Australia's National Science Agency

Preliminary procedure for performing QAQC checks on HyLogger Test rock data using TSG's "Headless mode"- NVCL QAQC report FY20

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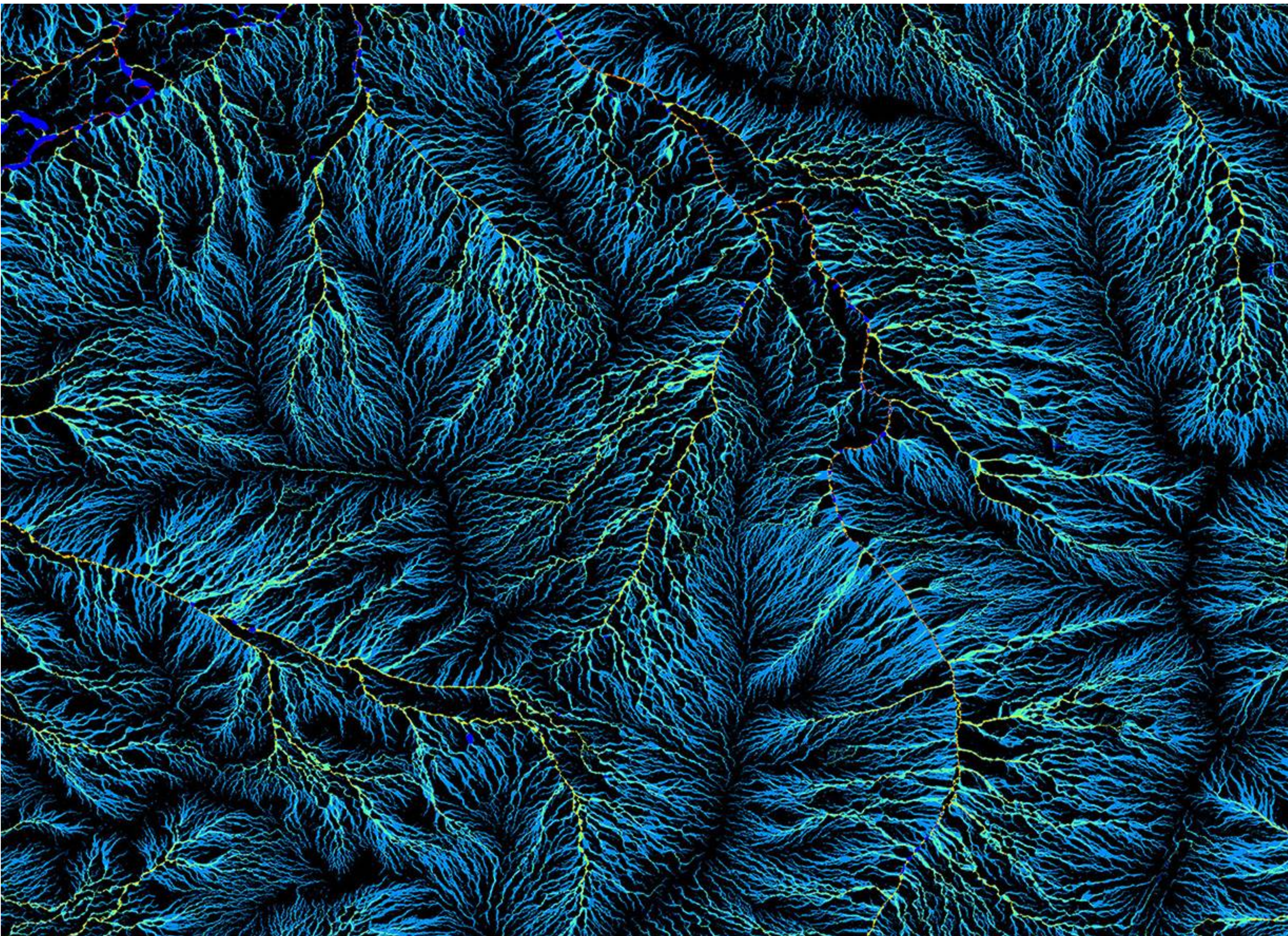

CSIRO Mineral Resources

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Acknowledgments

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Executive summary

The FY20 NVCL Project Plan identified the risk that the use of NVCL data by researchers was insufficient. A mitigation strategy to this is that improvements were needed to demonstrate cross-calibration, quantitative validation and publication of results which would lead to improvements in the quality and researcher trust of the NVCL data– a critical component in researcher uptake

The NVCL FY20 Activity 1 project aimed to improve the monitoring output from artificial standards by 1) proposing solutions towards automated monitoring of hardware, 2) identification and report on an intercomparison of test rocks & artificial standards for surveys to compare between them and within each HyLoggers variation for FY20, and 3) provide recommendations for how these differences can be addressed.

This report summarises the deliverables of the NVCL FY20 project and the key observations made from the newly collected QAQC data. With regards to the status of the above listed key deliverables:

1. Artificial standards were implemented in the Test rock panel. A method was developed for collecting Test rock and wavelength standard data, including the development of the PUCKWCAL script, which can be applied using TSG's *Headless mode*. The collected QAQC data are uploaded by each of the NVCL nodes to a designated server.
2. The analysis of Test rock and wavelength standard data collected over a 1-year timeframe (April 2019 to April 2020) showed that there are negligible differences between the reflectance spectra collected by the six NVCL nodes in the VNIR-SWIR wavelength region. The TIR features were broader than the VNIR-SWIR and showed larger variation in nanometres than the VNIR. However, if the data is viewed in wavenumbers (cm^{-1}) the variation is much smaller. All instruments showed low variation in the TIR, whereas the VNIR and SWIR showed more diurnal variation. Large changes(shifts) in wavelengths between dates could be explained by the change in the version of TSG and import settings used. It was found that the data needed to be standardised as the version of TSG QC and the settings for data import affected the wavelength results. This standardisation was also needed to be able to compare data between the nodes.

Analysis of the wavelength shifts of the VNIR and SWIR for the NIR puck over the 1 year of measurement were less than 0.5 nm and 2 nm, respectively, for each of the NVCL node HyLoggers and are negligible. Over the time period analysed the wavelength shifts in the TIR are also negligible, when comparing the ranges of wavelength shifts between the NVCL node HyLoggers for the VNIR and SWIR (1.4 nm, 3.5 nm). This means that, over the 1-year timeframe, HyLogger raw data produced by the six NVCL nodes are of the similar quality and comparable across jurisdictions.

The TIR shows that the longer wavelength features are broad and are not as accurate at tracking wavelength as the shorter (sharp) absorption features. The version of TSG and import settings of the data affected the results. The TIR for most nodes appeared to be less affected by diurnal variation. The scatter in daily values appears to be ~0.5 nm at 6245 nm and 9353 nm whereas it is between 1 to 2 nm at 11875 nm

The FY20 Activity 1 project found that the new standard holders enabled the collection of repeatable spectral measurements that is comparable between HyLogger instruments. The process of uploading of data on a regular basis by the nodes allowed comparisons on the data.

A recommendation of this report is the standardisation of the naming of the test rocks and the folders that they are kept in. The naming of the test rocks files should be standardised to allow them to be easily sorted, processed and stored. The recommended suggested nomenclature is YYYYDDMM_Testrocks_time. Thus 20200920_Testrocks_am for the first scan of the day and 20200920_Testrocks_pm for the last scan of the day. Folders should be named by year and then month, for example 2020_06 for June 2020.

The goal of the work in this Activity is to identify any differences in HyLogger outputs from the six NVCL nodes in real time. To achieve this, the following will be addressed in the next year (FY2021):

- Standardisation of the data's TSG version before processing. Improvements to the CLIMPORT function in headless to cope with nested folders.
- Batch extraction of metadata from the raw HyLogger data for tracking information using a Python script.
- Collation of each nodes instrument logs for identification of lamp changes/adjustments and mirror adjustments.
- Improved method of data upload to allow all nodes to use the same method.
- Repository of processed (standardised) data and results
- Automation of the standardisation and wavelength extraction, collation and report values on a website.
- Thresholds and warning values for HyLogger3 instruments which could be checked using a copy processing from a TSG file (template).
- Proposing a workflow/design for how level or differences in quality of respective data sets can be (pre-)viewed on AuScope portal by the NVCL community.

1 Introduction

The NVCL has collected hyperspectral drill core data, drill core imagery, laser profilometer data and associated meta-data of more than 3500 drill cores from across the Australian continent using various iterations of HyLogger technology over the past 13 years. The NVCL data are available to the research community and resources sector via AuScope's data infrastructure through various online portals. More key information about the upper 1 – 2 km of the Earth's crust is added by the NVCL nodes to this high value data set daily. The quality assurance (QA) of the HyLogger instruments has progressively evolved with increased user interaction and growth in knowledge of interpretation of reflectance spectra collected by means of hyperspectral drill core sensing technologies. There has been an increase in the awareness of the requirement to detect problems with the instrument and data in a timely manner, with a goal to consistently produce high quality reproducible data, with less need for time-consuming rescanning, and to reduce instrument downtime'. The AuScope 2018 Review Panel concluded that long-lived time series datasets have high value, but appropriate levels of QA/QC need to be funded across life of project to maximise this value.

In response to AuScope 2018 Review Panel's recommendation and in order to provide users of the HyLogger data with some indication of data quality, artificial standards were implemented in FY19. The NVCL FY20 project aimed to improve the monitoring output from these artificial standards by 1) proposing solutions towards automated monitoring of hardware, 2) identification and report on an intercomparison of test rocks & artificial standards for surveys to compare between them and within each HyLoggers variation for FY20, and 3) provide recommendations for how these differences can be addressed. The following document is part of the NVCL work on QA/QC of HyLogger data and outlines the procedure for performing QA analysis on HyLogger data using the "*Headless mode*" in TSG (https://research.csiro.au/static/tsg/tsg_headless_reference.pdf). This document is a preliminary document attempting to capture the basic method and will be built on with subsequent edits from comments and recommendations from other TSG/HyLogger users.

2 Current and proposed HyLogger QA/QC workflow

The HyLogger System consists of the instrument, control PC and software. The software for the HyLogger consist of engineering programs for checking the instrument health and data (e.g. EddieCPVE.exe,), operation software for controlling the instrumentation and the collection of data (e.g. HyLog3CoreTIR7-3-76.exe) and The Spectral Geologist (TSG) QC, for importing the measurements from the various sensors for checking immediately after a tray is scanned.

The HyLogger operation software, developed by CSIRO's HyLogger engineering team, now part of Corescan, contains a variety of QA checks that require some operator interaction (such as warning lights for spectrometer synchronisation errors and saturation), whereas the TSG QC software is used as the main determination of a successful scan, with its built in QA checks on the data. In TSG QC thresholds to detect problems in the data can be manually set and warnings of bad results can be turned off. The Eddie software can extract information from the ancillary files (Level 0 radiance and reflectance data) generated by the HyLogger software. This software is good for checking individual files but does not allow for export of results or the bulk processing and comparison of many days of measurements. Therefore, it is not a feasible routine solution for tracking quality of HyLogger-derived reflectance spectra. The need to quickly assessing multiple scans was required, with an ability to collate, display and report this information.

Thus, it was proposed that the HyLogger QC data could be:

1. Processed in a batch way to extract key information
2. Thresholds created to identify issues in the extracted information
3. The extracted information able to be displayed in a meaningful way to aid problem data identification and decision making
4. The extracted information collated and kept in an easily recounted online database/website
5. Users/operators could look at the collated information and compare with other HyLogger instruments.

3 Artificial standards

3.1 Description of artificial standards

Calibration standards were purchased from Middleton Spectral Vision in the U.S.A. (Figure 1) The standards are circular in shape and encased in a metal holder The size of the standards are 12 mm in height, 55 mm in diameter with a 41.5 mm diameter exposed area . The visible near (VNIR) to shortwave infrared (SWIR) standard (Figure 1) is based on the National Institute of Standards and Technology (NIST) Standard Reference Materials (SRM)-1920a standard, whereas the mid-infrared (MIR) to thermal-infrared (TIR) standard is based on the NIST SRM-1921 standard. It should be noted that the MIR-TIR standard NIST SRM-1921 is described by the supplier and NIST as MIR diffuse reflectance standard, as different spectroscopy communities use different terminologies for the wavelength region between 2500 and 15,000 nm. However, to be consistent with the terminology of wavelength regions used by the NVCL community, this report refers to it as the “MIR-TIR standard”.

The VNIR-SWIR standard has a clear window (possibly sapphire or other low-OH glass material) over the encapsulated, doped sintered polytetrafluoroethylene (PTFE) material, which protects it from dust and scratches, but does not allow longer wave infrared (i.e. TIR) wavelength radiation to pass through and reflect off the material. The doped material consists of Sigma Aldridge laboratory-grade rare earth elements and talc. This produces sharp absorption features in the VNIR to SWIR wavelength regions. The rare earth materials are dysprosium oxide (Dy_2O_3), erbium (Er_2O_3) and holmium oxide (Ho_2O_3). The inclusion of talc provides absorption features from 2000 to 2500 nm, which were lacking in the rare earth oxides. The MIR-TIR wavelength is a diffuse gold coated surface overlain by a polystyrene window. The standards were supplied with calibration reports, describing wavelengths of the strongest absorption features. On request, the spectral plots for each standard, measured with a Thermo Scientific Antaris FTIR spectrometer by the supplier, were obtained. The reported wavelengths of the absorption features were taken from the NIST publications (Appendix A: VNIR-SWIR: Table 1; MIR-TIR: Table 2).

Figure 1 Manufactured wavelength standards (VNIR -left, MIR-TIR -right) from Middleton Research.

3.2 Implementation of artificial standards

To standardise the information that was being analysed, a pair of reflectance wavelength standards were deployed to each survey in March 2019. The geological surveys with HyLoggers and the instrument serial numbers are shown in Table 1. The use of manufactured wavelength standards, at a set height was attempting to reduce variation due to the use of natural materials and the potential for problems due to humidity. The standards are held in a wooden holder which is designed to attach to the existing test rocks board and cover the iron ore samples on the left-hand side of the lower row (example shown in Figure 2). A template holder was 3D printed as a concept to determine if it was going to be feasible to mount the standards on the existing test rock board.

Table 1 NVCL Nodes and HyLogger serial numbers

Node	Serial Number
Commonwealth Scientific and Industrial Research Organisation (CSIRO)	HyLogger 3-1 (HL3-1)
Geological Survey of Western Australia (GSWA)	HyLogger 3-2 (HL3-2)
Geological Survey of South Australia (GSSA)	HyLogger 3-3 (HL3-3)
Geological Survey of New South Wales (GSNSW)	HyLogger 3-4 (HL3-4)
Geological Survey of Queensland (GSQ)	HyLogger 3-5 (HL3-5)
Mineral Resources Tasmania (MRT)	HyLogger 3-6 (HL3-6)
Northern Territory Geological Survey NTGS	HyLogger 3-7 (HL3-7)
Corescan (North Ryde, NSW)	

Figure 2 Example of the 'concept wavelength standard holder' mounted on a test rocks board, covering the iron oxide samples(left). The wooden wavelength standard holder being tested on a spare test rocks board (without rocks) before being placed on an operational test rocks board (right) on HyChips 6-2.

