The estimation of humification of exposed upland peat from HyMap and ASD spectra

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ABSTRACT

The degree of humification of the exposed upland peat in the Southern Pennines, UK, affects the colour of the water and the ease with which heavy metals, trapped from air pollution, are released into adjacent reservoirs used for drinking water supply. This paper reports on progress towards using HyMap data at 3m spatial resolution and laboratory spectroradiometry to estimate physico-chemical properties of exposed peat, notably the degree of humification.

Transmission, which is inversely related to humification, was measured colorimetrically for 33 peat samples. A strong relationship was observed between transmission and spectral indices calculated from HyMap reflectance for the sampling sites. Gravimetric moisture content of the samples showed no significant correlation with HyMap reflectance and a significant correlation with only one of the spectral indices, the depth of the band 52 absorption feature.

Whilst the transmission relationship provides a possible basis for estimating peat humification across extended areas, the confounding effect of moisture content cannot be ignored. To investigate this, contact probe spectra were acquired for dry peat samples in the laboratory using an ASD spectroradiometer. Preliminary results show that a humification signal remains at ASD scale, even in dry peat. The indices having strong correlations with transmission for both in situ HyMap (wet) spectra and ASD dry contact probe spectra were: the gradient of the near infrared slope between bands 62 and 31 (1337-873 nm); the gradient of the shoulders of the broad water, cellulose, lignin band 52 (1200 nm) at 1123-1281 nm; the depth of the band 52 absorption (negative for dry spectra); and the depth of the cellulose absorption index at band 103 (2100 nm).

Keywords: Peat, hyperspectral, humification, decomposition, moisture, uplands, moorlands, Pennines

1 INTRODUCTION

Severe erosion of upland peat bog in the Southern Pennines, UK, is a significant environmental problem that requires mapping and monitoring at regular intervals. Around 8\% of the total peat-covered area is now bare [1]. In addition to the spatial extent of erosion, the physico-chemical properties of the exposed peat are important, especially the degree of humification and moisture content. During the latter stages of decomposition, lignin down to humic acids, which are capable of discolouring the drinking water supply and releasing heavy metals into the ground water [2]. An estimate the degree of peat humification would therefore express the relative potential for the release of heavy metals into reservoirs.

At present, humification is determined by costly and time consuming point sampling and wet chemistry. Near infrared (NIR) reflectance spectroscopy offers an alternative method [3]. Previous work has shown that laboratory NIR-SWIR spectroscopy can be used to predict the stage of decomposition of dry, milled leaf litter [4, 5], decomposing grape and cattle manure [6] and dried peat from a stratigraphic core [7].

Decomposition involves biochemical changes, detectable by decreases in the depth of absorption features in the NIR and SWIR. The ratio of carbon to nitrogen decreases as organic matter decomposes. Soluble components are lost first, and then cellulose degrades, followed by lignins [8], so that the depth of cellulose and lignin absorption features reduces with humification [5]. Spectral indices such as the
cellulose absorption index (CAI) [9] and ligno-cellulose index [10] express the depth of absorption at 2100 nm relative to the shoulders at 2020 and 2200 nm, (HyMap bands 103, 99 and 110). Other significant cellulose or lignin absorptions occur at 1120 nm [11], 1203 nm, [6], and 2280 nm [10]. Broad band sensors can map the distribution of bare peat, but hyperspectral sensors such as HyMap are required to detect these narrow spectral absorptions.

2 METHOD

2.1 Laboratory analysis of physico-chemical properties
Peat samples, chosen for their within-site homogeneity and between-site variability, were collected concurrent with HyMap data for 16 peat sites and retrospectively for a further 17. Two sites which exhibited a burnt crust were excluded from the analysis reported here. Four physical properties were measured on the samples collected concurrent with the flight; particle size, gravimetric moisture content, percent organic matter (total and per size fraction) and percent transmission [12]. Moisture content is temporally dynamic so was not measured for the retrospective samples.

Percent transmission is commonly used as a proxy for peat humification and relative biochemical composition [13]. It is the optical density of alkali-extracted humic acids measured with a colorimeter, and is inversely related to the degree of peat humification. A Jencons spectrophotometer was used to measure transmission of light at 540 nm through a solution containing a mechanically homogenised peat sample digested in NaOH solution. Well humified samples have more humic acid and, therefore, lower transmission. Transmission was also measured on further samples collected for laboratory drying experiments with ASD, but using a Hach DR/4000 spectrophotometer at 540 nm, calibrated to the Jencons machine.

