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7 **Vegetation Cover Analysis of Hazardous Waste Sites in Utah**
8 **and Arizona using Hyperspectral Remote Sensing**

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19 *Received: / Accepted: / Published:*
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21 **Abstract:** Remote sensing technology can provide a cost-effective tool for monitoring
22 hazardous waste sites. This study investigated the usability of HyMap airborne
23 hyperspectral remote sensing data (126 bands at 2.3 × 2.3 m spatial resolution) to
24 characterize the vegetation at U.S. Department of Energy uranium processing sites near
25 Monticello, Utah and Monument Valley, Arizona. Grass and shrub species were mixed on
26 an engineered disposal cell cover at the Monticello site while shrub species were dominant
27 in the phytoremediation plantings at the Monument Valley site. The specific objectives of
28 this study were to: 1) estimate leaf-area-index (LAI) of the vegetation using three different
29 methods (i.e., vegetation indices, red-edge positioning (REP), and machine learning
30 regression trees), and 2) map the vegetation cover using machine learning decision trees
31 based on either the scaled reflectance data or mixture tuned matched filtering (MTMF)-
32 derived metrics and vegetation indices. Regression trees resulted in the best calibration
33 performance of LAI estimation ($R^2 > 0.80$). The use of REPs failed to accurately predict LAI
34 ($R^2 < 0.2$). The use of the MTMF-derived metrics (matched filter scores and infeasibility)
35 and a range of vegetation indices in decision trees improved the vegetation mapping when
36 compared to the decision tree classification using just the scaled reflectance. Results suggest
37 that hyperspectral imagery are useful for characterizing biophysical characteristics (LAI)
38 and vegetation cover on capped hazardous waste sites. However, it is believed that the

1 vegetation mapping would benefit from the use of higher spatial resolution hyperspectral
2 data due to the small size of many of the vegetation patches (< 1m) found on the sites.

3 **Keywords:** hazardous waste sites; hyperspectral remote sensing; HyMap; vegetation
4 mapping; LAI estimation; decision trees
5

6 1. Introduction

7 Humans produce large amounts of hazardous waste. In 2007, the United States generated 47
8 million tons of hazardous waste with Louisiana and Texas responsible for more than 50% of the total
9 [1]. Hazardous waste from current and historic activities is often isolated in landfills or disposal cells
10 using a capping system consisting of barriers that limit deep percolation of precipitation and
11 mobilization of the hazardous constituents [2, 3]. In addition to the thousands of capping systems in
12 existence, in 2004 the EPA estimated that almost 300,000 additional waste sites were expected to
13 require remediation [4]. Many of these sites, as well as the older sites contain residual contamination
14 or are undergoing some form of *in situ* remediation. In all cases, the management of water infiltration
15 into the waste area is a key issue to prevent the migration of the hazardous constituents into the
16 environment.

17 Historically, the vegetation component of a hazardous waste capping system has been viewed as a
18 means to stabilize the surface soils and prevent erosion. However, for some capping systems in arid
19 and semi-arid climates, the vegetative cover has taken an increasingly functional role through the
20 construction of evapotranspiration or water balance cover systems [5, 6]. In these systems, the
21 vegetative cover and soil system are constructed to maintain a hydrologic balance with the vegetation
22 withdrawing water from the underlying soils on an annual basis, thereby minimizing deep infiltration.
23 Proper functioning of these types of systems depends on the development and maintenance of a robust
24 plant community that can maintain water withdrawal capacity over the life of the capping system.

25 Some *in situ* remediation strategies are also being implemented whereby the migration of
26 subsurface contaminants is dependent on the water withdrawal capability of vegetation. Considered to
27 be a type of Phytoremediation [7], these strategies may be applicable where subsurface contaminants
28 are potentially mobile, and management of vegetation can result in reduced infiltration and subsequent
29 hydraulic control of the migration of contaminants in soils and shallow groundwater [8].

30 In all such cases, the maintenance of a high evapotranspiration capacity through well-adapted and
31 healthy plant communities is key to the proper and long term stabilization of the wastes. Monitoring of
32 these systems is commonly conducted by ground level observations by trained professionals and is
33 becoming a significant cost element in the management of such systems. Consequently, there is a
34 growing demand for an efficient and reliable approach to vegetation monitoring at waste remediation
35 and stabilization sites. Remote sensing technology can provide a cost effective tool for this type of
36 monitoring in harmony with information obtained from *in situ* investigation.

37 Multispectral (several bands) and hyperspectral (hundreds of narrow bands) remote sensing has
38 been used for monitoring hazardous sites [3, 9-11] as well as typical environmental resources such as
39 water, land, and vegetation [12-15]. In particular, remote sensing-derived vegetation products can

1 provide valuable information regarding vegetation health and dynamics when monitoring hazardous
2 waste sites [16]. Various classification approaches have been investigated for vegetation mapping,
3 including: maximum likelihood classification [17], subpixel analysis [18], machine learning [19], and
4 object-based methods [20]. The phenological cycle of vegetation has also been studied to better map
5 vegetation dynamics [21].

6 Several approaches have been investigated for modeling vegetation biophysical parameters such as
7 biomass and leaf-area-index (LAI) using remotely sensed spectral data. These approaches include:
8 empirical methods such as statistical regression, spectral positioning, and artificial intelligence, and
9 physical modeling [22]. Simple linear regression analysis has been widely adopted to correlate
10 vegetation biophysical parameters measured *in situ* with various vegetation indices such as the
11 Normalized Difference Vegetation Index (NDVI) [23]. More advanced regression techniques,
12 including principal component regression and partial least squares regression, have also been examined
13 [24, 25]. Some scientists have focused on identifying the spectral reflectance red-edge position (REP)
14 because of its close association with chlorophyll content and its seasonal variations, which directly
15 influence vegetation health [26]. Artificial intelligence methods such as neural networks and regression
16 trees can incorporate field training samples to estimate the vegetation parameters [27]. These methods
17 are relatively simple, but have some limitations, including the fact that the relationships are based on
18 representative training samples and the methods are sensitive to atmospheric conditions, sensor
19 viewing geometry, and the spatial resolution of the remote sensor data. Therefore, the methods
20 generally need to be calibrated each time a new remote sensing dataset is acquired [28].

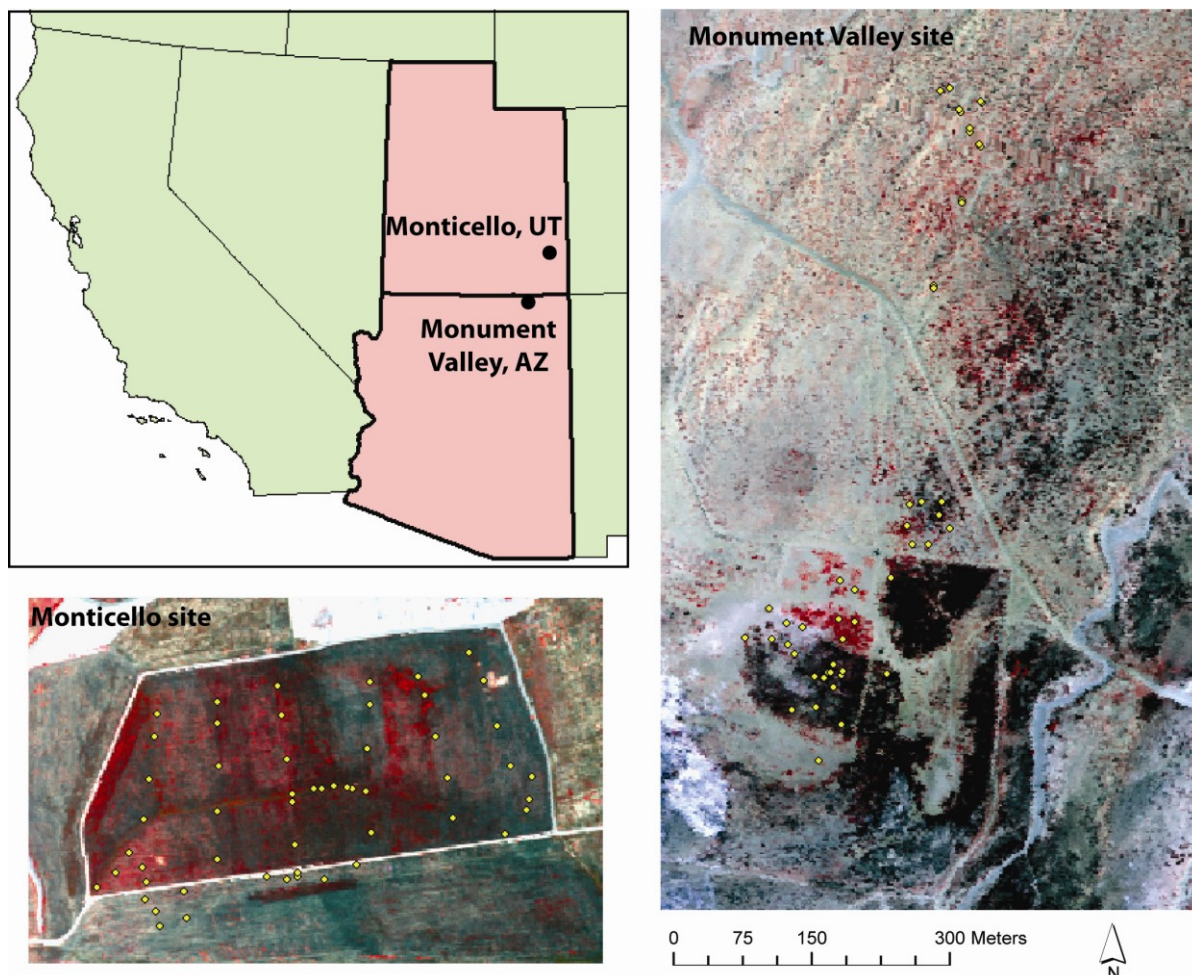
21 Physical models are theoretically based on leaf scattering and absorption mechanisms associated
22 with biochemistry [29]. A representative type of model is the radiative transfer model, which simulates
23 radiation transfer processes in vegetation by computing the interaction between plants and solar
24 radiation. Vegetation biophysical parameters can be retrieved through inversion of the radiative
25 transfer model (e.g., PROSPECT). Simulated reflectance databases have been frequently used with
26 model inversion techniques [30]. Model inversion approaches may result in a multitude of different
27 possible solutions increasing uncertainties [31].

