Improving the Interpretation of HyLogger Data Using XRF
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Introduction

The interpretation of HyLogging data is difficult in situations where the spectral data does not provide a unique identification of the contained mineralogy. In these situations we are often left to make difficult choices between two (or more!) mineral assemblages that explain the observed spectra equally well. Consequently we need to add other information to the interpretation to resolve the non-uniqueness. Geochemistry is perhaps the most obvious candidate in this regard and the potential availability of abundant pXRF and Minalyse data makes it even more attractive.

Theoretically, knowing the mineral composition (both abundance and species) completely allows us to compute chemical composition correctly. This calculation is a straightforward linear transformation but we need to be sure that the mineralogy that is produced by ummixing HyLogging data will be accurate enough model typical geochemical variability. In the same way, we need to check that rapid-scan geochemical data is accurate enough to track the mineralogical variation that HyLogging detects. Without some confidence in these two preconditions it will be hard to use either data set to aid the interpretation of the other.

To investigate how well HyLogging mineralogy can be correlated with XRF data, this note looks at the prediction of XRF wt% measurements using the mineralogy estimated by various unmixing methods. Because the thermal infrared has the potential to capture broader range of mineralogical content this comparison has only used the TIR spectrometer unmixing results. Further work will incorporate information from the SWIR.

Method

This note looks at the hole MSDP11 in South Australia and compares the results from:
- 496 Geochemical Assay (XRF wt% oxide) measurements with 1m samples.
- 3575 Minalyze (XRF wt% metal) measurements with 0.1m samples. No Minalyse data is available between ~95m and ~193m.
- Unmixed mineral estimates from Hylogging converted to wt% metal values via standard chemical compositions for each mineral. Unmixing was tested with both jCLST and dTSAT algorithms, more or less equivalent to those in the TSG software.
- The Minalyse results and the Hylogger results have been re-binned and averaged to 1m using the From/To data for the Assay data which were converted to wt% metal.

This note only looks at the major elements with appreciable variation[1] in the hole. These are:
- Assay data: Al, Si, K, Ca, Fe, Na, Mg
- Minalyse data: Al, Si, K, Ca, Fe

Even after averaging to 1m bins, the Minalyse data is more variable than the Assay data. Consequently I have used the Assay results as "Truth" in the following analysis.

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[1] There is some variation in Cl and S but it's not enough to worry about at this stage of the analysis.

Results

The figure below shows the Assay, Minalyse and HyLogger jCLST results for the seven assayed elements. Assay results are plotted in black, Minalyse results in red and the Hylogger estimated chemistry (hereafter called HLchem) in green. The hole has been divided into the seven spatial domains (separated by dashed lines) that were established during the TSG processing that led to the dTSAT results.
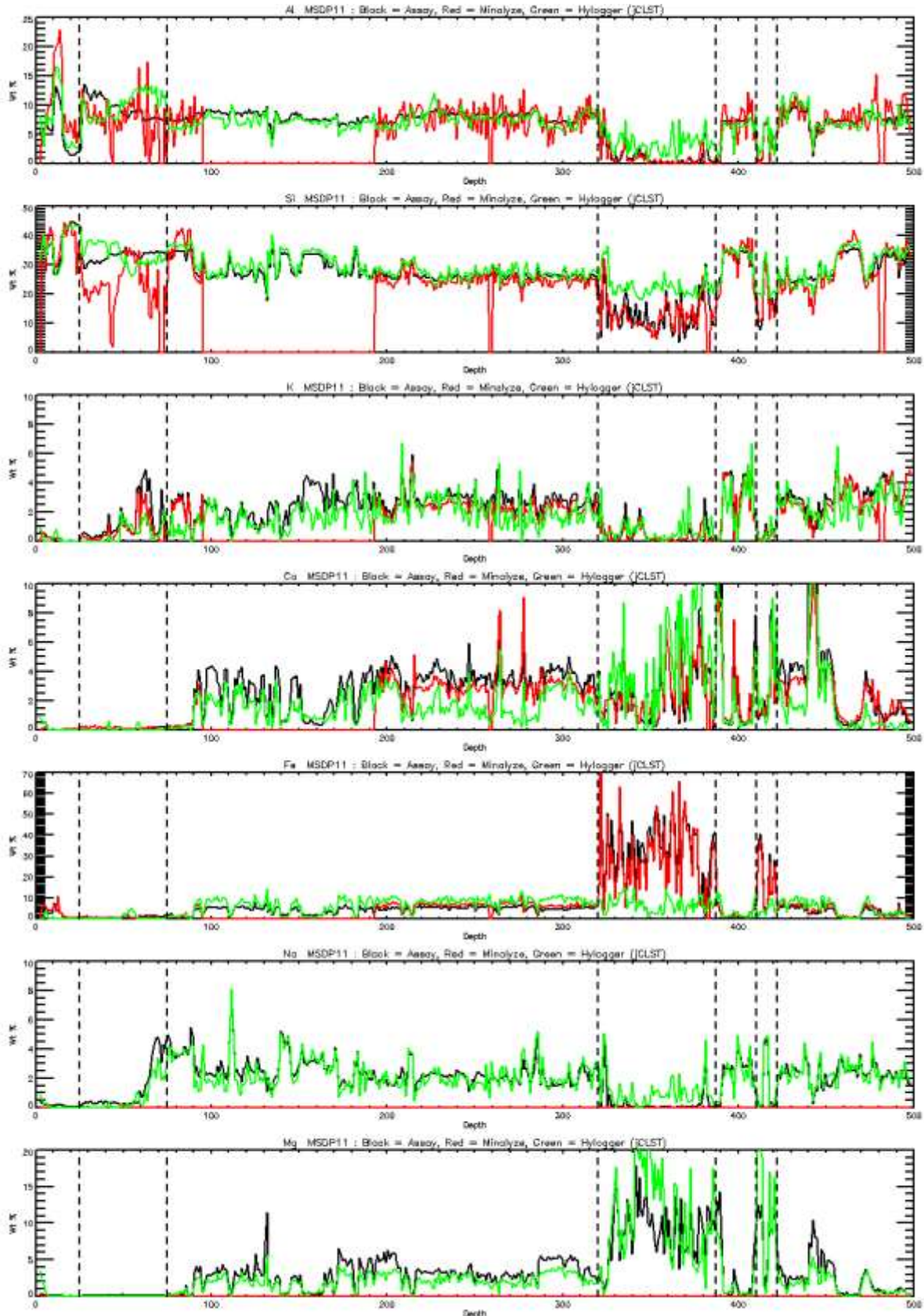
In most domains the Assay and HLchem show reasonable agreement but there are a number of places where there are obvious differences.

