collected from sites with a vertical range of some 620 meters, polynomial hypersurfaces (up to the third degree) were also calculated with the computer program published by Peikert (1963). Inclusion of elevation (W) as an independent variable results in marked increases in the total sums of squares associated with equations of the same degree (Table 11). Peikert (e.g., 1962, 1965) and Whitten (e.g., 1962) suggested that the increased proportions of the total sums of squares associated with third degree polynomials when elevation is included (in addition to geographic coordinates), implies that there is a significant amount of vertical mineralogical variability within the sampled populations studied. For some granites, it was suggested that the vertical rates of change are greater than those in the horizontal plane. It is important to recognize, however, that degree-three UVW -hypersurfaces involve 20 coefficients and that it is possibly more appropriate to compare them with the degree 5 UV -surfaces which have approximately the same number of coefficients.

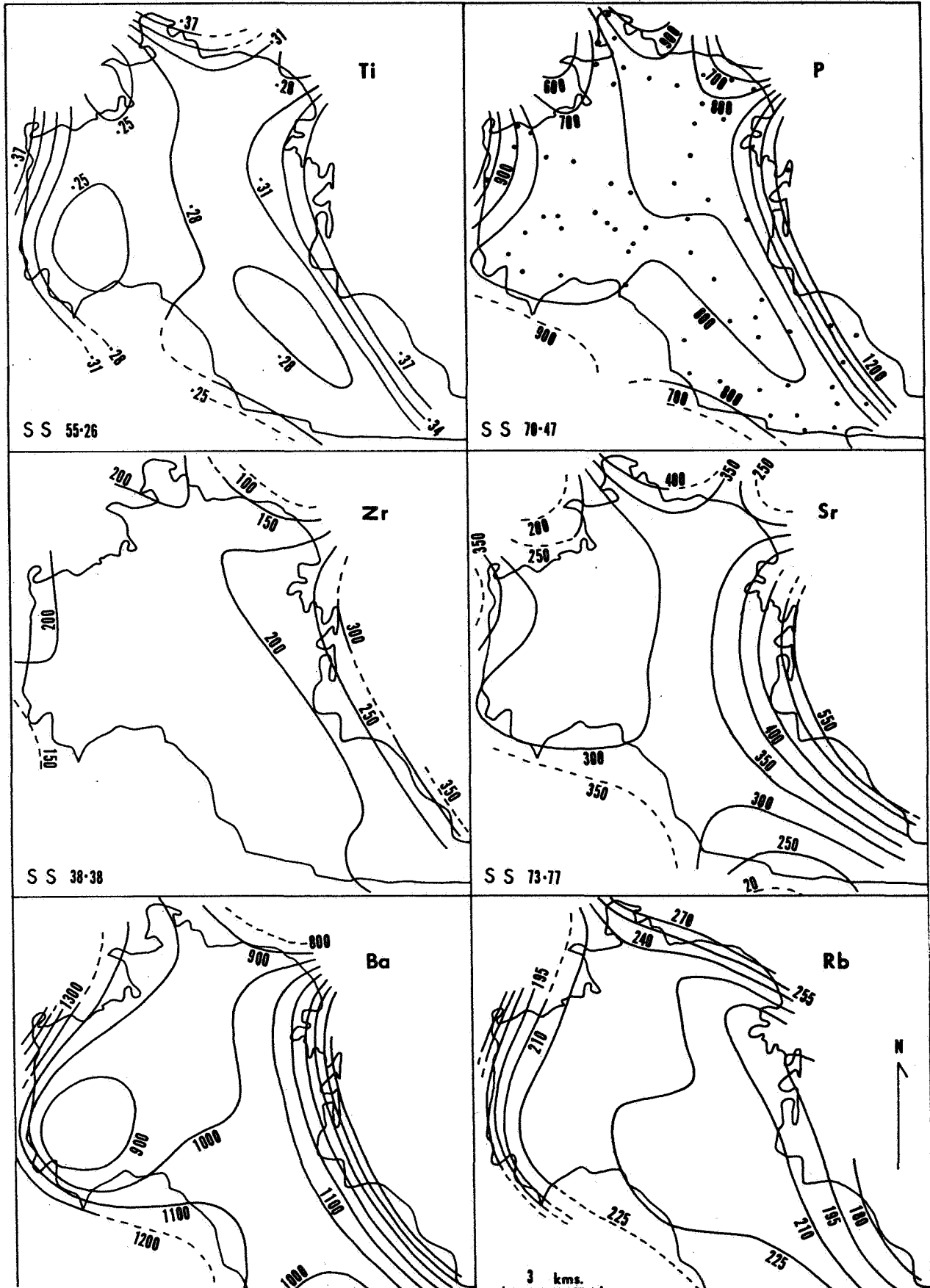


10. Degree 3 polynomial trend surfaces for the Malsburg Granite computed for \bar{U} , \bar{V} , and the analyses listed in Table 1; the 37 sample localities are shown on the specific gravity map and SS indicates the percentage of the total sum of squares associated with each surface.

