Study of carbonate concretions using imaging spectroscopy in the Frontier Formation, Wyoming

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ABSTRACT

Imaging spectroscopy is applied to study diagenetic processes of the Wall Creek Member of the Cretaceous Frontier Formation, Wyoming. Visible Near-Infrared and Shortwave-Infrared hyperspectral cameras were used to scan near vertical and well-exposed outcrop walls to analyze lateral and vertical geochemical variations. Reflectance spectra were analyzed and compared with high-resolution laboratory spectral and hyperspectral imaging data.

Spectral Angle Mapper (SAM) and Mixture Tuned Matched Filtering (MTMF) classification algorithms were applied to quantify facies and mineral abundances in the Frontier Formation. MTMF is the most effective and reliable technique when studying spectrally similar materials. Classification results show that calcite cement in concretions associated with the channel facies is homogeneously distributed, whereas the bar facies was shown to be interbedded with layers of non-calcite-cemented sandstone.

1. Introduction

Geologists use a variety of methods to determine composition and distribution of minerals, such as X-ray diffraction, electron microscope, and petrography. These traditional methods can be time consuming. Some methods have scale limitations (i.e. do not generate continuous data), and others are destructive (Zaini et al., 2012). Therefore, geoscientists use interpolation and generalization to estimate diagenetic effects and mineralogical variations.

Post-depositional mineralogical alteration due to fluid-flow can control flow paths by affecting rock porosity and permeability in reservoirs (hydrocarbon and/or groundwater). After deposition, depending on the fluid chemistry, new minerals can fill up pores spaces, reducing the porosity of the rock. Alternatively, the mineral phase can be dissolved, increasing porosity and permeability (Taylor and Merchant, 2011). In reservoir analog studies, high resolution quantitative mineral mapping can be an excellent way to understand complex diagenetic processes and reduce uncertainty. In particular, the presence of calcite concretions and clay cements might change flow dynamics and reduces the quality of the reservoir (Dutton et al., 2000).

In recent years, portable hyperspectral cameras have opened up new horizons for mineralogical characterization at different scales, from hundreds of meters (outcrop) to millimeters (laboratory specimens) (Kurz et al., 2012; Zaini et al., 2014; Krupnik et al., 2016; Sun et al., 2017). Imaging spectroscopy and traditional methodologies can be combined to understand diagenetic processes and reduce uncertainty in reservoir characterization.

For this study, the Wall Creek Member of the Frontier Formation, in Wyoming was studied because of prominent geochemical variations due to diagenetic processes (Nyman et al., 2014). The studied outcrop is located in a gully, locally known as “Raptor Ridge” that was scanned by Visible Near-Infrared (VNIR) and Shortwave-Infrared (SWIR) hyperspectral cameras. Representative samples and core samples were used for laboratory analyses (Fig. 1). In addition, hyperspectral scanning and spectral data were collected in the laboratory for confirmation of remote sensing data.

This study used imaging spectroscopy for high-resolution mapping of diagenetic cements and their secondary-mineral distribution at different scales. Facies distribution and abundance are compared with previous published sedimentological data. Following are the specific objectives of this study; (i) evaluate the accuracy of carbonate concretion detection using imaging spectroscopy in comparison to traditional fieldwork studies (ii) compare commonly-used classification techniques to evaluate the best one for rocks of deltaic facies; (iii) evaluate the accuracy of outcrop classification using spectral endmembers from cores.
2. Study area

The study area is located between the Powder River Basin and the Wind River Basin in Wyoming (Fig. 1). The Frontier Formation consists of, at least, three unconformity-bounded members (from oldest to youngest): the Cenomanian Belle Fourche Member, the Emigrant Gap Member of Middle Turonian age, and the Upper Turonian Wall Creek Member (Gani and Bhattacharya, 2007). The Wall Creek Member of the Frontier Formation is Upper Cretaceous (Turonian 93.5 Ma) in age and deposited under fluvial-deltaic conditions. Parasequence #6 of the Wall Creek Member spectacularly crops out at the study area (43° 17' 30.85"N, 106° 47' 27.65"W). Parasequence #6 presents a lobate geometry with a shore parallel elongation, interpreted to have a mixed-influence (river and tide) deltaic origin (Gani and Bhattacharya, 2007).

