Long-wave infrared (LWIR) hyperspectral analysis of the Duvernay Formation on the micrometer and centimeter scale

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Introduction

Long-wave infrared (LWIR: 6 to 15 µm) hyperspectral techniques are capable of distinguishing between carbonates, clay minerals, and different silica polymorphs in a non-destructive manner, while also providing information about total organic carbon (TOC). Utilizing new data processing approaches, LWIR hyperspectral data collected using Fourier-transform infrared (FTIR) instruments can be used to in-situ identify and quantify minerals in a rapid manner with very little sample preparation. To evaluate the applicability of this technique in regards to the analysis of fine-grained sediments, hyperspectral data were collected from seven Duvernay samples using two LWIR instruments. One instrument collected hyperspectral data on the centimeter scale (macro-scale) and the other instrument collected data on the micrometer scale (micro-scale). The hyperspectral data were analyzed to identify the presence and abundance of quartz, Al-clay, Mg/Fe-clay, carbonate, lithic fragments, and TOC to provide information about compositional trends and to identify micro-structures in these fine-grained sediments. The results obtained using the hyperspectral techniques were compared to results collected using more traditional sedimentological analyses.
Materials and methods

Hyperspectral data were collected from seven polished thick sections from the Duvernay Formation (Kaybob area). The polished thick sections were created to have a thickness of at least 500 micrometers, which ensured that the samples were optically thick. With optically thick samples, all incident infrared energy is reflected back to the detector and no infrared energy is transmitted through the sample. Due to the limited working distance between the stage and the detector for the micro-scale instrument, it was not possible to use slabs of polished drill core for this study, but in principle, this is possible.

Two LWIR instruments were used to collect the hyperspectral data. Micro-scale imaging data were collected at the University of Innsbruck in Austria using a Bruker Vertex 70 FTIR spectrometer, which was coupled to a Hyperion 3000 IR-microscope equipped with a Focal Plane Array (FPA) detector. This instrument operates over a spectral range of 6 to 11 µm, collecting images that contain approximately 100,000 pixels over an area of 0.8 x 0.8 millimeters, producing pixels with a size of 2.7 x 2.7 µm. It is important to note that the pixel size of this instrument is very close in size to the size cut-off for clays, meaning that this instrument is very useful for identifying different clays and their mineral constituents.

Macro-scale point data were collected at the Agilent facilities using a handheld Agilent 4300 FTIR instrument, which collects hyperspectral point data over a spectral range of 2.5 to 15 µm with an approximate spot size of 1 x 1 cm. Three spectra were collected from each sample at the macro-scale.

The hyperspectral data were analyzed by Hyperspectral Intelligence Inc. (HII) (Gibsons, BC). HII uses customizable, modular tools to build advanced automated processing chains that work efficiently with large hyperspectral datasets. Using a modular approach, the hyperspectral data were subjected to a rigorous pre-processing protocol that reduced the influence of the spectral noise commonly produced by hyperspectral instruments. This de-noising step is an important part of every pre-processing protocol and is adapted for each instrument and sample type as required. After the pre-processing phase, the hyperspectral data were analyzed to extract compositional information and to identify relationships between the different compositional groups that were identified.

The micro-scale hyperspectral imagery were analyzed to identify the presence of quartz, Al-clay, Mg/Fe-clay, carbonate, and lithic fragments. The end result was the production of compositional maps that show the distribution of these compositions in different colours. Each compositional group represents a specific mineral (a pure pixel) or a spectrally uniform assemblage of two or more minerals (a mixed pixel). Using this approach, it was possible to analyze the composition of grains larger than the resolution of the instrument (2.7 x 2.7 µm), while also being able to determine the mineralogical composition of the matrix and the cement, which has a grain size of <2.7 x 2.7 µm. The abundance of each compositional group was compared to the TOC value obtained over the respective intervals.

The macro-scale hyperspectral point data collected using the handheld Agilent 4300 instrument were analyzed to identify the presence of quartz, clay, and carbonate, and these results were compared to the TOC values obtained for the intervals at which these samples were collected.

Results and discussion

Considering that crystalline quartz, amorphous silica, clay, and carbonate generally fulfill different rolls in sedimentary rocks (e.g., crystalline quartz is often found as detrital clasts, whereas amorphous silica is typically found in the matrix and cement), it is conceivable that TOC, porosity, and permeability are directly or indirectly governed by the presence, abundance, and physical arrangement of these different minerals in sedimentary rocks.
Analysis of the micro-scale hyperspectral imagery from the seven samples from the Duvernay revealed that crystalline quartz is observed in >95% of the pixels (Figure 1), with two quartz populations observed. These two quartz populations are very different. They differ in their overall grain size, their modal abundance, and their compositional purity. Herein, these two quartz populations are named based on their overall grain size.