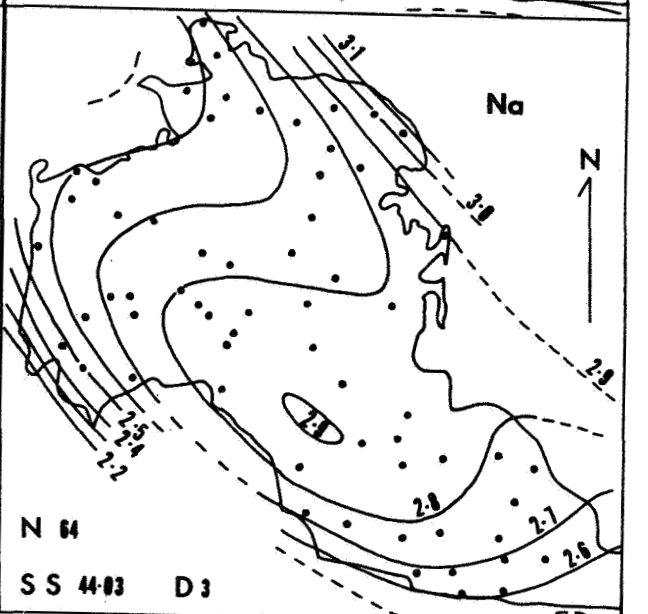
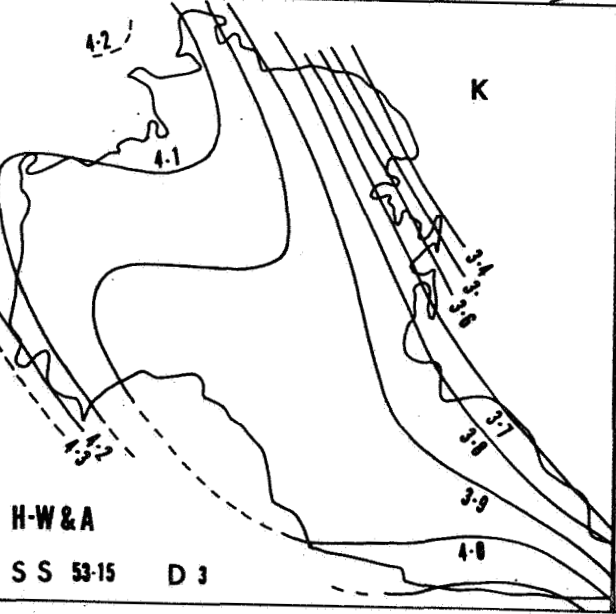
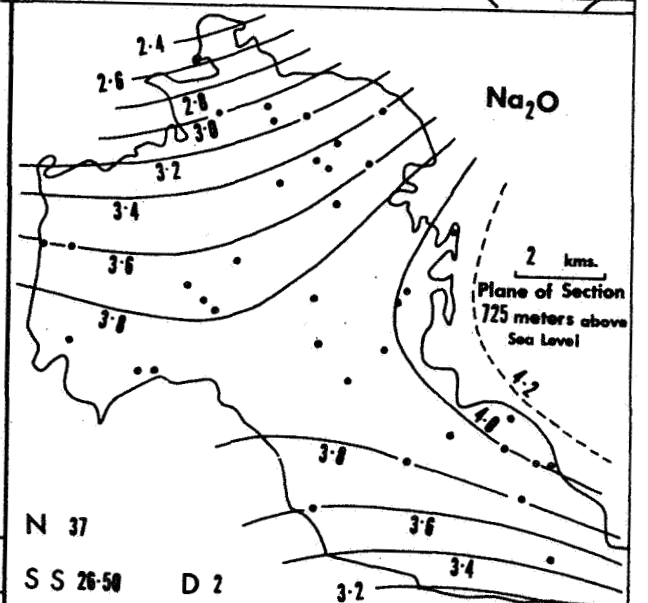
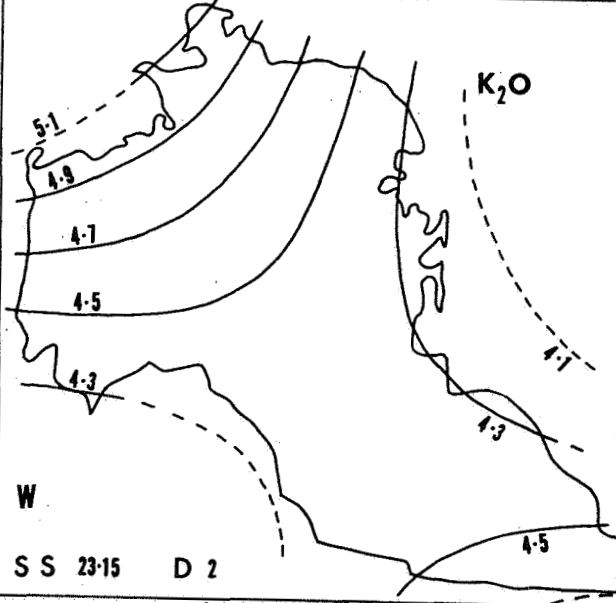
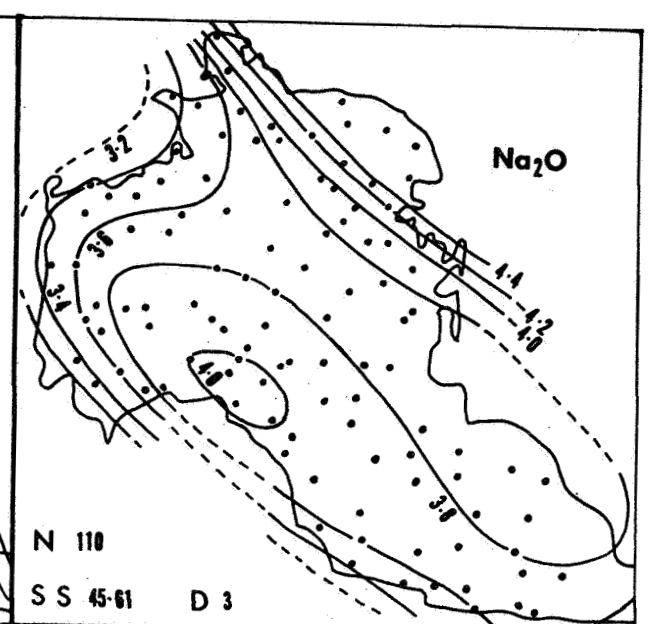
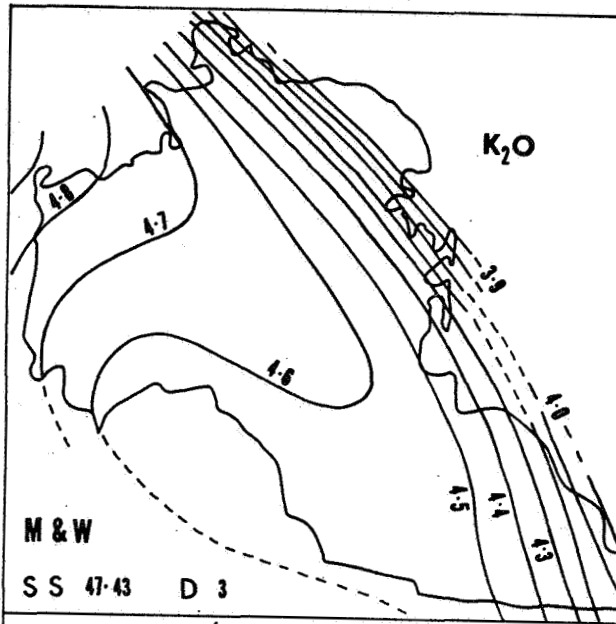
11. Polynomial trend surfaces for the Malsburg Granite: computed for U, V, and the three independent sets of alkali analyses by Mehnert and Willgallis (M & W), Whitten (W), and Hahn-Weinheimer and Ackermann (H-W & A); degree 5 (D5) and degree 3 (D3) surfaces are illustrated and SS refers to the percentage of the total sum of squares associated with each surface. N is the number of sample localities used for each pair of maps (the actual sites are shown on the Na₂O or Na map).