- In Domains 4 (320m – 384m) and 6 (410m – 419m) there is an obvious problem with the HLchem iron results which is also reflected in some of the other elements.
- From 150 m to 165 m the Assay potassium concentration is substantially higher that found by HLchem
- From 210 m to 290 m the Assay calcium concentration is higher than found by HLchem.
- In Domain 2 (25m - 72m) there are marked differences in the silicon and aluminium results.

The corresponding plot for the dTSAT HLchem results are basically the same as above except there is a little improvement in the iron results in Domains 4 and 6.

The correlation between the Minalyse wt% and Assay wt% was calculated for all samples where the Minalyze data was available. The Assay/HLchem wt% correlation was calculated over the whole hole and includes the elements not available in the Minalyse data (Na and Mg). The correlations for each element are below. The Assay v Minalyse correlation is first and the Assay v HLchem correlation second, (e.g. 0.74/0.78 for aluminium with jCLST).

	Al	Si	K	Ca	Fe	Na	Mg
jCLST	0.74/0.78	0.82/0.83	0.96/0.78	0.94/0.81	0.97/0.19	----/0.89	----/0.86
dTSAT	0.74/0.66	0.82/0.87	0.96/0.76	0.94/0.84	0.97/0.76	----/0.91	----/0.85

In looking at correlations it needs to be recalled that correlation does not measure agreement where the two records are offset by a constant bias. Nevertheless it is interesting that, for aluminium and silicon the HLchem results are as well-correlated with the Assay results as the Minalyse results and the performance for potassium and calcium is not that much worse. However the results for iron are substantially worse because of problems in Domains 4 and 6. A detailed breakdown of the correlations by domain is available in the Appendix.
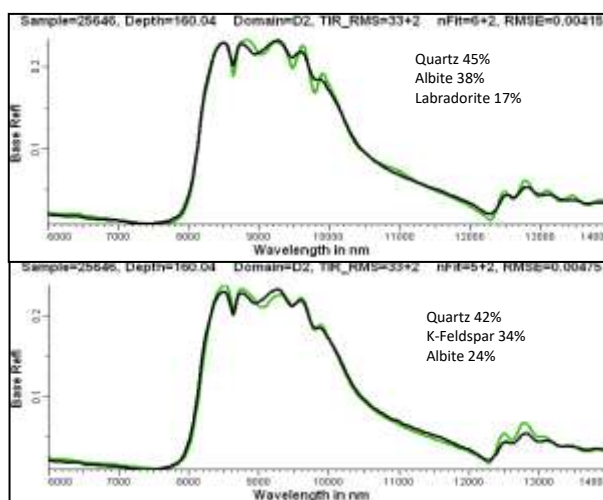
Discussion

The availability of Minalyse data is an exciting prospect for the future of the NVCL. However it is apparent that the Assay/Minalyse correlations for the lighter elements are (as expected) worse than for the heavier metals. Silicon and aluminium are the major components in the minerals most commonly detected by the HyLogger and, even when they are averaged to 1m bins, the results are probably not as good as we would like for comparison with HyLogger data.

