

SPECTROSCOPIC ANALYSIS OF TEPHRA AS A SITE CHARACTERIZATION TOOL

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ABSTRACT

Tephra (ash) deposits from Sunset Crater volcano, Arizona, were investigated to understand the relationship between visible near-infrared reflectance and physical properties of volcanic material as related to the erosion and weathering of a 900-year-old deposit in a semiarid climate. Quantitative and qualitative analyses were performed on tephra modified by aeolian (i.e., wind) processes to investigate the effects of grain size, shape, texture, and weathering on spectral response. Reflectance spectra were collected from homogeneous sample splits separated by sieve fraction. Principal component analysis was applied to decompose data by finding maximum variances, so the complexity of the spectral response of tephra samples could be more easily interpreted. Partial least squares analysis was used for developing a linear calibration model between grain size and spectral reflectance of sieve fractions. The model was used to estimate grain-size distributions of other tephra samples collected from the study area. The trends observed in the spectral reflectance of these samples showed that a complex relationship exists between reflectance and geometry/grain size of the analyzed fractions. The first and second principal components were useful to separate the samples based on shape, texture, and the amount of weathering. As expected, the grain size of a homogeneous sample affects the reflectance properties such that an increase in grain size produces a decrease in reflectance. This trend is noticeable for grain-size sieve fractions less than 0.6 mm [0.02 in]. Through this research, we have improved understanding of the relationships between physical properties and spectral response of volcanic material in the visible and near-infrared regions. These relationships may be used to support site characterization and the investigation of the extent of tephra deposit remobilization and redistribution, resuspension, rates of weathering and erosion, and grain-size characteristics.

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: All CNWRA-generated original data contained in this report meet the quality assurance requirements described in the Geosciences and Engineering Division, Quality Assurance Manual. Sources for other data should be consulted for determining the level of quality for those data. Field measurement data and laboratory analyses have been recorded in CNWRA Scientific Notebooks 747E and 748E (Necsoiu, 2005; Hooper, 2005).

ANALYSES AND CODES: No scientific and engineering software was used in the analyses contained in this report.

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Necsoiu, M. "Spectral Field Measurements, Post-Fieldwork Analysis, Lab Processing of Geologic Samples and Remote Sensing Data Analysis in Support of the Airborne Transport of Radionuclides Project (DIRECT2)." Scientific Notebook No. 747E. San Antonio, Texas: CNWRA. 122 pp. 2005.

1 INTRODUCTION

Remote sensing (e.g., satellite and airborne image data) is a potentially valuable tool for site characterization because it affords an opportunity for a reconnaissance-scale analysis of the surface geology of large geographic areas in a short timeframe. However, spectroscopic data that characterize a sample of a mineral or rock type in a laboratory setting may differ from remotely sensed information from the same material in a natural setting. For example, differences in grain size, variations in mineral distribution in rocks, and alteration of rocks due to weathering will affect the spectroscopic data. As part of U.S. Nuclear Regulatory Commission precicensing activities related to the proposed high-level waste repository at Yucca Mountain, Nevada, to enhance understanding of the factors that influence the above variations, Center for Nuclear Waste Regulatory Analyses staff conducted field and laboratory investigations of heterogeneities in physical properties such as grain size, shape, texture, and weathering of tephra from Sunset Crater volcano in north-central Arizona. Sunset Crater is a suitable analog for volcanic processes and post-eruption surface processes at Yucca Mountain, Nevada. The focus of the investigation was to contrast the physical properties of the tephra with measured variations in the visible and near-infrared reflectance of the samples. Volcanic ejecta includes scoriaceous ash {<2 mm [0.08 in]}, lapilli (or cinders) {2–64 mm [0.08–2.5 in]}, and blocks and bombs {>64 mm [2.5 in]}. When transported through the air, these ejecta are collectively termed tephra. Aeolian tephra deposits were sampled because they offer the opportunity to examine basaltic volcanic material that has been reworked by surface processes and redistributed. The techniques used in this investigation and the improved understanding of factors that affect such measurements may be useful for future site characterization applications. This approach is not restricted to volcanoclastic deposits or volcanic (igneous) rock types, but can be expanded to other sediment and rock types and/or other locations as part of a comprehensive site characterization.

2 BACKGROUND

2.1 Sunset Crater Volcano

Sunset Crater is a 900-year-old (Smiley, 1958; Champion, 1980; Ort, et al., 2001) scoria-cone volcano composed of alkali olivine basalt (Holm and Moore, 1987). The volcanic cone stands 314 m [1,030 ft] in height and is interpreted to have been created by a Strombolian-type eruption (Figure 2-1). These volcanoes are also known as cinder cones because of the abundance of vesicular cinder or scoria.