Previous studies at the outcrop scale mapped and described the sedimentological and ichnological characteristics (3D concretion distribution is studied using Ground Penetrating Radar core data, and outcrop description show that concretions are elongated and tabular in shape (Gani and Bhattacharya, 2007). Based on previously published petrographic studies major diagenetic cements are calcite and authigenic chlorite, also kaolinite, iron-oxide, and quartz overgrowth can be found as minor diagenetic cements phases. The concretions are entirely cemented by calcite with minor authigenic, kaolinite, and chlorite co-existing in the margins forming pore-filling and pore-lining phases (Nyman et al., 2014).

3. Data and methods

VNIR and SWIR data were acquired from the depositional dip direction of the Parasequence # 6 at Raptor Ridge. In addition, SWIR
presence of carbonate concretions both in channel and bar facies.

3.1. Point spectral data

ASD FieldSpec Pro spectroradiometer was used in the laboratory to acquire spectral reflectance data from core samples. The spectroradiometer collects 2151 bands with a spectral bandwidth of 1 nm from 350 to 2500 nm. In the cores, only the portions that contain the carbonate concretions were scanned. Thirty-seven such areas in core-8 and nineteen spots in core-9 were selected for spectral data acquisition with the spectroradiometer. A systematic sampling was performed every 5–10 cm at the central area of the core.

3.2. Imaging spectral data

The field work was carried out during the summer of 2015 under clear sky conditions. Ground-based hyperspectral imaging data were acquired with VNIR Specim V106 sensor and SWIR Specim ImSpector N25E (Specim, Finland). VNIR camera collects 840 bands from 400 nm to 1000 nm with a bandwidth of ∼1.4 nm. SWIR camera collects 256 bands from 896 to 2,503 nm with a bandwidth of 6 nm. At Raptor Ridge, the cameras were set ∼ 50 m perpendicular to the outcrop wall. The pixel size was 5 cm and 15 cm for VNIR and SWIR, respectively. The cameras were mounted on a rotating stage and tripod that was remotely controlled by the user. For data calibration, a white reference calibration panel made of polytetrafluoroethylene (PTFE) with a known reflectance of 99% was placed within the sensor’s field of view at the center of the scanned area, parallel to the outcrop face, and in directly sun-illuminated area. (Okay and Khan, 2016; Khan et al., in press).

At the laboratory, the same cameras were installed in a custom laboratory configuration to scan the cores. Core samples were scanned on a moving stage at a distance of about ∼ 35 cm. The cameras were remotely controlled and data were acquired under similar illumination conditions created by a four direct-current bulbs perpendicular to the scanned area. For every image, a white reference panel (Labsphere Spectralon ® ) is scanned for calibration. The imaging sensor was configured to record continuous spectra at a high spatial resolution of 0.06 mm and 0.2 mm for VNIR and SWIR, respectively.

For image correction purposes both at the field and at the laboratory, a parallel dark image, using the same image parameters, was taken after every image by blocking the sensor input. Preprocessing steps were applied to hyperspectral images to transform raw data from at-sensor radiance into reflectance values. Standard tools available in ENVI 5.3 software were used for hyperspectral image processing. Besides in-house solutions developed in Matlab 2014 (Mathworks Inc.) were used for dark current subtraction from raw data (Okay and Khan, 2016). Preprocessing steps are described in more detail in (Alonso de Linaje and Khan, 2017). Preprocessed hyperspectral images were classified using the Spectral Angle Mapper (SAM) (whole pixel analyst) (Kruse et al., 1993) and Mixture Tuned Match Filtering (MTMF) (sub-pixel analyst) (Boardman, 1998) image processing algorithms. Workflow of processing steps is shown in Fig. 2.

SAM is a physically based spectral technique that treats the spectra as vectors in n-dimensional space and measure the angular similarity (in radians) between a given reference spectra and image pixel spectra. Smaller angles represent closer match. In this study, the angular similarity threshold was 0.1, SAM classified image was transformed into a binary classified image. This method was selected because it is relatively insensitive to reflectance intensities caused by illumination effects (Kruse et al., 1993). Endmembers for SAM classification were selected from isolated spectra image (from 2115 nm to 2360 nm) in the continuum-removed image. Limiting the input wavelength to diagnostic absorption features greatly increase the accuracy when comparing spectrally different minerals (Hecker et al., 2008).