28 Vegetation is typically characterized by slow rates of change and affected by other slow processes
29 such as climate change or soil acidification. However, the vegetation cover on a hazardous waste site
30 may rapidly change due to the unanticipated conditions (e.g., soil subsidence, biointrusion). This
31 change must be quickly detected. The objective of this research was to demonstrate the usefulness of
32 hyperspectral remote sensing to provide long term monitoring capability for Department of Energy
33 (DOE) remediation and waste sites. This study investigated characteristics of vegetation cover on
34 hazardous waste sites with regard to species type and LAI distribution using various technical
35 approaches.

36 2. Study Area and Data

37 Two U.S. Department of Energy sites were investigated in this study (Figure 1): a) a uranium mill
38 tailings disposal cell capping system near Monticello, UT, and b) a phytoremediation planting of desert
39 shrubs near Monument Valley, AZ.

1 **Figure 1.** The HyMap imagery of two study sites (RGB = Hyperspectral bands 24, 17, 11). The
 2 yellow symbols are *in situ* sampling locations.



3
4

5 To limit percolation into underlying tailings, the Monticello capping system relies on the water-
 6 storage capacity of a 163-cm sandy clay loam soil and rock “sponge” layer overlying a 38-cm coarse
 7 sand capillary barrier, and native sagebrush steppe vegetation to seasonally remove stored precipitation
 8 [32]. The capillary barrier increases the water-storage capacity of the soil “sponge” [33]. The topsoil
 9 has favorable edaphic properties for a sustainable plant community. Percolation flux, measured within
 10 a 3-ha embedded lysimeter, was approximately 0.5 mm yr^{-1} from 2000 through 2009 [32]; the capping
 11 system has performed well in the short term. Detecting temporal changes and spatial patterns in plant
 12 species and LAI on a landscape scale will be important for performance monitoring in the long term.

13 At the arid Monument Valley site, two deep-rooted native shrubs, *Sarcobatus vermiculatus* (black
 14 greasewood) and *Atriplex canescens* (fourwing saltbush), are part of the remedy for nitrate
 15 contamination in soil where a uranium mill tailings pile once stood, and in an alluvial aquifer
 16 spreading away from the source area soil [8]. When protected from livestock grazing, populations of
 17 these phreatophytic shrubs transpire enough water from the source area soil to limit recharge and
 18 nitrate leaching [34], and from the alluvial aquifer to slow the spread of the nitrate plume [35].
 19 Monitoring the long-term performance of phytoremediation at Monument Valley will include tracking
 20 responses of phreatophyte health and transpiration rates to changing land management practices over

1 many hectares [36].

2 HyMap hyperspectral remote sensing data were collected by *HyVista, Inc.* at Monument Valley,
 3 AZ on 2 June 2008 and Monticello, UT on 3 June 2008. Ground reference data were collected at these
 4 sites at the same time as data acquisition. An additional ground level dataset was collected at the
 5 Monticello, UT, site the previous week. Field data included vegetation composition (percent canopy
 6 cover) and LAI ($n = 54$ on the Monticello site and $n = 19$ on the Monument Valley site; refer to Table
 7 1). The dominant species included *Artemisia tridentata* (big sagebrush), *Ericameria nauseosa* (rubber
 8 rabbitbrush), and *Pascopyrum smithii* (western wheatgrass) on the Monticello site and *Sarcobatus*
 9 *vermiculatus* (black greasewood) and *Atriplex canescens* (fourwing saltbush) on the Monument Valley
 10 site.

11 The HyMap hyperspectral data consisted of 126 bands from 440 to 2500 nm at 2.3×2.3 m nominal
 12 spatial resolution. The HyMap radiance data were radiometrically corrected to scaled reflectance using
 13 the HYCORR algorithm with EFFORT spectral polishing [37]. The scaled reflectance data were then
 14 geometrically rectified to a Universal Transverse Mercator (UTM) projection using 15 to 20 GCPs
 15 collected from the 2006 National Agricultural Imagery Program (NAIP) Digital Orthophoto Quarter
 16 Quadrangle (DOQQ) data (1 x 1 m spatial resolution) over the two study sites resulting in root-mean-
 17 square-error (*RMSE*) < 1 pixel.

18 **Table 1.** Field data characteristics for vegetation mapping and leaf-area-index (LAI) estimation.

	Monticello site	Monument Valley site
Strata (classes)*	Big sagebrush ($n = 8$) Rubber rabbitbrush ($n = 12$) Western wheatgrass ($n = 16$) Litter (dead plant materials; mostly grass species) ($n = 17$)	Black greasewood ($n = 12$; percent cover available for 8 out of 12) Fourwing saltbush ($n = 14$; percent cover available for 9 out of 14) Soil ($n = 17$)
LAI range	0.09 – 5.1 ($n = 54$)**	0.95 – 6.26 ($n = 19$)***

19 * A dominant class at a sampled location was determined based on percent canopy cover.

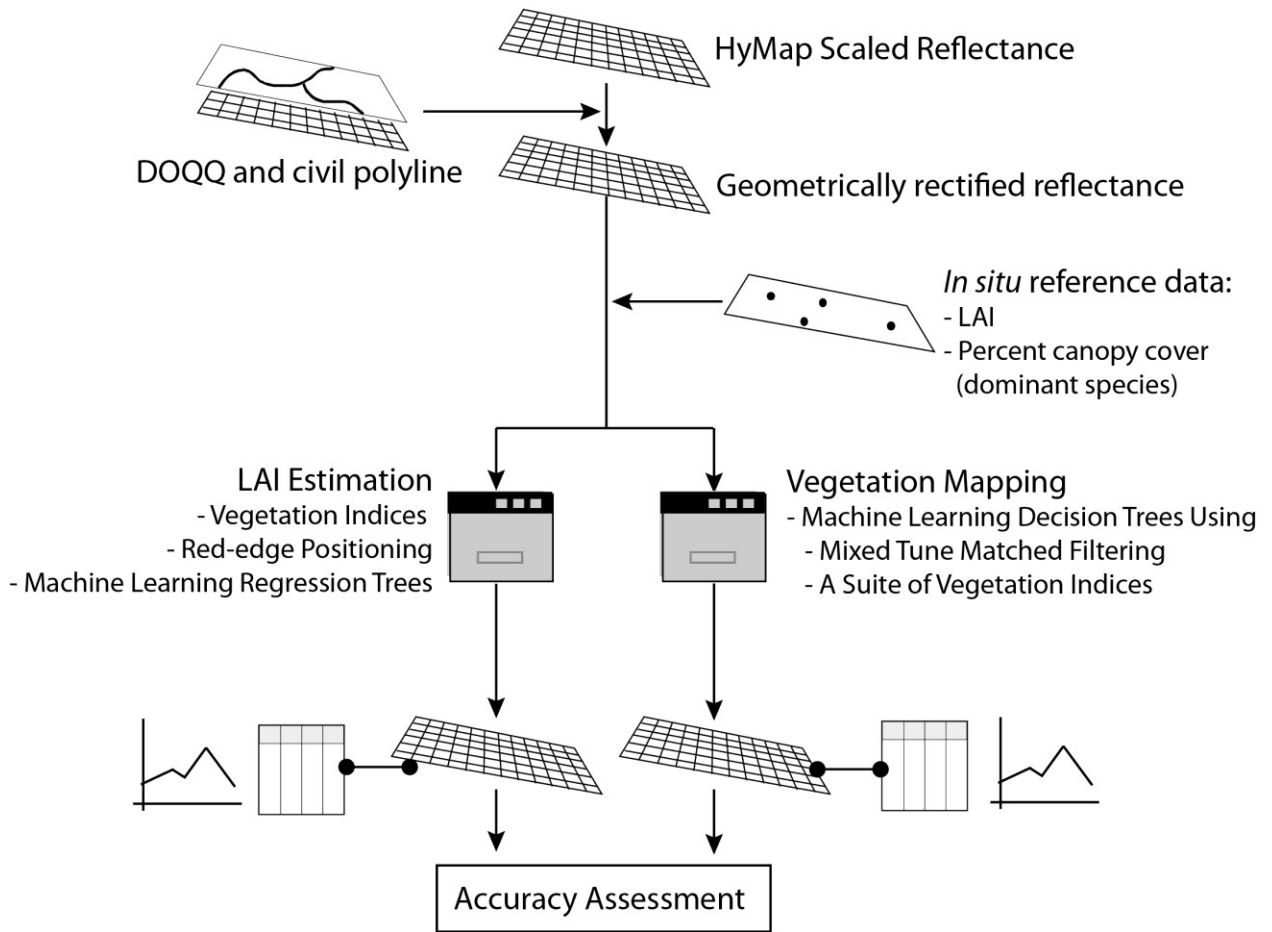
20 ** One of the samples was not used for the classification since the dominant class (soil) was other than the four.

21 *** LAI was measured at only 19 sample locations of greasewood and saltbush plots.

22 3. Methods

23 Figure 2 is a flow diagram of the digital image processing methods used to a) predict the spatial
 24 distribution of LAI, and b) map the vegetation species present on the two hazardous waste sites.

25 **Figure 2.** Digital image processing flow diagram.



1
2

1 3.1. Leaf-area-Index (LAI) Estimation

2 One of the major goals of this research was to map the spatial distribution of vegetation biomass
 3 on the waste sites using remote sensing-derived indices and algorithms in conjunction with *in situ*
 4 derived LAI used as a surrogate for vegetation biomass. LAI, the total area of one-sided green leaves
 5 in relationship to the ground below them, directly quantifies the vegetation canopy structure and is
 6 highly-related to diverse canopy processes including water interception, photosynthesis,
 7 evapotranspiration, and respiration.

8 Three approaches were investigated to estimate vegetation LAI, including: 1) vegetation index
 9 (VI)-based methods, 2) the red-edge positioning (REP) methods, and 3) the use of machine learning
 10 regression trees. Although there are numerous vegetation indices, we evaluated two basic vegetation
 11 indices:

$$12 \quad VI1 = \frac{B_2}{B_1} \quad (1)$$

$$13 \quad VI2 = \frac{B_2 - B_1}{B_2 + B_1} \quad (2)$$

14 These are extended versions of the simple ratio (SR) and normalized difference vegetation index
 15 (NDVI), respectively [14, 38]. Unlike SR and NDVI which only use one red band and one near-
 16 infrared band, we evaluated VI1 and VI2 with all $126 \times 125 (= 15,750)$ possible band combinations in
 17 the entire spectral range from 400 to 2,500 nm as long as the value of B_1 was smaller than B_2 . While
 18 the correlation between the VI2 and LAI results in a symmetric pattern when B_1 and B_2 are switched,
 19 the correlation between the VI1 and LAI is a bit asymmetric with the switch of B_1 and B_2 . However,
 20 the asymmetric characteristic of the VI1-LAI relationship were not considered in the study because the
 21 asymmetry was slight and we were only interested in the band combinations that resulted in the highest
 22 correlation.

