APPLIED INFORMATION SYSTEMS RESEARCH PROGRAM

PROGRESS REPORT, April 23, 2004

PROPOSAL: NRA 01-OSS-01 NAG5-12001

PROPOSAL TITLE: Autonomous Mineral Detectors for Mars Rovers
and Landers

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1. Proposal Summary

We are developing onboard intelligence sufficient to extract geologically meaningful data from VIS/NIR spectrometer measurements of soil and rock samples, and thus to guide the selection, measurement and return of these data from significant targets at Mars. This work builds on a multi-layer feedforward neural network supervised classification system that was successfully trained using synthetic data generated from combinations of laboratory spectral data to detect carbonate minerals in spectra collected in the field. Here we proposed to 1) improve the neural net by a) evaluating the algorithm's ability to identify feasible, useful, and detectable environmental properties, b) establishing detection limits, particularly under martian conditions (*e.g.*, dusty) and c) adding nonlinear mineral mixing models; 2) develop a new set of detectors targeting minerals that, like carbonates, signal the presence of water and possibly life, and 3) develop a 'novelty detector' that autonomously identifies mineralogies that have not been previously detected during the mission. Each of these tasks will contribute to the full functionality of a landed instrument suite given the limited resources of time, data storage, downlink data rate and uplink opportunity, thus enabling the autonomous detection of scientifically important minerals by rovers and landed instruments at Mars.

Our proposed implementation plan included the following Year 2 tasks:

- To improve the carbonate detector by evaluating the effects of dust coatings and mixtures. This will determine how much carbonate is required in a sample to yield a positive identification by the neural net.

- Develop addition mineral detectors for minerals of high priority for Mars. Collect laboratory data for these minerals and train the neural net on these laboratory data. Analyze results of new mineral detectors.

- Field collection of mineral spectra at Yellowstone and their analyses.

- Develop detailed theoretical nonlinear mixing model and develop empirical powder based spectral model.

2. Year 2 Accomplishments

A major accomplishment this year was the identification of an able graduate student, Matt Merrill, who has been working on the experiments described below.

Effects of dust coatings on detection of carbonate spectra

A primary concern for remote sensing on Mars is the ability to detect primary mineralogy through the ubiquitous ferric dust on the planet's surface. A primary task in this proposal was to measure visible/near-infrared (350-2500 nm) spectra of calcite (a carbonate mineral: $CaCO_3$) coated with different thicknesses of dust and evaluate the performance of the carbonate detector. We devised an experiment where JSC-Mars-1 Martian soil simulant (palagonite; *Allen et al.*, 1998) was air fall deposited onto a calcite crystal in the laboratory within a bell jar (Fig. 1). A glass slide positioned against the calcite crystal allowed for repeated thickness measurements to be taken without altering the position of the calcite crystal during the length of the experiment. The palagonite was initially manually ground and sieved to 45μm to simulate martian surface dust. Each layer of dust was deposited by elevating 0.1g of dust into the air. After each deposit, spectra were taken of the calcite crystal. Average layer thickness was determined using a vertically calibrated petrographic microscope by averaging dust thickness at 100 grid points in a 1 cm^2 region of the slide; thickness measurement error is ≤15μm. Aerial coverage of dust on the slide was determined by averaging 5 counts of all non-white (non-slide) pixels on digital photomicrographs of different regions of the slide. The spectra were run through the carbonate detector, where the output (activation value), in the range 0 to 1, indicates the degree to which the input spectra fits the prototypical carbonate represented by the network weights. An activation of 0.3 was selected empirically in initial experiments [*Gilmore et al.*, 2000] as our positive identification threshold for carbonate minerals. The activation values were compared to the depth of the 2300 nm carbonate absorption (continuum depths (D=1-Reflectance at trough center/Reflectance of continuum)), a standard tool for comparison on spectra.