MTMF is partial spectral unmixing algorithm that was applied to map sub-pixel abundance of the user-defined end-members. Spatially coherent MNF components were used as input for MTMF classification. For every end-member MTMF results are divided into (a) a score image that represent the proportion of the end-member material (MF) and (b) a infeasibility image (in noise sigma units) that are used to reduce the false positives. In this study, a threshold of 0.5 for MF results and pixels with infeasibility values below 30 were used.

The reflectance spectrum can be divided into three basic components, (a) a continuum (b) absorption bands and (c) residuals or noise (Asadzadeh and de Souza Filho, 2016). The continuum is described as the overall albedo of the reflectance curve and could be the manifestation of non-selective multiple scattering and presence of inactive minerals (e.g. microcrystalline quartz). The removal of the continuum allows the comparison between different characteristics of absorption features related to mineral abundance/or grain size changes (Zaini et al., 2012; Asadzadeh and de Souza Filho, 2016).

Continuum removal methodology provides better results when applied just to those areas of the spectra where absorption features are located (Hecker et al., 2008; Asadzadeh and de Souza Filho, 2016). The characteristics of the absorption features (i.e. position, depth, width, and asymmetry) were calculated using the continuum from previously isolated regions (from 2115 nm to 2360 nm) of the spectral where diagnostic absorption features of carbonate and clay minerals are located. Such characteristics were determined based on Van der Meer, 2004; Clark and Roush, 1984. The position of the absorption band is described as the wavelength where the maximum adsorption or minimum reflectance occurred. The depth, D of the absorption feature corresponds to the reflectance value at the shoulders minus the ratio of reflectance value at the position of absorption wavelength, Rb is the reflectance at the band bottom and Rc is the reflectance of the continuum at the same band as Rb (D = 1-(Rb/Rc)). The width, W, of the absorption feature is determined as the sum of the area left (Aleft) of absorption position and the area right (Aright) of absorption position divided by two times the depth value of the feature (W = [(Aleft + Aright)]/2D). The asymmetry (S) of the absorption band is represented as the ratio of (Aleft) and
(Aright) \( S = \frac{A_{\text{left}}}{A_{\text{right}}} \) (Asadzadeh and de Souza Filho, 2016; Van der Meer, 1995).

### 4. Results

#### 4.1. Point spectral data

In Figs. 3 & 4 the reflectance spectra of different lithologies found in the Raptor Ridge deltaic wedge are depicted. Reflectance results were divided into, bar facies, channel facies, carbonate concretions in bar facies, carbonate concretions in channel facies, and distal facies. However, sometimes the similarity between facies (similar composition although chlorite was previously described as a cement phase (Nyman et al., 2014), its presence is not recognized in the spectral data. Some erroneous results are reported for spectroscopic analysis in rocks with chlorite, due to the dark color and hence lower signal to noise ratios; low precision and high detection-limits (Zhang et al., 2001).

A closer look at specific parameters (e.g., depth, width, and asymmetry) of the reflectance spectra of kaolinite and calcite (major cement constituents) in the SWIR wavelength region is shown in Fig. 5. Blue and red shaded areas are correlated with carbonate concretions in channel facies and bar facies, respectively. The depth of the absorption where the minimum reflectance is related to mineral abundance. Additionally, physical properties such as grain size reduce the overall re-
480–550 nm, and 850–1000 nm has been previously related to hematite (Haest et al., 2012). These absorption features were found in all the core measurements but are more prominent in the carbonate concretions. Alternatively, these features can be explained by dominance or absence of ferrous iron.

The absorption feature, located at around 2200 nm, is related to the presence of clay minerals (Clark et al., 1990; Haest et al., 2012) (Figs. 3 and 4). This absorption feature can be found in both the sandstone host rock (bar and channel facies) and in the carbonate concretions (Fig. 5).

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Additionally, this drop, in combination with a smaller absorption feature at 2165 nm, creates a doublet that is characteristic of well-ordered kaolinite. This doublet is somewhat more prominent in the bar and channel facies versus the distal facies and carbonate concretions (Fig. 3 and 4). As shown in the graphs (Fig. 5), the width of the kaolinite absorption feature was relatively constant along the measured sections. The position of the absorption feature remains constant along the core section at ~2205 nm. The depth of the absorption feature decreases at ~2205 nm in the areas of carbonate concretions, meaning that the kaolinite abundance is lower (except, in core-8 points: 115 & 116). Apart from some anomalies in the host rock (i.e., in core-8 points: 66 & 95), the asymmetry of the absorption feature at 2205 nm was relatively constant with major anomalies found at the edges of concretions (e.g., in core-8 points: 35 & 66). The asymmetry of calcite was slightly reduced at the edges of concretion (i.e., in core-8 points: 41, 66 & 78) (Fig. 5). Overall, the absorption position varies from 2333 nm to 2335 nm (Fig. 5).