1. **Silt-sized quartz** (3.9 to 62.5 µm in size): This population of quartz is comprised of larger grains that have a pure composition. This population is shown in bright yellow in Figure 1 and produces a classic quartz spectrum. This population is a minor form of quartz in these samples (<5%), and it is found distributed throughout all samples except E, which is dominated by carbonate.

2. **Clay-sized (0.98 to 3.9 µm) and colloidal-sized quartz (<0.98 µm)**: This population of quartz is comprised of much smaller quartz grains that always occur in close association with clay minerals. This quartz population is shown in dark yellow, orange, pink, and purple in Figure 1 and displays a highly variable quartz spectrum. These quartz spectra are mixed with different clay minerals within a single pixel (2.7 x 2.7 µm) indicating that the grain size of this quartz population is very small. This type of quartz is the dominant form of quartz in these samples, and it is found distributed throughout all samples except E, which is dominated by carbonate.

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**Figure 1**: Compositional maps of seven samples from the Duvernay Formation (04-19-064-22W5) obtained from Micro-FTIR imaging and hyperspectral analysis. Each map consists of more than 100,000 individual spectra, and each pixel is 2.7 x 2.7 µm in size, which is close to the size cut-off for clays. Pixels with similar spectra (i.e., similar mineralogical compositions) are shown in the same colour. Multiple colour shades for a single mineralogical assemblage illustrate the natural spectral variation observed within that assemblage, which is due to small compositional variations. The term Al-Clay refers mainly to kaolinite, whereas the term Mg/Fe-Clay mainly refers to saponite and/or chlorite.
In the seven samples analyzed for this study, each sample has a different relative abundance of quartz, clay, carbonate, and lithic fragments (Figures 2A). This shows that the upper Duvernay is dominated by clay-sized quartz mixed with Al-clay, the middle Duvernay is dominated by carbonate compositions, and the lower Duvernay is dominated by clay-sized quartz mixed with Mg/Fe-clays.

TOC measurements conducted on the intervals in which these samples were collected revealed that the areal abundance of silt-sized quartz directly and linearly correlates with %-TOC abundance with an $R^2$ value of 0.86 (Figure 2B). This means that as the number of large, pure silt-sized quartz grains increases, the amount of TOC increases as well.

The macro-scale LWIR spectra collected from these samples show a wide range of spectral variability (Figure 3A), and these spectra are dominated by the spectral features of quartz, clay, and carbonate. TOC values collected for these samples were used to derive a Duvernay spectral metric that can be used to obtain non-destructive TOC abundance information from samples in a rapid manner using a handheld LWIR spectrometer (Figure 3B).

Figure 2: (A) Abundances of different compositional groups or mineral assemblages in samples from the upper, middle and lower Duvernay Formation (see Figure 1 for legend). (B) Areal abundance of silt-sized quartz versus TOC content for seven samples from the Duvernay. A linear regression line ($R^2=0.86$) is shown in red
Conclusions

Preliminary research conducted on sedimentary rocks from the Duvernay Formation using micro- and macro-spectroscopic techniques shows that these techniques can be used to obtain important compositional information from fine-grained sedimentary rocks. The micro-scale compositional maps capture the mineral content and the in-situ arrangement of the minerals while providing information that may be used to correlate lithology to TOC content. In addition, the macro-scale results can be used to define TOC content and assist with stratigraphic correlations that are not easily defined in fine-grained lithologies with high clay content as the radioactivity and uniform grain size inhibit the use of geophysical well logs to confidently define sedimentary packages. The lithology changes in fine-grained reservoirs, which are produced through fracking, must be understood in order to develop fracking strategies and to determine the composition of fluids that will be effective and not plug fractures.

Fine-scale changes in mineralogy cannot be mapped using whole rock geochemistry or handheld XRF instruments, but micro-scale hyperspectral techniques can be used to characterize fine-scale compositional changes. Unlike current destructive whole rock analytical techniques, micro-FTIR hyperspectral imaging is capable of identifying minerals and determining their in-situ distribution at the micron scale, providing unparalleled information about textures in fine-grained reservoir rocks. The technique may be used on drill core and also on rock chips, and it is particularly useful when studying fine-grained rocks where the composition of the rocks change on a sub-millimeter scale. Given the high costs associated with drilling and producing from unconventional reservoirs, hyperspectral techniques have the potential to provide information that can help reduce drilling and production costs.

Figure 3. (A) Reflectance spectra collected from polished thick sections from the Duvernay Formation using a handheld LWIR spectrometer. The spectra from samples B, A, and F are dominated by the spectral features of quartz. The spectrum from Sample E is dominated by carbonate. (B) A spectral metric was derived for the Duvernay samples that linearly correlates with TOC. This means that TOC can be extracted from spectra collected using a handheld LWIR spectrometer.