Reflectance spectra for 35 layers of dust deposition (up to 270 μm thick) are provided in Fig. 2. Dust was deposited until the activation value calculated for the spectrum matched and exceeded that of pure palagonite. The reflectance at the blue wavelengths is greatest in the calcite and decreases dramatically with the initial layers of dust deposited. Carbonate vibrational features at 1700 nm and 2300 nm and the water absorption bands at 1400 nm and 1900 nm are deepest in the calcite and become reduced with successive palagonite layers.
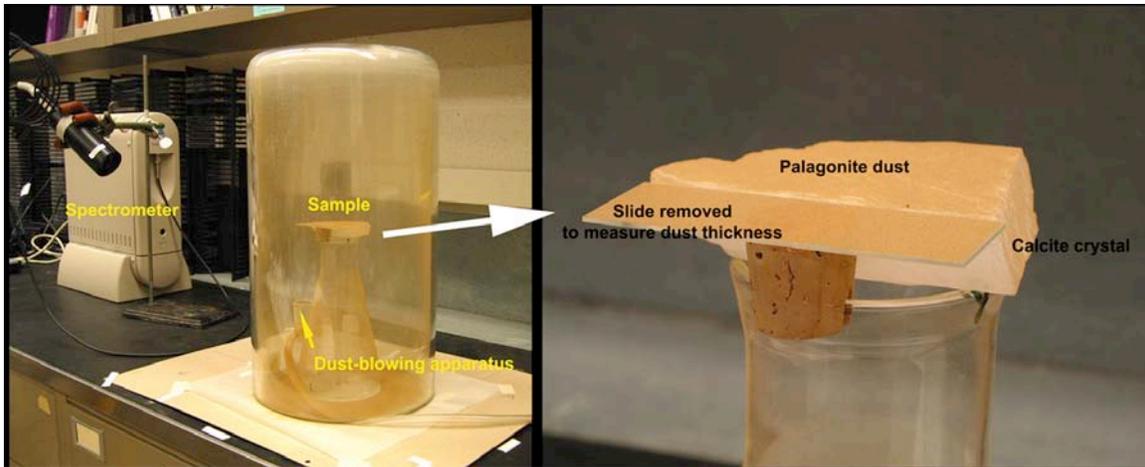
Figure 1. Dust coating experiment. Aliquots of palagonite are air fall deposited onto calcite crystal and glass slide. Spectra are taken of the crystal after each deposit; the slide is removed for dust thickness and coverage measurements.
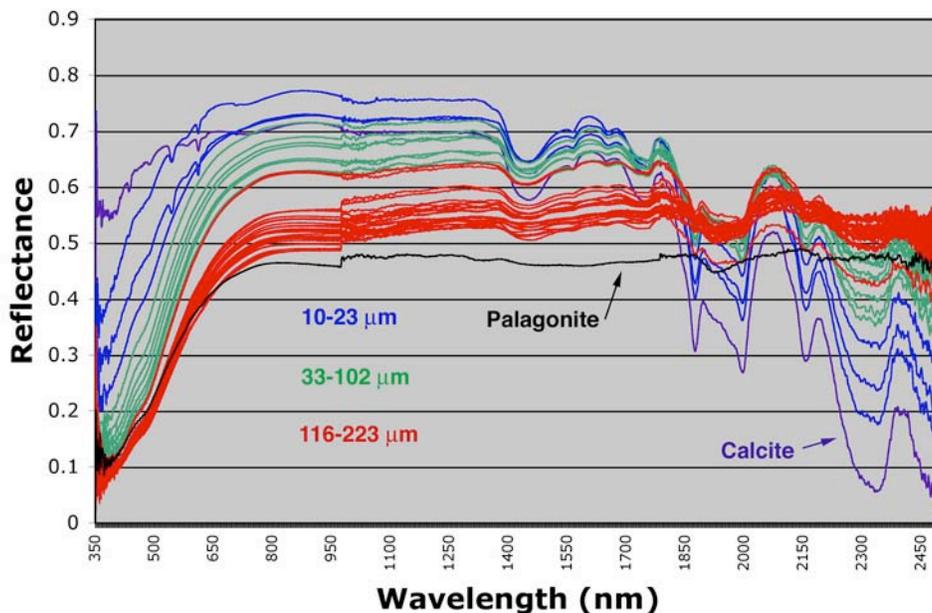

Figure 2. Spectra of all experiments. Blue spectra: activation values >0.6; green: 0.3-0.4 and red <0.3 (no carbonate detected; see Fig. 4). Numbers correspond to thickness of dust layer within color group.