12. Degree 5 polynomial trend surfaces for the Malsburg Granite: computed for \bar{U} , \bar{V} , and the 64 sets of analyses from Hahn-Weinheimer and Ackermann. The 64 sample localities are shown on the P map; SS indicates the percentage of the total sum of squares associated with each surface.



13. Horizontal sections (at 725 meters above sea level) through the polynomial trend hypersurfaces for U, V, W, and the three independent sets of alkali analyses by Mehnert and Willgallis (M & W), Whitten (W), and Hahn-Weinheimer and Ackermann (H-W & A); degree 3 (D3) and degree 2 (D2) surfaces are illustrated and SS refers to the percentage of the total sum of squares associated with each hypersurface. N is the number of sample localities used for each pair of maps (the actual sites are shown on the Na₂O or Na map).



The restraints applying to interpretation of the UV-maps obviously apply to the UVW-trend components and make it difficult to draw meaningful conclusions for the present data set. The degree 5 UV-surfaces and degree 3 UVW-hypersurfaces (Table 11) show that inclusion of elevation yields important sums of squares increases for SiO_2 , MgO , TiO_2 , and Zr and important decreases for Fe_2O_3 , CaO , Whitten's K_2O , Ba , Na , and Mehnert and Willgallis' Na_2O . For the variables showing increases, there is possibly important vertical variability. By contrast, the decreases suggest variables for which vertical variability is relatively less important and for which a greater proportion of the total variability of the sampled population is accounted for by more complex areal variability patterns.

To illustrate the effect of including elevation, horizontal sections through the polynomial hypersurfaces at 725 meters above sea level (roughly the mean elevation of the sample sites) for the three sets of alkali analyses are given in Figure 13. These maps should be compared and contrasted with those in Figure 11 for the same data, but with elevation ignored. Of course, Figure 13 reflects vertical as well as horizontal extrapolations because the 725 meter plane is either above or below the sample surface (ground level) over most of the map area.

The limitations of polynomial trend surfaces (particularly when interpolation and extrapolation are involved) have been widely discussed (e.g., Whitten, 1966a, Merriam and Cocke, 1967, Chayes, 1970). A wide range of problems that affect the usefulness of individual surfaces has been recognized (e.g., selection of the trend, evaluation of deviations, boundary effects, spacing of data points, change of variance over map area, etc.). The limited amount of data available for the Malsburg Granite makes it uncertain (or even unlikely) whether Figures 10, 11, 12, and 13 provide a realistic picture of the regional variation of either the sampled or the target population.* Even

* For this purpose, the target population is defined as all those hand-sample size samples that theoretically comprise the whole mapped extent of the Malsburg Granite.

if high confidence could be associated with the trend components, statistical inferences cannot be made about the target population on the basis of trend components; substantive geological reasoning can be used, but this (as in most other petrographic studies) is fraught with immense problems because so little is known about the levels of variance of the several variables involved. Also, it would be difficult to integrate a generalized picture of granite variability on the basis of separate maps of 19 different variables. A multivariate approach, permitting simultaneous consideration of some, or all, of the measured variables, would have distinct advantages. Such a method is outlined in the next section.

Mapping several variables simultaneously

In a preceding section attempts were made to determine the efficiency with which the available data for the sampled populations permit retrieval of Mehnert and Willgallis' (1961) mapped zones of the Malsburg Granite. An alternative approach is to use Q-mode factor-vector analysis to detect, emphasize, and map the natural relationships between the available samples. In Q-mode factor analysis, n significant factors are selected and the specimens that most closely correlate with each of the n factors are found. Each other sample is then expressed numerically as proportions of the n samples chosen to approximate each of the n factors. Maps can be prepared for each factor by plotting and contouring the numerical values for each specimen on the base map. The mathematical bases for such analyses were restated by Imbrie (1963) and Krumbein and Graybill (1965, pp. 368, 402).