23 The REP is the spectral position between the red (~680 nm) and near-infrared (~800 nm)
 24 wavelengths where the maximum slope is found [29]. The REP is sensitive to the biophysical and
 25 biogeochemical properties of vegetation such as LAI and leaf nitrogen content. Phenological change
 26 and/or vegetation stress can affect the REP. There are several methods for computing REP, including:
 27 derivative function-based methods [39] and Gaussian model-based methods [40]. Some studies have
 28 reported that the REP is not a single location, but multiple wavelengths [39, 41]. In this study, three
 29 REP techniques were tested to estimate LAI, including: 1) a linear four-point interpolation (LI_REP)
 30 [42], 2) a three-point LaGrange interpolation (LG_REP) [43], and 3) a linear extrapolation (LE_REP)
 31 [26].

32 LI_REP assumes that the reflectance curve at the red-edge can be simplified to a straight line
 33 centered near the midpoint between the NIR reflectance and the minimum reflectance of the
 34 chlorophyll absorption. It was computed using:

$$35 \quad LI_REP = 700 + 40 \left[\frac{\rho_{red\ edge} - \rho_{70nm}}{\rho_{40nm} - \rho_{70nm}} \right], \text{ where } \rho_{red\ edge} = \frac{\rho_{70nm} + \rho_{30nm}}{2} \quad (3)$$

36 LG_REP uses the point with the maximum first derivative reflectance FDR_{λ} , (λ , FDR_{λ}), and two
 37 points on both sides, (λ_{-} , $FDR_{\lambda_{-}}$) and (λ_{+} , $FDR_{\lambda_{+}}$). A second-order polynomial was fit using the

three points and the wavelength where the second derivative equals zero was determined to be the REP:

$$LG_REP = \frac{A(\lambda_1 + \lambda_2) + 3(\lambda_2 + \lambda_3) + 3(\lambda_3 + \lambda_4)}{2(A + 3 + 3)} \quad (4)$$

where $A = \frac{FDR_{\lambda_1}}{(\lambda_1 - \lambda_2)(\lambda_2 - \lambda_3)}$, $B = \frac{FDR_{\lambda_2}}{(\lambda_2 - \lambda_3)(\lambda_3 - \lambda_4)}$, and $C = \frac{FDR_{\lambda_3}}{(\lambda_3 - \lambda_4)(\lambda_4 - \lambda_5)}$.

LE_REP was based on a double-peak feature in the first derivative reflectance resulting from the discontinuity in REP and foliar-nitrogen relationship. Four points, two at the far-red peak (680 to 700 nm) and two at the NIR peak (725 to 760 nm), were used to create two straight lines. The wavelength corresponding to the intersection of the two lines was the REP:

$$LE_REP = \frac{-c_{far-red} - n_{NIR}}{(m_{far-red} - n_{NIR})} \quad (5)$$

where c and m were the intercept and slope of the lines, respectively.

Machine learning regression trees typically use a binary recursive partitioning process to generate rule-based models based on user-supplied training samples for estimating a target variable such as LAI [27, 44]. Cubist by *RuleQuest Inc.* was used in this study. The usefulness of Cubist for creating robust regression trees has been documented in the remote sensing literature [27, 45, 46].

The coefficient of determination (R^2), representing the goodness-of-fit of a model, and *RMSE* were used to measure calibration performance. Due to the limited number of field data points, it was not possible to perform cross-validation associated with the three approaches.

3.2. Vegetation mapping

Two different classification approaches were investigated to map vegetation on the Monticello, UT, and Monument Valley, AZ, hazardous waste sites. Both approaches employed machine learning decision trees, but one used scaled reflectance data as input variables while the other used mixture-tuned-matched-filtering (MTMF)-derived metrics and a suite of vegetation indices as input variables.

Decision trees have wide application for classification problems because they divide a complex decision into a hierarchy of simple and interpretable decisions [47-52]. See5 by *RuleQuest Research Inc.*, a widely used machine learning decision tree software, was used to generate decision trees for image classification.

MTMF is a hybrid classification method based on a combination of linear mixture theory and matched filtering, which is based on a partial unmixing approach with user-defined targets [53]. One of the advantages of MTMF is that the endmembers (i.e., spectral reflectance characteristics for spectrally pure materials) within a scene do not need to be identified because MTMF uses each endmember independently and models the pixel at each endmember as a mixture of the endmembers and an undefined background material [54, 55]. MTMF typically uses the minimum noise fraction (MNF) results extracted from the reflectance data. In this study, the cumulative 80% variation threshold was used to determine the subset of MNF results to be used in the MTMF analysis for each site. Consequently, the first 18 and 25 MNF transformed images were used in the MTMF analysis for the Monticello and Monument Valley sites, respectively. The MTMF output includes a matched filter (MF) score and an infeasibility value for each endmember. Ideally, pixels with a high MF score value

1 and a low infeasibility value have a high percent cover of each endmember (e.g., sagebrush). Pixels
 2 with high MF score values and high infeasibility values may be false alarms. We used two image-
 3 derived endmembers for each class based on the percent cover data, which resulted in 8 endmembers
 4 for the Monticello site and 6 endmembers for the Monument Valley site.

5 The MF scores and infeasibility values were used as input variables along with a suite of
 6 vegetation indices. A total of 11 vegetation indices were used and two (i.e., VI1 and VI2) of them were
 7 developed from the LAI estimation in this study (Table 2). The original scaled reflectance data (126
 8 bands) were also used as input variables in the decision tree classifications for comparison.

9 **Table 2.** Vegetation indices used in the decision tree classification.

Index	Equation	Reference
Simple ratio (SR)	$\frac{R_{845}}{R_{665}}$	Tucker [55]
Normalized difference vegetation index (NDVI)	$\frac{R_{845} - R_{665}}{R_{845} + R_{665}}$	Tucker [55]
Modified NDVI (MNDVI)	$\frac{R_{750} - R_{705}}{R_{750} + R_{705}}$	Fuentes et al. [56]
Photochemical reflectance index (PRI)	$\frac{R_{531} - R_{570}}{R_{531} + R_{570}}$	Gamon et al. [57]
Normalized difference water index (NDWI)	$\frac{R_{860} - R_{1240}}{R_{860} + R_{1240}}$	Gao [58]
Water band index (WBI)	$\frac{R_{900}}{R_{970}}$	Penuelas et al. [59]
Normalized difference nitrogen index (NDNI)	$\frac{\log(R_{1680}/R_{1510})}{\log(1/R_{1680}R_{1510})}$	Serrano et al. [60]
Normalized difference lignin index (NDLI)	$\frac{\log(R_{1680}/R_{1754})}{\log(1/R_{1680}R_{1754})}$	Serrano et al. [60]
Cellulose absorption index (CAI)	$\frac{R_{2020} + R_{2220}}{2} - R_{2100}$	Nagler et al. [61]
(VI1) for the Monticello site	$\frac{R_{1583.8}}{R_{1746.6}}$	From this study
(VI2) for the Monticello site	$\frac{R_{1746.6} - R_{1583.8}}{R_{1746.6} + R_{1583.8}}$	From this study
(VI1) for the Monument Valley site	$\frac{R_{1329.5}}{R_{1187.8}}$	From this study
(VI2) for the Monument Valley site	$\frac{R_{1329.5} - R_{1187.8}}{R_{1329.5} + R_{1187.8}}$	From this study

10 Decision trees are known to be sensitive to the characteristics of the training samples, especially
 11 when there are a limited number of training samples [47]. To improve the stability of the decision tree
 12 classifier, an aggregation approach was introduced [55, 63-66] where multiple decision trees were
 13 generated with different sets of training samples and a majority rule was used to determine the class for
 14 each pixel. Due to the relatively small number of training data samples, we used 50% of the reference

1 data through random selection to train the decision tree and the remaining 50% to test the decision tree.
2 A total of 40 decision trees were generated and 20 trees were selected based on the testing results for
3 each site (i.e., the decision trees with higher testing accuracy were selected). These 20 trees were used
4 for the voting process to generate the final vegetation map for each site.

5 Accuracy assessment of the vegetation maps included the determination of commission and
6 omission errors for each class, overall accuracy (%), and the Kappa Coefficient of Agreement (κ). A
7 Kappa Z-test was used to determine if there was a significant difference between two Kappa
8 Coefficients associated with each site.