2.2 HyMap spectra
A HyMap image with a spatial resolution of 3.2 m was acquired on 18 June 2000 for the SAR and Hyperspectral Airborne Campaign (SHAC). HyMap spectra cover 126 bands of 15-20nm wide from the visible to the SWIR (450 to 2500 nm). Data were supplied with an ATREM atmospheric correction [14] and an ephemeris geometric correction, but required further correction with GPS-derived control points. Bands 1-3, 63-64, 95 and 120-126 were excluded from further analysis after examination of signal to noise ratios. HyMap reflectance spectra were extracted for the 33 sample sites and imported into Excel and SPSS. The spectra were visually compared with physico-chemical properties.

Various spectral indices were developed to express the features observed in the reflectance spectra and the first derivative of reflectance (R'), such as the gradient of the right shoulder of the 1400 nm water absorption, from band 68 to 82 (1477-1660 nm). Published indices for plant litter decomposition, such as CAI [9] which characterise the depth of absorption features due to cellulose, lignin, nitrogen and water below their continuum were also used. A simplified continuum removal method was used to measure the depth of other absorption features:

\[ d = \frac{0.5 \times (L_{\text{ref}} + R_{\text{ref}}) - F_{\text{ref}}}{d_{\text{depth below continuum}}} \]  

where \( d \) is depth below continuum, \( L_{\text{ref}} \) is the reflectance of the left shoulder, \( R_{\text{ref}} \) is the reflectance of the right shoulder and \( F_{\text{ref}} \) is the reflectance minimum of the absorption feature. The typical position of the shoulders and reflectance minimum were identified using \( R' \) and applied to all spectra. Where the reflectance minimum (absorption maximum) was not at the midpoint between the shoulders, an adjusted constant was applied to replace 0.5 in equation 1.

A difference index, normalised difference index and a simple ratio were also calculated for each pair of shoulders and for major observed variations in gradient elsewhere in the spectrum. Difference indices and ratios are similar to \( R' \), but express the reflectance gradient calculated over a lag of several bands instead of at a single point. For instance, r17_25 represents the red edge, the gradient between bands 17 and 25 (677 to 799 nm). In total, 49 indices were calculated and correlated against physico-chemical properties [15]. In this paper we report on the correlation of transmission at 540 nm with nine of the most significant spectral indices (Table 1).

2.3 ASD spectra
To test the confounding effect of moisture content on peats of different humification, laboratory spectra were acquired for further peat samples collected from field sites in the two years following the HyMap flight. Some sites were those used for HyMap, but the range of humification matched that for the HyMap samples. The samples were not ground in this experiment to better match in situ surfaces recorded by HyMap. Measured amounts of water were added to an optically thick sub-sample of
0.5cm deep until saturation was achieved (approximately 90% water by mass). The wet samples were oven dried in stages at 20°C. Every hour, the reflectance was measured at 10 points over the sample using a FieldSpec-Pro Analytical Spectral Device (ASD) in contact probe mode, with an integral light source and a 2 cm field of view. In this paper we analyse spectra from the driest stage in an attempt to decouple moisture and humification effects.

Mean ASD spectra were calculated for each sample and simulated to HyMap using a filter based on the spectral band passes for HyMap during the SHAC Europe flights. At this stage, no atmospheric noise has been added. The same 49 indices derived for HyMap were calculated for the simulated spectra.

The features of the HyMap (wet) in situ spectra were compared against dry, unground ASD spectra to gain an insight into the effect of moisture. The strength and direction of correlation coefficients for transmission against HyMap and ASD spectral indices was compared.