This setup created problems due to its height (approximately 60 mm, whereas the test rock board is 30 mm and the Teflon white-reference is approximately 50 mm) and the issue of not being able to check iron ore materials in TSG for the test rocks. A new holder for the wavelength standards was designed in Q1 FY20 and the standard test plate was manufactured by the same company who made the standards in Q2 FY20. It is designed to hold three round standards and sit along the right-hand side of the existing test rocks board (Figure 4). The new calibration plate was deployed to each HyLogger3 in December 2019 with its own package to keep it clean (Figure 5).

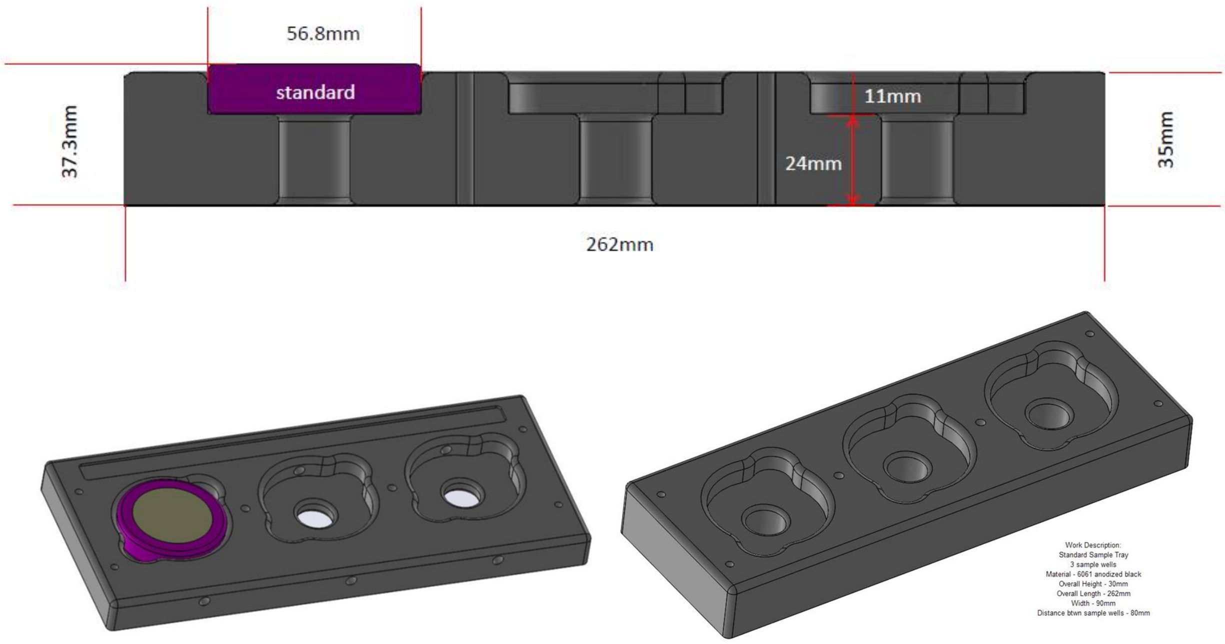


Figure 3 Concept drawings of the wavelength standard holders by Middleton Research.

Figure 4 Test rocks plate with the wavelength standard plate alongside being scanned by a HyLogger3. A quartz pebble has been placed in the 3rd slot in this example because this particular test rocks board lacks a quartz-rich sample.

Figure 5 The wavelength standard holder in its case. In this example there is only a VNIR-SWIR wavelength standard (for a HyLogger1, which lacks a TIR sensor and, therefore, does not need the polystyrene on gold wavelength standard).

4 Calibration data collection and processing

4.1 Scanning the test rock and wavelength standard plates

The standard test rocks plate, which has been used as a HyLogger testing material since early in its development, is scanned along with an additional metal plate containing two wavelength standards (Figure 6). The metal plate has an additional space for a third material or sample if required (such as if the node’s standard test rock plate is missing a mineral or material). An adjustment to the standard test rocks template is required to capture the extra plate, with a slight increase in the length of the X-direction of the scan and changes to the base height to prevent abundant profilometer PZ errors occurring in TSG QC. The gaps between the standard and the holder can be filled by adding black electrical tape. This will also lessen the possibility of TSG reporting saturation on the metal edges of the standard.

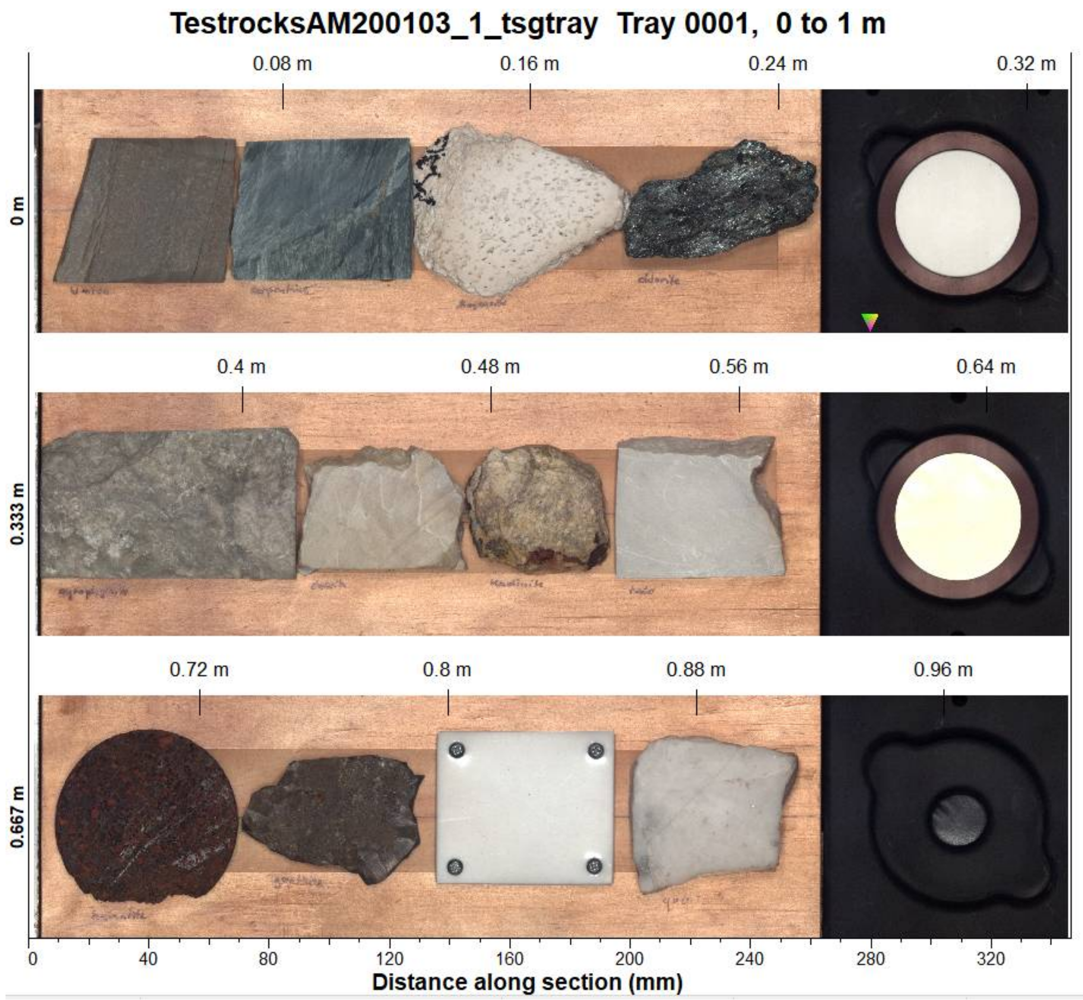
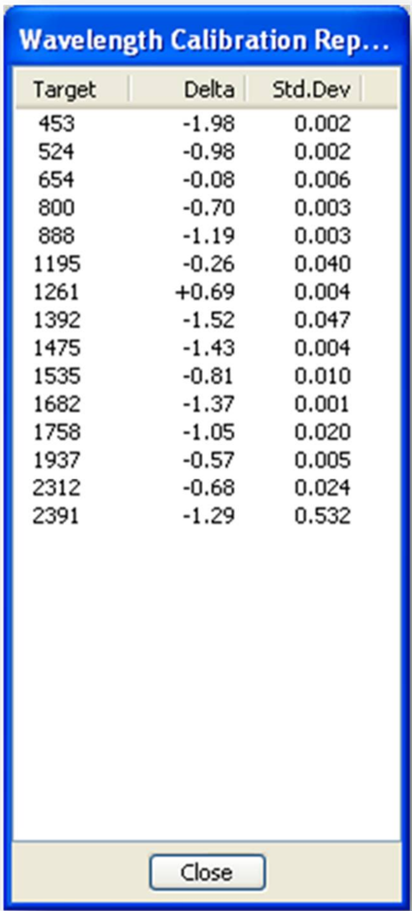


Figure 6 Test rocks from GSSA on wooden plate with the calibration standards holder containing the wavelength standards. Note this example does not have strips of tape on the black metal outer-rings of the wavelength standards.

4.2 Wavelength calibration check of single files

TSG QC (from TSG version 8.0.3.21 February 2019) detects the presence of the wavelength standards and identifies the key absorption features in the VNIR-SWIR and TIR. The results of the wavelength calibration check are shown on the screen as a popup (Figure 7) after the data is imported (at the end of the scan) and this information is captured in the dataset information (Figure 8). The dataset information results show the target spectral feature's wavelength, the difference of the average of multiple spectra, collected on the puck, from the reference wavelengths for that feature, the standard deviation of the multiple spectra used in the check for that feature and the number of spectra found on the puck and used in the calculation. If, instead of TSG QC a full version of TSG is used to import the raw HyLogger data the popup will not be shown, but the wavelength results can be found in the dataset information (Figure 8).



Target	Delta	Std.Dev
453	-1.98	0.002
524	-0.98	0.002
654	-0.08	0.006
800	-0.70	0.003
888	-1.19	0.003
1195	-0.26	0.040
1261	+0.69	0.004
1392	-1.52	0.047
1475	-1.43	0.004
1535	-0.81	0.010
1682	-1.37	0.001
1758	-1.05	0.020
1937	-0.57	0.005
2312	-0.68	0.024
2391	-1.29	0.532

Figure 7 Popup in TSG QC after automatically importing HyLogger scan showing the results of the wavelength calibration check (for HyChips 6-2, only showing VNIR-SWIR).

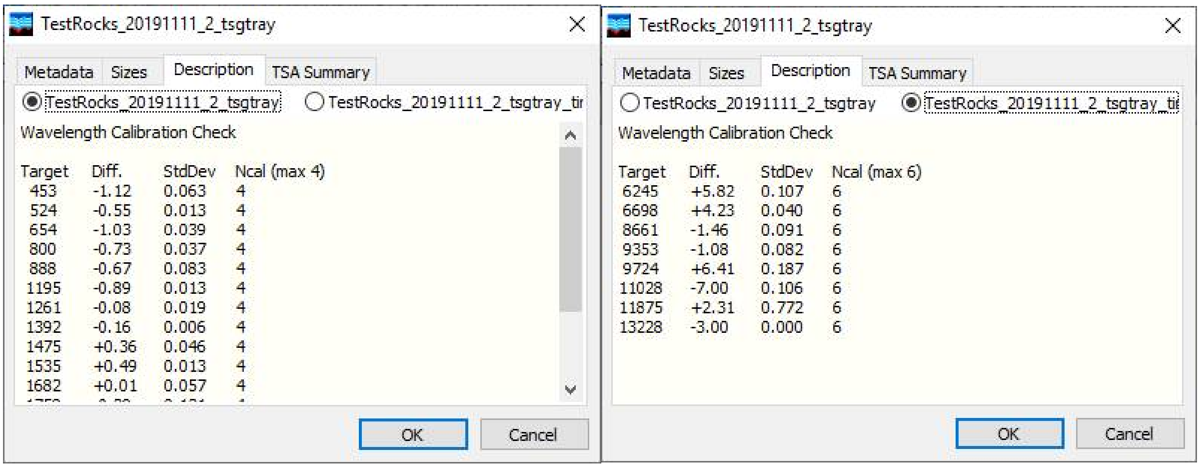


Figure 8 Wavelength calibration check results recorded in the dataset Information in TSG after import of a test rocks scan with the wavelength calibration pucks for the VNIR-SWIR (left side) and TIR data (right side). In each screenshot, results from left to right comprise1) "Target": the target absorption feature's wavelength, 2) "Diff.": the difference of the average of multiple spectra, collected on the puck, from the reference wavelengths for that feature, 3) "StdDev": the standard deviation of the multiple spectra used in the check for that feature and 4) "Ncal": the number of spectra found on the puck and used in the calculation.

Currently there is no warning message if the wavelength differences are excessively large or if a large standard deviation occurs. It should be noted that the absorption wavelengths of the standards are taken from NIST SRM-1920x (https://www-s.nist.gov/srmors/certificates/1920A.pdf) and NIST SRM-1921b (https://www-s.nist.gov/srmors/certificates/1921b.pdf) for TIR. Official wavelength accuracy figures of the HyLogger3 instrument (from Schodlok *et al*. 2016) are less than ±1 nm across the 400–2500 nm and to be within ±1 nm at 6000 nm, rising to about ± 5 nm at 14500 nm.

4.3 Data sharing/upload

A shared directory has been created on Cloudstor to keep all the HyLogger Test rock data. The address is https://cloudstor.aarnet.edu.au/plus/s/K0FECELeDP9SMKw. This allows the NVCL nodes to upload their Test rock data. A folder exists for each HyLogger/node and these have sub folders for years and months. Data can be uploaded as separate files but zipping the data into separate zip files for each month is the most effective method.

Currently the data is being downloaded from the Cloudstor shared drive and processed manually using headless TSG.

4.4 Processing multiple scans of the test rocks and wavelength standards using TSG's *Headless mode*

The processing of multiple scans of test rocks containing the wavelength standards, such as when QAQC of historic/batch measurements is required, is done with *Headless mode* of TSG (see Running the script file below). 'Headless' is an automated process within the TSG software that can be done without supervision, and can be set up to run while the TSG application is not open. A routine called

PUCKWCAL ("Puck-wavelength-calibration") was written into the TSG software for identifying the presence of the wavelength standards (pucks) and extracting the wavelengths of their spectral features.