Sunset Crater rests on the edge of the Colorado Plateau at an elevation of 2,135 m [7,000 ft]. Mean annual precipitation in the region is approximately 500 mm [20 in] (Sellers and Hill, 1974; Staudenmaier, et al., 2007). The climate is semiarid and supports pine forests at higher elevations and pinyon-sagebrush communities at lower elevations where precipitation amounts are lower. The prevailing wind direction is from the southwest, but it becomes more northerly during the winter months (Sellers and Hill, 1974; Staudenmaier, et al., 2007).

2.2 Tephra Deposit

The fall deposit from the Sunset Crater eruption is a widespread blanket of fresh black and subordinate red tephra. Pyroclasts are typically vitreous, highly vesicular, and aenelithic in morphology. Individual fall units are unconsolidated, well sorted, and demonstrate both reverse and normal grading. Grain size range is typical of Strombolian style eruptions (i.e., coarse scoriaceous ash to lapilli). Granulometric analyses are described in a previous report (Hooper, et al., 2008). Secondary mineralization of Sunset Crater pyroclast surfaces by carbonate and/or silica is rare. Lithic fragments within the tephra are uncommon. When lithics are present, they make up an extremely low percentage ($\sim <0.5$ percent) of their associated tephra package (Amos, 1986; Hooten, et al., 2001). Amos reports occasional carbonate lithic fragments from the Kaibab Formation. Amos (1986) identified eight discrete tephra-fall units associated with the Sunset Crater eruption with an estimated total volume of 0.75 km^3 [0.18 mi^3] {dense rock equivalent volume of 0.41 km^3 [0.10 mi^3]}. Each unit ranges in thickness from 10 mm to over 1 m [0.4 in to 3.3 ft] and represents a separate phase of the eruption.

Sunset Crater tephra drapes preexisting scoria cones, and the older pyroclasts are noticeably more weathered and oxidized. When pits were dug to the base of the tephra-fall deposit, a substrate of oxidized, cohesive material usually was encountered (Hooper, et al., 2008). This is the preeruption surface (or paleosol) comprising a red-colored, clay-rich layer that sharply contrasts with the black, fine-grained and coarse-grained tephra layers.

Tephra dispersal from the Sunset Crater eruption can be divided into a continuous and discontinuous deposit. The continuous tephra-fall deposit mantles the preexisting landscape in the proximal and medial regions and covers an area of approximately 260 km^2 [100.4 mi^2] (Amos, 1986; Colton, 1967, 1932). In the distal region, tephra grades into a discontinuous deposit contingent upon local topography, erosion, and initial deposition (dependent upon wind direction). Hooten, et al. (2001) supplemented the study by Amos (1986) with additional data points and generated a new isopach map (Figure 2-2). Hooten, et al. (2001) is the full technical report, but a general discussion of tephra dispersal, complete with an isopach map, can be found in Elson and Ort (2003). Hooten, et al. (2001) proposed that preexisting local topographic features played a significant role in the distribution and thickness in the proximal zone.



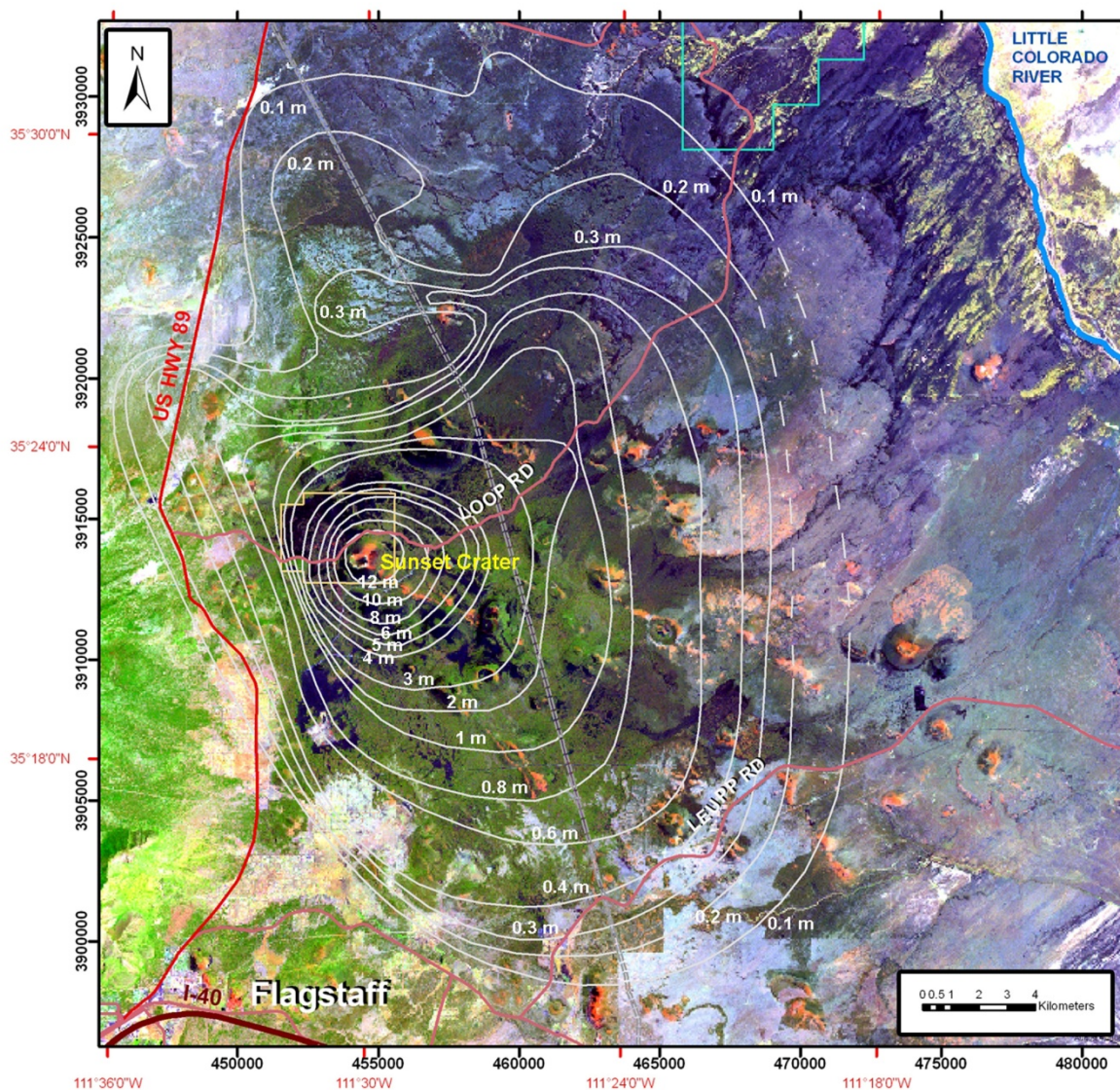
Figure 2-1. Sunset Crater Scoria Cone Viewed From the South. A Deposit of Black Tephra Covers the Surrounding Landscape.