9 4. Results and Discussion

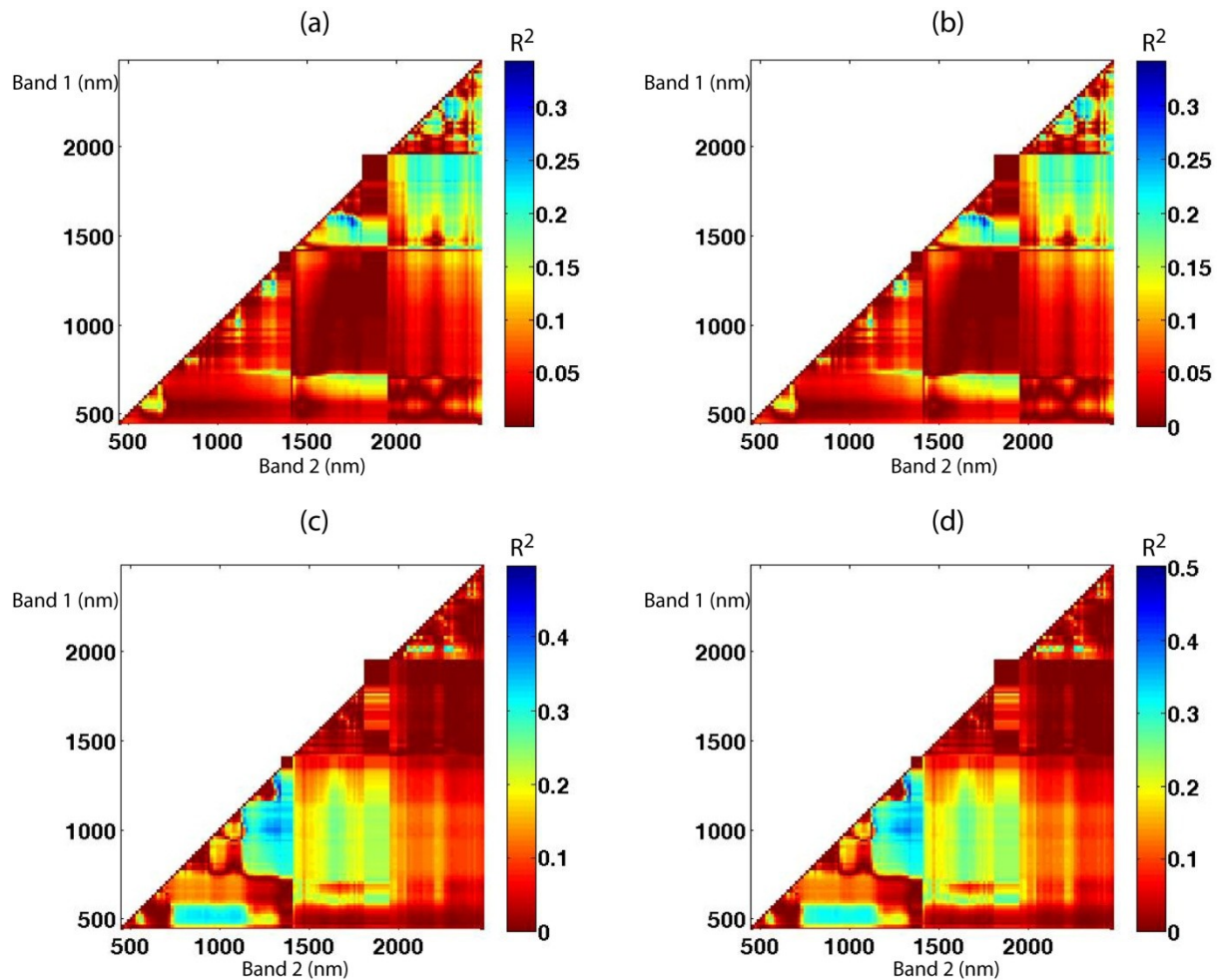
10 4.1. LAI Estimation

11 The results of the correlation matrices produced between the vegetation indices and LAI for all
12 possible band combinations are shown in Figure 3. The greater the correlation of the ground reference
13 LAI value with the two bands used to compute the vegetation index, the more blue the pixel in the
14 diagram. Both VI1 and VI2 exhibited very similar patterns for each site. While relatively high
15 correlations between the vegetation indices and LAI were found in the region between 1500 and 1800
16 nm for the Monticello site, they were found in the region between 900 and 1400 nm for the Monument
17 Valley site (Figure 3). Interestingly, the bands in the red and near-infrared regions, which are assumed
18 to have more information regarding vegetation health, did not produce higher correlations than the
19 bands in the middle-infrared region. This might be because the study sites are located in semi-arid/arid
20 areas and thus the spectral response of each vegetation type may be distinguishable in the middle-
21 infrared region, where the spectral response of vegetation to water is more sensitive.

22 Table 3 summarizes the best band combination and associated statistics (i.e., R^2 , $RMSEs$ from
23 calibration and cross-validation) of the two vegetation indices for each site. It was not surprising that
24 one of the two best bands was found in the water absorption region ($\sim 1,200$ nm) [67] for the
25 Monument Valley site because some of the sample locations were irrigated while the others were not
26 at this site. The vegetation index approach resulted in better performance for the Monument Valley site
27 than the Monticello site (e.g., $R^2 = 0.501$ accounting for 50% of the variance with $r = 0.7$). This might
28 be because the vegetation distribution and structure were more dynamic in the Monticello site than in
29 the Monument Valley site. In particular, the grass and shrub species were highly mixed in the
30 Monticello site, and this made it difficult to calibrate the *in situ* LAI data with the HyMap data at the
31 2.3×2.3 m resolution. Slight difference between the field and the pixel location might have also
32 introduced errors in LAI estimation.

33

1 **Figure 3.** The correlation matrices using the vegetation index approach to estimate LAI:
 2 using (a) VI1, and (b) VI2 for the Monticello, UT site; and using (c) VI1 and (d) VI2 for
 3 the Monument Valley, AZ site.



4
 5 **Table 3.** The best band combination and associated statistics of both VI1 and VI2 for the Monticello
 6 and Monument Valley sites.

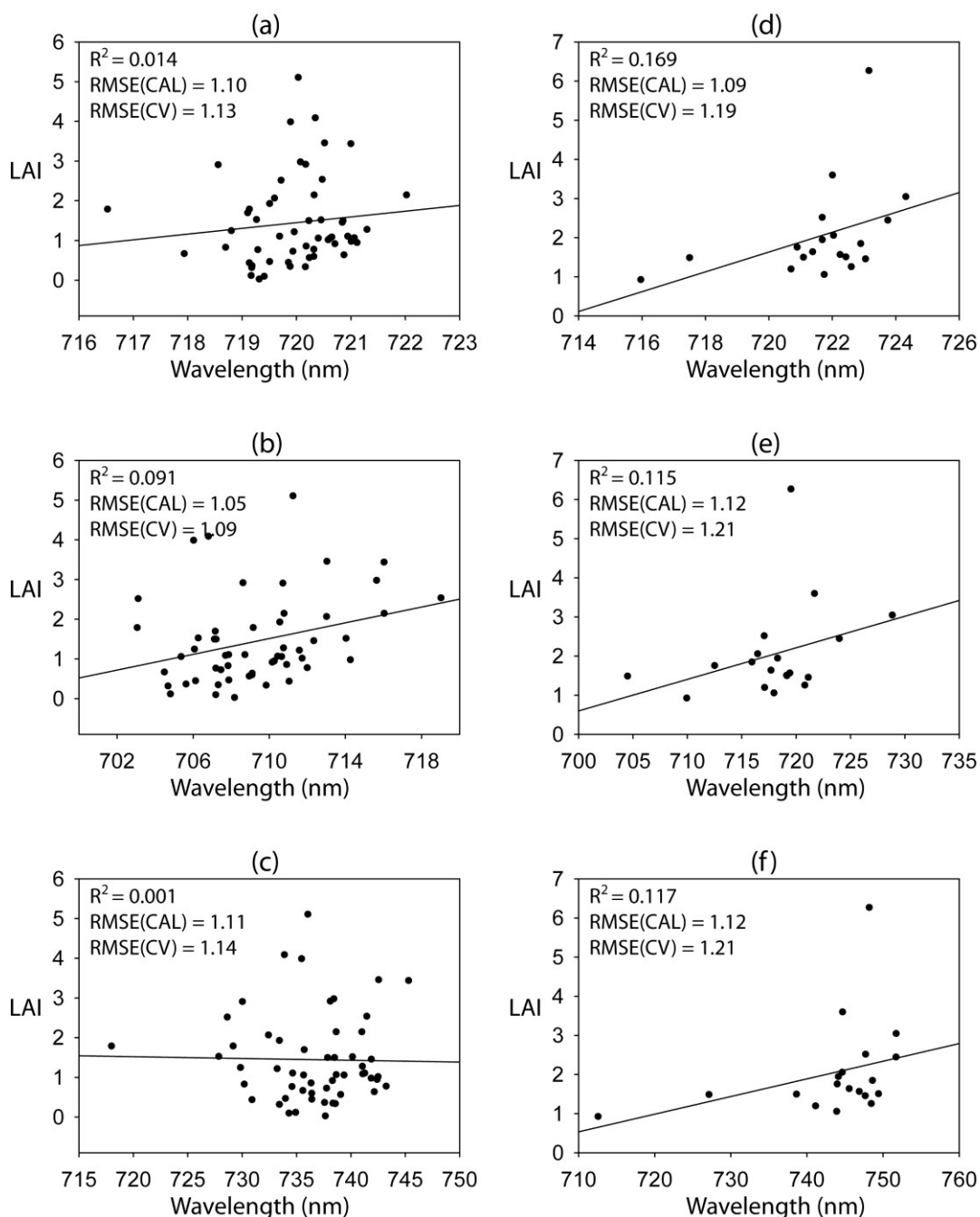
Site	Vegetation index	Band 1 (nm)	Band 2 (nm)	R ²	RMSE
Monticello	VI1	1583.8	1746.6	0.343	0.90/0.93*
	VI2	1583.8	1746.6	0.341	0.90/0.93
Monument Valley	VI1	1187.8	1329.5	0.495	0.85/1.03
	VI2	1187.8	1329.5	0.501	0.84/1.03

7 * RMSE from calibration/RMSE from cross validation

8 The scatterplots between each of the three REP approaches and LAI are shown in Figure 4. The
 9 REP approach did not predict LAI well, resulting in low correlations (< 0.2). Similar to the vegetation
 10 index approach, REP methods resulted in better performance for the Monument Valley site than the
 11 Monticello site. While the LG_REP resulted in the best performance for the Monticello site, the
 12 LI_REP produced the highest accuracy in LAI estimation for the Monument Valley site. However,

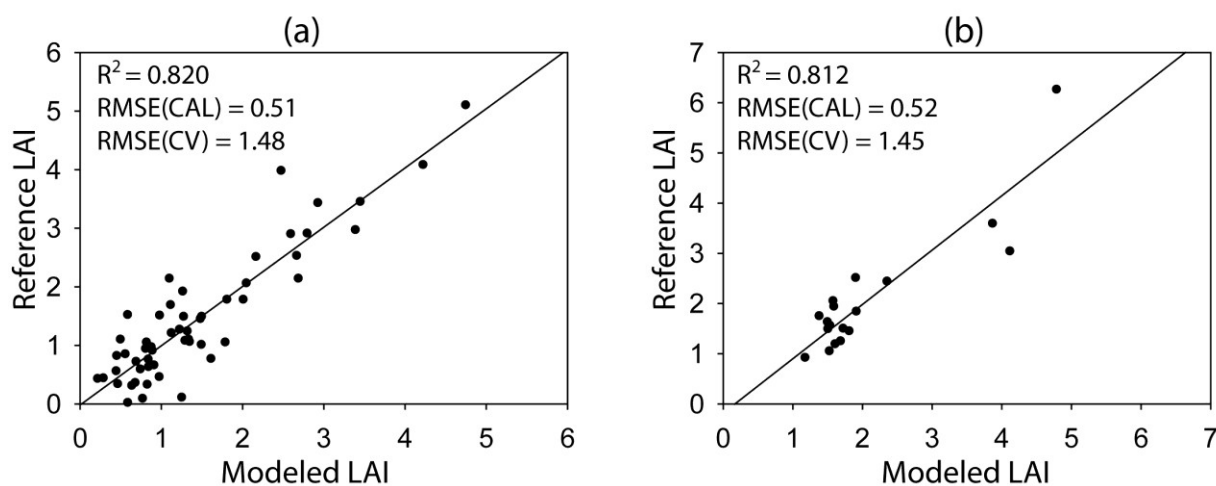
1 there was no significant relationship between any of the REPs and LAI ($p > 0.05$). One of the reasons
 2 for the poor performance of the REP approach might be background soil spectral influence within
 3 pixels. The REP approach typically works well for vegetation with full canopies [68, 69]. Many of the
 4 sample pixels had vegetation cover between 70% and 90%, and thus the background soil could have
 5 influenced the spectral response associated with the red-edge. That most of the sample pixels contained
 6 multiple vegetation species may have also caused the REP approach fail to estimate LAI because each
 7 species typically has a unique REP characteristic.