The TSG QC data that is being uploaded has been generated with different versions of TSG over the course of the trial period by different NVCL Nodes. The version of TSG QC can change with annual service or a requirement to update the HyLogger PC to gain features and fix bugs. Thus there is a need to standardise the version and import settings of the data if meaningful information is to be obtained from a HyLogger and when comparing between the various nodes.

Before initiating the PUCKWCAL routine, all the pre-digested trays should be imported and processed with the same version of TSG. This may require all the L0 raw HyLogger files (.SDS) to be reimported into TSG, which can be done using the *Headless mode* of TSG. Failure to do this may cause some differences in the wavelength results, as seen when an older version of TSG was used (NTGS) and when comparing data (i.e. Chunking by 2 vs Chunking data by 1 with a different HyLogger). For this, the "CLIMPORT" routine (Appendix B) was developed, which reimports SDS (and associated SDT) with set options, such as chunking size, thresholds etc.

As of Q4 of FY 2020, it is not possible to reimport multiple SDS test rocks files into separate TSG files using the *Headless mode* CLIMPORT command (see https://research.csiro.au/static/tsg/tsg_headless_reference.pdf). It would be possible to use TSG's *Headless mode* to import multiple SDS test rocks files into a single file if the depth are sequential, but this may only be done for multiple measurements on a single day if there is no depth overlap (i.e. tray 1 scan in the am is 0-1 m, midday scan tray 2 is 1-2 m, and tray 3 in the pm scan is 2-3 m) and they have the same name. Import of these data together will only produce one averaged result for each absorption (along with its standard deviation) when using the PUCKWCAL routine.

Thus, the naming of the test rocks files should be standardised to allow them to be easily sorted, processed and stored. The recommended suggested nomenclature is YYYYDDMM_Testrocks_time. Thus 20200920_Testrocks_am for the first scan of the day and 20200920_Testrocks_pm for the last scan. This would allow multiple files to be kept together and sorted by their date. The data could be further sorted into folders by year and month. However, the naming should be as numbers YYYY_MM (i.e. 2020_05) and not MM_YYYY or MMM_YYYY as text (i.e. May_2020).

After the data has been standardised it can then have the wavelength information extracted. For this, the "PUCKWCAL" routine (Appendix B) was developed, which records the mean wavelength values of important diagnostic features of the artificial wavelength standards (explained in the previous chapters) and their standard deviations.

The PUCKWCAL routine (and other QA routines) can open existing TSG files (such as individual TSG QC pre-digested trays) within folders and extract the wavelength information

The following PUCKWCAL routine script for reporting wavelengths of absorption features of the calibration standards can be run using the *Headless mode* in TSG:

```
MULTIOPTIONS swir
multifile C:\TestRocks\*.*
```

task_begin

operation puckwcal

report_file1 C:\TestRocks\swircalrep.csv

report_file2 C:\TestRocks\tircalrep.csv

task_end

In this basic example, all the test rocks files in the folder Testrocks on C:\ will be evaluated to check if the calibration standards are present, and the wavelengths extracted. The term 'Multioptions swir' is required or the TIR data will be interleaved with VNIR-SWIR columns of data in the swircalrep.csv file. The 'operation puckwcal' is the command that will be run on the files found in the folders above. The extracted wavelength results will be placed in two csv files in C:\Testrocks\ along with the log file. If the csv files already exist, the script will append the results onto the existing files. Thus, wavelength values from measurements of the same dates could occur multiple times in the same file, if the multifile option did not preclude the data that the script had previously been run on.

When the example script above is run 'multifile C:\TestRocks*.*' may be used, but subsequent runs the script file will need to be edited to, for example, 'multifile C:\TestRocks\2020_05*.*' to only run on test rocks data in the folder for May 2020. Otherwise the *Headless mode* will run again on the previous TSG files and append the results onto the CSV.

The *Headless mode* can also be used to perform the other QC analysis, such as 1) the extraction of the wavelength of the Mylar, kaolinite, pyrophyllite and talc SWIR absorption features in test rocks/drill core data or 2) the extraction of the wavelength of the quartz and apatite TIR absorption features in test rocks/drill core data

Prior the development of the PUCKWCAL Further scripts of interest for QA that can be run using the *Headless mode* include:

- TESTROX (wavelength-calibration checking on "test rocks" items)
- WVLCAL (generalised but very limited wavelength-calibration checking)

Examples of these headless scripts are shown in Appendix B . These scripts can be run on other HyLogger data (for example HyLogger1 instruments or older NVCL data) or other spectral data (for example CoreScan, ASD or Bruker FTIR spectra) which have the necessary wavelength range and spectral features (i.e. kaolinite, talc features in the SWIR or Quartz in the TIR).

4.5 Running the script file

The *Headless mode* in TSG can be selected via File -> Special -> Schedule a script for unsupervised TSG (Figure 9), which will prompt for a script file. Alternatively, the *Headless mode* can be run from a command line (see https://research.csiro.au/static/tsg/tsg_headless_reference.pdf) or by drag-and-drop of a script txt file (ASCII ANSI, not Unicode) into TSG. If the 'TSG File Menu' method is used, a window will pop up to request a script file (Figure 10) and then the schedule window will appear (Figure 11).

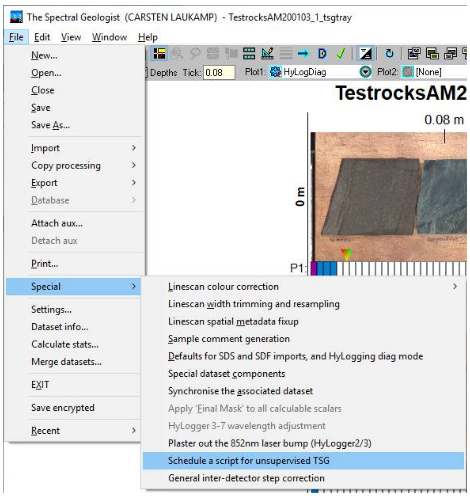


Figure 9 Menu location in TSG for running scripts in the *Headless mode*

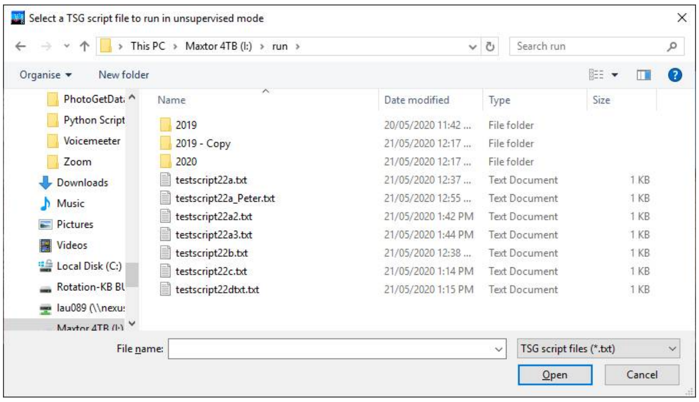


Figure 10 Popup window requesting the script for processing in TSG's *Headless mode*

A time can be set for when the script is run by selecting the time and pressing Schedule, or it can be run straight away by selecting Run now!, as shown in Figure 11 A scheduled scan requires the computer login and password information to be entered.

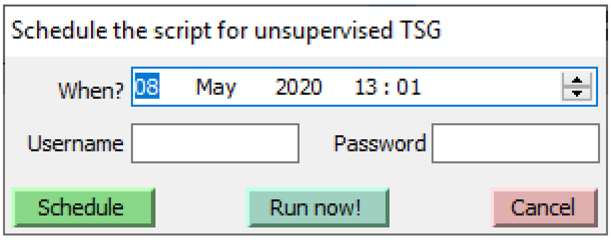


Figure 11 The script window, once a script file has been selected

There is no notification that the script is running or has completed, besides looking for the generation of a log file in the same location as where the script file is located. On completion the (ASCII) log file will include a line stating the finish time. The log file will report if the script was successful on each file that it has found and processed.

The output comprises two CSV files, one for the VNIR-SWIR and one for the TIR, with a selection of the average results from the NIST wavelength absorption features, the standard deviation, number of spectra found and the HyLogger instrument, sorted by date (including time). An example of the VNIR-SWIR wavelength csv file is shown in Figure 12. The names of these files are determined in the script.

HyLogger	Scan_Date	Dataset_file	453_mean	453_stddev	524_mean	524_stddev	654_mean	654_stddev	800_mean	800_stddev
HyLogger 3-2	29/05/2018 9:23	C:\00me\0cust\Mi	453.357	0.00219139	524.089	0.00826803	653.959	0.0570906	799.552	0.0273681
HyLogger 3-2	29/05/2018 15:43	C:\00me\0cust\Mi	453.309	0.0498661	524.08	0.00539197	653.879	0.0455521	799.548	0.0256349
HyLogger 3-2	30/05/2018 15:47	C:\00me\0cust\Mi	453.294	0.0426556	524.107	0.00766042	653.888	0.0545779	799.489	0.0326576
HyLogger 3-2	30/05/2018 8:17	C:\00me\0cust\Mi	453.312	0.0161911	524.182	0.0181742	653.904	0.0552887	799.503	0.0398767
HyLogger 3-2	31/05/2018 15:28	C:\00me\0cust\Mi	453.281	0.0235907	524.081	0.00652029	653.891	0.0432969	799.504	0.0284309
HyLogger 3-2	31/05/2018 8:18	C:\00me\0cust\Mi	453.312	0.0280683	524.168	0.0110209	653.869	0.0150826	799.466	0.011335
HyLogger 3-2	1/06/2018 14:42	C:\00me\0cust\Mi	453.304	0.0320609	524.066	0.0156064	653.911	0.0250781	799.494	0.0304242
HyLogger 3-2	1/06/2018 8:10	C:\00me\0cust\Mi	453.328	0.00835682	524.154	0.00293498	653.908	0.0411231	799.468	0.0350697

Figure 12 Example of the VNIR-SWIR csv created by PUCKWCAL on test rocks TSG files containing the pucks

CSV files do not keep formulas, plots or colouring in Excel and thus the data needs to be saved as an Excel file. Once a ‘working’ Excel file has been created the formulas for calculating the ongoing statistics on the data can be performed and plots created tracking changes. Further information can be gained from the results by determining the minimum, maximum, mean and median for each wavelength. Colour coding each column using colour scales in Excel can quickly identify outliers (under Styles -> Conditional Formatting -> Colour Scales) or diurnal variation.

5 Results of one year's test rocks and wavelength standard analysis using currently available scripts and data

A total of 1000 test rock scans from 7 HyLogger3 instruments between April 2019 and April 2020 were processed with the PUCKWCAL script using the *Headless mode* in TSG. The whole dataset was analysed for mean, median, standard deviation, maximum, minimum and the differences between max/min from median and max/min from mean using Microsoft Excel. The data was also subset into each NVCL node. For this Initial processing the test rock data was not standardised to the same version of TSG. The need to undertake standardisation of the HyLogger data to the same TSG version-build and using the same import settings for the raw was not discovered until after results were analysed and is a recommendation for work in the next year of the project.

5.1 VNIR-SWIR data

The results show a small difference between AM and PM scans for most of the nodes, with a slight shift in the CCD spectrometer (VNIR) to shorter wavelengths (~0.02-0.2 nm) between 7 am and 3 pm measurements. This is shown in Figure 13, with a shift of 0.2 nm at 524 nm between the morning and afternoon measurements. The exception of this HyLogger 3—5 (GSQ) which shows the least variation in wavelength. Some NVCL nodes displayed lower standard deviations and differences between average and the min/max values compared to other NVCL nodes. Further work should be done to check if the unmixing results and scalar results are different between NVCL node test rock data. The reason for the difference in variation between the NVCL nodes is unclear at this stage, but could be due to the different thermal properties of the rooms used (exterior walls) and air conditioning. A method for checking the metadata of the raw HyLogger data is proposed for future work.

HyLoggers 3-4, 3-6 and 3-7 (GSNSW, MRT and NTGS) and possibly 3-1 (CSIRO) have similar wavelengths for the 524 nm feature at ~523.8 nm, whereas HyLogger 3-2, 3-2 and 3-5 (GSWA, GSSA and GSQ) have an average longer wavelength at 524 nm (~524.4 nm).

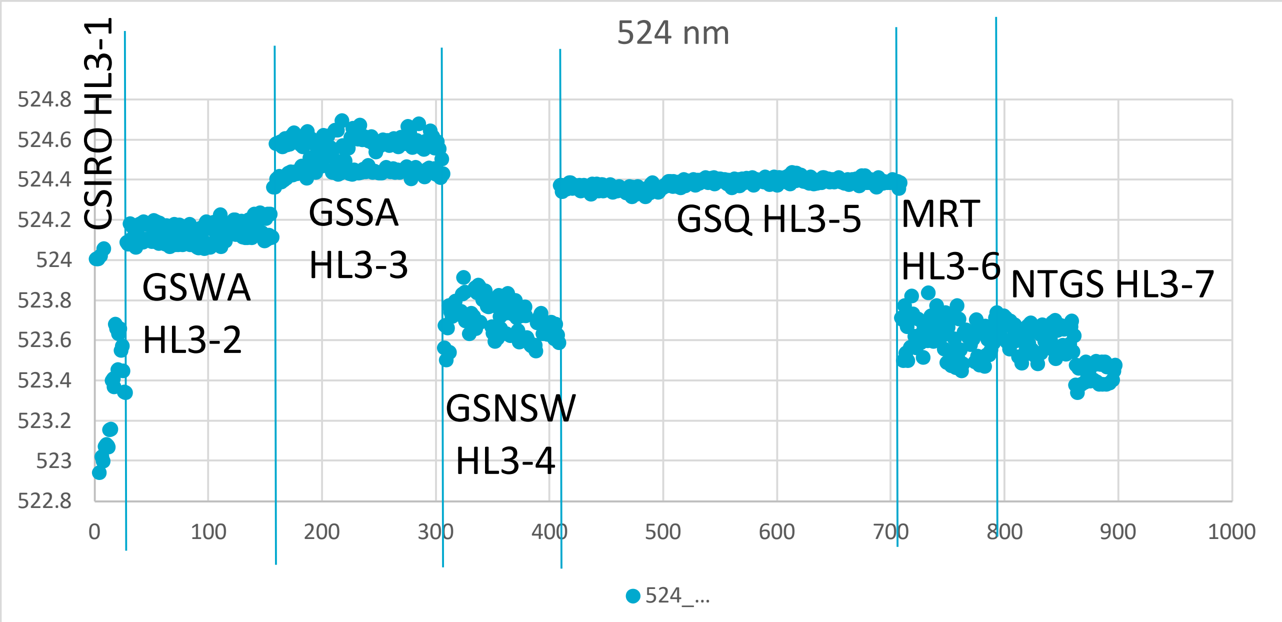


Figure 13 Wavelength position (y-axis) of the 524 nm VNIR absorption feature due to Er in NIST standard (SRM)-1920a for a total of 2775 test rock scans from 7 HyLogger3 instruments between April 2019 and April 2020. Diurnal variation in VNIR wavelength indicated by two "parallel" trends are evident especially in the GSWA 3-2, and GSSA HL3-3. This data has not been standardised for TSG QC version and shows a sudden wavelength shift in NTGS HL3-7 data.