Rapid decreases in thickness likely correspond to older volcanic edifices acting as a topographic barrier to initial tephra deposition.

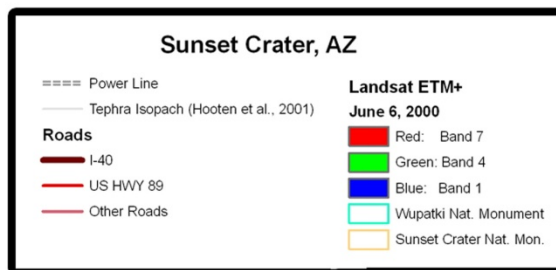
2.3 Tephra Redistribution

Primary tephra is recognizable in the field because it is glassy, vesicular, and unconsolidated. In contrast, fluvially reworked tephra is abraded, rounded, and often mixed with older sediment. Tephra that has been reworked by aeolian processes is usually finer grained, well sorted by wind transport, and often remobilized into dune forms.

The top of the Sunset tephra sequence, especially in the proximal region, is exposed directly on the surface without an overlying distinguishable soil horizon and is subjected to active surface processes. Because of the potential for erosion after 900 years since the time of emplacement, the initial thickness of tephra is unknown and the amount present today is only a measure of the minimum thickness immediately after the eruption. Careful inspection of the sequence reveals a topmost layer of bioturbated tephra mixed with aeolian fines (or potentially colluvium). This horizon is a surficial layer of scoria (cinder) with mixed quartz-rich sediment ranging from 8 to 15 cm [3.2 to 5.9 in] in thickness as measured in numerous pits (Hooper, et al., 2008). In other locations, the primary tephra is covered by a protective layer of alluvium—usually mixed with Sunset scoria—of the same thickness.



Satellite Imagery: Landsat
ETM+, Bands 741
June 6, 2000
Path 037, Row 035
Source: Global Land
Cover Facility
<http://www.landcover.org>



Projection: UTM, Zone 12N
Datum: NAD83

Figure 2-2. Map of Tephra Thickness Reproduced From Hooten, et al. (2001) and Superimposed Upon Landsat ETM+ Satellite Data of the Study Area

The U.S. Geological Survey has mapped areal distribution of alluvial and aeolian deposits as part of the geologic map of the eastern San Francisco Volcanic Field (Moore and Wolfe, 1976). As is typical for this semiarid region, the drainage system is ephemeral or intermittent and is characterized by dry, flat-floored channels (i.e., washes or arroyos). The regional slope for the study area is to the east-northeast toward the Little Colorado River. However, the coarse and porous nature of the Sunset Crater tephra deposit prohibits significant fluvial activity such as overland flow and runoff. Overland flow is more significant in the distal portion of the Sunset Crater fall deposit where the tephra covering is thin or intermittent and a weathered, preeruption surface dominates.