8 **Figure 4.** The scatterplots between each of the Red-edge position (REP) and LAI: using (a)
 9 LI_REP, (b) LG_REP, and (c) LE_REP for the Monticello, UT site; and using (d) LI_REP,
 10 (e) LG_REP, and (f) LE_REP for the Monument Valley, AZ site. The R^2 and RMSEs from
 11 calibration (CAL) and cross-validation (CV) are also provided.



1 Unlike the results of the VI- and REP-based LAI estimation, the regression trees resulted in very
 2 good LAI estimation performance ($R^2 > 0.8$) (Figure 5). The regression trees generated three rules for
 3 the Monticello, UT, site and two rules for the Monument Valley, AZ, site. Interestingly, one of the
 4 three rules for the Monticello site were associated mainly with the grass species samples (i.e.,
 5 wheatgrass and litter) while the other two rules were applied to most of shrub species samples (i.e.,
 6 sagebrush and rabbitbrush). Eight bands were used to generate the multivariate equations for the
 7 Monticello site, which was not efficient and resulted in inflation of the fitness of the models.
 8 Conversely, only two bands (709 and 754 nm) in the red-edge region were used to generate the
 9 multivariate equations in the regression trees for the Monument Valley site. One rule was applied to
 10 relatively high LAI (> 2) samples for the Monument Valley site, while the other was applied to the
 11 lower LAI samples. The red-edge bands effectively divided the samples into the two groups.

12 **Figure 5.** LAI estimation using the regression tree approach for (a) the Monticello, UT site,
 13 and (b) the Monument Valley, AZ site. The R^2 and RMSEs from calibration (CAL) and
 14 cross-validation (CV) are summarized in the plots.

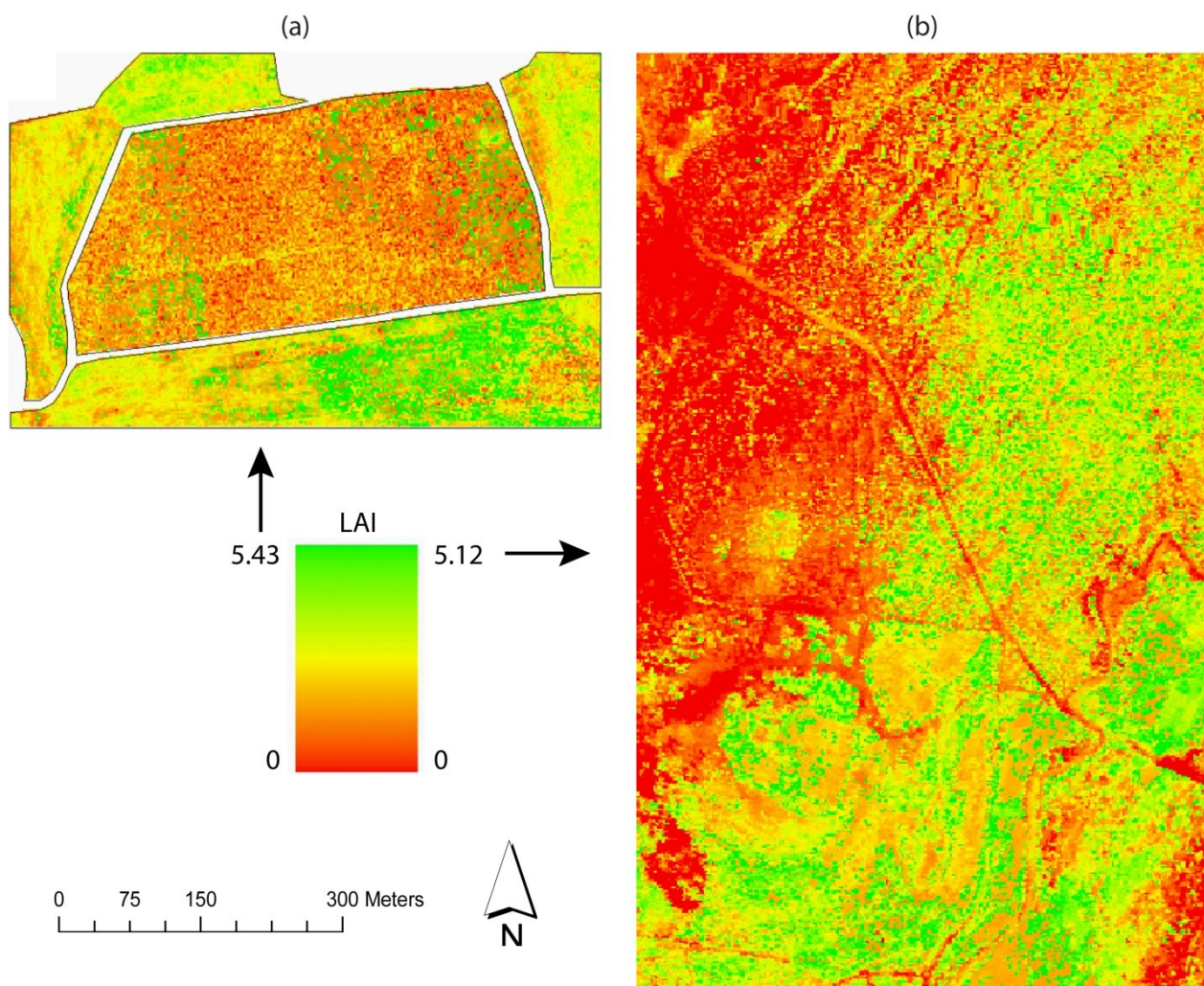


15

16 Although the calibration using the regression trees outperformed those using the vegetation index
 17 and REP data, the cross validation did not correspond to the calibration results. The RMSEs through
 18 cross-validation using the regression trees were higher than those using the other approaches. While
 19 most of the folds for cross-validation generally resulted in low errors, some of the folds ($\sim 25\%$)
 20 resulted in high LAI estimation errors (e.g., > 2), which consequently increased the total RMSE. The
 21 overfitting problem of the regression trees, especially when a small number of samples are used, often
 22 occurs [27]. This is also related to the well known problem of decision/regression trees, which are
 23 sensitive to the training data configuration [70]. Glenn *et al.* [71] investigated black greasewood and
 24 fourwing saltbush over the Monument Valley site using 2007 MODIS data. They measured LAI using
 25 the traditional direct method and found a good agreement with the scaled Enhanced Vegetation Index
 26 (EVI) from MODIS data based on a simple linear regression ($R^2 = 0.77$; $n = 55$; $P < 0.001$). Figure 6
 27 shows the LAI distribution maps estimated using the regression trees for the Monticello and
 28 Monument Valley sites.

1 Although all possible two-band combinations were tested for the VI1 and VI2 in this study, the
 2 most valuable VI might consist of more than two narrow hyperspectral bands. We tested a few narrow
 3 band-derived VIs such as the Vogelmann Red Edge Index 2 [72], which uses spectral data at more than
 4 two wavelengths. However, the additionally tested indices did not outperform the VIs used in this
 5 study. Optimization of multiple wavelengths associated with such narrow band-derived VIs might
 6 further improve the performance of LAI estimation.

7 **Figure 6.** The estimated LAI distribution maps for (a) the Monticello site, and (b) the
 8 Monument Valley site. The dirt road and other land cover classes were masked out for the
 9 Monticello site.



10

11 4.2. Vegetation Mapping

12 Figures 7 and 8 show the relationship between the percent cover and the matched filter scores for
 13 the Monticello, UT, and Monument Valley, AZ, sites, respectively. The percent covers of wheatgrass
 14 and litter were correlated with the matched filter scores at the 90% and 95% confident levels,
 15 respectively. However, the percent covers of sagebrush and rabbitbrush failed to be significantly
 16 correlated with the corresponding matched filter scores. There might be two reasons for this: the
 17 spectral separability of sagebrush and rabbitbrush from other species was not strong. In addition, most
 18 of the sagebrush and rabbitbrush samples were dominated by the corresponding species (i.e., percent

1 cover > 70%), while a few of them were mixed with other species (i.e., percent cover < 60%). MTMF
 2 is known to be sensitive to the amount of green vegetation present within a pixel [38, 55]. Litter (dead
 3 plant materials) for the Monticello site and soil for the Monument Valley site could affect determining
 4 the matched filter scores of the healthy vegetation species. Locational errors could also influence the
 5 relatively lower correlation between the percent covers and the matched filter scores. Interestingly, the
 6 percent covers of saltbush were well correlated with the matched filter scores (Figure 8b). Excluding
 7 one outlier, the percent covers of greasewood were also well correlated with the scores. The MTMF
 8 approach has been successfully applied to map single vegetation species resulting in good relationships
 9 between percent cover and matched filter scores [73], but it typically results in more variation and
 10 confusion between species when multiple species are considered [74]. In this study, while several
 11 vegetation species were mixed at each sampling location in the Monticello site, one species was
 12 dominant at each sampling location in the Monument Valley site. Consequently, there was less
 13 influence from other species in the relationship between the percent cover and the matched filter scores
 14 for the Monument Valley site than for the Monticello site. However, because the matched filter scores
 15 were not sufficient for separating each species from the others, the use of a suite of vegetation indices
 16 was expected to improve classification accuracy using decision tree logic.

17 **Figure 7.** The relationships between the matched filter scores and the percent cover of the
 18 vegetation species for the Monticello site: (a) sagebrush, (b) rabbitbrush, (c) wheatgrass,
 19 and (d) litter.