<table>
<thead>
<tr>
<th>Spectral feature (wavelength, nm)</th>
<th>HyMap band</th>
<th>Index and formula</th>
<th>Correlation with transmission at 540 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>HyMap Dry simulated</td>
</tr>
<tr>
<td>Absorption feature at 2137 nm</td>
<td>105</td>
<td>Ab_105, 0.5(Hy98+Hy110)-Hy105</td>
<td>-0.908 0.629</td>
</tr>
<tr>
<td>Cellulose absorption at 2100 nm</td>
<td>103</td>
<td>Cai_nagl Cellulose Absorption Index, CAI. Depth of absorption at Hy103 0.5 (Hy99 + Hy110) – Hy103</td>
<td>0.562 0.765</td>
</tr>
<tr>
<td>Absorption feature at 2083 nm</td>
<td>Ab-102, 0.5(Hy98+Hy110)-Hy102</td>
<td>0.522 0.750</td>
<td></td>
</tr>
<tr>
<td>Gradient between shoulders of 2100 nm cellulose absorption</td>
<td>110 to 99</td>
<td>N110_99 Normalised difference index: (Hy110 – Hy99)/(Hy110 + Hy99)</td>
<td>0.907 -0.132</td>
</tr>
<tr>
<td>Lignin and water absorption at 1450 nm; Lignin at 1420 nm; Water at 1400 nm</td>
<td>66, 63, 63</td>
<td>Gradient of right limb of water absorption: N82_68 Normalised difference index, (Hy82 – Hy68)/(Hy82 + Hy68).</td>
<td>0.899 0.180</td>
</tr>
<tr>
<td>Water, cellulose and lignin absorption at 1200 nm</td>
<td>52</td>
<td>Ab2_52 0.5 (Hy46 + Hy58) – Hy52</td>
<td>0.638 0.746</td>
</tr>
<tr>
<td>Gradient between shoulders of absorption at 1200 nm (NIR shelf)</td>
<td>47 to 58</td>
<td>R58_47 Ratio: Hy58/Hy47 N58_47 Normalised difference index (Hy58-hy47)/(Hy58+Hy47)</td>
<td>-0.759 -0.809</td>
</tr>
<tr>
<td>Gradient of NIR slope</td>
<td>31 to 62</td>
<td>N62_31 Normalised difference index, (Hy62 – Hy31)/(Hy62 + Hy31).</td>
<td>-0.818 -0.640</td>
</tr>
<tr>
<td>Red edge gradient, 677 to 799 nm</td>
<td>17 to 25</td>
<td>R25_17 Ratio, H25/Hy17</td>
<td>-0.501 0.384</td>
</tr>
</tbody>
</table>

3 ANALYSIS OF HYMAP AND DRY SIMULATED HYMAP REFLECTANCE

3.1 VIS/NIR region

Both HyMap and dry simulated HyMap peat spectra (Figure 1) were more similar to plant litter than to soil spectra published in Ref 9. Spectra in the visible and near infrared (VNIR) were not concave between bands 5 and 60 (500 and 1300 nm), as expected for organic rich soils [16], even though the organic content was over 80%. They were sigmoidal, with a steep red edge from band 17 to 25 (677 to 800 nm), then a gentler, linear NIR shelf to band 46 (1108 nm) followed by a variable flat to steep gradient between bands 46 and 62 (1108-1337 nm) (Figure 1).
3.2 1200, 1400 and 1900 water absorption regions

The most prominent absorption features of the HyMap spectra were the 1400 and 1940 nm water absorptions at bands 63 and 94, as expected for wet in situ peat. Although moisture content showed expected negative correlations with single band HyMap reflectance at major water absorption features, for instance, band 65 \( r = -0.41 \), band 94 \( r = -0.32 \) and band 119 \( r = -0.42 \) (1434, 1806 and 2376 nm, respectively), these correlations were not statistically significant [12].

There was a significant positive correlation between moisture content and only one index, the depth of the band 52 absorption feature, \( ab_{2,52} \) \( r = 0.624, p = 0.030 \). The lack of further significant correlations between moisture itself and indices expressing the depth of water absorptions may be explained by the small sample size, as only moisture data concurrent with the flight were used, and the fact that samples unavoidably included some peat from below the outer surface skin seen by the sensor. Particle size and percent organic matter were also not significantly correlated with single band reflectance.

One of the highest correlations of HyMap indices with transmission was \( n_{110,99} \) \( r = 0.907, p = 0.000 \), the normalised difference index of bands 110 and 99 (2225 and 2008 nm) (Table 1). It expresses the gradient of the right shoulder of water absorption. There were other strong correlations with the gradient of the right limb of the band 65 absorption feature; for instance, \( n_{82,68} \), the normalised difference index of reflectance at 1660 and 1477 nm \( r = 0.899, p = 0.000 \). One of the problems is that other biochemicals have absorptions at these two water features, including lignin at band 64 (1420 nm) and cellulose at bands 69 and 94 (1490 and 1820 nm). However, neither of these gradients had significant correlations for the dry simulated spectra and \( n_{110,99} \) actually had an opposite sign \( r = -0.132 \), suggesting that water, not transmission, was the primary cause for the correlation in the HyMap spectra. Water absorptions were still present although much shallower in the dry simulated spectra. This reinforces the idea that O-H bonds in other chemicals in addition to water were responsible for absorptions in the 1400 and 1900 nm regions.
3.3 NIR slope