Dust layer thickness (Fig. 3) increases linearly through the first 14 (119 μm, 84% coverage) experiments for which it was measured. In the first set of experiments, the final thickness underestimates what is expected for the linear trend and may indicate some settling at thicknesses >119 μm. A second run of experiments verified this was the case. Aerial coverage increased exponentially throughout the experiment to a final value of 99.5% coverage. The nonlinear effect of dust thickness on continuum depth and activation value is evident in this figure. Activation and continuum depth values drop

markedly with the first 3 layers of dust, a rate that decreases with each successive layer. This logarithmic relationship elucidates the potential signal contamination of thinner dust coatings.
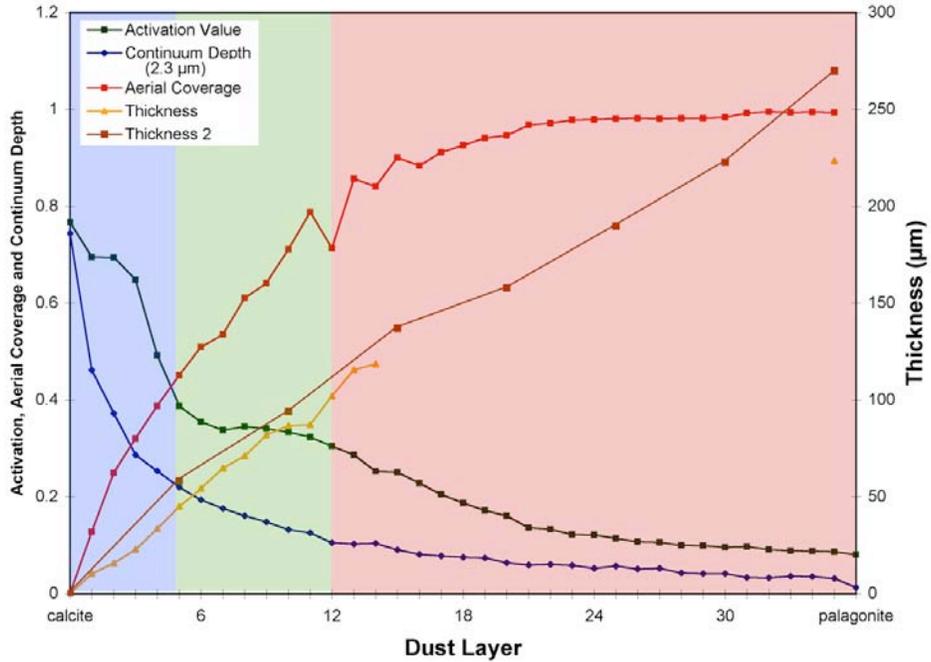

Figure 3. Experiment parameters. A linear increase in dust thickness results in exponential increase in aerial coverage and a exponential decrease in the continuum depth and activation values of the detector. Background colors correspond to spectra in Fig. 2.
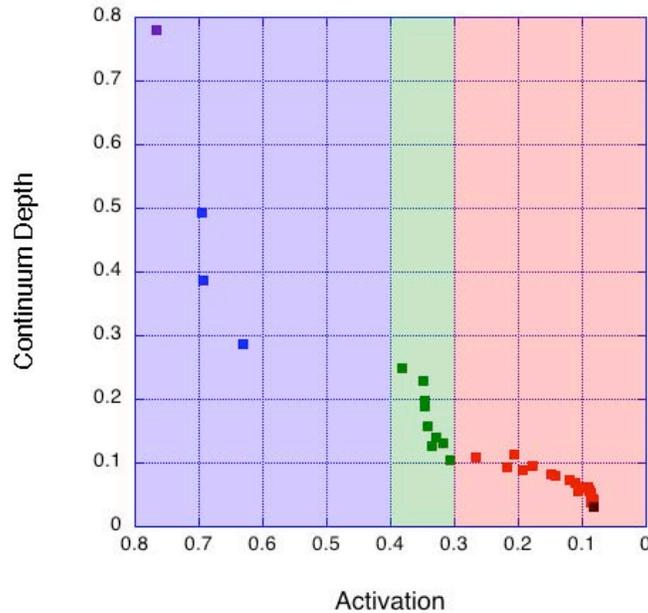

Figure 4. Continuum depth of 2300 nm feature vs. activation values computed by the neural net for individual spectra. Colors correspond to spectra in Fig. 1. Carbonate is detected by the neural net for all spectra with activation values > 0.3.

Activation values and continuum depths were calculated for the 2.3 μm feature of each spectrum and are plotted in Fig. 4. In this experiment, the carbonate detector reached the 0.3 threshold at a dust coating of 102-116 μm (78-85% aerial coverage). This coincides with a change in the slope of the continuum depth values in Fig. 4 where the depth of the 2300 nm band changes less with each layer of added dust. The neural net converges to the 0.3 threshold value due to this change in band depth response. Importantly, lower threshold values would not improve the detector's ability to resolve carbonate.