Garrett (1967) published the computer program (limited to use with 100 samples and 25 variables) used in the present work. The program permits data for each variable to be transformed into a 0-100 scale so that each variable has an equal weight in the Q-mode analysis.* The number of factors adequate

*Data normalization is necessary when major and trace components are used together, but it is questionable whether equal weight should be given to each variable. If analytical accuracy is not the same for all variables, some would favor giving extra weight to the more accurate (cf., Rhodes, 1969); more complete variance information for each variable (for samples of the size analyzed) might justify assigning unequal weights to variables.

to describe all of the samples is commonly decided on the basis of the size of the eigenvalues of the sample correlation matrix; three representative sets of eigenvalues are listed in Table 13. Maps were prepared for several data subsets on the basis of two, three, or four factors. However, Table 13 shows that one factor accounts for an overwhelming proportion of the total variability; analogous (or even more marked) situations occur for the other data subsets tested. Thus, for the present data for the sampled population of the Malsburg Granite, it appears that use of two factors provides an adequate representation of their spatial variability.

Slightly dissimilar results are obtained when different subsets of the measured data are used. Three of the many subsets examined are described here, viz:

- (i) 25 variables for 36 specimens: specific gravity, 10 Whitten's chemical analyses, 7 Rein's modal values, and 7 normative values.
- (ii) 8 variables for 64 samples: Hahn-Weinheimer and Ackermann's chemical analyses.
- (iii) 7 variables for 100 samples: Rein's modal values.

Table 13. - Eigenvalues of some sample correlation matrices used for Q-mode factor analysis of the Malsburg Granite.

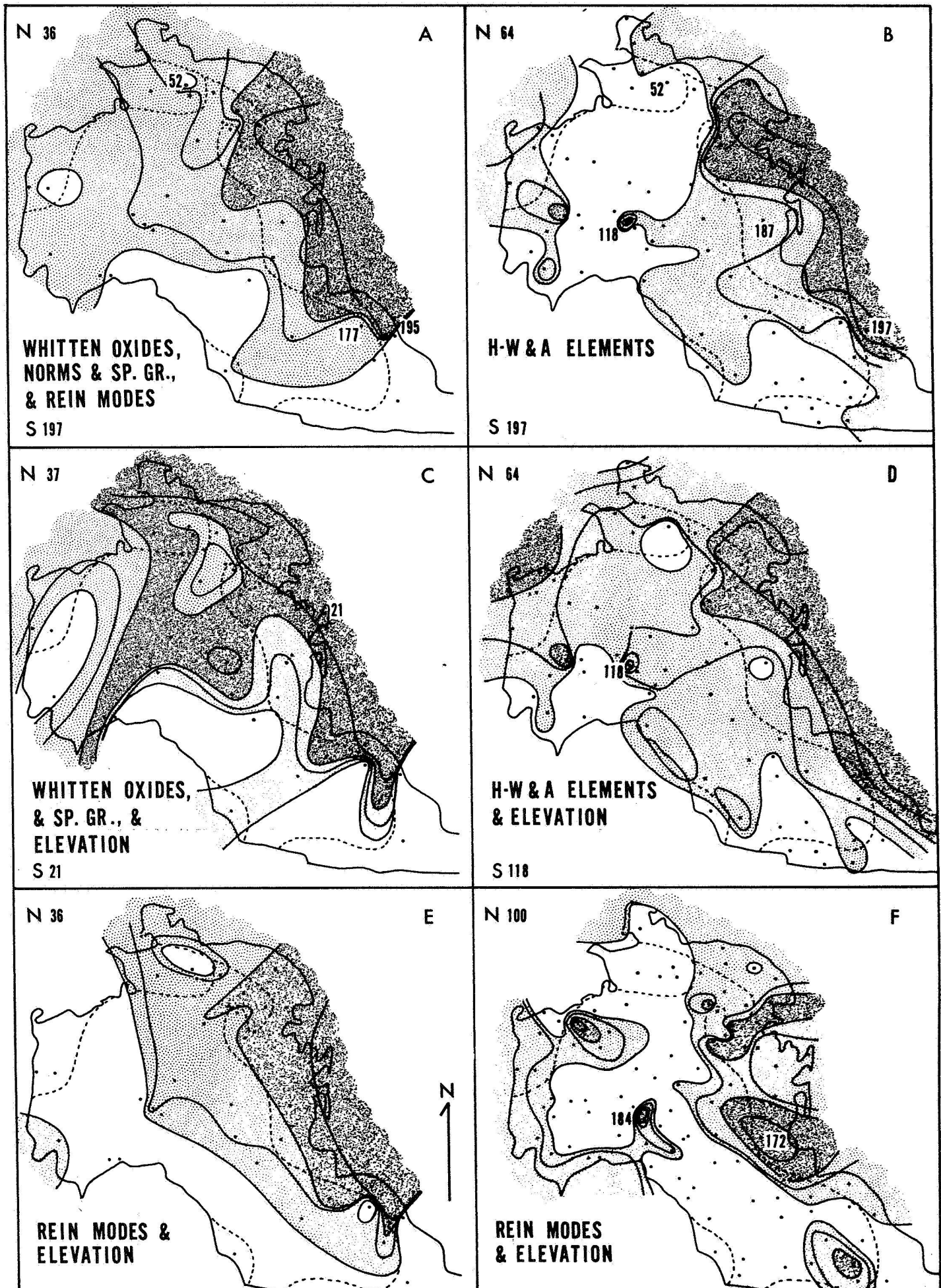
Factor	Data subset (i)		Data subset (ii)		Data subset (ii) with elevation included	
	Eigenvalue	Cumulative % of communality over 36 factors	Eigenvalue	Cumulative % of communality over 64 factors	Eigenvalue	Cumulative % of communality over 64 factors
1st	31.316	87.0	57.429	89.7	56.287	87.9
2nd	1.647	91.6	3.360	95.0	3.083	92.8
3rd	.735	93.6	1.825	97.8	2.173	96.2
4th	.573	95.2	.755	99.0	1.402	98.3
5th	.431	96.4	.258	99.4	.539	99.2
6th	.337	97.3	.204	99.7	.213	99.5
7th	.200	97.9	.126	99.9	.175	99.8
8th	.192	98.4	.043	100.0	.093	99.9
9th	.140	98.8	.000	100.0	.036	100.0