Wind action has subsequently redistributed and reworked the tephra into a variety of dark-colored, aeolian deposits and dune forms (Figure 2-3). Aeolian dunes accumulate when a supply of sand-sized granular material is carried downwind by bouncing or jumping motions (saltation) and is deposited when these winds weaken below the threshold for transport. Aeolian deposits composed of basaltic sediment from the Sunset Crater eruption include coppice dunes, falling dunes, wind ripples, and sand streaks (Hooper and Necsoiu, 2008; Hooper, et al., 2008). Coppice (nebkha) dunes form where clumps of vegetation trap saltating particles and create small mounds or hummocks. The spatial distribution of aeolian deposits relates to patterns of sedimentary deposition and erosion of source materials. In the vicinity of Sunset Crater, topographic barriers, such as mountains, escarpments, mesas, boulders, and the margins of lava flows generate zones of airflow turbulence, acceleration, and deceleration. This in turn strongly influences the accumulation or transport of the sand-size particles. Identifying the type and pattern of aeolian deposition can provide insight into sedimentary processes and paleotopography.

Wind and human activity can disturb fallen fine-grained volcanic deposits for months or years after an eruption, presenting a long-term health hazard. Airborne particle mass concentrations were measured using a personal sampler under a variety of surface-disturbing activities within different depositional environments at both volcanic and nonvolcanic sites surrounding Sunset Crater (Hooper, et al., 2008; Benke, et al., 2009). Light surface-disturbing activities include walking or setting up equipment, while heavy surface-disturbing activities include digging and hoeing. The level of surface-disturbing activity was found to be the most influential factor affecting the measured airborne particle concentrations, which increased over three orders of magnitude relative to ambient (i.e., without human activity) conditions. Under ambient conditions, the total airborne particle concentration in the Sunset Crater region is 0.1 to 0.4 mg/m³ [6.2×10^{-9} to 2.5×10^{-8} lb/ft³] (Benke, et al., 2009).



Figure 2-3. Aeolian-Reworked Sunset Crater Tephra in the Distal Area. Black-Colored Tephra, Which Has Been Remobilized by the Wind, Drapes the Non-Volcanic Red-Colored Moenkopi Formation. The Sedimentary Rock is Capped by an Old Basaltic Lava Flow on the Skyline. Kana-a Wash Is in the Foreground.

3 SAMPLE DATA COLLECTION AND PREPARATION

The erosional change over time (i.e., geomorphologic evolution) of a basaltic tephra deposit in a semiarid climate can be evaluated by studying the relationship between visible near-infrared reflectance and physical properties of aeolian (volcaniclastic) material. Several previous studies (e.g., Leu, 1977; Johnson, et al., 1992; and Okin and Painter, 2003) have investigated the relationship between reflectance spectroscopy and the grain size of unconsolidated or powdered rocks and minerals. The goal for spectroscopic analysis is to understand the relationship between physical properties of tephra and near-infrared reflectance and compare these results to the expected relationship noted by previous studies. This analysis provides a basis for future site characterization applications.

3.1 Granulometric Analyses

Granulometric analyses are the main source of data when examining the grain-size variations in unconsolidated pyroclastic (tephra) deposits. Systematic measurements of maximum particle size are also used to analyze the energetics of pyroclastic fall eruptions. Samples were first dried and then placed in a set of stacked sieves with standard mesh sizes. The stack of sieves was placed on a shaking machine (Ro-Tap) for 10 minutes. For aeolian deposits, analyses focused on a grain-size range from 0.106 to 2 mm [0.004 to 0.078 in]—the desired range for spectroscopic analyses (Table 3-1). The sample volume for fractions less than 0.106 mm [0.004 in] were too small for the collection of spectral data.

Because of the broad distribution of grain sizes found in many geologic materials, it is common to use a logarithmic transformation of grain diameters called the phi (Φ) scale (Wentworth, 1922)

$$\Phi = -\log_2(d_{\text{mm}}) \quad (3-1)$$

for which d_{mm} is the grain diameter in millimeters [1 mm = 0.04 in]. For example, -4Φ is equal to 16 mm [0.63 in], -2Φ is equal to 4 mm [0.16 in], 0Φ is equal to 1 mm [0.04 in], 2Φ is equal to 0.25 mm [0.01 in], and 4Φ is equal to 0.062 mm [0.0024 in].

3.2 Spectroscopic Analyses

The geologic samples collected in the field were analyzed in the laboratory with an Analytical Spectral Devices FieldSpec® 3 portable spectroradiometer which is designed to collect reflectance (solar or built-in light source), radiance, and irradiance measurements. This instrument collects a high volume of quality data in a short time interval and performs contact and noncontact National Institute of Standards and Technology-calibrated reflectance measurements of soil, vegetation, and rock samples over a wide spectral range. For these analyses, diffuse-reflectance spectra were collected from five samples (MN62406-5, MN62406-6, MN62606-13, MN62706-27, MN62906-32) with each of the samples being sieved into eight different sieve fractions or splits (Figure 3-1). Each spectral measurement was performed without interference from noise (in this case specular reflectance). The setup configuration, such as the angle of incident light and the distance of light illumination and sample surface, were consistent throughout the measurement process. A large number of samples (e.g., 60) were averaged per measurement because random noise is reduced by spectral averaging (as the square root of the number of averaged spectra). In addition, several measurements were performed on different locations of the sample to obtain measurement results that are representative of the entire sample.