That ~100μm of palagonite dust obscures a carbonate signal in this experiment is consistent with studies of dust coatings conducted by several groups, which find that ~40 - 400μm of dust obscures the Vis/NIR (and TIR) spectral signal of other substrates [*Wells et al.*, 1984; *Fischer and Pieters*, 1993; *Morris et al.*, 2001]. Atmospheric opacity modeling derived from the Pathfinder radiometric calibration target concludes the annual rate of dust deposition on Mars is about 20-45 μm per Earth year [*Johnson et al.*, 2003]; similar results were obtained by the Pathfinder MAE experiment [*Landis and Jenkins*, 2000]. Dust layers of this magnitude may be expected on rocks within regions of aeolian activity and dust mobilization.

In conclusion, these experiments 1) demonstrate the ability of the detector to correctly recognize carbonate under dust layers of up to ~100μm; 2) link the detector performance to specific behavior of the 2.3 μm band; and 3) confirm the significant effects of even thin (~10-20 μm) palagonite dust layers on spectral response of substrate. This work was presented at the Lunar and Planetary Science Conference in March 2004 and a manuscript is in progress.

Creation of detectors for additional minerals

In Year 1 of this task, we compiled a list of minerals that are of high priority for detection at Mars due to their association with water (evaporites, hydrothermal minerals, sulfates). We have also identified minerals that are common on Mars (silicate minerals of basalt and similar igneous rocks) in order to spectroscopically discriminate what are expected to be the majority of rocks from minerals of interest.

In Year 2 of this task, we attempted to develop a general phyllosilicate detector. We used our generative model to create several thousand positive (phyllosilicate) and negative (not phyllosilicate) synthetic spectra. The majority of these spectra were used to train several artificial neural networks (ANNs) and support vector machines (SVMs) of varying configurations. The detectors that converged to a low error rate on the training set were applied to the test set, *i.e.*, the remainder (unseen portion) of the synthetic spectra. As a final validation step, the top performing detectors on the test set were applied to laboratory spectra of minerals collected by PI Gilmore. Unfortunately, all detectors performed poorly on this real data. Further analysis suggests our linear generative model is insufficiently similar to real data for this class of minerals because of the degree of variability between minerals in this class (dissimilar to carbonates).

An alternative to developing a single detector for a general class of minerals is to develop several detectors tuned to recognize specific minerals within a specific class. We believe constructing such specialized mineral detectors will be more feasible using our current linear generative data model. To test this theory, we chose to focus on sulfates and specifically jarosite, as this mineral has been found at the Opportunity landing site.

We followed a process similar to previous detectors, in this case, generating 5000 positive (jarosite) and 5000 negative (distinctively not-jarosite) synthetic spectra to train both ANNs and SVMs. The synthetic jarosite were linear combinations of nine spectra from the JPL ASTER database, three each of jarosite, plumbojarosite, and natrojarosite. The other spectra were meant to be representative of both not-jarosite and the other ground-truth laboratory spectra we have collected. They were linear combinations of zero or more of the following minerals: clinchlore, biotite, kaolinite, montmorillonite, nontronite, talc, hematite, ilmenite, cerussite, calcite, and dolomite, all from JPL ASTER. The top performing detector was an ANN comprised of 53 input units, two layers of 25 and 10 hidden units (much like our original carbonate detector) and a single real valued (0, 1) output unit. Output values near 0.1 indicate the sample does not contain jarosite while values near 0.9 indicate the presence of jarosite. The detector inputs are reflectances (averaged over 0.01 μm windows) in three wavelength ranges: 1.40–1.50 μm, 1.70–1.85 μm, 2.15–2.40 μm. When we tested the detector on 208 laboratory spectra collected at Wesleyan, it correctly identified all jarosites and rejected nearly all non-jarosites (8 of 17 kaolinite samples were misclassified as jarosite). Given this initial positive result, we plan to further test and refine the jarosite detector.

Collection of field data

The field excursion has been postponed to Year 3 for several reasons: 1) the late arrival of the graduate student made planning difficult for Yellowstone where permits were required essentially when the student began work. 2) Data from the Opportunity rover show a specific set of minerals formed via precipitation from groundwater/ surface water brines. These minerals are not available at Yellowstone. We are in the process of identifying field sites which contain the minerals observed at the Opportunity site. The identification and planning for a field excursion is the number one priority for the initial months of Year 3.