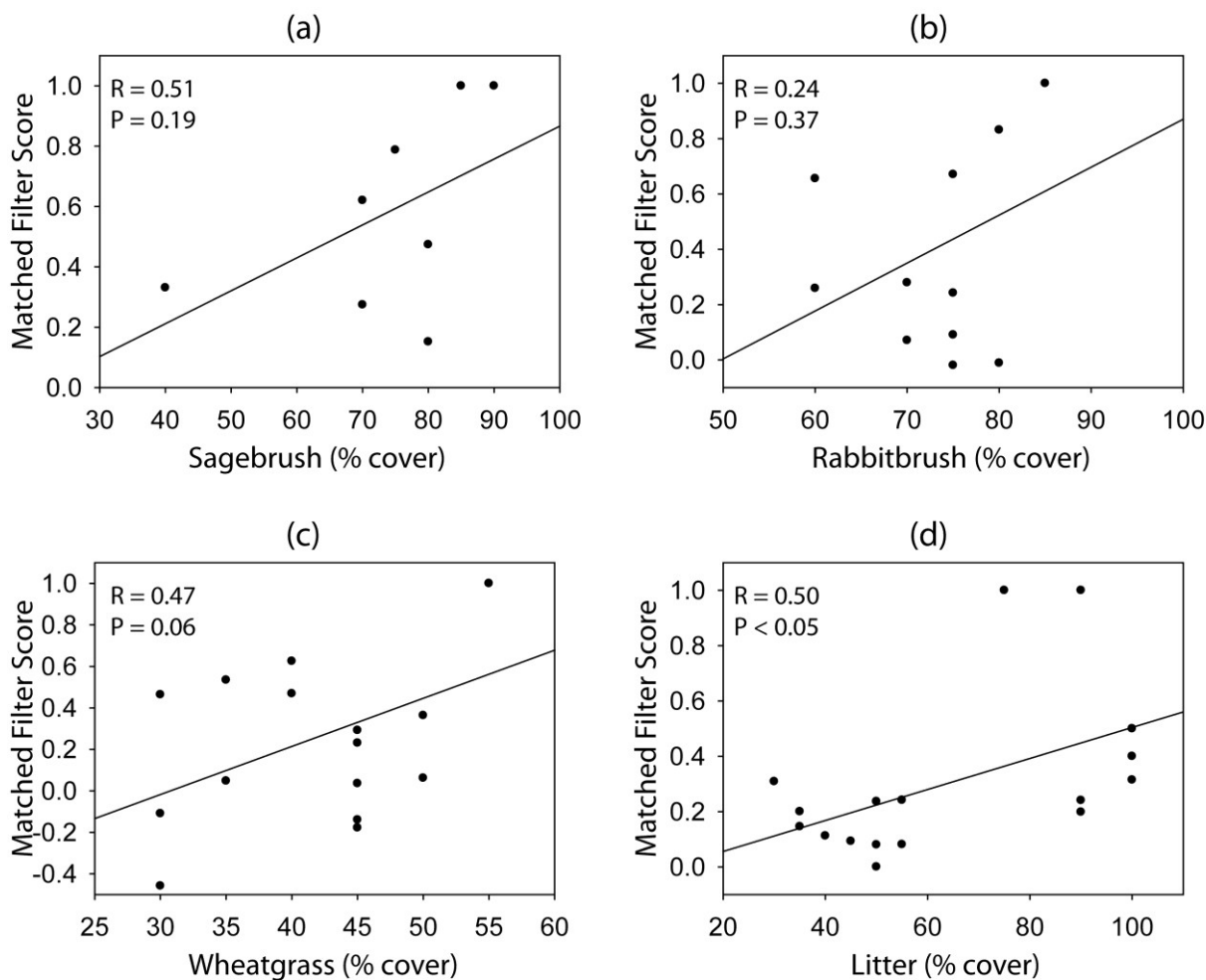


Figure 8. The relationships between the matched filter scores and the percent cover of the vegetation species for the Monument Valley site: (a) greasewood and (b) saltbush.

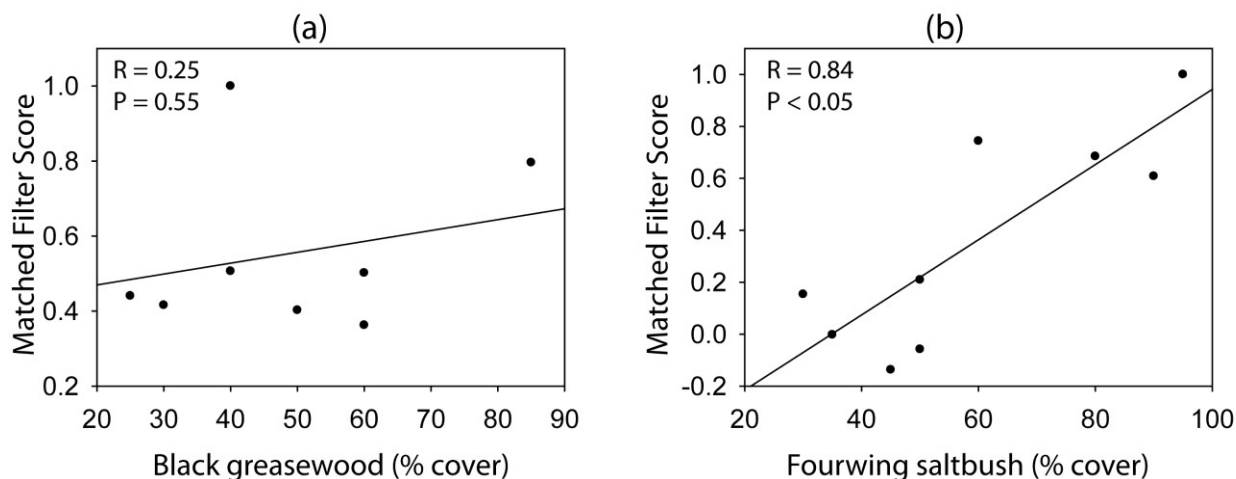


Figure 9 shows the performance variations of the multiple (i.e., 20) decision trees using different sets of training samples for each site. Since the size of the reference data was small (i.e., 53 samples of four classes for the Monticello site and 43 samples of three classes for the Monument Valley site), the performance variation of the multiple decision trees for training and testing was a bit large. For both sites, the MTMF-derived metrics and the vegetation indices (labeled MV in Figure 9) resulted in better performance (for both training and testing) than the original scaled reflectance (labeled REF in Figure 9) in decision tree classification.

Table 4 lists the key input variables to the decision trees classifications for each site. The PRI and NDNI among the vegetation indices were very useful in the decision tree classification for the Monticello site. The MF scores of sagebrush and rabbitbrush also contributed to the decision tree generation for the Monticello site. When the original scaled reflectance data were used in the decision tree classification for the Monticello site, the red (663.4 nm) and red-edge bands (709 nm) contributed most to the classification, followed by the blue (443.3 nm) and middle-infrared band (2477.5 nm). A different pattern of contributing variables was found for the Monument Valley site: The WBI, NDLI, and NDWI contributed most to the MTMF and vegetation index-based decision tree classification. The infeasibility of greasewood was also very useful. When the reflectance data were used, the bands near the water absorption features (i.e., around 1400 and 1940 nm) contributed most to the classification. This may be because the Monument Valley site is located in an arid area and some of the sampling locations were irrigated while others were not. That is why the water-related vegetation indices and reflectance were very useful in vegetation mapping for the Monument Valley site. The chlorophyll absorption features and related vegetation indices contributed moderately to the decision trees for both sites.

1 **Figure 9.** Box plots showing the performance variation of the multiple decision trees using
 2 different sets of training and testing samples: (a) for the Monticello site, and (b) for the
 3 Monument Valley site. MV represents the decision trees using the MTMF-derived metrics
 4 and vegetation indices and REF represents the decision trees using the original scaled
 5 reflectance data.

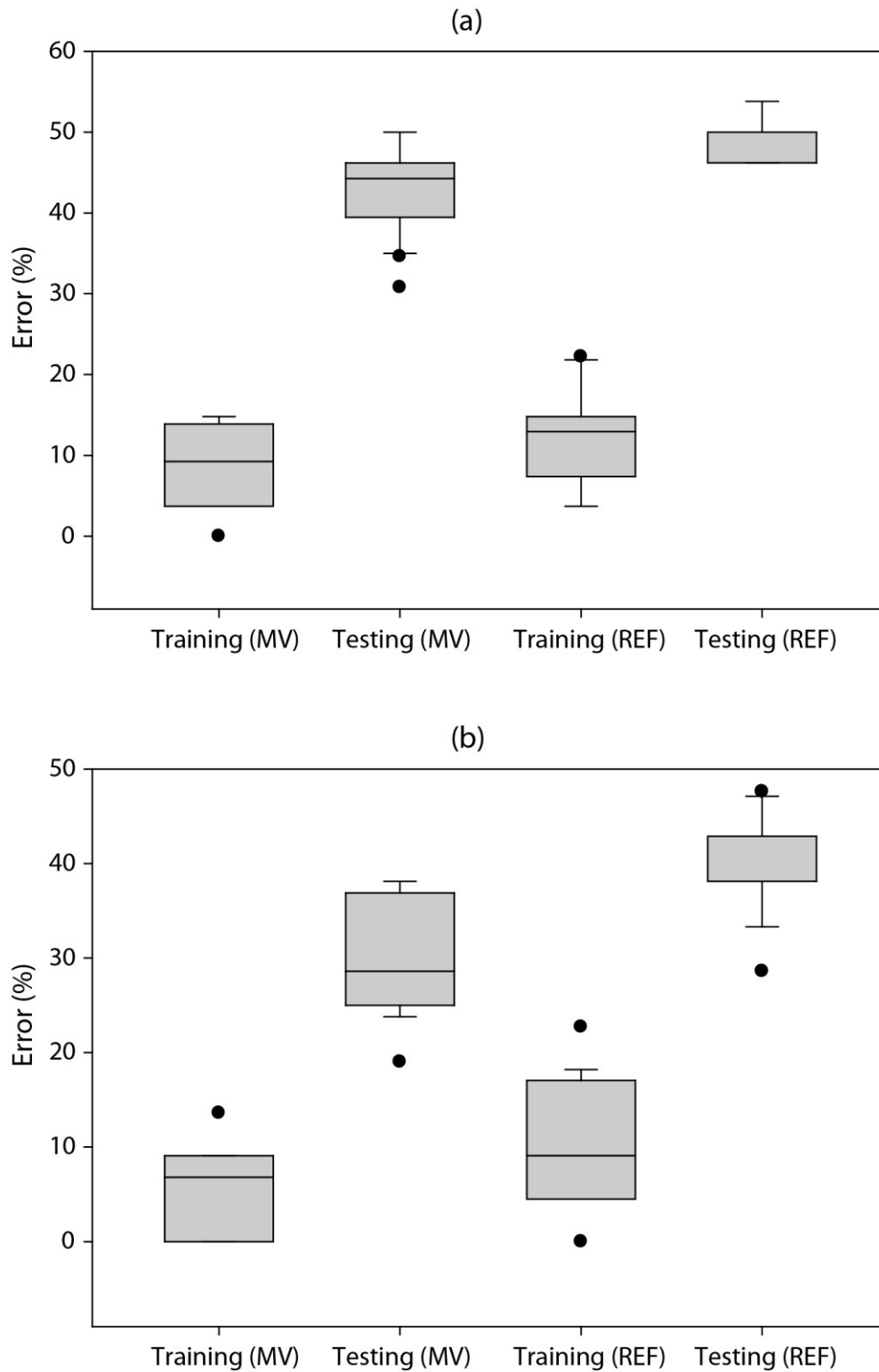


Table 4. Key input variables to the decision trees classifications: (a) for the Monticello site, and (b) for the Monument Valley site.