Each subset represents a different sampled population. Whitten's chemical analyses and subsets (ii) and (iii) were also re-run with elevation included as an extra variable.

Figure 14A is based on subset (i) and the zonation from northeast to southwest is clear, although there are significant differences and anomalies when these zones are compared with the subdivisions of Mehnert and Willgallis (1961). Because it was possible that either the chemical components or the modes might have been controlling the map pattern (Fig. 14A), these groups of variables were analyzed separately (Figs. 14C and 14E); the latter maps show that, for both groups of variables (combined with elevation as an additional variable), this sampled population yields patterns remarkably similar to Figure 14A. For the modal map (Fig. 14E), specimens 52, 177, and 195 are very anomalous in terms of the regional pattern of variability. Specimen 195 (and to a lesser extent 177) are also anomalous in the oxide map (Fig. 14C).

The effect of elevation as an additional variable is appreciable. Figure 14B shows the Q-mode map for Hahn-Weinheimer and Ackermann's analyses of eight variables for 64 samples (subset ii); the same data together with elevation are the basis of Figure 14D. Although these maps have analogies, dissimilarities in the central and southeastern areas indicate that there is significant chemical variability in the limited vertical dimension exposed and represented by this sampled population. In these two maps, specimens 52, 118, and 187 are anomalous (but 177 is not); specimen 195 was not included in this subset.

Figure 14F is based on 100 of Rein's modes and the elevations of each sample site (subset iii); the 36 specimens used for Figure 14E are all included together with 64 other samples chosen (with the aid of a random number table) from the 110 samples analyzed by Mehnert and Willgallis. Much of the complexity near the southwest margin of the granite in Figure 14F occurs in areas that are dataless for Figure 14E. Geologically, it would seem to be significant that, when the data used for Figure 14F are represented by three factors, the highs



are accounted for by two separate factors. The high on the eastern margin (Fig. 14F) is due to factor 2 and that at the western margin to factor 3; the small high at the south is produced by a combination of factors 2 and 3. Specimens 52 and 177 have very small values in Figure 14F by comparison with neighboring specimens, although 47 (immediately southwest of 52) has an almost identical value to 52. This suggests that similar rock composes 47 and 52 and that it is different from the rock of surrounding areas, rather than that the modal analyses (and chemical analyses in Figure 14D) are in error.