Additionally, the PI will accompany Co-I Greenwood to St. Lucia in the summer of 2004, which contains a hydrothermal system atop a simmering volcano. Spectral data will be collected for this site and used to test the mineral detectors and mixing models. Samples will be returned and analyzed in the laboratories at both Wesleyan and Yale to identify constituent minerals.

Development of empirical and theoretical mixing models

Our carbonate detector has been thus far tested on rocks that are 100% carbonate or 0% carbonate. The substrate in the dust experiment was also 100% carbonate. We now turn to the goal of the detection of carbonate within a mixture, which is a more geologically

realistic state. Initially, we seek to simply determine the detection limits of the carbonate detector on mineral mixtures of known percentages. The characterization (composition, size and modal % of end-members) for all mineral mixtures in the study will be utilized to derive empirical mixing relationships of constituents. Linear mixtures of synthetic data will then be used to train a supervised classifier to deconvolve the mineral mixtures into its end-members. We are empirically measuring the non-linear mixing effects. After linear deconvolution, we will use non-linear mixture models to perform the deconvolution. The performance of linear vs. nonlinear deconvolution algorithms will then be compared.

We have prepared mixture of known amounts of palagonite and calcite at several grain sizes (Fig. 5). Preliminary analysis of the mixtures by the carbonate detector were surprising, in that the detector failed to identify carbonate in samples with high percentages. Examination of the spectra shows that small grain sizes increase the overall reflectance values of the carbonate and the carbonate absorptions are reduced (Fig. 6); overall reflectance is one factor in the training set. We hypothesize these factors are contributing to the performance of the detector and we are presently taking steps to solve for these issues (e.g., normalize the reflectance).
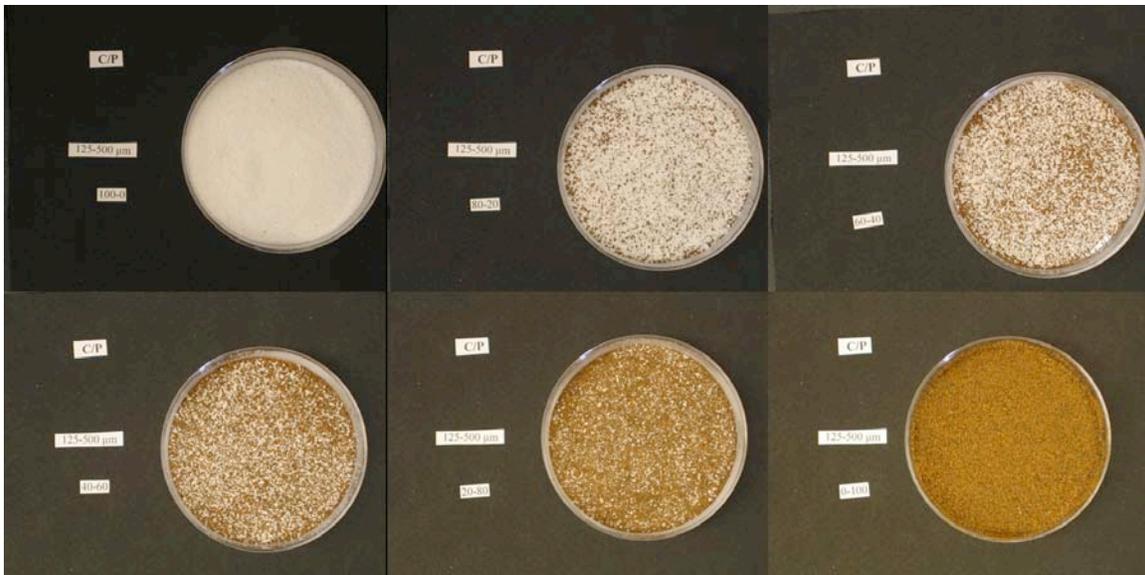