(a)

Ranking	MTMF + Vegetation indices		Reflectance	
	Variable	Average contribution (%)	Variable	Average contribution (%)
1	PRI	65.9	Band 16 (663.4 nm)	30.0
2	NDNI	50.0	Band 19 (709.0 nm)	26.9
3	MF-Sagebrush 1	49.4	Band 1 (443.3 nm)	25.9
4	CAI	35.0	Band 126 (2477.5 nm)	25.2
5	MF-Sagebrush 2	31.1	Band 21 (739.2 nm)	22.8
6	MF-Rabbitbrush 1	21.3	Band 2 (451.1 nm)	22.4
7	MF-Rabbitbrush 2	15.9	Band 3 (464.5 nm)	16.7
8	INF-Sagebrush 2	14.8	Band 28 (844.4 nm)	14.1
9	VII	11.9	Band 64 (1419.9 nm)	11.3
10	MF-Litter 1	10.2	Band 94 (1805.8 nm)	10.2

(b)

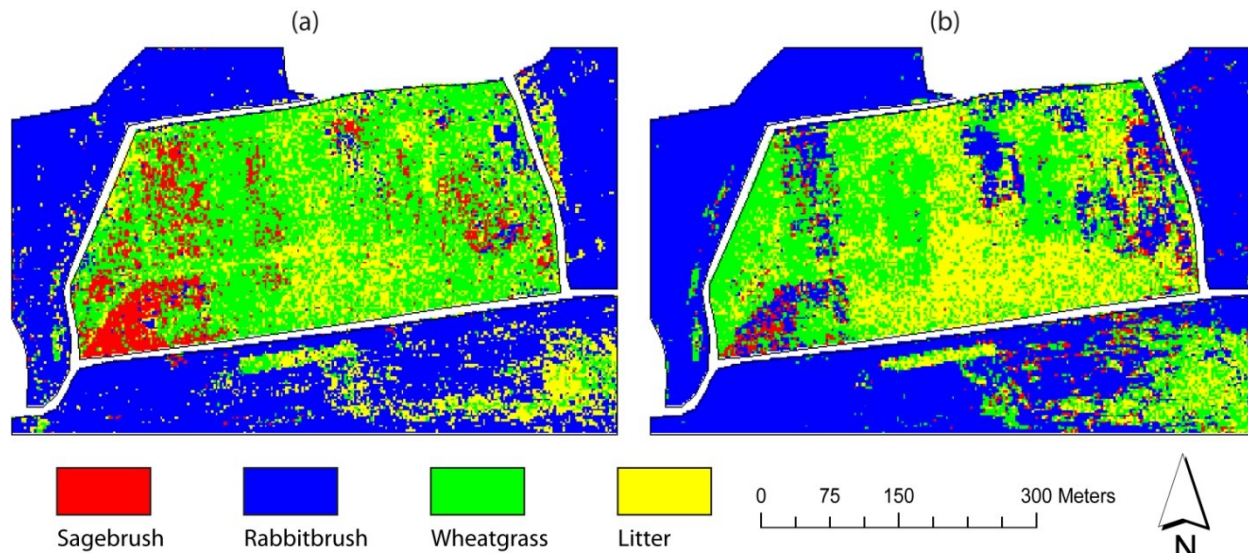
Ranking	MTMF + Vegetation indices		Reflectance	
	Variable	Average contribution (%)	Variable	Average contribution (%)
1	WBI	50.0	Band 63 (1405.4 nm)	35.0
2	NDLI	38.0	Band 97 (1987.0 nm)	30.0
3	NDWI	30.0	Band 31 (892.3 nm)	20.5
4	INF-Greasewood 2	20.5	Band 1 (443.3 nm)	17.5
5	MF-Saltbush 1	18.7	Band 17 (678.4 nm)	15.0
6	NDNI	15.0	Band 61 (1329.5 nm)	15.0
7	VII	6.9	Band 4 (480.6 nm)	12.1
8	MF-Greasewood 1	6.0	Band 22 (754.1 nm)	10.0
9	INF-Greasewood 1	5.5	Band 94 (1805.8 nm)	10.0
10	MF-Soil 1	5.0	Band 23 (769.3 nm)	8.4

A majority rule was applied to produce the final species distribution map based on the multiple decision trees. Because some pixels had multiple maximum votes, additional processing was necessary. A three-step approach was used: a majority rule was first applied using all of the 20 decision trees, and then another majority rule was applied to the undecided pixels using the top 10 decision trees based on their testing performance. Finally, the best decision tree was used to determine the classes for the still undecided pixels and the final vegetation maps were created for each site.

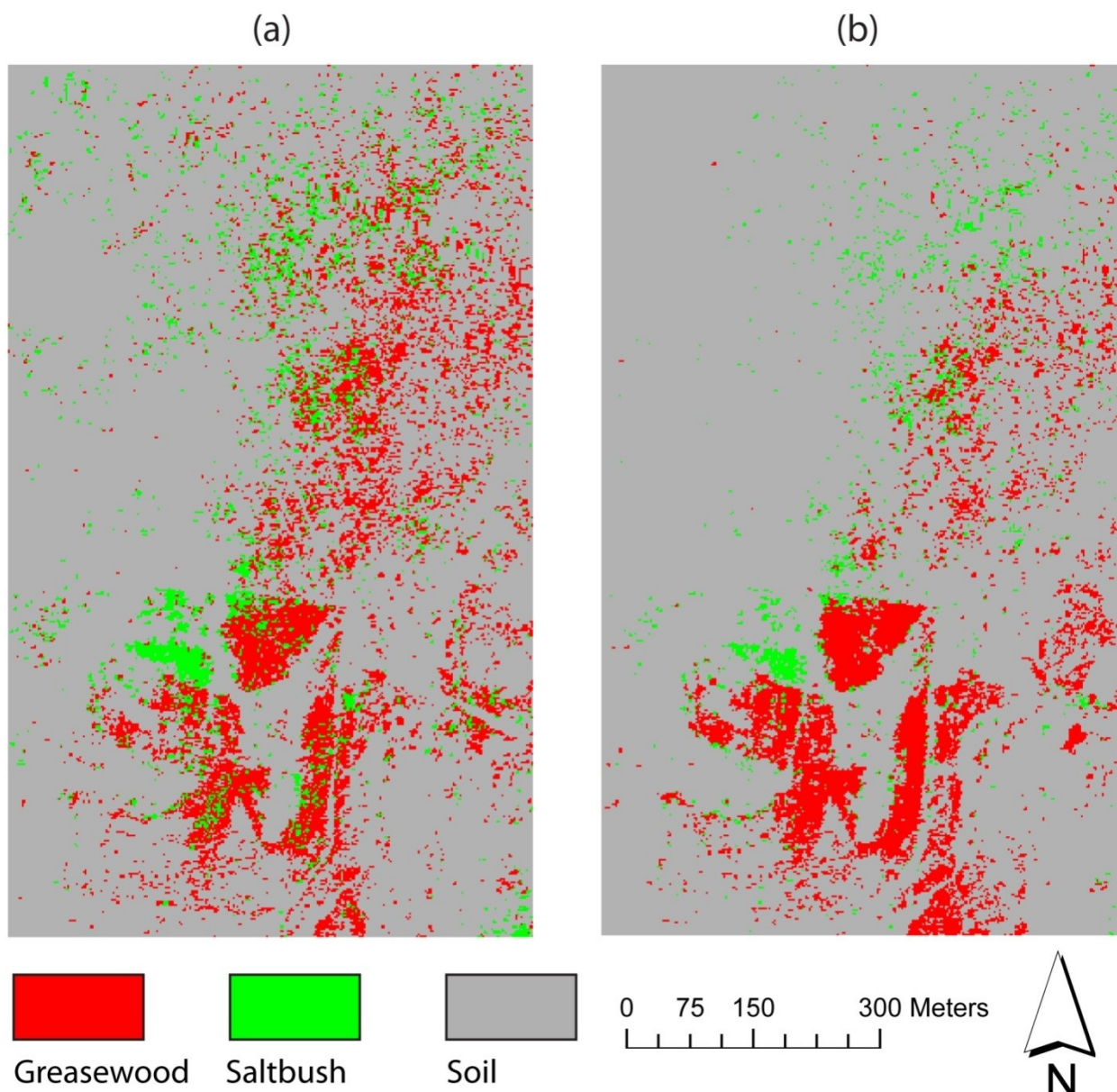
Figure 10 shows the vegetation maps over the Monticello site using the two sets of decision trees

1 (i.e., one set using the MTMF variables and vegetation indices and the other using the scaled
2 reflectance). Sagebrush appeared to be somewhat overestimated through visual inspection when the
3 MTMF variables and vegetation indices were used (Figure 10a). On the other hand, rabbitbrush and
4 litter were generally overestimated when the scaled reflectance data were used for decision tree
5 classification (Figure 10b). The vegetation maps of the Monument Valley site using the two sets of the
6 decision trees are shown in Figure 11. The classes were more clumped in the map using the scaled
7 reflectance than using the MTMF variables and vegetation indices. Soil appeared to be overestimated
8 when the reflectance data were used. These classification maps exhibited some discrepancies with the
9 actual field conditions. For example, while the disposal cell cover (central region) in Figure 10 appears
10 close to the field conditions, a monoculture of rabbitbrush on the side slopes does not agree with the
11 field conditions. At the Monument Valley site, greasewood appears to be over classified. The limited
12 quantity and quality of the field reference data might account for the discrepancies, including 1) the
13 small sample size resulted in variations in performance for multiple decision tree classifications; and 2)
14 each ground reference sample was measured using a circular plot with a diameter of 1 m, which is
15 smaller than the hyperspectral image pixel size (2.3 x 2.3 m). Given the small shrub and grass patches
16 in the sites, this could result in significant confusion in classification.