Table 3-1. Sieve Characteristics for Sampling Protocol			
Sieve No.	Mesh Size (Diameter, inches)	Mesh Size (Diameter, mm)	Phi Units ($-\log_2$ Diameter)
10	0.078	2	-1.0
18	0.039	1	0.0
30	0.024	0.6	0.75
40	0.017	0.425	1.25
50	0.012	0.300	1.75
70	0.008	0.212	2.25
100	0.006	0.150	2.75
140	0.004	0.106	3.25

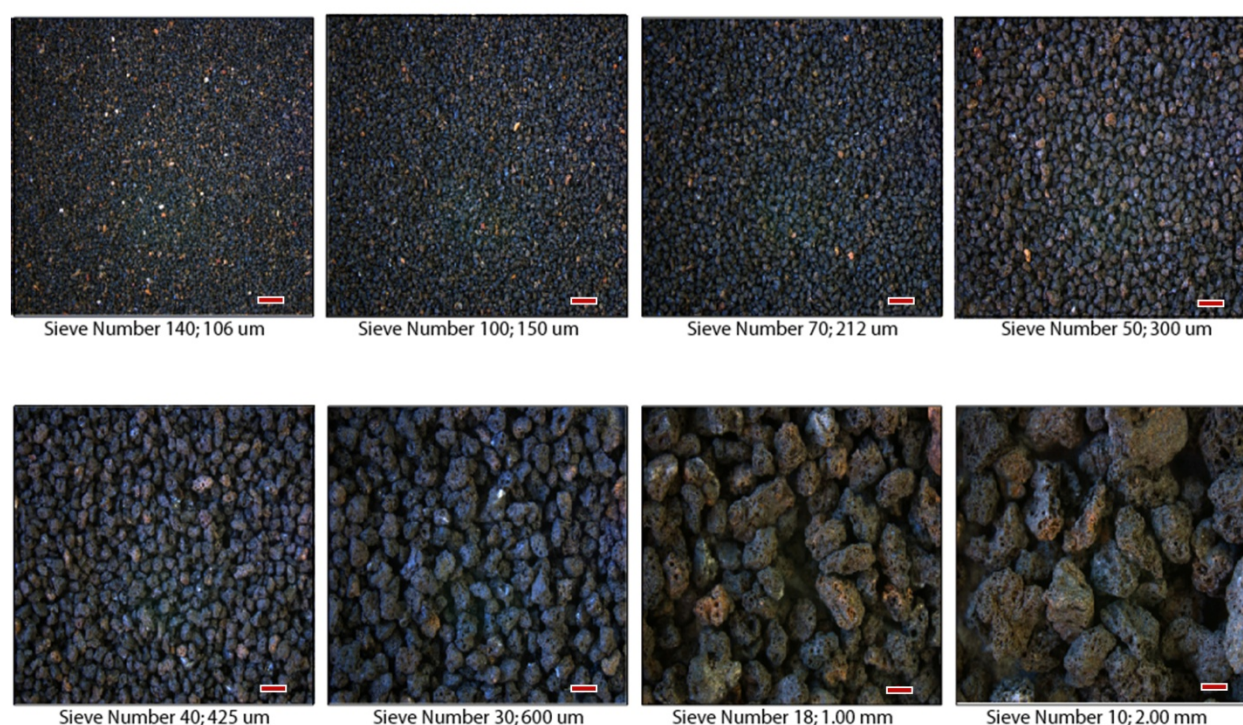
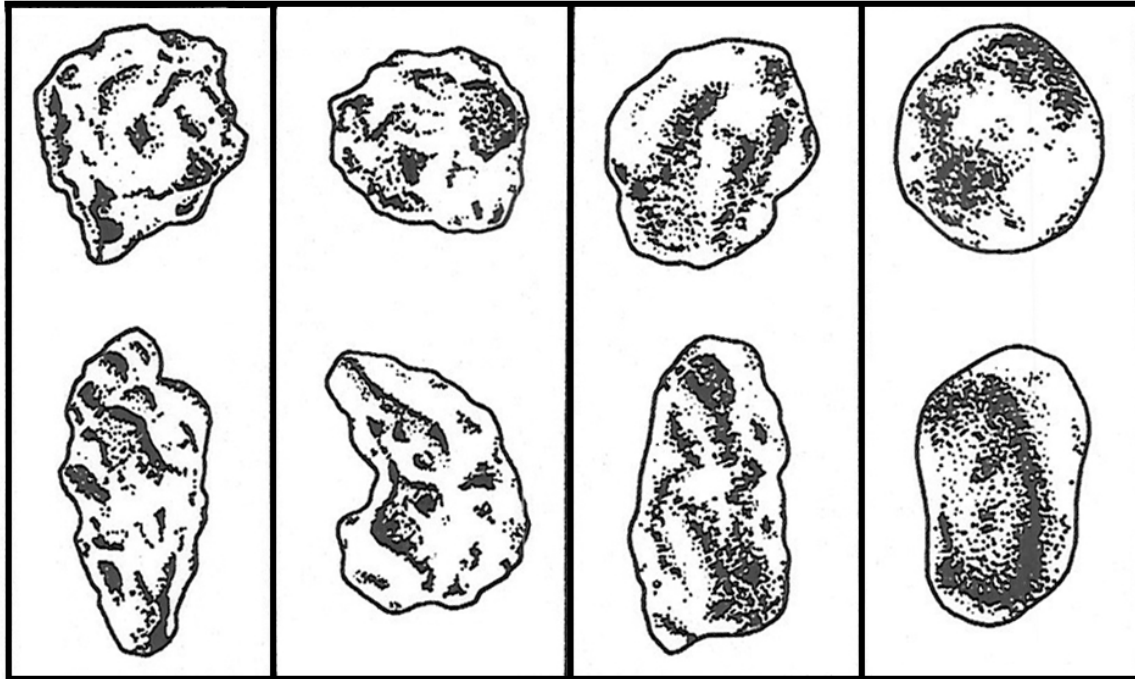


