Section S1: Systematic core analysis method for coal and non-coal coal bearing sedimentary lithotypes

Suggested Materials

- Viewing table with measuring tape
- Core logging form or digital logging software (WellCAD, Strater)
- Hand lens and 100x dissecting scope
- Measuring tape and appropriate scale bars
- Grain size scale
- Spray bottle with water to increase visibility of geological structures.
- 10% HCl solution to identify carbonate minerals
- Hammer, putty knives, and chisels
- Drillers Log, maps, and cross sections.
- Core wire logs (gamma and resistivity)

Procedure for general lithologic description

- Lay out the core to be analyzed on the viewing table.
- Check the amount of core with the coring report and ensure that no core material has been lost or missing, note breaks, damage, and missing sections.
- Check the numbering and order of boxes or containers against cumulative depth.
- Check core continuity and orientation with respect to the top of the core. Mark top of core.
- Check the order of core segments in the boxes; look for matching "breaks" or scribe marks from one piece to the next and from one box to the next.
- Measure and mark footage on each box. Mark core to the nearest 1 /2 inch (1 centimeter).
- If downhole gamma-ray logs are available, a comparison should be made with the core gamma-ray logs to verify that the cored interval depths are consistent with well log depths.
- Assess the entire cored sequence before commencing. Seek out and mark distinguishing features such as units, contacts, and unique markers (e.g., coal, mineralization, cementation).
- Record major features using standardized nomenclature and abbreviations
    - Core lithology (sandstone, siltstone, claystone, coal, limestone, etc.).
    - Color.
    - Bedding (thickness, bed contacts, erosional markers).
    - Obvious sedimentary structures.

- Texture (grain size, angularity/roundness and sorting).
- Composition (grains, cement, fossils).
- Porosity types.
- Diagenetic and tectonic features.

Coal Bed Descriptions

Visual descriptions of core are difficult to make unless the core is broken. Visual descriptions can be complemented with data from common down-hole, geophysical measurement techniques, such as gamma, gamma-gamma (density), and resistivity (Lavers and Smits, 1976). A high-resolution geophysical density log can provide data that aid in the identification of coal facies. High-resolution density logging also can provide measurements of thickness to the nearest 3 cm and a profile of the quality of the coal bed. X-ray radiography, combined with visual observation of the core and density log, provides another tool for recognizing the dominant facies in a core. Comparison of an X-ray radiograph to a density log can be used to: (1) discriminate between layers of pyrite, clay, impure coal, and coal; (2) determine which parts of the coal bed were not recovered in the core; and (3) identify the different facies of the coal bed.

Identification of carbonaceous shale

High-ash coal or mineral-rich partings generally are visually distinct in a coal bed. However, in most cases, criteria or tests cannot be applied objectively in the field to differentiate impure coal (25 to 50 weight percent ash) from carbonaceous shale (>50 weight percent ash). Any classification that involves such terms as "bone," "billy coal," or "rash" generally has only local significance and is not useful for coals of different rank or type (Schopf, 1960). Some field methods may provide aid in discriminating carbonaceous shale from coal. In surface mines, a gamma-ray scintillometer (a hand-held instrument) is used to locate impure layers in low-ash coal. For the drill core, an X-ray radiograph and a gamma-gamma (density) down-hole geophysical log can be compared with the coal core.

For sample collection from deep mines, no comparable instrument that is "mine safe" is available. This deficiency in instrumentation creates difficulty when applying the exclusionary procedure. However, even if this procedure is not followed, another difficulty exists in precisely sampling a coal bed at the points of contact with adjacent rock strata. Commonly, coal bed contacts between the floor and roof rocks are sharp. However, in places, contacts are interbedded, transitional, or located in a non-banded layer, particularly at the top of the bed.

These procedures (Procedure A, B, and C) have been adapted from *METHODS FOR SAMPLING AND INORGANIC ANALYSIS OF COAL U.S. Geological Survey Bulletin 1823 Edited by D.W. Golightly and F.O. Simon. Major differences from the U.S.G.S. procedure referenced herein have been developed by the University of Wyoming Center for Economic Geology Research in collaboration with the National Energy Technology Laboratory to better achieve high resolution depth profiles of collected core to pair with state of the art geochemical evaluation in use for NETL-URC and related coal assessment strategies currently in development.