The most promising indices of humification were those expressing the gradient of various parts of the NIR slope. The upper part coincides with shoulders of the band 52 feature and was shallower for well humified samples in both sets of spectra. This gradient between 1123 and 1281 nm, expressed as r47_58, the ratio of bands 47 and 58, was the index which was strongly correlated with transmission for both sets of spectra (r 0.768, p 0.000, HyMap; r 0.816, p 0.000, dry simulated spectra). Indeed, the whole of the NIR slope is very diagnostic of humification; the normalised difference index expressing the gradient between 873 and 1337 nm, n62_31, had an r value of -0.818 for HyMap and -0.640 for the dry simulated spectra. Ref. 17 found the slightly shorter wavelength region from 900 to 1220 nm good for estimating soil organic matter. The reason is not clear, but it appears that, as humification proceeds, either reflectance increases around band 47, or an absorption feature develops at or beyond band 58.

3.4 SWIR features

Both sets of spectra showed that peats were best separated at longer wavelengths, especially the SWIR. Strong positive correlations were found between HyMap single band SWIR reflectance and percent transmission; for instance, band 96 (1971 nm) had an r of -0.75 (p <0.01) [12].

Small absorption features were superimposed on the HyMap spectra, but were especially prominent on the dry simulated spectra, as they were no longer masked by water. The simulated spectra had more pronounced absorption features in the SWIR beyond band 97 (1990 nm) at bands 102, 104 to 105, 115 and 118 (2083, 2119-2137, 2310 and 2360 nm, respectively). For instance, the cellulose absorption at band 103 (2100 nm), expressed as the cellulose absorption index, cai_nagl [9], had a significant positive correlation with transmission for both sets of spectra (r 0.562, p 0.001, HyMap; r 0.765, p 0.000, simulated). As expected, the absorption at 2100 nm is shallower for more humified peat with less remaining cellulose.

Other relationships are less easy to explain. The depth of the feature at band 105 (2137 nm), ab_105, has a very significant negative correlation with transmission for HyMap spectra (r -0.908, p 0.000) yet an equally significant positive correlation for dry simulated spectra (r 0.629, p 0.000).

4 CONCLUSIONS

The strong relationship of HyMap SWIR reflectance and derived indices with transmission provides a possible basis for estimating peat humification across extended areas, but the confounding effect of moisture content cannot be ignored. It is possible that higher moisture content was reinforcing the lower SWIR reflectance observed in poorly humified peats, especially as poorly humified peats in the study area tend to be associated with wetter sites. The of the albedo differences between HyMap spectra may also be partly due to surface texture effects, such as smooth surfaces for peat re-deposited in pools compared to rougher, in situ peat. However, any such albedo effects are reduced by the use of normalised difference indices.

Preliminary work at the ASD scale does suggest that a humification signal remains even in dry peat. The best indices of humification with the confounding effect of water should be those which are strongly correlated to transmission for both wet, in situ HyMap spectra and dry simulated spectra obtained with the ASD. This is true of two indices: the r47_58, the index, which expresses the shallowing gradient of the NIR slope between 1123 and 1281 nm; n62_31, the normalised difference index covering the whole of the NIR slope. A third, the ab2_52 index, is also valuable even though it is negative for dry peat; it expresses the change from absorption to reflectance in dry peats of increasing humification.

5 FURTHER WORK

To better characterise the shape of the absorption features, other indices are being calculated based on the shape of the absorption feature and the changing position of its reflectance minimum and shoulders. They are being applied to all drying stages for over 200 samples, so that the effect of moisture on the identical samples can be directly compared [18]. HyMap spectra will also be extracted for the ASD sampling sites and compared against mean ASD contact probe spectra to examine scaling effects.

Transmission has been recorded at 624 and 651 nm and the greater range of values at these wavelengths appears to provide a more sensitive colorimetric index of humification. Lignin-cellulose ratio and carbon-nitrogen ratio are also available and will be used as an alternative to transmission.

The confounding relationship between indices, humification and moisture is being further investigated using approaches such as multiple regression modelling and artificial neural networks to
account for noise. As an alternative to prediction of single physico-chemical variables, a classification approach with combined broad humification-moisture classes is also being explored.

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7 REFERENCES