4.2. Imaging spectral data

MTMF and SAM algorithms were employed to classify SWIR images of the core and outcrop data. Based on facies associations description and field observations (Gani and Bhattacharya, 2007), four end-members were selected: channel facies, bar facies, carbonate concretions, and clay minerals. SWIR absorption features of clay minerals and calcite in spectral data collected for core-8 and core-9. For locations refer to Figs. 3 and 4. The red rectangles and green triangles correspond to calcite and kaolinite reflectance. Also, blue and red areas correlate with carbonate concretions in channel facies and bar facies, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Fig. 6. Four different facies found at Raptor Ridge outcrop and used for outcrop classification. Images were derived from a high resolution photomosaic image with a resolution of \( \sim 0.5 \) cm. (a) Carbonate concretions in channel facies. (b) Bar facies and carbonate concretions in bar facies. (c) Channel facies and distal facies. For complete image of Raptor Ridge please refer to Fig. 8.

Fig. 7. Core-8 and core-9 from Raptor Ridge; (Column a) core photograph; (Column b) false-color composite image with spectral bands 2195 nm, 2334 nm and 2152 nm displayed in RGB; (Column c) SAM classified image using U.S. Geological Survey spectral library from calcite and kaolinite; (Column D) normalized spectral depicting depth at band 2334 nm (calcite); (Column E) normalized spectra depicting depth at band 2200 nm (kaolinite). In column D and E, darker red means deeper absorption features, hence greater abundance. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
and distal facies (Fig. 6). Due to the high similarity between carbonate concretions in bar and channel facies they are classified together.

4.2.1. Core Samples

Core-8 and core-9 were only scanned with the SWIR camera where calcite concretions were located. SWIR images were acquired, pre-processed and classified using the methodology described in Fig. 1. Photographs of the scanned-core are shown in Fig. 7: column A. Fig. 7: column B depicts a false color SWIR image with spectral bands 2195 nm, 2334 nm and 2152 nm displayed as RGB. As a preliminary observation, carbonate concretions are displayed in pink and host rock sandstone (bar facies and channel facies) in green. Results of core image analysis revealed that the calcite cement in channel facies was homogeneously distributed from the edges to the center of the concretions, whereas, calcite cement at the concretions located in proximal and distal bar facies was less homogeneous and show interbedded thin layers of non-calcite cemented sandstone, where kaolinite was more abundant. The low abundance of clay minerals in the carbonate concretions of Core-9 can be observed in (Figs. 4 D, 5, and 7). This is not the case of Core-8 at around ~4.8 m, where inhomogeneity of the concretion is related to a contemporary fracture, where water could have dissolved the calcite.

4.2.2. Outcrop

For an initial interpretation of the outcrop data, true-color VNIR and coherent transformed MNF components were first examined (Fig. 8A & B). In Fig. 8B, spectral differences between carbonate concretions (depicted in bluish color) and the host rock (depicted in yellowish colors) are highlighted. In Fig. 8B, carbonate concretions are shown in cold colors (green/blue), whereas the host rock is shown in warm colors (yellow/red). With very similar spectra, channel and bar facies are not distinguished with this technique. Grey and black areas in Fig. 8 correspond to non-outcrop pixels and shadowed areas, and were removed for further classifications steps, to avoid misclassifications. The SWIR outcrop image was classified using SAM and MTMF classification algorithms (Figs. 9 & 10). The results were compared to each other and to previous studies to determine which technique performs better in siliciclastic rocks for hyperspectral image processing.

The spectra of end-members derived from the outcrop SWIR image itself, core SWIR, and ASD were used for SAM classification. MTMF classification results are illustrated in Fig. 9A. Carbonate concretions represent 10% of the outcrop while channel facies represent 54%, bar facies represent 32%, and distal facies represent 4%. In Fig. 9B, SAM classification results are shown based on end-members selected from the outcrop hyperspectral image. Similar to MTMF results, carbonate concretions represent 10% of the outcrop. Comparatively, bar facies were 28%, channel facies were 59%, and distal facies were 3% of the total outcrop exposure.