Figure 3-1 Sieved Sample MN62906-32. Grain-Size Range From 0.106 mm to 2 mm [0.004 to 0.089 in] Scale Bar Represents 2 mm [0.089 in].

3.3 Classification Scheme

In addition to grain size, grain shape, texture (vesicularity), and degree of weathering were measured for the sieve fractions. Grain shape was based on standard visual charts (e.g., Lindholm, 1987) and consisted of subdivisions representing angular, subangular, subrounded, and rounded (Figure 3-2). Grain texture was defined by degree of vesicularity. Vesicularity was classified as very high when the majority of grains are significantly covered in vesicles (bubble voids). Vesicularity grades through high, medium, low, and very low. For very low vesicularity, most grains have no or very few vesicles. For these cases, vesicles are smaller and the surface area is smooth and usually lustrous or shiny. The degree of weathering or amount of weathered material in vesicles or on the grain surface

Modified from Lindholm (1987)



ANGULAR SUBANGULAR SUBROUNDED ROUNDED

Figure 3-2. Grain Shape Visual Chart

was classified as very high when most grains were predominantly or totally coated in weathered material, grading through high, medium, low, and very low when most grains had little or no weathering. Typical weathering products include precipitation of calcium carbonate and clay mineralization and alteration.

4 DATA RESULTS AND ANALYSIS

Quantitative and qualitative analyses were performed on tephra modified by aeolian processes to investigate the effects of grain size, shape, texture, and weathering on spectral response (Necsoiu, et al., 2007a,b). Each reflectance spectra was jump-corrected at 1,000 and 1,800 nm [4.0×10^{-5} and 7.0×10^{-5} in] (i.e., spectral discontinuities due to the spectrophotometer), and multiple measurements were averaged per sieving. Principal component analysis was applied to decompose data by finding maximum variances so the complexity of tephra samples could be interpreted. A partial least squares method was used for developing a linear calibration model between grain size {0.106 to 0.6 mm [0.004 to 0.024 in]} and spectral reflectance of sieve fractions (Figures 4-1 and 4-2). Chemometric techniques were used for quantitative analysis. These techniques were utilized to extract the information hidden in a complex data set and involved collecting a sufficient number of representative and diverse samples and then performing reference analyses for the parameters of choice. The resulting scores were used to detect sample patterns, groupings, similarities, or differences. Over 98 percent of the variance in the data was explained by the first two components of the principal component analysis. Reflectance spectra, which were collected from homogeneous sample splits separated by sieve fraction, displayed a complex relationship between spectral responses and the geometry and grain size of the analyzed fractions (Figure 4-3).

The trends observed in the spectral reflectance of the analyzed fractions of tephra samples showed that an orderly relationship exists between reflectance and geometry, grain size, and mixing with nontephra grains. In the near-infrared wavelength range, the grain size of a homogenous sample generally affects the reflectance properties such that an increase in grain size produces a decrease in reflectance (Clark, 1999). This observation seems to generally agree with our aeolian-modified samples such that an increase in grain size produces a decrease in reflectance. This trend is particularly true for grain-size sieve fractions less than 0.6 mm [0.024 in]. For grain-size sieves greater than 0.6 mm [0.024 in], the effect is reversed, probably due to the presence of weathering material on the surface of individual grains.

The analysis reveals a subtle grain shape change from angular to subangular as grain size decreases from 2 to 0.106 mm [0.078 to 0.004 in], which may be related to the change in vesicularity and its overall effect on grain texture and morphology (coarser particles being more vesicular than finer particles). This trend agrees with the observation by Sandia National Laboratory (2007) that larger particles tend to have a higher fraction of vesicles than small particles.