17 **Figure 10.** The vegetation species distribution maps for the Monticello site based on the
18 decision trees (a) using the MTMF-derived metrics and vegetation indices, and (b) using
19 the original scaled reflectance data. The road and other land cover classes were masked out.



1 **Figure 11.** The vegetation species distribution maps for the Monument Valley site based
 2 on the decision trees (a) using the MTMF-derived metrics and vegetation indices, and (b)
 3 using the original scaled reflectance data.



Since all of the reference data might have been used to train decision trees (50% on average), the classification accuracy based on the assessment using the reference data might be a bit inflated. The classification accuracy assessment for the Monticello site is presented in Table 5. Interestingly, although the MTMF variables and the vegetation indices outperformed the original scaled reflectance based on the individual decision trees for both training and testing (refer to Figure 9), the accuracy assessment results were similar between the two maps, resulting in the overall accuracy around 87% and Kappa around 0.82. Similar to the visual inspection of the classification maps, the commission error of sagebrush when using the MTMF variables and vegetation indices was large (~36.4%), while the omission error of sagebrush when using the reflectance data was large (~37.5%). Due to the small size of the reference data, the overestimation of rabbitbrush and litter when using the scaled reflectance was not clearly indicated by the error matrix. Wheatgrass was confused with sagebrush and litter in the

1 classification using the reflectance data. There was no significant difference between the two Kappa
2 values (Table 5c).

3 **Table 5.** Accuracy assessment results of the decision tree classifications for the Monticello site: (a)
4 using the MTMF variables and vegetation indices, (b) using the scaled reflectance data, and (c) Kappa
5 Z-test between the two classifications.

6 (a)

Class. \ Ref.	Sagebrush	Rabbitbrush	Wheatgrass	Litter	Sum	Commission Errors (%)
Sagebrush	7	2	1	1	11	36.4
Rabbitbrush	0	10	1	0	11	9.1
Wheatgrass	1	0	14	1	16	12.5
Litter	0	0	0	15	15	0
Sum	8	12	16	17	53	
Omission Errors (%)	12.5	16.7	12.5	11.8		

Overall accuracy: 86.79%
Kappa Coefficient of Agreement: 0.821

7

(b)

Class. \ Ref.	Sagebrush	Rabbitbrush	Wheatgrass	Litter	Sum	Commission Errors (%)
Sagebrush	5	1	1	0	7	28.6
Rabbitbrush	1	11	0	0	12	8.3
Wheatgrass	2	0	15	2	19	11.1
Litter	0	0	0	15	15	0
Sum	8	12	16	17	53	
Omission Errors (%)	37.5	8.3	6.3	11.8		

Overall accuracy: 86.79%
Kappa Coefficient of Agreement: 0.819

8

(c)

	Kappa	ASE	MTMF + VIs	Reflectance
MTMF + VIs	0.821	0.0622	NA	
Reflectance	0.819	0.0629	0.0276*	NA

9 * no significant difference between the two Kappa values at the 95% confidence level

10 Table 6 presents the accuracy assessment results of the classification maps for the Monument
11 Valley site. Saltbush was confused with soil for both maps. This might be because some of the saltbush
12 sample locations were grazed and not irrigated, causing their spectral response to be similar to soil.
13 Saltbush was also confused with greasewood when the reflectance data were used in the decision tree
14 classification. However, the confusion was much improved when the MTMF variables and vegetation

1 indices were used in the decision tree classification. There was no significant Kappa difference
 2 between the two classifications due to the relatively large asymptotic standard errors (ASE), a
 3 measurement of uncertainty, even though there was a 10% difference between the two Kappa values
 4 (Table 6c).

5 **Table 6.** Accuracy assessment results of the decision tree classifications for the Monument Valley site:
 6 (a) using the MTMF variables and vegetation indices, (b) using the scaled reflectance data, and (c)
 7 Kappa Z-test between the two classifications.

8

(a)

Ref.	Greasewood	Saltbush	Soil	Sum	Commission Errors
Class.	Greasewood	Saltbush	Soil	Sum	Commission Errors
Greasewood	10	1	0	11	9.1
Saltbush	1	10	1	12	16.7
Soil	1	3	16	20	20
Sum	12	14	17	43	
Omission Errors	16.7	28.6	5.9		
Overall accuracy: 83.72%					
Kappa Coefficient: 0.751					

9

(b)

Ref.	Greasewood	Saltbush	Soil	Sum	Commission Errors
Class.	Greasewood	Saltbush	Soil	Sum	Commission Errors
Greasewood	11	3	1	15	26.7
Saltbush	1	7	0	8	12.5
Soil	0	4	16	20	20
Sum	12	14	17	43	
Omission Errors	8.3	50	5.9		
Overall accuracy: 79.07%					
Kappa Coefficient: 0.682					

10

(c)

	Kappa	ASE	MTMF + VIs	Reflectance
MTMF + VIs	0.751	0.0856	NA	
Reflectance	0.682	0.0905	0.5541*	NA

11 * no significant difference between the two Kappa values at the 95% confidence level

12 For vegetation mapping over hazardous waste sites, the omission errors of shrub could be more
 13 serious than the commission errors. The commission errors could be false alarms for biointrusion on
 14 the capped materials, but the omission errors might indicate undetected biointrusion, which requires
 15 quick response and treatment. From this point of view, the use of the MTMF-derived metrics and
 16 vegetation indices was better than the use of the scaled reflectance for vegetation mapping. The
 17 omission errors of rabbitbrush and saltbush (both shrub species) were relatively large when the scaled
 18 reflectance data were used.

1 At the Monticello site, rabbitbrush is an early successional shrub adapted to disturbed, unstructured
2 soils. Sagebrush is a later successional shrub that appears to be increasing in abundance as soil
3 structure develops in the engineered soil cover, creating preferential flow pathways for water to move
4 deeper in the profile and, hence, gradually creating a more favorable habitat for sagebrush. The
5 phytoremediation study at the Monument Valley site was designed, in part, to compare the two
6 dominant native desert phreatophytes: the obligate black greasewood and facultative four-wing
7 saltbush. Consequently, for long-term monitoring of these sites, differentiating rabbitbrush and
8 sagebrush at the Monticello site, and greasewood and saltbush at the Monument Valley site are critical.

9 When considering the small shrub and grass patches (~ 1 m and sometimes < 1 m in size) found in
10 the study sites, the spatial resolution of the HyMap imagery (2.3 × 2.3 m) appears to be a bit coarse.
11 Although there is a concern that higher spatial resolution data may actually reduce classification
12 accuracy by increasing within-class spectral variability [75], the Monticello and Monument Valley
13 sites should benefit from higher spatial resolution data (e.g., ~ 1 × 1m) for vegetation mapping because
14 small grass and shrub patches (not tall vegetation) are dominant and their cover is relatively dense
15 (percent cover > 70%).

16 5. Summary and Conclusions

17 This study evaluated the usefulness of HyMap hyperspectral data for characterizing the vegetation
18 cover (i.e., LAI estimation and vegetation species mapping) on two hazardous waste sites. The
19 findings of this study are:

- 20 • The vegetation index approach to estimating LAI revealed that reflectance data in the middle-
21 infrared region were more useful than reflectance data in the red or near-infrared region. The
22 REP approach failed to estimate LAI mainly because the 2.3 x 2.3 m pixels often contained
23 multiple species and background soil spectral influence. The regression trees resulted in the
24 best calibration accuracy for estimating LAI ($R^2 > 0.80$), but the instability of the models due to
25 the small sample size was a concern. More sophisticated narrow band-derived vegetation
26 indices need to be investigated further.
- 27 • Aggregated decision trees were successfully used to map the vegetation species with a limited
28 amount of reference data. Overall accuracies exceeded 85% in both study areas with Kappa
29 Coefficients of Agreement > 0.81. The MTMF approach and the associated metrics improved
30 the classification accuracy. However, if the endmember pixels contained only one species (i.e.,
31 they were pure pixels), the MTMF approach resulted in improved classification. In other words,
32 the MTMF approach would benefit from the use of higher spatial resolution hyperspectral
33 remote sensor data. A suite of vegetation indices were also useful for the vegetation mapping.
34 In particular, the water-related indices were especially useful for classification of the
35 Monument Valley site.
- 36 • The site characteristics influenced the performance of the LAI estimation and vegetation
37 mapping. While multiple species were generally found in the individual pixels in the
38 Monticello site, only two species were dominant within the scene in the Monument Valley site,
39 which was more arid than the Monticello site and included irrigation/non-irrigation treatments.
40 These site characteristics affected the performance of the LAI estimation and vegetation

1 mapping, and provided an explanation of the performance to some extent.

2 *Automated monitoring of vegetation cover on hazardous waste sites using hyperspectral remote*
3 *sensing data and modeling techniques appears feasible, but requires further investigation using*
4 *different remote sensing data sources, higher spatial resolution hyperspectral data, and more*
5 *advanced modeling techniques.* Site characteristics must be carefully considered when determining the
6 remote sensing data to be collected and the approaches to be used. Future research includes
7 applications of multi-sensor data fusion (e.g., high density LiDAR data + hyperspectral imagery)
8 and/or different modeling techniques (e.g., artificial immune networks, support vector machines, and
9 artificial neural networks) for monitoring hazardous waste sites. In addition, while this study provided
10 the preliminary results and single-date baseline data associated with monitoring of the
11 phytoremediation systems at the Monticello and Monument Valley sites, linking remote sensing
12 methods with actual monitoring tasks in a hazardous waste context should be further examined. Such
13 links include: (1) detecting changes in the spatial distribution of plant species and LAI through time at
14 the landscape scale using < 1 x 1 m multiple-date hyperspectral remote sensor data, and (2) tracking
15 the response of phreatophyte health and evapotranspiration rates to changing land management
16 practices.

17 Acknowledgements

18 This research was funded by the Department of Energy.

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