For the SWIR data (Figure 13), HyLogger 3—4 (GSNSW) displayed the greatest variation of up to 0.5 nm, with most Nodes showing very small variations of ~0.1 nm at 1535 nm. The CSIRO results include initial measurements with HyChips 6-2 using an ASD FieldSpec 3, which has a lower spectral resolution than the HyLogger 3 FTIR spectrometers. From the 1535 nm results there appears to be 3 groups of wavelengths. A majority of instruments (HyLogger 3-1, 3-2, 3-4, 3-5 and 3-6) show a wavelength of 1535.5 nm, whereas HyLogger 3-3 has a slightly longer wavelength (1536.2 nm) and HyLogger 3-7 a shorter wavelength (1534.5 nm), which changes to a wavelength similar to the majority of the instruments at a specific date in September 2019. The explanation for this is described below.

After interpreting the first pass input of the data, a change in the wavelength was observed in HyLogger 3-7 (NTGS NVCL node) between the 4th of September and the 12th of September 2019 in both the VNIR (Figure 13) and SWIR data (Figure 14). This shift was attributed to the change in the TSG QC version after a service, with differences in the handling of the data on import. Test rock data that had been manipulated with a full version of TSG after scanning (reimported the raw HyLogger files, or reopened the TSG QC file and updated) displayed the newer version of TSG. An example is shown in Figure 15. The information about the version of the TSG file can be found by using a text editor (notepad for example) to open the .tsg file.

Another noticeable difference between the nodes was the chunking. Chunking is the downsampling of the HyLogger3 scans. Typically the HyLogger3 measures every 4 mm, which can be downsampled/chunked by 2 to 8 mm. GSSA's data was not chunked, whereas GSQ had the largest chunking. Interestingly GSQ's HyLogger data showed the lowest variation, whereas GSSA was about average. The GSQ TSG QC data was generated with TSG QC version 7 and could have influenced the results. It was these discoveries that initiated the standardisation of test rocks TSG files, which will be undertaken in work in the next part of the project. HyLogger 3-4 shows the largest scatter in values at 1535 nm, as it did in the VNIR.

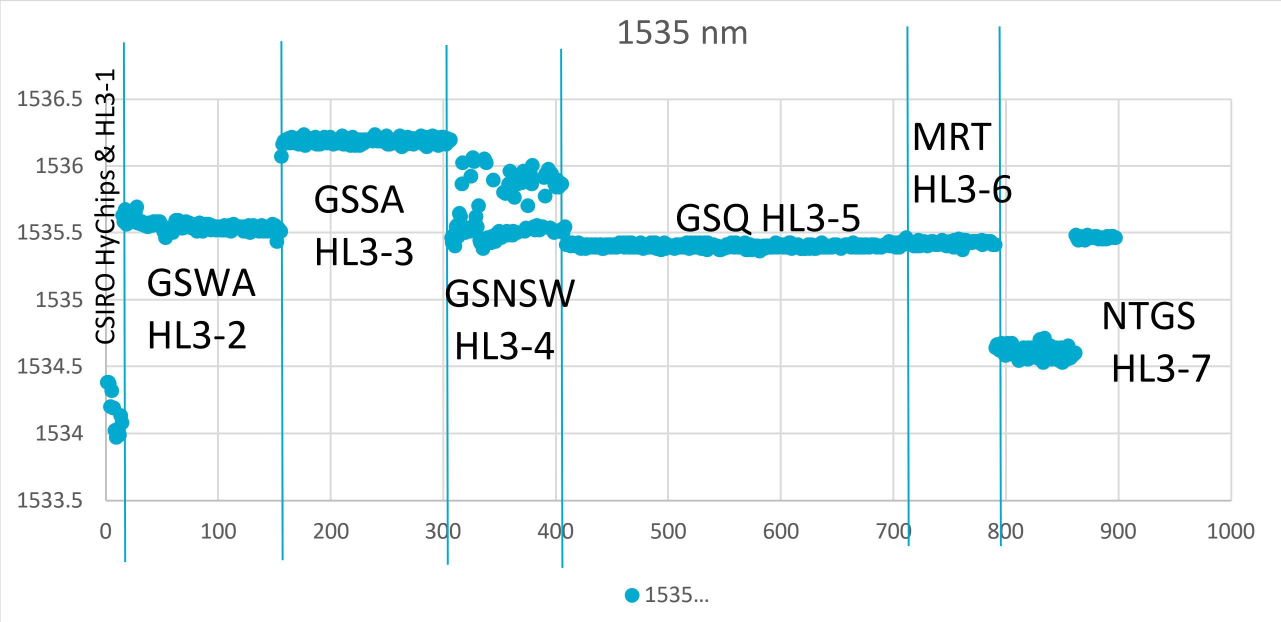
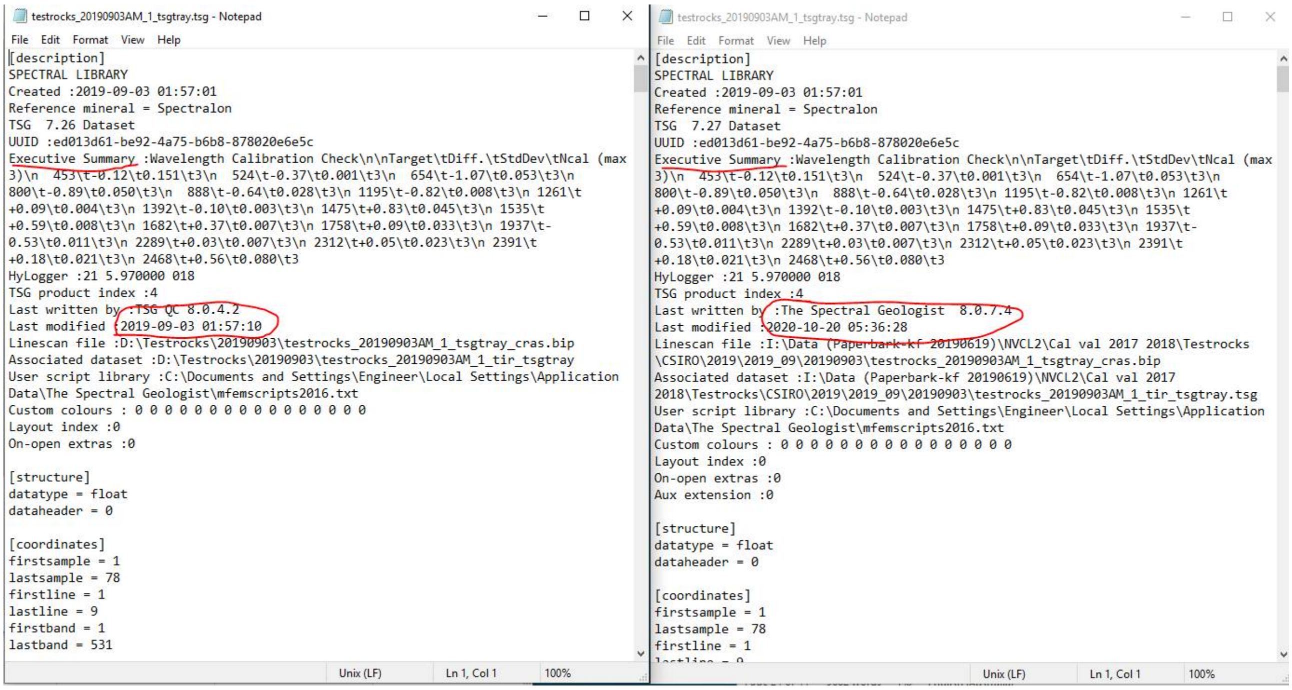


Figure 14 Wavelength position (y-axis) of the 1535 nm SWIR absorption feature due to hydroxyl-related combination band in talc in NIST standard (SRM)-1920a for a total of test rock scans from 7 HyLogger3 instruments between April 2019 and April 2020. This data has not been standardised for TSG QC version and shows a sudden wavelength shift in NTGS HL3-7 data.


```
testrocks_20190903AM_1_tsgtray.tsg - Notepad
File Edit Format View Help
[description]
SPECTRAL LIBRARY
Created :2019-09-03 01:57:01
Reference mineral = Spectralon
TSG  7.26 Dataset
UUID :ed013d61-be92-4a75-b6b8-878020e6e5c
Executive Summary :Wavelength Calibration Check\n\nTarget\tDiff.\tStdDev\tNcal (max
3)\n  453\t-0.12\t0.151\t3\n  524\t-0.37\t0.001\t3\n  654\t-1.07\t0.053\t3\n
800\t-0.89\t0.050\t3\n  888\t-0.64\t0.028\t3\n 1195\t-0.82\t0.008\t3\n 1261\t
+0.09\t0.004\t3\n 1392\t-0.10\t0.003\t3\n 1475\t+0.83\t0.045\t3\n 1535\t
+0.59\t0.008\t3\n 1682\t+0.37\t0.007\t3\n 1758\t+0.09\t0.033\t3\n 1937\t-
0.53\t0.011\t3\n 2289\t+0.03\t0.007\t3\n 2312\t+0.05\t0.023\t3\n 2391\t
+0.18\t0.021\t3\n 2468\t+0.56\t0.080\t3
HyLogger :21 5.970000 018
TSG product index :4
Last written by :TSG QC 8.0.4.2
Last modified :2019-09-03 01:57:10
Linescan file :D:\Testrocks\20190903\testrocks_20190903AM_1_tsgtray_cras.bip
Associated dataset :D:\Testrocks\20190903\testrocks_20190903AM_1_tir_tsgtray
User script library :C:\Documents and Settings\Engineer\Local Settings\Application
Data\The Spectral Geologist\mfemscripts2016.txt
Custom colours : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Layout index :0
On-open extras :0

[structure]
datatype = float
dataheader = 0

[coordinates]
firstsample = 1
lastsample = 78
firstline = 1
lastline = 9
firstband = 1
lastband = 531
Unix (LF)   Ln 1, Col 1   100%
```

```
testrocks_20190903AM_1_tsgtray.tsg - Notepad
File Edit Format View Help
[description]
SPECTRAL LIBRARY
Created :2019-09-03 01:57:01
Reference mineral = Spectralon
TSG  7.27 Dataset
UUID :ed013d61-be92-4a75-b6b8-878020e6e5c
Executive Summary :Wavelength Calibration Check\n\nTarget\tDiff.\tStdDev\tNcal (max
3)\n  453\t-0.12\t0.151\t3\n  524\t-0.37\t0.001\t3\n  654\t-1.07\t0.053\t3\n
800\t-0.89\t0.050\t3\n  888\t-0.64\t0.028\t3\n 1195\t-0.82\t0.008\t3\n 1261\t
+0.09\t0.004\t3\n 1392\t-0.10\t0.003\t3\n 1475\t+0.83\t0.045\t3\n 1535\t
+0.59\t0.008\t3\n 1682\t+0.37\t0.007\t3\n 1758\t+0.09\t0.033\t3\n 1937\t-
0.53\t0.011\t3\n 2289\t+0.03\t0.007\t3\n 2312\t+0.05\t0.023\t3\n 2391\t
+0.18\t0.021\t3\n 2468\t+0.56\t0.080\t3
HyLogger :21 5.970000 018
TSG product index :4
Last written by :The Spectral Geologist  8.0.7.4
Last modified :2020-10-20 05:36:28
Linescan file :I:\Data (Paperbark-kf 20190619)\NVCL2\Cal val 2017 2018\Testrocks
\CSIRO\2019\2019_09\20190903\testrocks_20190903AM_1_tsgtray_cras.bip
Associated dataset :I:\Data (Paperbark-kf 20190619)\NVCL2\Cal val 2017
2018\Testrocks\CSIRO\2019\2019_09\20190903\testrocks_20190903AM_1_tir_tsgtray.tsg
User script library :C:\Documents and Settings\Engineer\Local Settings\Application
Data\The Spectral Geologist\mfemscripts2016.txt
Custom colours : 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Layout index :0
On-open extras :0
Aux extension :0

[structure]
datatype = float
dataheader = 0

[coordinates]
firstsample = 1
lastsample = 78
firstline = 1
Unix (LF)   Ln 1, Col 1   100%
```

Figure 15 Examples of the .tsg opened with a text editor showing the changes in versions after updating with a full version of TSG. Note the wavelength calibration check results are shown in the Executive Summary field.

Therefore, it was proposed that the raw data be reimported into TSG using the same version and chunking settings and then the PUCKWCAL be rerun to check the results. This was initially performed on a small subset (2 months) of NTGS data and the wavelength shift that was previously observed between the 4th and 12th of September 2019 data was no longer evident. Averaging of the daily scans reduced the daily (diurnal) variation and resulted in a flatter plot (as shown by the light blue line in Figure 16). Similarly, the NTGS TSG QC data showed a wavelength shift on the 15th of June 2020, corresponding to a change in TSG QC version from TSG QC 8.0.5.3 to TSG QC 8.0.7.4.

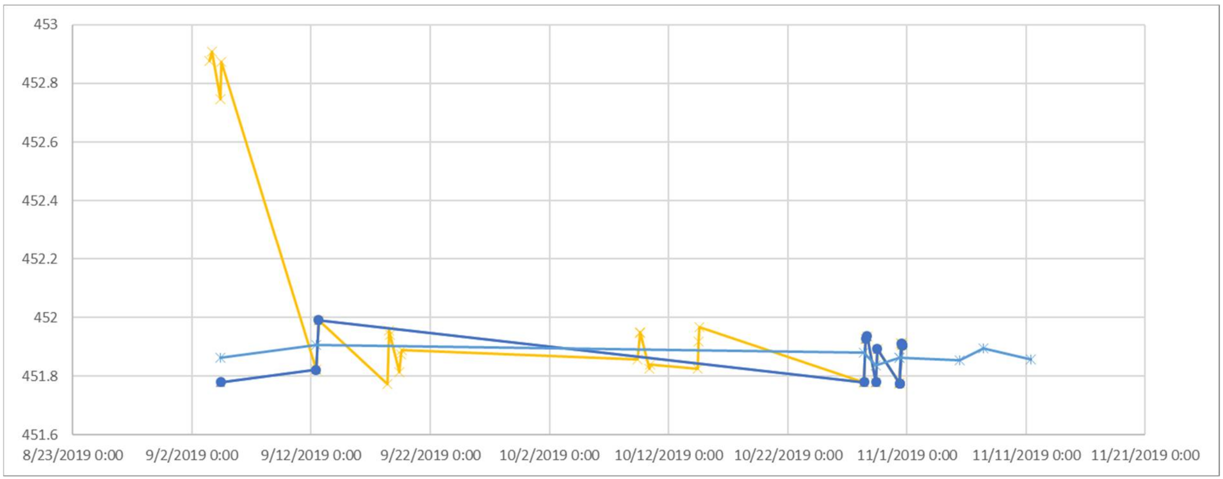


Figure 16 HyLogger 3-7 (NTGS) wavelength check for the 453 nm absorption feature, showing raw TSG data (orange crosses), averaged reprocessed TSG data (light blue asterisk) and reprocessed TSG data (blue dots).