High spectral response of the fine grain sizes is also related to the degree of mixing. The percentage of nontephra grains increases in the finer grain-size splits, where the finest grain-size split is the most mixed. This is due to fine-grained aeolian sand and dust (mostly quartz), which is not related to the basaltic tephra from Sunset Crater. The coarser grain-size splits display slightly more weathering. Broadly, this includes oxidation, possible development of a weathering rind (usually best observed on larger particles), mineralization and cementation (may include clay minerals or a calcium carbonate coating), and similar processes that coat individual grains and fill vesicles or other pores. The observation that coarser grains are more weathered may be connected to another observed relationship, that coarser grains are more vesicular than fine-grained particles. These bubble voids appear to be the focus of most postdepositional mineralization.

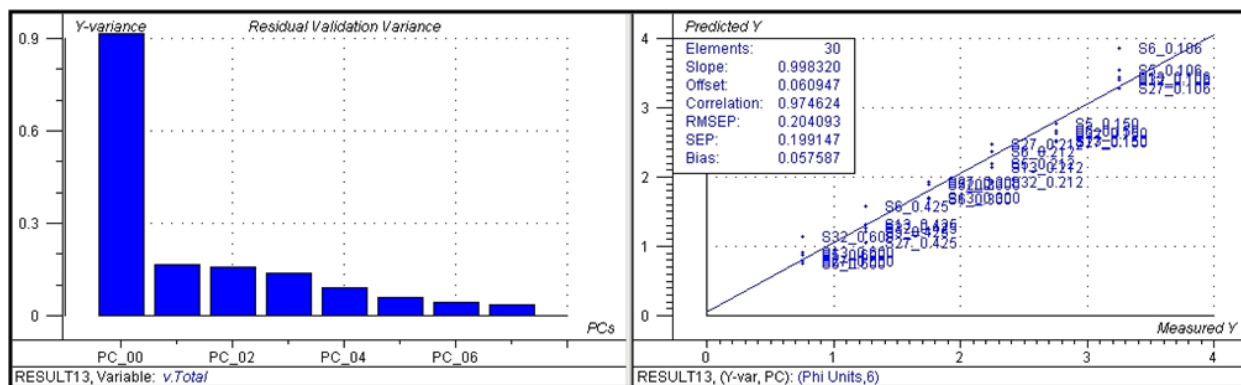


Figure 4-1. Residual Validation Variance for the Model and Predicted Versus Measured Y Plots