The six maps in Figure 14 were manually contoured and quite different contour configurations could be drawn without violation of the data (cf., Fig. 9); the information contoured in these Q-mode maps could have been smoothed by trend surface methods. In any analysis of the Malsburg Granite, or discussion of the petrogenetic development of the pluton, the detailed similarities and differences shown by the six maps need to be examined in detail. Despite local differences, the marked similarity of the regional zonation shown by all six maps is impressive. The results presented earlier in this paper (e.g., discriminant analyses, correlations, etc.) had suggested that the available variables do not strongly support the zonation proposed by Mehnert and Willgallis. However, Figure 14 seems to justify the claim that, considered in a multivariate framework, zonation is real and distinct.

Because there are six different maps in Figure 14, it remains to be determined which is the "best" approximation of the zonation that actually occurs in the sampled populations. The answer is not clear at this time. Further numerical analysis may indicate the answer, but it seems more likely that critical re-examination of the outcrops in the field in the light of Figure 14 would throw significant light on the problem. It is geologically important to elicit more information about the levels of variance for the several variables in order to permit more-realistic subjective extrapolation of the results to the target population. Probably a small selection of the

many variables actually employed (or a few different variables) would be adequate to define the zonation; work is proceeding to identify such subsets of variables and to determine whether the same variables are equally useful in mapping the internal variability of other lithic units.

CONCLUDING STATEMENT

Considerably more attention needs to be given to the significance of collected data and to the nature of the internal variability of granitic plutons and other lithic units. Study of the independent sets of analyses for the Malsburg Granite suggests that great care needs to be used in basing conclusions upon any single set of published analyses. In most published studies, insufficient is known about the levels of variance of the several analyzed variables and about the precise mode of sampling that was used; as a result, generalizations about the spatial variability of a complex become hazardous. In the absence of much more complete variance information than is commonly available, it is commonly difficult to assess the significance of a trend surface in terms of the actual spatial variability of the whole lithic unit.

Multivariate Q-mode maps, in which a large number of dissimilar variables can be considered simultaneously, appear to offer significant advantages in defining the spatial variability of sampled populations of granitic plutons and other rock bodies. Because each variable included in the analysis has, in general, a different pattern and amount of variance, some variables are undoubtedly sampled more appropriately than others. Intuitively, it seems reasonable to anticipate that Q-mode maps based on many variables will permit the gross variability of a sampled population for a lithic unit to be assessed with greater confidence than is possible with monivariate maps. However, insufficient emphasis is currently given to the fact that all such mapping techniques relate to a sampled population whereas, in most cases, the geologist wishing to draw petrogenetic conclusions is interested in a target population that is quite distinct from the sampled population for which data happen to be available.

Unfortunately, at this time, it is not known how representative the Malsburg Granite and its variability are. The pattern of variability of a granite mass needs to be known with accuracy in order to provide sound bases for quantitative petrogenetic models. With current knowledge of the thermodynamic factors underlying magmatic and metamorphic crystallization phenomena, it will soon be possible to develop quantitative computer-based non-linear models for the petrogenesis and three-dimensional compositional variability of simple granitic masses. It would be unfortunate if such models are available before sufficient is known about actual granitic complexes to test and refine the petrogenetic predictions.

This paper is offered as a progress report. It is hoped that it will demonstrate that, in spite of the analytical technology and ability currently available (cf., Baird, et al., 1967, Chappell, 1966, Rhodes, 1970), for petrology as a whole, there is a tremendous lack of knowledge about commonly-measured variables of granitic masses. Petrographers commonly find significance in many other textural, mineralogical, and compositional variables than those discussed in this paper -- several hundred such variables can be listed. It is quite possible that some unmeasured variables, in addition to (or in place of) some, or all, of those considered in this paper, might be highly critical in establishing an adequate quantitative basis for testing the accuracy of petrogenetic models. It is important to recognize that adequate description of a lithic unit is extremely important but not an end in itself; it is a necessary step in establishing the validity of petrogenetic models.

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