5.2 TIR data

The nodes can be classed into 3 groups of wavelengths. When comparing the 6998 nm absorption from all the HyLoggers, HyLogger 3-1 (CSIRO) and 3-7 (NTGS) show similar (longer 6701 nm) wavelengths in the TIR, whereas HyLogger 3-2 (GSWA) and 3-6 (MRT) showed shorter wavelengths (6699 nm), whereas HyLogger 3-3 (GSSA), 3-4 (GSNSW) and 3-5 (GSQ) were in between (6700.5 nm). A comparison of the 6245 nm absorption features wavelength for each node is shown in Figure 17. The results show considerable variation between each instrument but low within instrument variation. The variation was approximately 0.5 nm, which compares well with the reported value of ±1 nm in Schodlock *et al.* (2016).

Although HL3-4 (GSNSW) displayed the greatest standard deviations in the VNIR-SWIR, this instrument displayed average standard deviations in the TIR wavelength range (typically below 0.8 nm for wavelengths less than 11875 nm). In comparison, HL3-5 (GSQ) which displayed very low VNIR-SWIR differences had high TIR wavelength differences for almost all wavelengths. Examination of the TSG header files from the data downloaded from Cloudstor revealed the version of TSG used. Most files were TSG QC but from many different versions, which changed as the software on the HyLogger acquisition PC was updated. Some of the data was full version TSG, which had been post processed after scanning before being uploaded. The data from HyLogger 3-5 (GSQ) was found to be TSG 7.1.0.71 until November 2019. HyLogger 3-3 (GSSA) showed a change in the wavelength due to the replacement of their TIR FTIR in June 2020. HyLogger 3-7 (NTGS) displayed a step change (0.5 to 2 nm shorter) in wavelength in December 2019.

The wavelength tracking of the 13228 nm absorption feature showed a large variation for all HyLoggers. This may be because the absorption feature is quite broad, but also due to the decreasing spectral resolution of the TIR mercury cadmium telluride (MCT) detector with increasing wavelength. Figure 18 shows the polystyrene puck spectrum measured with HyLogger 3-2, with the broad feature at 13200 nm. The highest values were 25 nm greater than the mean (as seen for HL3-7 and 3-5) with the lowest being 6 nm, with the average ~14 nm.

The wavelengths appear to show little variation for each instrument in the TIR, with differences found when the TSG QC version was changed.

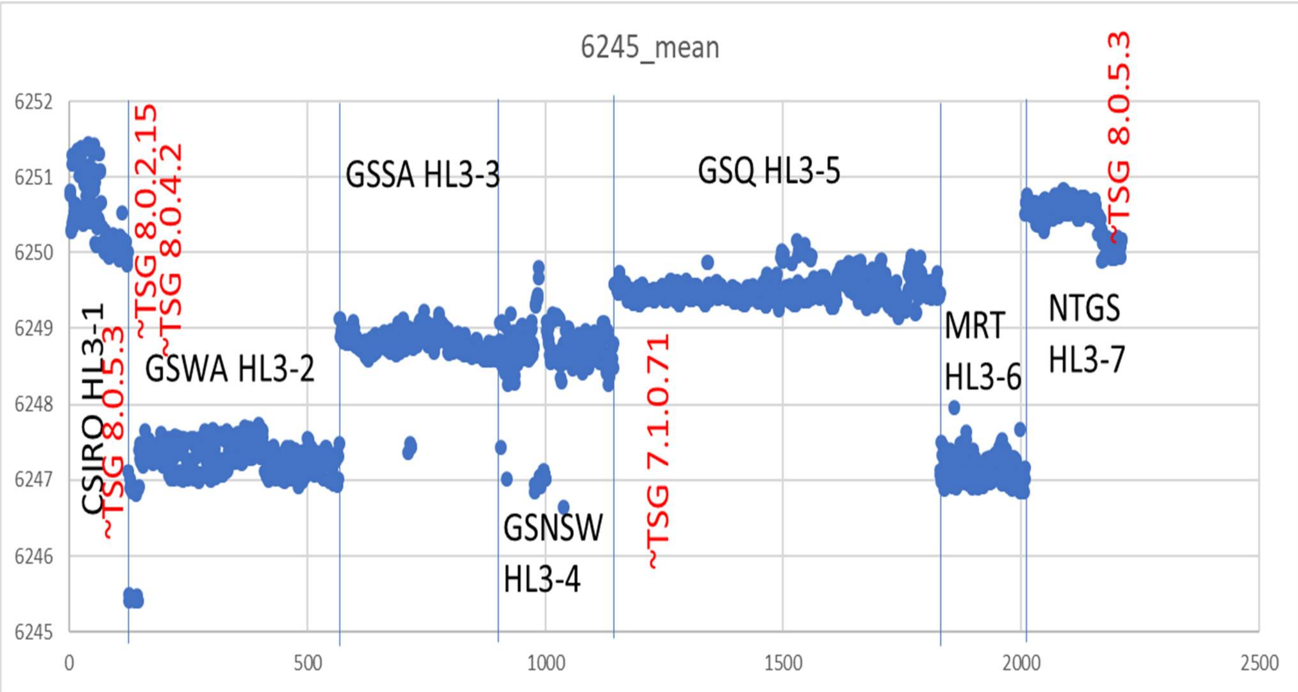


Figure 17 Wavelength position (y-axis) of the 6245 nm TIR absorption feature in NIST SRM-1921 for a total of 1000 test rock scans from 7 HyLogger3 instruments between April 2019 and April 2020. The red vertical lettering is the version of TSG in the TSG header files of the un-standardised data from Cloudstor.

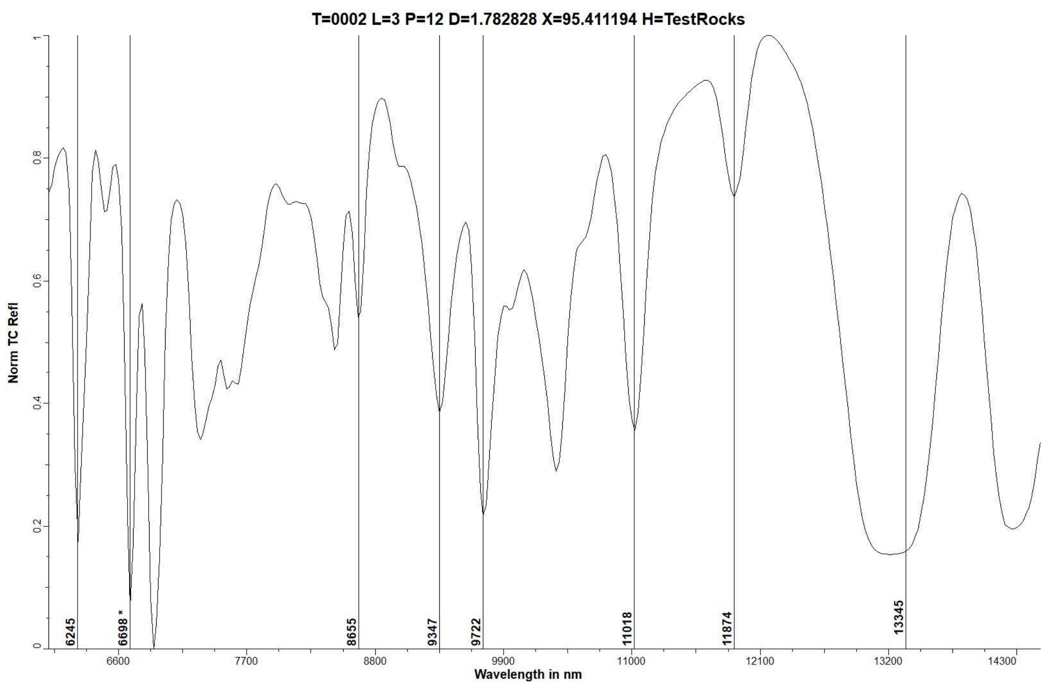


Figure 18 Example of the MWIR (polystyrene on gold) puck by HyLogger3-2 showing the broad 13345 nm feature.

6 Summary

The NVCL FY20 project aimed to improve the monitoring output from artificial standards by 1) proposing solutions towards automated monitoring of hardware, 2) identification and report on an intercomparison of test rocks & artificial standards for surveys to compare between them and within each HyLoggers variation for FY20, and 3) provide recommendations for how these differences can be addressed.

This chapter summarises the deliverables of the NVCL FY20 project and the key observations made from the newly collected QAQC data. With regards to the status of the above listed key deliverables:

1. Artificial standards were implemented in the Test rock panel. A method was developed for collecting Test rock and wavelength standard data, including the development of the PUCKWCAL script, which can be applied using TSG's *Headless mode*. The collected QAQC data are uploaded by each of the NVCL nodes to a designated server.
2. The analysis of Test rock and wavelength standard data collected over a 1-year timeframe showed that there are negligible differences between the VNIR and SWIR reflectance spectra collected by the six NVCL nodes. The TIR features were broader than the VNIR-SWIR and showed larger variation in nanometres than the VNIR. However, if the data is viewed in wavenumbers (cm^{-1}) the variation is much smaller. All instruments showed low variation in the TIR, whereas the VNIR and SWIR showed more diurnal variation. Large changes/shifts in wavelengths between dates could be explained by the change in the version of TSG and import settings used. A summary of the comparison is provided in chapter 6.3
3. It was found that the data needed to be standardised as the version of TSG QC and the settings for data import affected the wavelength results. This standardisation was also needed to be able to compare data between the nodes. Prior to running the headless routine to extract the wavelengths a routine is needed to reimport the raw HyLogger data using the same settings to ensure that it is standardised and can be compared between instruments and dates of acquisition. A Python script has been drafted for extraction of the metadata from the raw HyLogger files. This script will be written and tested in the next FY to determine if more information about the HyLoggers (i.e. albedo for the 3 spectrometers, temperatures) can be obtained to help with determining faults or tracking of changes.

6.1 Engineering and implementation of artificial standards

Artificial standards were added to the Test rock panels that have been used by the NVCL nodes over the previous years. The addition of the artificial standards was deemed to be necessary because the Test rock plates previously only comprised natural samples, which differ in composition and shape between the Test rock plates used by the NVCL nodes. The artificial standards are NIST-traceable and present distinct and sharp absorption features that improve efforts towards wavelength calibration and intercomparison of the HyLoggers employed by the NVCL nodes and the CSIRO. The Test rock plate was not replaced with artificial standards but complemented. This was done to enable QAQC checks on historically collected HyLogger data.

After several options of implementing the artificial standards onto the Test rock plate, it was found that a separate holder for the calibration standards would be the best option for collecting QAQC data from Test rock samples and artificial standards. This required an update of the standard test rocks template, which is part of the HyLogger data acquisition routine.

It should be noted that only two slots of the new calibration standard holder are occupied by the VNIR-SWIR and TIR calibration standards, respectively. A third slot can be used to add further artificial standards if deemed necessary of for adding other natural samples (such as quartz in the case of when no quartz-rich sample is present on the Test rock plate).

6.2 Method

The method for collecting and processing the QAQC data for multiple data sets comprise the following steps:

1. Scanning the test rock and wavelength standard plates. TSG QC automatically checks for the wavelength standards and reports the wavelengths. Uploading the HyLogger data to a central repository (Cloudstor) for further analysis: https://cloudstor.aarnet.edu.au/plus/s/K0FECELeDP9SMKw
2. Processing collected Test rock and wavelength standard data using the CLIMPORT (to standardise the data, which will be further developed in FY21) and PUCKWCAL scripts (developed as part of this project for this FY) in TSG's *Headless mode*, and
3. Uploading the results of the Test rock and wavelength standard data. The method for this reporting will be developed in FY 21.

6.3 Observations from QAQC-check of data collected over 1 year

Test rock and wavelength standard data from HyLoggers of the six NVCL nodes and the CSIRO that were collected for the April 2019 to April 2020 timeframe, were processed using the PUCKWCAL script. This provided information about how the respective HyLoggers were performing but also how they compare with each other over that 1-year timeframe:

- Wavelength shifts of the VNIR and SWIR are less than 0.5 nm and 2 nm, respectively, for each of the NVCL node HyLoggers and are negligible.
- Over the time period analysed the wavelength shifts in the TIR are also negligible, when comparing the ranges of wavelength shifts between the NVCL node HyLoggers for the VNIR and SWIR (1.4 nm, 3.5 nm). This means that, over the 1-year timeframe, HyLogger raw data produced by the six NVCL nodes are of the similar quality and comparable across jurisdictions.
- The TIR shows that the longer wavelength features are broad and are not as accurate at tracking wavelength as the shorter (sharp) absorption features. The version of TSG and import settings of the data affected the results. The TIR for most nodes appeared to be less affected by diurnal variation. The scatter in daily values appears to be ~0.5 nm at 6245 nm and 9353 nm whereas it is between 1 to 2 nm at 11875 nm.

- From the VNIR-SWIR calibration standard, a small difference was observed between AM and PM scans, with a slight shift in the CCD spectrometer (VNIR) to shorter wavelengths (~0.02-0.2 nm) between 7 am and 3 pm measurements. The range of these diurnal variations differ between the various HyLoggers, with GSSA and GSNSW showing the largest diurnal variations. GSQ's HyLogger shows the smallest (negligible) diurnal variation. The reason for the diurnal variation could be heat related. Information in the raw HyLogger data files may allow some tracking of temperatures which could be used to track these changes. A method for batch extraction and reporting of the metadata will be developed in FY21.
- TSG QC files from the nodes were found to have some variation in the version of TSG QC used.

6.4 Further work

In the next FY (2021) the following will be addressed:

- Standardisation of the data's TSG version before processing. Improvements to the CLIMPORT function in headless to cope with nested folders.
- Testing the use of other scripts of interest for QA that can be run using the *Headless mode*, on older test rock and drill hole data
    - TESTROX (wavelength-calibration checking on "test rocks" items). This can be run on test rocks without the calibration standards and looks for mineral absorption features.
    - WVLCAL (generalised but very limited wavelength-calibration checking), which can be run on any dataset.
- Batch extraction of metadata from the raw HyLogger data for tracking information using a Python script.
- Collation of each nodes instrument logs for identification of lamp changes/adjustments and mirror adjustments.
- Improved method of data upload.
- Automation of the standardisation and wavelength extraction, collation and report values on a website.
- Thresholds and warning values for HyLogger3 instruments which could be checked using a copy processing from a TSG file (template).
- Proposing a workflow/design for how level or differences in quality of respective data sets can be (pre-)viewed on AuScope portal by the NVCL community.
- Checking the results of applying scalars and unmixing on test rocks of different versions.