In general, the agreement between the HLchem and the Assay results are quite good. This provides some confidence that our unmixing methods are working reasonably well. However it is worth looking at the problem areas in more detail.

Domains 4 and 6 are dominated by serpentine and magnetite. Magnetite is a difficult target for spectral measurement in all our wavelength regions and it is hard for unsupervised (system-level) algorithms like jCLST to distinguish it from ΔT effects. (dTSAT, the supervised unmixing algorithm had slightly more success but it still badly underestimates the iron content of these

domains.) Obviously it would be wonderful if we could get a magnetic susceptibility measurement to characterize the rock in such situations but it seems clear that having good iron chemistry would also be of great assistance.

In the zone of elevated (~4%) potassium concentration between 150 m and 165 m the jCLST unmixing does show increased K-Feldspar abundance but it is not enough to match the Assay result. A close examination of the unmixing results shows that about half the samples are unmixed using K-Feldspar while others, like the sample shown on the upper right, use no K-Feldspar. However, the plot below shows that when K-Feldspar replaces Labradorite the spectrum can be modelled almost

equally well and in a way that would also model the observed amount of potassium. This is an example of the well-known problem of recognizing K-feldspar with quartz/albite mixtures. However, when potassium XRF is available to this interpretation this ambiguity, and others like it, can be confidently resolved.

Accurate identification of plagioclase chemistry is also a well-recognized problem in HyLogging interpretation. The TIR spectra for the interval 210m to 290m are ambiguous can often be equally well modelled as quartz/chlorite/oligoclase or quartz/chlorite/labradorite and the automatic algorithms choose them with approximately equal probability. In this part of the hole the XRF calcium provides a strong indication that the latter assemblage is correct.
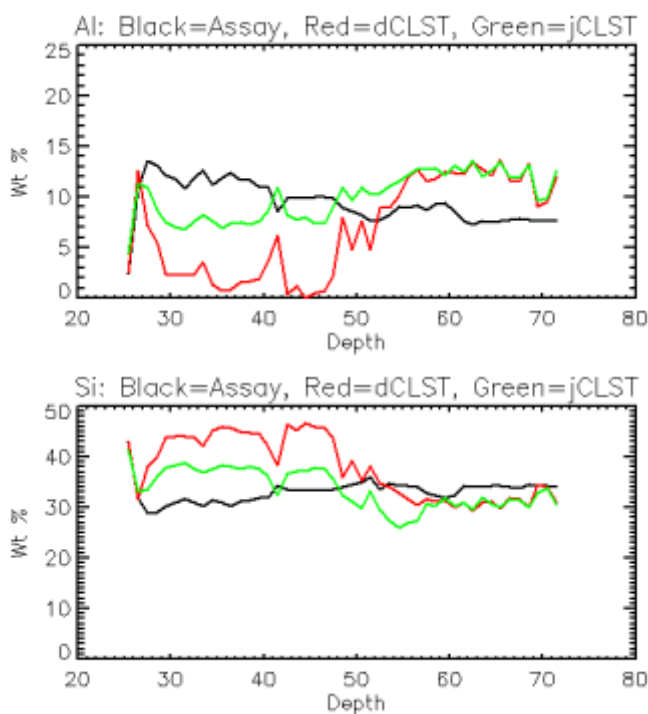
The figure to the left enlarges the aluminium and silicon results for Domain 2 and compares the performance of jCLST and dTSAT. The first half of Domain 2 is a quartz/kaolinite region where the spectra show substantial non-linear mixing behaviour which can't be modelled by the usual linear models.

The latest version of jCLST (used here and in CorStruth) has a modified algorithm for dealing with these non-linear mixtures and although the jCLST results in this region are somewhat better than the dTSAT results there is still room for improvement.

XRF data in this quartz/kaolin domain is now being used to calibrate the non-linear model so that it can be applied with confidence.

Other types of spectral non-uniqueness could also be susceptible to resolution with the addition of XRF data. For example, in the SWIR, the confusion of chlorite and epidote at low abundances could be aided with calcium measurements from XRF.