Figure 5. Set of mixtures of calcite (white) and palagonite (orange) for grain size of 125-500 microns.
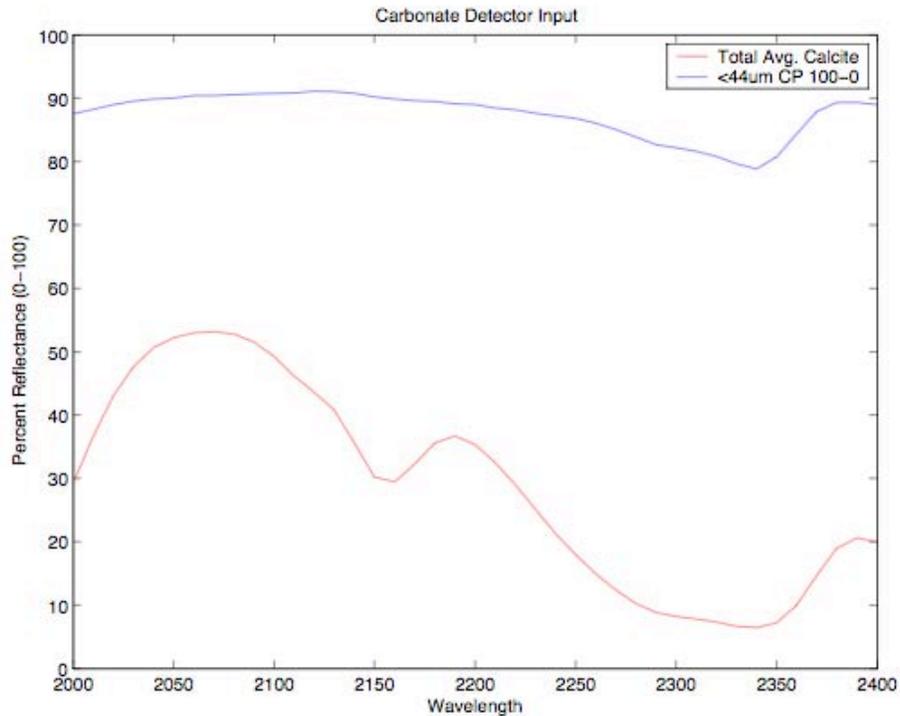
Figure 6. Sample spectra for a single calcite and palagonite mixture experiment. The first number in the legend for the experiment (blue) refers the percentage of calcite in the sample. The red spectrum is an average of several spectra of a single calcite crystal. The dissimilarity between the two spectra may be due to grain size. The carbonate detector failed to detect carbonate in the experiment.

3. Year 3 Schedule of Work

We will continue the development and testing of new detectors that will identify hydrothermal minerals relevant to the martian surface. We are exploring both the detection of broad classes of minerals and of specialized classes. Initial experiments indicate the higher accuracies can be obtained when the classes are more restricted. The classifier then has more constraints to distinguish between samples belonging to the target class and those that do not. In the final year of work, we will implement and test the nonlinear models that are under development, as described above.

We will complete our planning and collect spectra and rock samples in the field in the summer of 2004. Once the data are collected, samples will be returned and analyzed in the laboratories at both Wesleyan and Yale to identify constituent minerals. The sample spectra will be analyzed using the detectors and the accuracy assessed using the results from the lab analyses conducted at Wesleyan and Yale.

Our final algorithm to be developed and tested is a novelty detector. The novelty detector will identify signatures that are anomalous with regard to the collection of samples. This may be due to the target containing an unusual mineral or due to the target consisting of an unusual combination of more common minerals. The novelty detector will not

distinguish between these two scenarios. It will identify the sample and indicate that it should be further studied by the science team. Two algorithms will be tested. The first is based on an unsupervised clustering. The known samples will be clustered together. A new sample that has a signature which would be statistically unlikely to occur given the set of past samples will be marked as novel. The second method will be to use a supervised (Support Vector Machine) method to model the set of samples as a known class. The test sample will then be evaluated to determine the distance (in feature space) from the set of training samples. Samples that are far away from the rest of the set will be marked as novel. Both methods will be tested on the lab data and using the field data.

4. Budget

There are no changes to the original budget.

5. Conference Presentations/ Publications

Gilmore M. S., Merrill M. D., Castaño R., Bornstein B. and Greenwood J. (2004) Effect of palagonite dust deposition on the automated detection of carbonate Vis/NIR spectra, *35th Lunar and Planetary Science Conf.*, Abstract #1335 (CD-ROM).
Gilmore M. S., Merrill M. D., Castaño R., Bornstein B. and Greenwood J. (2004) Effect of palagonite dust deposition on the automated detection of carbonate Vis/NIR spectra, *Geophysical Research Letters,* in prep.

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