References

Schodlok, M. C., Whitbourn, L. Huntington, J. (2016). HyLogger-3, a visible to shortwave and thermal infrared reflectance spectrometer system for drill core logging: functional description. AJES 63 (8): 929-940.

Appendix A Calibration wavelengths of NIST standards

Wavelengths highlighted in red have a value that is +/- 5 nm different from the literature wavelength.

Table 1. List of wavelengths and features used for the VNIR-SWIR standard.

Calibration Wavelength	Source	Literature wavelength	Recommended by NIST
453 nm			
488 nm			
524 nm	Er	525	*
539 nm	Ho	536.4	*
654 nm			
744 nm	Dy	743	
800 nm	Dy	799	*
888 nm	Dy	887.2	
975 nm	Er	970.6	
1196 nm	Dy	1192.9	*
1261 nm	Dy	1262.063752	*
1322 nm	Dy	1321.319893	
1392 nm	Talc	1391.683854	
1475 nm		1478.056769	
1536 nm		1536.027526	*
1643 nm		1643.301656	*
1683 nm		1682.600897	
1757 nm		1758.14593	*
1939 nm		1931.975155	
1971 nm		1971.2435	*
2009 nm			
2289 nm	Talc	2290.258158	
2312 nm	Talc	2313.122808	
2391 nm	Talc	2391.589259	
2468 nm	Talc	2467.0586	

Table 2. List of wavelengths used for the MIR-TIR polystyrene standard.

Calibration Wavelength	Source	Recommended by NIST
6245 nm	SRM-1921b	6244.964997
6698 nm		
8655 nm	SRM-1921b	8660.708099
9347 nm	SRM-1921b	9352.612185
9722 nm	SRM-1921b	9722.991959
11018 nm	SRM-1921b	11029.49286
11874 nm	SRM-1921b	11881.70574
13345 nm		13217.37291

Appendix B Example of the headless scripts

See https://research.csiro.au/static/tsg/tsg_headless_reference.pdf for more information.

Example of the puckwcal script with #explanations

MULTIOPTIONS swir

#if not put in the VNIR-SWIR and TIR results are combined

multifile C:\TestRocks*.*

directory to start in where files exist, will dive into folders (unless nodive is specified in MULTIOPTIONS).

task_begin

#start of script

operation puckwcal

#name or command that will be performed, puckwcal.

report_file1 C:\TestRocks\swircalrep.csv

#Location and name to place the SWIR wavelength results. If the file already exists the file will be appended and multiple dates may be added to the same file.

report_file2 C:\TestRocks\tircalrep.csv

Location and name to place the TIR wavelength results.

task_end

#finish

Example of test rock script (Mylar, kaolinite, pyrophyllite and/or talc)

TESTROX

TASK_BEGIN
OPERATION **TESTROX**
TSG_DATASET *path+filename of .TSG file (overridden by MULTI_SPEC)*
TESTROCKS_JOB **(***space-delimited options) MYLAR PYRO KAOLIN TALC*
BKREM **(***nothing or), GLOBAL or LOCAL*
REPORT_FILE *path+filename of report file to generate*
TASK_END

Example

MULTIOPTIONS swir noassoc testrocks
multifile c:\00me\swift*.*
task_begin
operation testrox
testrox_job mylar pyro kaolin talc
bkrem local

report_file c:\00me\swift\0rep.csv
task_end

Example of wavelength script for minerals (kaolinite features, quartz absorption features or apatite absorption)

WVLCAL

TASK_BEGIN
OPERATION **WVLCAL**
TSG_DATASET *path+filename of .TSG dataset (overridden by MULTI_SPEC)*
HWCOPT (*nothing or), K2206 (default), K2160, Q8625, Q12625, A9200 (apatite)*
REPORT_FILE *path+filename of report file to generate*
TASK_END

Example

MULTIOPTIONS swir noassoc
multifile c:\00me\swift*.*
task_begin
operation wvlcal
report_file c:\00me\swift\0kcrep.csv
hwcopt k2206
task_end
MULTIOPTIONS tir noassoc
multifile c:\00me\swift*.*
task_begin
operation wvlcal
report_file c:\00me\swift\0q12crep.csv
hwcopt q12625
task_end

Example of re-import HyLogger data script to update TSG version (used to make sure all test rock data is from the same version of TSG)

MULTIOPTIONS dirs

multifile I:\run\2019*.*

will look down directories in the folder "2019", which will include subfolders of months and then subfolders of days.

task_begin

operation climport

format sds

will also re-import the TIR data. SDF can be used to import HyLogger1/HyChips data or HyLogger3 chip data. HCI3 data can also be imported.

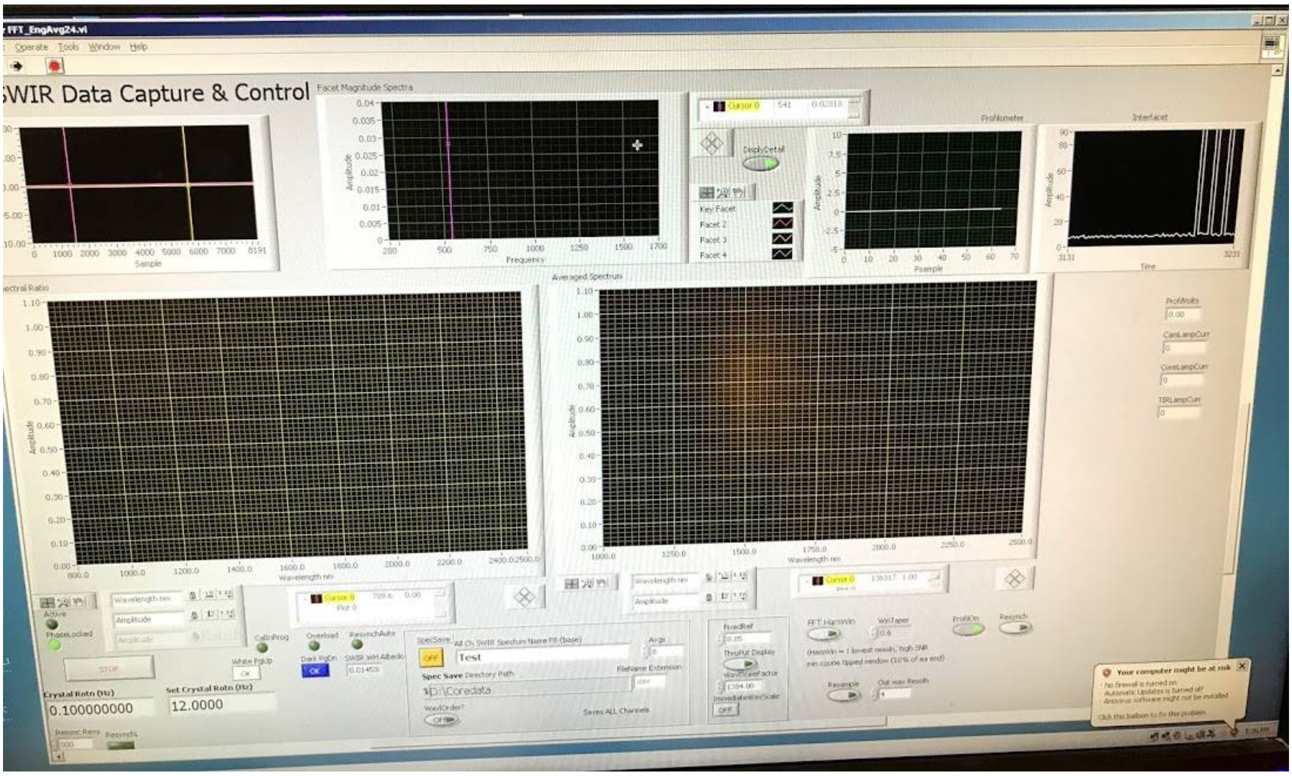
#cprocfile can be used to copy the scalars and layout from another TSG file.

sdschunk 2

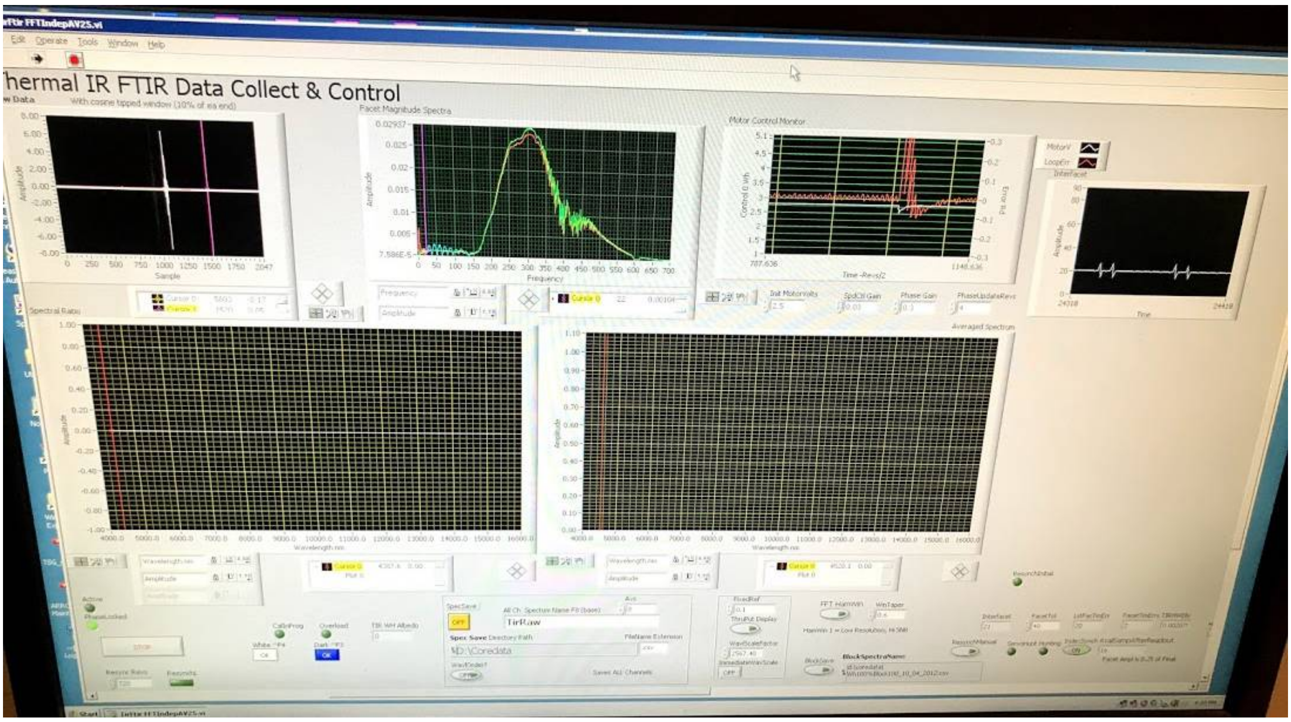
```
sdxgamma 0.72
jpqual 80
sdsopt doimg black white oladj revlon wtrim ttcor dogam doloc dotir tircal
sdscrit maxcl whitestep albrat
sdsthresh maxcl=20 darkmax=17 whitemina=160 whiteminm=125 maxsat=17 whitestep=40 whiteclip=1
sdstefalb v=0 s=0 t=0
sdsthermc tirscat=0.02 tirbktemp=10 tirtmtmp=10 tirtdtmp=15 tirdtmp=18
sdsalbrat 3.5
sdspdtray y
task_end
#the settings above can be changed to change the thresholds.
```

Appendix C

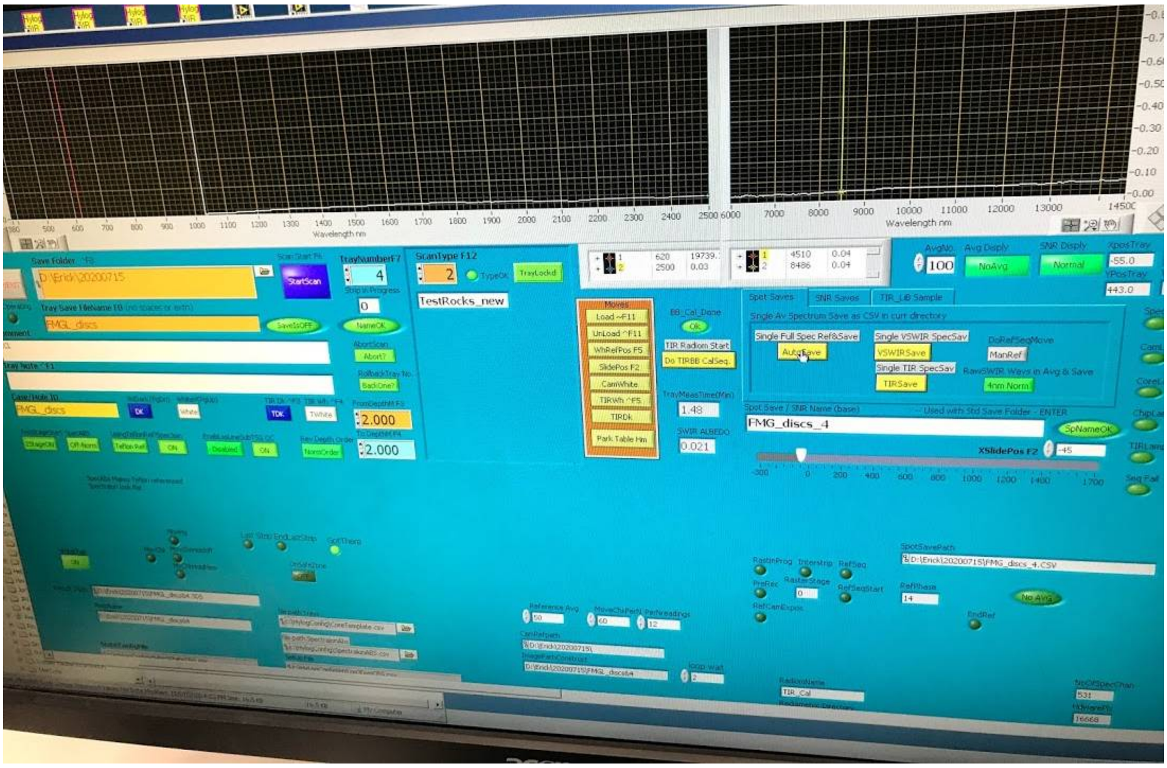
The HyLogger3 has an Engineering software called SWIR for investigating the SWIR FTIR spectrometer:

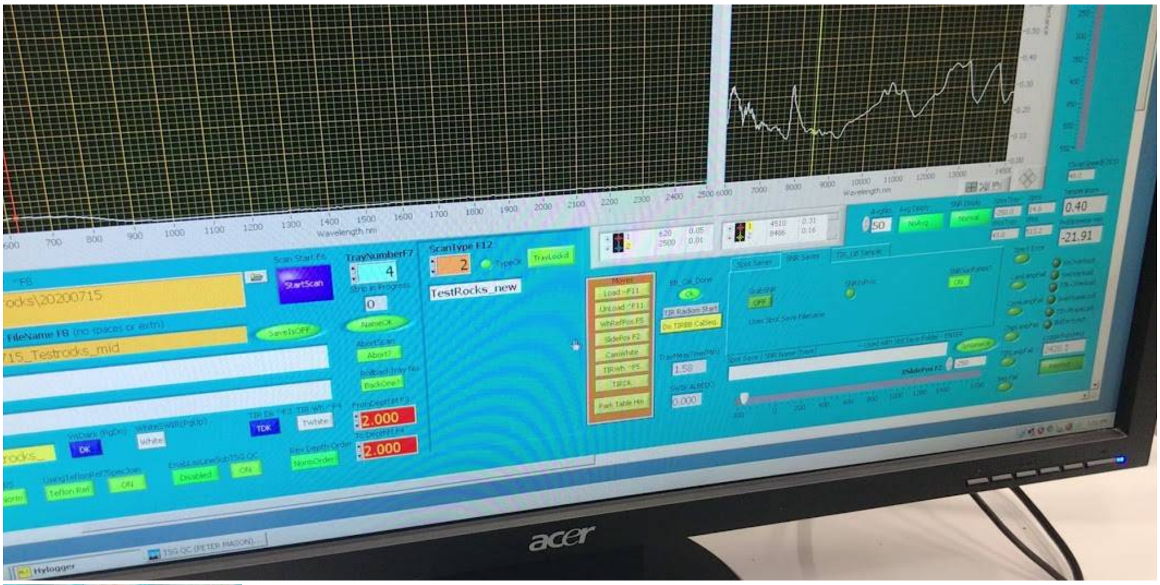


The TIR engineering software:



The HyLogger3 control software:





The green lights on the right-hand side of the screen which go red when there are errors with the HyLogger.