The SAM classification algorithm was applied using the hyperspectral data and spectral data collected in the laboratory from core samples as end-members (Fig. 9C & D). For the SAM classified image for the hyperspectral data collected in the laboratory, carbonate concretions also represent 10% of the outcrop. Bar facies are 48%, channel facies are 41%, and distal facies are 1% (Fig. 9C). These results were comparable with the ones obtained applying the SAM algorithm, with spectral data as end-members (Fig. 9D), where carbonate abundance is
15%, bar facies are 47%, channel facies are 37% and distal facies represent 1% of the outcrop exposure.

From the classification results, carbonate concretions are distributed subparallel to the outcrop as elongated and heterogeneous patches. Overall, all classification methods show a lateral change in facies at the NW part of the outcrop from bar facies to a more channelized sandstone. Channel facies are predominantly located at the base of the Raptor Ridge outcrop with a sharp contact at the base and top of each channel.

In order to visualize the relative cement abundance, well-ordered kaolinite, calcite, and artificial spectral mixtures of calcite and kaolinite (50/50) were extracted from U.S. Geological Survey spectral library data (Fig. 10). To create the artificial spectral mixture the reflectance spectra of both minerals were added. The reflectance spectra of well-ordered kaolinite (100% abundance), calcite (minimal abundance) and VNIR part of the spectra increases (e.g., Fig. 4D). The overall spectral reflectance of channel facies were slightly lower than bar facies, probably related to a slightly greater grain size (Figs. 3 & 4). The higher absorption minimum depth of kaolinite in bar facies vs. channel facies cannot be related to greater abundances in clay minerals, since there was a difference in grain size between the two facies. Besides, the depth of the absorption minimum of the kaolinite in carbonate concretions vs. sandstone host rock could be related to abundance. The presence of an absorption minimum at ~2335 nm in the concretions matches with the existence of calcite cement (Fig. 5). The depth of these absorption minimum values slightly increased at the edges and could be associated with a greater abundance of calcite.

Bar facies are tidally influenced deposits, which show interbedded-thin mudstones between sandstone beds. Calcite cement only precipitated in the sandstone host rock, giving a heterogeneous cement distribution throughout the core section. Calcite cement, which
5. Discussion

In general, when calcite is present, the overall reflectance at the spectral library), which matches previous sedimentological studies that suggested 10.9% abundance (Fig. 11). In the field characterization of cement was tedious and time consuming due to visual similarity with the host rock. Cement mapping using hyperspectral is a reliable and faster technique, and when combined with outcrop observations, improves characterization results.

Geometric variabilities due to the natural erosion nature of the outcrop might create inaccuracies in the classification results. Ground-based hyperspectral data can be draped over existing topography, providing integrated spectrally and geometrically accurate information (Okyay and Khan, 2016). Geometric reconstruction of the outcrop is beyond the scope of this study. Outcrop areas, which do not receive direct sun light, cannot be correctly classified, due to the lack of spectral information in these pixels. It was assumed that shadows are randomly distributed and classification results were normalized to obtain the final statistics and facies abundance. In this study, outcrop classification using endmembers from cores proved successful for facies that are spectrally different. However, spectrally similar facies (channel facies vs. distal facies) were difficult to classify.

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References


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6. Conclusion

In this study, datasets with different spectral and spatial resolutions were combined to extract information about diageneis in deltaic sandstone. The high accuracy of laboratory spectral data allowed a precise mineralogical characterization that was compared with other techniques and carbonate concretions are classified. Analysis of the spectral data revealed accurate information about mineralogical variations between facies association in Parasequence # 6 of the Frontier Formation. The study of Parasequence # 6 of the Frontier Formation at Raptor Ridge revealed that better classification results were achieved when using spectra from the image itself.

Classification results using ASD spectra and hyperspectral data collected in the laboratory were still comparable but far less accurate. Reflectance spectral studies revealed that calcite cement is homogeneously distributed within concretions in channel facies and is the major diagenetic constituent. Concretions at the bar facies present a more heterogeneous distribution with noncalkite interbedded layers following the direction of the bedding.

Normalized (shadowing and unclassified-removed pixels) classification results showed that the outcrop wall was composed of approximately 87 m² of bar facies, 150 m² of channel facies, 11.6 m² of distal facies, and 26.7 m² of carbonate concretions. This work demonstrates capabilities of imaging spectroscopy as a technique for geochemical characterization at the outcrop and laboratory scales.

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