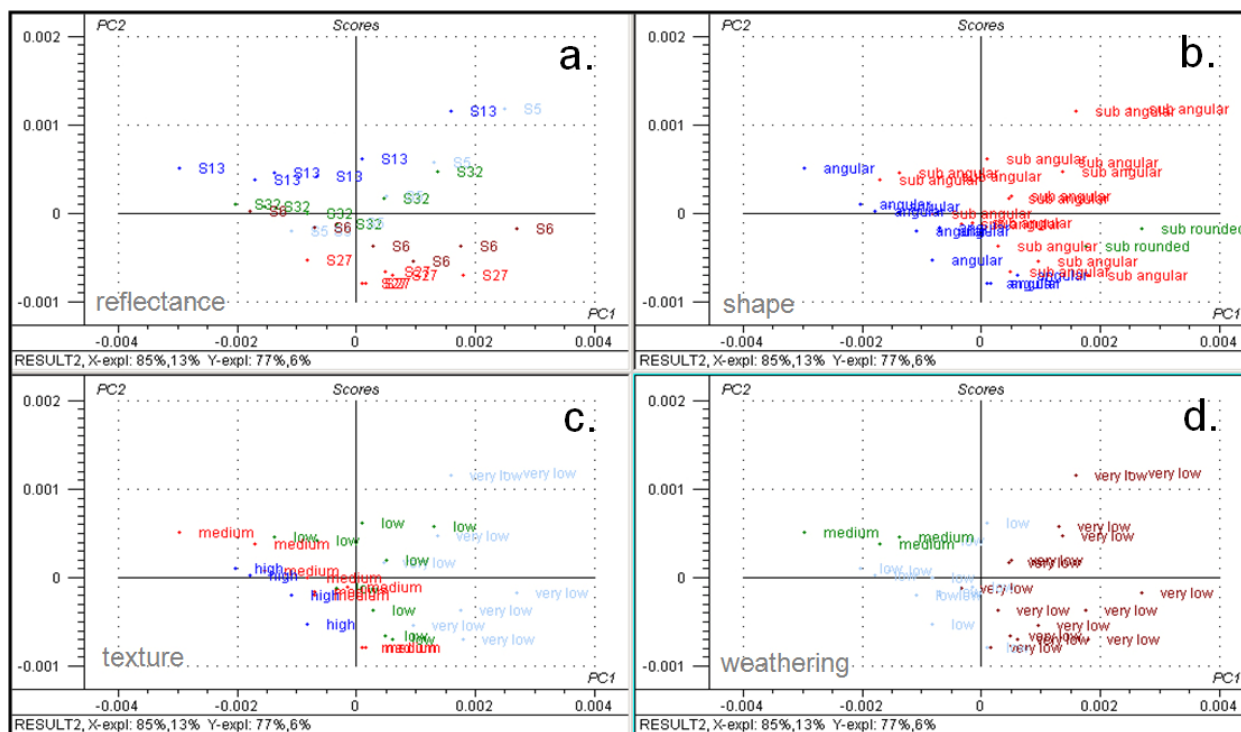


Figure 4-2. Plots Demonstrating the Results From Principal Component Analysis. After Quantitative Analysis, Reflectance Spectra of Sieved Samples Were Grouped by (a) Sample Number, (b) Shape, (c) Texture, and (d) Degree of Weathering.

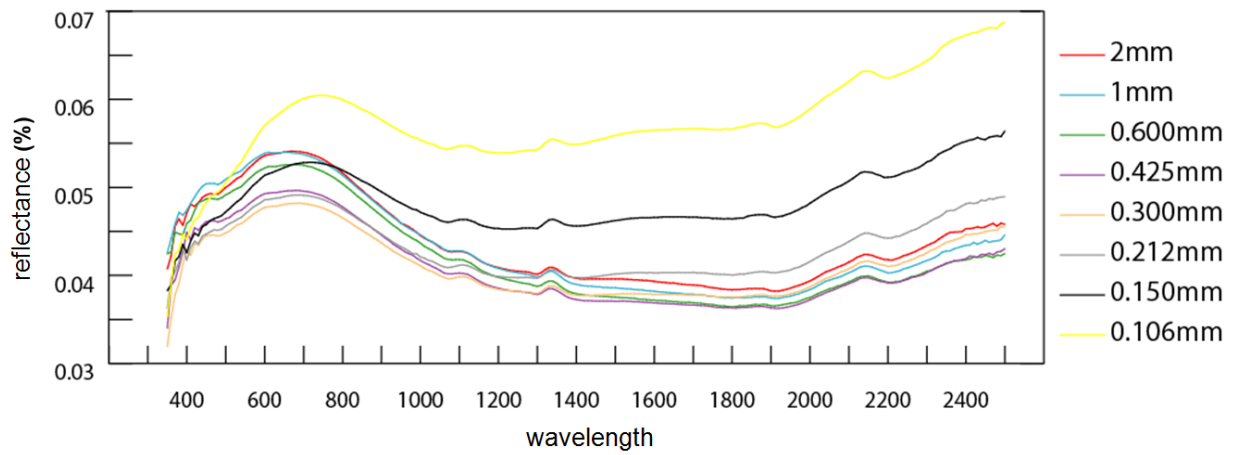


Figure 4-3. Spectral Response of Sieved Tephra Sample (MN62906-32) Over Spectral Range (wavelength) From 350–2,500 nm [1.4×10^{-5} – 9.8×10^{-5} in].

5 CONCLUSIONS

Given the considerable areal extent of the fall deposits at Sunset Crater and the vegetation patterns within the depositional area, the use of satellite and airborne image data for reconnaissance mapping is time-efficient and cost-effective. Geomorphologic and structural relationships can be discerned over large areas with minimal ground control, and the identification of lithologic and vegetation units can be extrapolated on the basis of spectral characteristics. Furthermore, satellite and airborne image data can be used to evaluate uncertainties in published tephra deposit patterns and distribution characteristics.

The complex relationships among tephra thickness, vegetation, elevation, lithology, and weathering in the Sunset Crater area can also be assessed using field and laboratory spectroscopy. Using a portable instrument, field spectroscopy includes studies of reflectance or radiance properties of vegetation, soils, rocks, and water bodies under solar illumination. Near-infrared spectroscopy is a successful technique to characterize volcanic materials based on their physical properties. A model that relates spectral response to grain size was developed and successfully validated using a systematic cross-validation method; however, the test was performed on a small number of samples from the Sunset Crater tephra. Results indicate that physical characteristics of analyzed samples—shape, texture, and weathering—are intercorrelated. Samples with a high degree of weathering were identified as being angular with high vesicularity. These characteristics appear to be independent of the percent of black tephra mixing with oxidized tephra and nonvolcanic material. Tephra samples appear to be distinguishable based on the degree of oxidized tephra and nontephra material. An approach using a combination of near-infrared spectroscopy and airborne/satellite image data is a powerful tool for distinguishing lithological variations over a large areal extent.

This research improves understanding of the relationship between physical properties and spectral response of basaltic tephra in the visible and near-infrared regions. These relationships can be used to support investigations of a broad range of volcanic deposits and eruption types, models of tephra dispersal, the extent of tephra deposit remobilization and redistribution, rates of weathering and erosion of tephra deposits, and grain-size characteristics. Finally, these relationships and analyses are not restricted to volcanoclastic deposits or volcanic (igneous) rock types, but can be expanded to other sediment and rock types as part of a comprehensive site characterization.

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