Appendix D

From 00what's new in tsg.doc by Peter Mason:

- I wrote a small standalone program called Eddie, to assist in TIR blackbody measurements. (It is available on request.) Give it a blackbody measurement file (.rad or .csv) and it displays some plots and calculations devised by Andy Green. Once you're used to it, it'll help you judge whether or not the measurements are okay.

6.5 **Eddie** (Sec 35.3 in 00what's new in TSG.doc by Peter Mason -September 2014)

Eddie (the HyLogger operator's companion) has been updated. The current version is "Ed the knife CPVE". It knows two new tricks: batch generation of a kind of summary, and image handling.

6.5.1 Batch summary

This option was requested by one of our researchers.

If you drop a *directory* onto Eddie, it is expected to contain a collection several core trays' worth of HyLogger-3 (VSWIR and TIR) raw data files and Eddie sets about preparing a summary file called **`eddie.csv`**. Eddie flashes through its usual VSWIR and TIR plots as it processes each tray's SDS and SDT files.

`Eddie.csv` is created within the dropped directory. It is a table with one row per core tray and the following columns: tray's filename (minus extension), Vis albedo, Vis noise[1], SWIR albedo, SWIR noise, TIR albedo, TIR noise.

6.5.2 Image support

You can drop individual .JPG image files or .JPM HyLogger section files onto Eddie.

[1] The SWIR and TIR items are the same as the ones shown in Eddie's plots. The Vis items don't appear in the SDT plot but are calculated in the same way as the SWIR items, only over the Vis wavelength range. Albedo is the white-reference average; noise is the white-reference standard deviation.

Individual .JPG files

Although you can drop any old JPEG image file onto Eddie, support is geared towards HyLogger -1 / -2 / -3

white / black calibration images and HyLogger-1 image frames. The display of a HyLogger-3 white calibration frame is shown above. Some of the plot's attributes and features:

- The image is scaled to fit Eddie's plot window.
- The text "`Iso`" at bottom left shows that the image is being displayed isometrically (square pixels). There are big black borders above & below because the image has a much thinner aspect than the plot window. (The borders would have been grey if the image were dark.) Isometric display can be toggled with the **"I" keypress**.
- The text "`FullXY`" at top left shows that the whole image is displayed. A rectangular subset can be selected via clicking the **mouse** LMB and dragging out a rectangle. The full view can be restored by double-clicking. If an .aux file was found then the **"A" keypress** can also be used to change the view.
- The three **R G B** readout sets in the top-left line are the maximum, minimum and average colours for the *section of image that's displayed*.
- The **R G B** % readout at top right shows the colour and colour-saturation percent for the image pixel under the mouse pointer.
- There is a *second line of stuff* at top left because Eddie has figured out that it has a special calibration image. This line has readouts for the *section of image that's displayed*, and they relate to TSG's HyLogger import image diag codes and thresholds. (Eddie shows different readouts for white & black calibration frames.)
- Red, green and blue histograms are shown. They are calculated over the *section of image that's displayed*. They go from 0 on the left to 255 on the right, and are "scaled to fit" vertically. The dot on the right end of the blue histogram shows that blue maxed out somewhere in the image. Histogram display can be toggled with the **"H" keypress**.
- The **red rectangle** over the middle of the image demonstrates that Eddie managed to find an .AUX file to pair off with the image file. Using the .AUX file, Eddie had a crack at calculating the image's "**active subset**" – the bit that would be retained by a TSG import. The **"A/Z" keypress** is active. Typing **A** or **Z** goes through a zoom cycle: the active X subset, then the active X & Y subset, then back to the full image. You should know this, especially when working with a calibration image. Some of the image diags (top left, second line) should be calculated over the active X range if they are to relate to a TSG import.
- Although you probably can't tell, the image's colour has not been "stretched". The **"S" keypress** toggles a hard-coded colour stretch of Eddie's choosing. The colour stretch does not affect the histograms or readouts.

HyLogger .JPM files

The “big HyLogger” saves its imagery in .JPM files, one per core-tray section. A .JPM file contains lots and lots of image frames, one after the other. You might be surprised at how many there are. One reason is that the HyLogger normally records one frame for each 4mm of travel. Another reason – and please stare for a moment while this sinks in – is that there are *lots* of excess frames at the start & end of the JPM file. As the HyLogger has three or four instruments along the direction of travel, it needs additional measurements so that the “innermost” instrument catches the start properly and the “outermost” instrument catches the tray end properly. Note I didn’t say “tray start”; I said “start”. The big HyLogger measures the calibration block for each section. And another thing: The big HyLogger measures “snakewise” – even and odd sections in different directions, one of which can safely be called “backwards”. The calibration block is near the start of the .JPM file for an even section and near the end for odd. Keep all this in mind.

W h e r e a a a a s s s. Eddie’s .JPM display is much like the .JPG display. One image frame is displayed at a time. Just about the only difference I can think of is the second readout line around top left. It’s always present in a JPM display and shows you which frame you’re looking at.

The .JPM display would be almost useless if there weren’t a way to navigate through the frames. This subject will get some attention shortly.

Mouse zoom

To zoom into a rectangular subset of the image, just click and drag with the mouse. I just wouldn’t believe you if you said that you don’t know what I mean.

You can zoom in more than once.

Readouts, histograms and colour stretches are calculated on the *section of image that’s displayed*.

Double-click to get back to the full image.

If a related .AUX file was found then there’s also the hotkey “A” or “Z” zoom. I told you about that already.

When zoomed in, the readout at top left will report the zoom region (instead of saying “`FullXY`”).

Navigating through images or frames

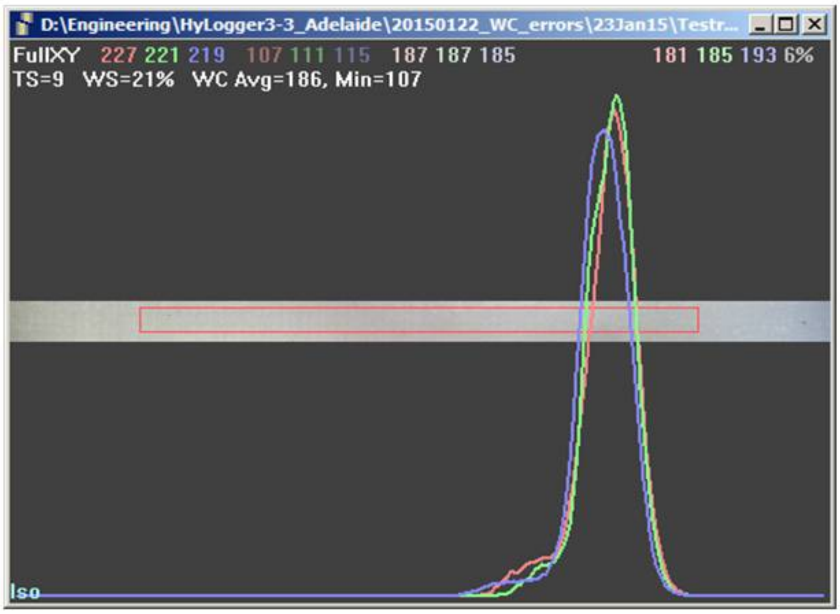
If you gave Eddie any old JPEG image or a black calibration image then there’s none of this. If you gave a white calibration frame then there probably is, for these things usually come in threes. If you gave a frame from a section’s directory of HyLogger-1 frames, or a big HyLogger’s .JPM file, then there is navigation through the tray section.

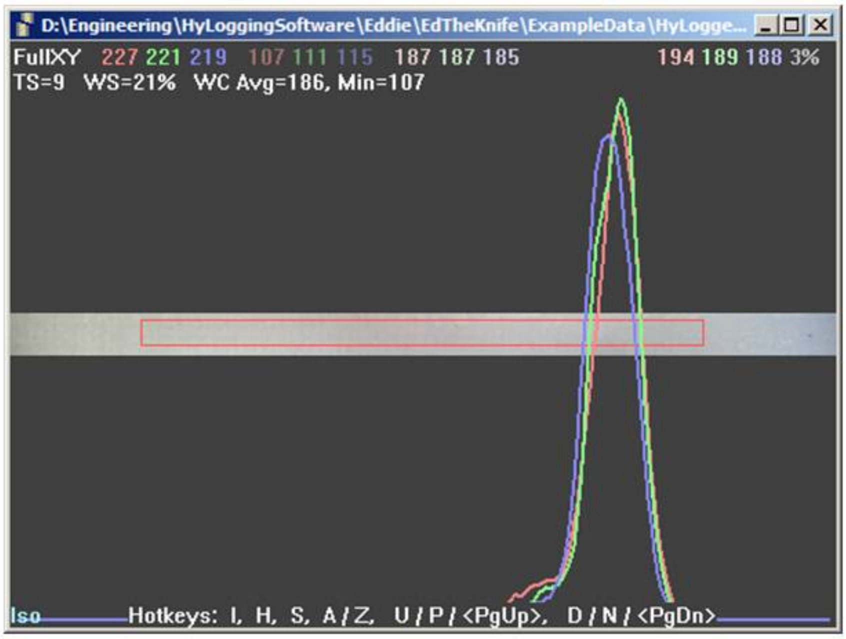
- **U** or **P** or **<PgUp>** displays the previous image / frame if there is one
- **D** or **N** or **<PgDn>** displays the next image / frame if there is one

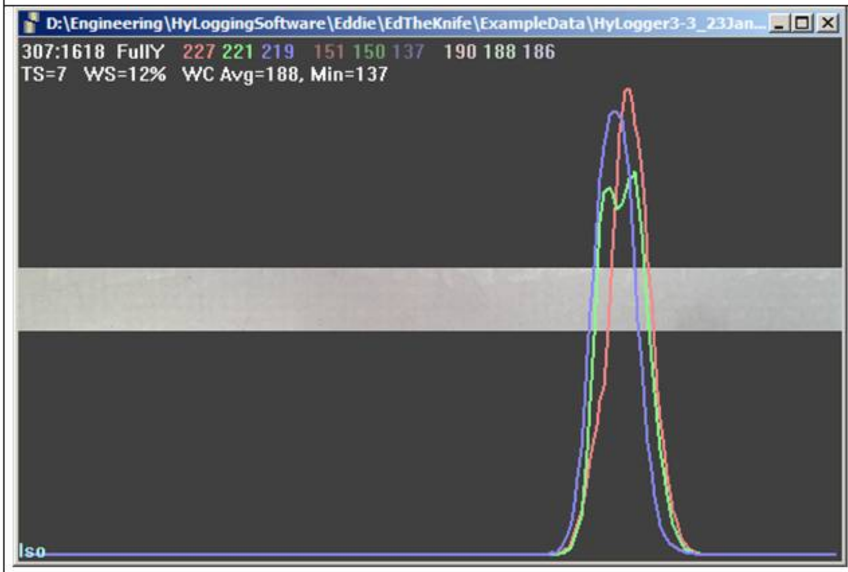
Notes by Lew Whitbourn 11th February 2015

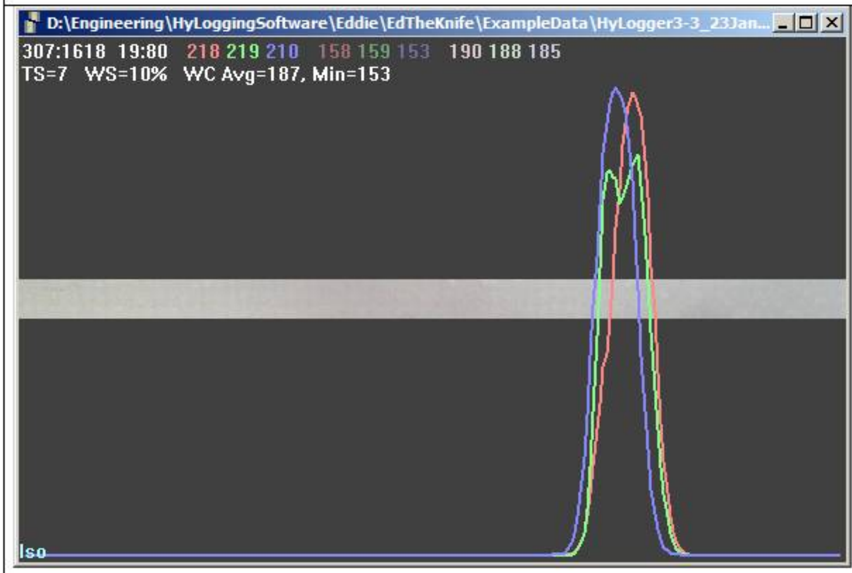
Eddie_CPVE.exe (Ed the Knife: 23 Sep 2014)