It should also be noted that the algorithm used to convert the estimated mineralogy to geochemistry could be substantially improved by making better use of SWIR scalars. Currently the estimation of iron and magnesium content of the chlorites uses only information from the TIR and we know this is vastly less sensitive than the SWIR for this purpose. Likewise the geochemistry of the carbonates is similarly limited.

These results suggest that there is considerable potential for XRF results to be used to improve HyLogging interpretation. However it is clear that we are unlikely to get adequate XRF data with the spatial resolution of the HyLogger any time soon. This means interpretation techniques, both expert and automated, will have to bear this in mind. If they have access to some simple software tools, this should not be a problem for expert interpreters but improved algorithms will be necessary if our TSG system-level tools are to take advantage of the new information. This is an important area for research.

In situations where only a pXRF instrument is available it would still be worthwhile to make XRF measurements out if advanced real-time pre-processing in TSG could recommend locations for the pXRF measurements. This is another profitable area for research.

Conclusions

- Elemental concentrations determined from HyLogging TIR mineralogical unmixing results compare quite well with Assay XRF results in situations where we are confident about our unmixing algorithms.
- Where we have known problems in unmixing the comparison breaks down.
- There is considerable potential to improve the conversion from estimated mineralogy to geochemistry by using scalar measurements from the SWIR.
- There is a big opportunity to use XRF results to better control the unmixing mineralogy we produce from HyLogger data
- Routine acquisition of high-quality XRF data with HyLogger data should be an important objective for an expanded NVCL scope.
- The Minalyse noise levels for the lighter elements indicate that it will be difficult to use this data for controlling HyLogger interpretation at the 0.1m sample interval.
- If high quality XRF data is not available in a routine manner we should investigate real-time automated methods of selecting pXRF sampling locations while the core still laid out.

Appendix - Correlations to Assay Results Minalyse/Hylogger by domain

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jCLST
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Whole hole	Al 0.74/0.78	Si 0.82/0.83	K 0.96/0.78	Ca 0.94/0.81	Fe 0.97/0.19	Na 0.00/0.89	Mg 0.00/0.86

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By Domain
From  To
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From	To	Al	Si	K	Ca	Fe	Na	Mg
0	22	0.89/0.98	0.60/0.97	0.96/0.54	0.56/0.95	0.83/0.44	0.00/0.90	0.00/0.92
25	72	0.12/-0.14	0.35/0.00	0.93/0.64	0.16/-0.11	0.56/-0.10	0.00/0.94	0.00/0.31
75	317	0.34/0.76	0.82/0.94	0.97/0.68	0.90/0.79	0.96/0.88	0.00/0.88	0.00/0.93
320	384	0.74/0.67	0.75/0.29	0.73/0.47	0.92/0.87	0.91/-0.24	0.00/0.84	0.00/0.67
387	407	0.81/0.96	0.93/0.90	0.98/0.88	0.95/0.97	1.00/0.45	0.00/0.94	0.00/0.89
410	419	0.93/0.94	0.96/0.87	0.93/0.85	0.96/0.90	0.99/-0.47	0.00/0.99	0.00/0.89
422	495	0.58/0.82	0.93/0.95	0.91/0.70	0.96/0.94	0.95/0.71	0.00/0.79	0.00/0.96

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dTSAT
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Whole Hole	Al 0.74/0.66	Si 0.82/0.87	K 0.96/0.76	Ca 0.94/0.84	Fe 0.97/0.76	Na 0.00/0.91	Mg 0.00/0.85

```
By Domain
From  To
```

From	To	Al	Si	K	Ca	Fe	Na	Mg
0	22	0.89/0.96	0.60/0.95	0.96/0.87	0.56/0.92	0.83/---	0.00/0.89	0.00/0.93
25	72	0.12/-0.37	0.35/-0.14	0.93/0.51	0.16/-0.18	0.56/0.25	0.00/0.91	0.00/0.42
75	317	0.34/0.66	0.82/0.91	0.97/0.62	0.90/0.78	0.96/0.84	0.00/0.84	0.00/0.87
320	384	0.74/0.89	0.75/0.67	0.73/0.77	0.92/0.82	0.91/0.56	0.00/0.97	0.00/0.60
387	407	0.81/0.97	0.93/0.96	0.98/0.85	0.95/0.96	1.00/0.87	0.00/0.93	0.00/0.96
410	419	0.93/0.92	0.96/0.92	0.93/0.73	0.96/0.90	0.99/0.62	0.00/1.00	0.00/0.92
422	495	0.58/0.63	0.93/0.95	0.91/0.56	0.96/0.95	0.95/0.61	0.00/0.83	0.00/0.73