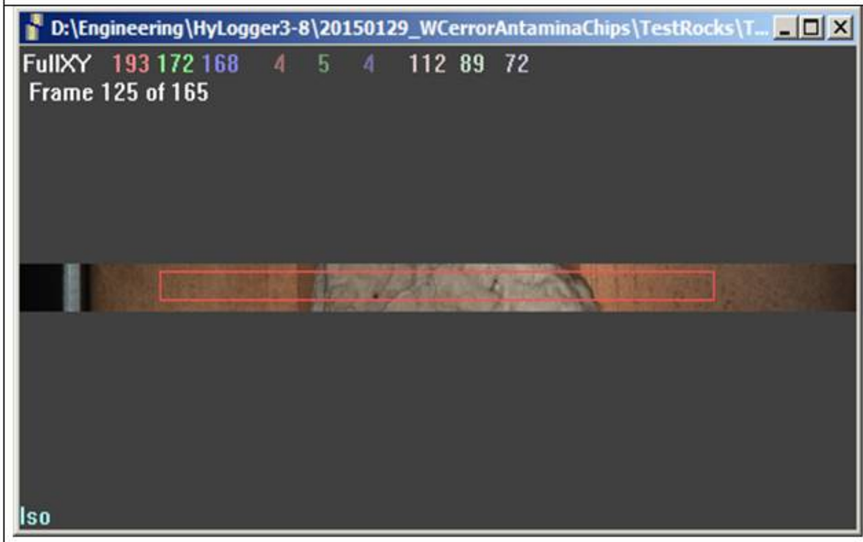
Lew Whitbourn 11 February 2015

Camera white reference images, e.g. TestRocks&1_WhRef0.JPG, TestRocks&1_WhRef2.JPG & TestRocks&1_WhRef3.JPG	Horizontal Range is 0 – 255 DN (digital numbers)
	This view results from dropping a JPM file onto Eddie. **Red Green and Blue** traces: histograms of red, green and blue in the Teflon reference images. These histograms from Sam in Adelaide on 29Jan15 are just about as good as you can get. **Legend on top left of screen:** **FullXY:** full field of view of the camera (other options described below) and corresponding histograms and data. The **Region Of Interest** (**ROI**) is shown by the red box if the **AUX** file is found. **227 221 219:** DNs at the right hand edges **107 111 115:** DNs of the darkest pixels **187 187 185:** DNs at the left hand edges **TS (Teflon Step check):** The largest change in DNs in 10 pixels horizontal or vertical throughout the frame. TSG compares this with a default threshold of 40. **WS:** Check for "colour" in white image. TSG compares this with a default threshold of 15%. **WC Avg:** Average brightness in the current field of view on the camera. TSG compares the average brightness in the **Region Of Interest** with a default value of 160. **WC Min**: Minimum brightness in the field of view. TSG compares the minimum brightness in the **Region of Interest** with a default value of 120.

Camera white reference images, e.g. TestRocks&1_WhRef0.JPG, TestRocks&1_WhRef2.JPG & TestRocks&1_WhRef3.JPG	Horizontal Range is 0 – 255 DN (digital numbers)
	**Legend of Hotkeys on bottom of screen:** This legend only displays briefly after the file is dropped onto Eddie. **I:** Toggle stretch white image to full height of window. **H:** Toggle histograms on/off. **S:** Stretch the brightness of the image. **A or Z:** Cycle through: **FullXY:** The whole field of view of the camera, which is approximately 1980 pixels across x 100 high, from which TSG uses the**ROI** to create its stitched images. The **ROI** is shown as a red outline in this view, only of the AUX file is in the same directory as the JPG file that was dropped onto Eddie. **307:1618 FullY:** See next plot.

Camera white reference images, e.g. TestRocks&1_WhRef0.JPG, TestRocks&1_WhRef2.JPG & TestRocks&1_WhRef3.JPG	Horizontal Range is 0 – 255 DN (digital numbers)
	**307:1618 FullY:** The images and histograms in this plot are for a reduced area, specifically 1618 of a total of 1608+307 camera pixels across the screen (corresponding to the width of the red box in the plots above), but still showing the full height of the image. It is clear that this cuts off the low-intensity "stragglers" from the left-hand edges of the histograms. This results in much better DNs for the darkest pixels; 151 150 137 in this plot, versus 107 111 115 in the plots showing the full field of view of the camera (**FullXY**).

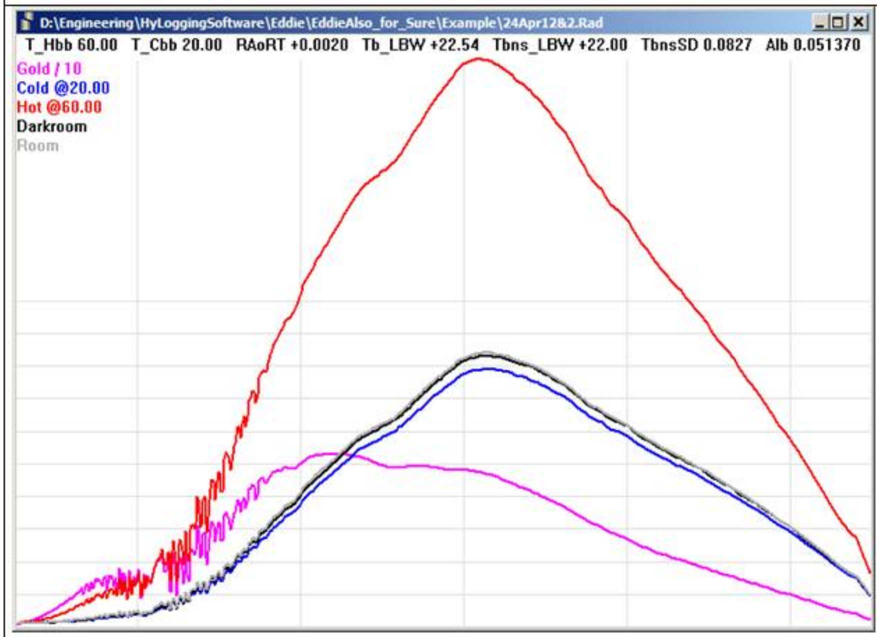
Camera white reference images, e.g. TestRocks&1_0.JPG, TestRocks&1_2.JPG & TestRocks&3_0.JPG	Horizontal Range is 0 – 255 DN (digital numbers)
	**307:1618 19:80:** The images and histograms in this plot are for the ROI of interest to TSG, i.e. 1618 of a total of 1608+307 camera pixels across the screen X 80 of a total of 80+ 19 pixels vertically (corresponding exactly to the **ROI** shown by the red box in the first two plots above). **THIS IS THE PLOT THAT YOU WANT IN ORDER TO SEE HOW YOUR CAMERA WHITE IMAGE WILL PERFORM AGAINST THE TSG THRESHOLDS:** WC Avg=187 and Min=153 easily easily meet the TSG defaults of 160 and 120 respectively. Note that these histograms could be improved by adjustments to the camera exposure time and RGB balance, moving all histograms to the right, and improving the registration of blue with red/green. This would further increase **WC Avg** and **Min**, and reduce the **WS** (colour) score.

<table>
<tr><td>Composite images for tray sections,
e.g. TestRocks&1_0.JPM, TestRocks&1_2.JPM & TestRocks&3_0.JPM</td><td></td></tr>
<tr><td>
</td><td>This view shows all the image "tiles" that get stitched together to produce the final tray images in TSG. You can scroll through them using the PageUp and PageDown buttons. Only the parts in the ROI (red box) get stitched, of course.

In this TestRocks JPM file there are 165 overlapping tiles, or Frames, each about 6 mm high. For a typical 1-meter long core tray, there are typical 380 image tiles. In core logging mode, the width of the ROI varies with template parameters, specifically the spacing between core or TestRocks sections, but the height is ALWAYS 4 mm.

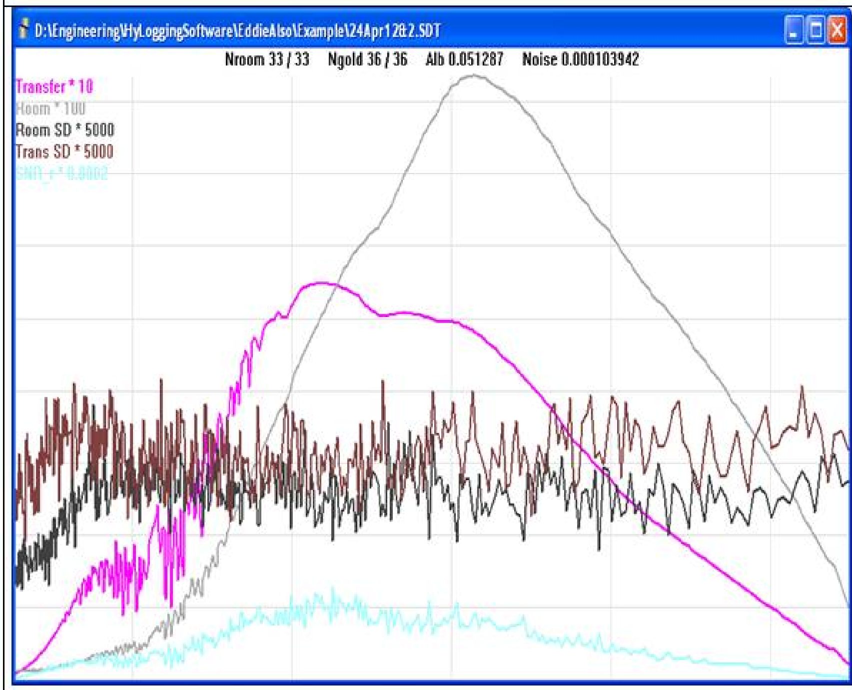
In chip logging mode, because the machine moves in 25-mm steps, the vertical height of the ROI is 25 mm. It is harder to achieve sufficiently bright and uniform lighting over this much larger area, and it is sometimes appropriate to relax the TSG WC Avg and Min thresholds accordingly (e.g. from 160/120 to say 140/100).</td></tr>
</table>

Eddie13.1397.exe (Eddie also for sure and then some: 20 Feb 2013) HyLogger 3-2 TestRocks2 24 April 2012: Lew Whitbourn 10 February 2015

<table>
<tr><td>Daily RAD file 24Apr12&2.RAD 10:24 AM</td><td>Wavelength Range is 4.5 um to 15 um approx.
Vertical lines are at 6, 8, 10, 12, 14 um</td></tr>
<tr><td>
</td><td>Red: Raw TIR signal from hot blackbody at temperature T_Hbb (which comes from config file)
Blue: Raw TIR signal from cold blackbody at temperature T_Cbb (which comes from config file)
Black: Raw TIR signal from the room ("background"), with the sources off.
Grey: Raw TIR signal from the room, with the TIR sources on (should be just above black).
Pink: Raw TIR signal from gold transfer target with TIR sources on, divided by 10. 5 divisions of height is about normal.

RAoRT = estimated fraction of scattered source
Tbns = estimated room temperature with the source off
Tb = estimated room temperature with the source on
TbnsSD = a measure of noise
Ralb = TIR Albedo
This should be about 1.5 times the current albedo threshold in TSG.</td></tr>
</table>

Tray SDT (TIR data file) 24Apr12&2.SDT 10:30 AM



Wavelength Range is 4.5 um to 15 um approx.
Vertical lines are at 6, 8, 10, 12, 14 um.

Grey: Raw TIR signal from the room, with the TIR sources on

Pink: Raw TIR signal from gold transfer target with TIR sources on.

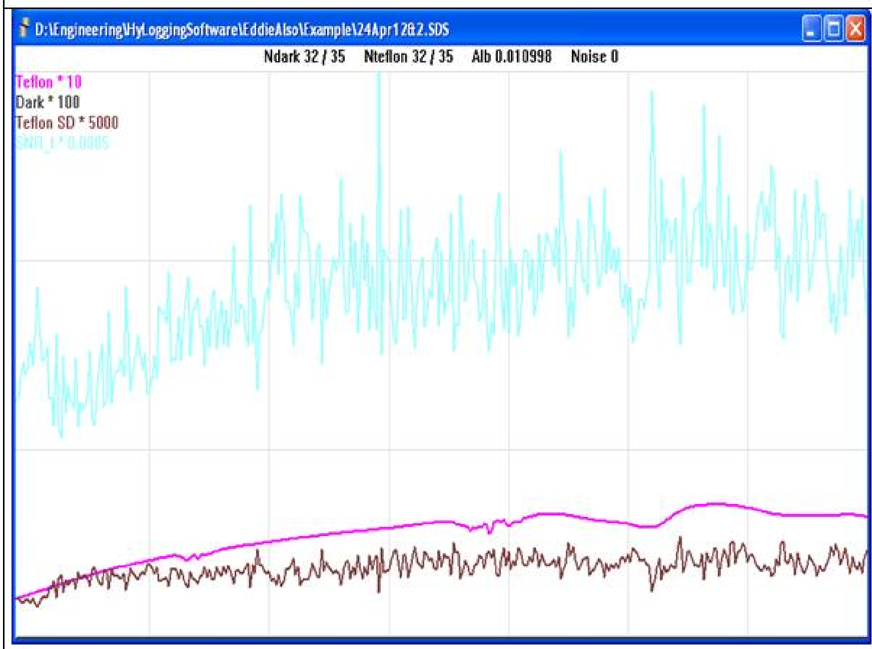
Black: Noise in raw TIR signal from the room

Brown: Noise in Raw TIR signal from gold transfer target with TIR sources on.

Blue: Signal to noise ratio (SNR: Pink/Black) **One vertical division is 1000**, so the peak SNR here is 1000. Current (Feb 2014) peak TIR SNR for HyLogger 3-2 is closer to 3000.

Note: Correct wavelength scale depends on correct WVT file being in the same directory as the TIR data (SDT) file that is being "dropped" onto Eddie. Otherwise, the plots appear in frequency space and are much harder to interpret.

Tray SDS (SWIR data file) 24Apr12&2.SDS 10:30 AM



Wavelength Range is 850 nm to 2500 nm approx.
Vertical lines are at 1000, 1250, 1500, 1750, 2000 & 2250 nm.

Pink: Raw SWIR signal from Teflon transfer target with SWIR lamps on

Brown: Noise in Teflon signal

Blue: Signal to noise ratio (SNR: Pink/Brown). **One vertical division is 400**, so the peak SNR here is about 800. Current (Feb 2014) peak SWIR SNR for HyLogger 3-2 is closer to 1000.

Note 1: Correct wavelength scale depends on correct WVL file being in the same directory as the SWIR data (SDS) file that is being "dropped" onto Eddie. Otherwise, the plots appear in frequency space and are much harder to interpret.

Note 2: SNR estimates in the SWIR are systematically less than that for TIR, because the noise used for SWIR SNR includes noise from the source caused by fluctuations in atmospheric absorptions. This is avoided in TIR by using noise from the room (i.e. background) radiance.

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