Procedure for high resolution sampling of drill core

Drill core collected for purposes of high-resolution spatial and geochemical data should be representative of the coal sediment system including both the coal seam(s) itself and over- and under-burden sediments. Newly collected core is the most useful despite core segments often being lost during coring operations. If the complete bed is not represented by the recovered drill core, the missing intervals need to be noted. Often, this will be critical information provided by the driller on site, or by the mine geologist who is most familiar with the coal being targeted. Therefore, the most useful data comes from coal core collected while a member of the analysis team is present. Down hole geophysical log techniques should be used to compare the total coal sediment system thickness to recovered core thickness.

Once the coring barrel is brought to the surface, collection of core will involve one or all of the following procedures depending on how much of the core is retained by the owner, and how much made available to the analysis team:

I. Full Core Collection:

In this method an entire core is collected and will be sent to the analysis team's laboratory for additional analysis. That is, no splits nor segments are removed in field.

- Split the core barrel open by removing top core barrel segment and arrange tape measure along the bottom core barrel at the correct depth from surface to the core barrel top end. This measure will carry over to each subsequent core barrel, moving the bottom measurement to the top of the next core barrel etc. Take precise notes from the driller as to any depth corrections noted by the drill rig including lost interval(s). Likewise note any core barrels which are not completely full, as these could also indicate lost intervals.

- Photograph core in its entirety and along segment sections of the core. Make sure the tape measure is visible in all photographs.
- Describe the core using major features of the coal sediment system noting observations to specific depths (bedding, lithology, pyrite horizons, contacts, etc…). These field descriptions will be used as reference later in the assessment process. More detailed core descriptions will take place in the laboratory using Appendix A of this document as a guide.
- Segment the core into usable vertical lengths dictated by the core box/core storage system size. This is usually 2 or 3 foot segments to fit standard core box sizes.
- Slide each core segment into core sleeves, seal to prevent moisture loss and/or contamination, and mark core bags for top and bottom, and core depths per foot interval. Then transfer to core boxes arranging each segment so core is organized top to bottom.
- Record core name, core depth interval, and any relevant notes on core box. Label each core box with a unique number (i.e. 1, 2, 3…) and record in field book. Take a photograph of each loaded core box with label showing.
- Tape lids on core storage boxes to guarantee safe transport to laboratory.
- Once in the laboratory, use Section C for Direct Core Material Sampling methods and/or Section B for Partial Core Split procedures.

II. Partial Core Split:

In this method the core is split along its length in the field so half can satisfy archival sample collection and/or reporting requirements for coal mines providing core materials. The other half of the core segments will be sent to the analysis team's laboratory for additional analysis.

- Once core has been segmented in to 2 or 3 foot segments for core boxes, identify and take notes on segments that are competent vs incompetent to plan for core splitting.
- For competent core, it may be necessary to use a wide blade chisel and hammer to lightly tap the core in half along the mid line. Be careful to not disrupt adjacent core or throw material into other segments (avoid contamination). Once split, slide the interval down the core barrel for collection in core bag. For incompetent core, brace the material in the core barrel with a clean gloved hand and slide it in the core barrel for collection in

a core bag. You may need several helpers for this step if the coal is highly fractured.

- Place a 2 or 3 foot long straight painters' edge into the middle of the split core to physically divide the core in half.
- For each segment of core, slide a core collection bag over the end of the coring barrel half and carefully push the core into the collection bag.
- Seal each core collection bag to prevent moisture loss and/or contamination, and mark core collection bags for top and bottom, and core depths per foot interval. Then transfer to core boxes arranging each segment so core is organized top to bottom.
- Record core name, core depth interval, and any relevant notes on core box. Label each core box with a unique number (i.e. 1, 2, 3…) and record in field book. Take a photograph of each loaded core box with label showing.
- Tape lids on core storage boxes to guarantee safe transport to laboratory.

III. Direct Core Material Sampling:

Once core boxes have been brought into the laboratory, a number of preparation steps are required prior to taking individual samples. Moisture content of coals is a standard measurement. However, for state of the art geochemical analysis, moisture should be removed the core material to stop any geochemical reactions currently underway in the core and also inhibit mold and other biological processes that have the ability to alter elemental/isotopic measurements.

1. Place core boxes in order of depth and open lids with core bags remaining inside the core boxes.
2. Slice vertical incisions down the length of each core collection bag. Be careful to not contaminate core collection bags from the previously cut segment. Clean the cutting blade between each bag.
3. Once the core bags have been opened, proceed with detailed observations/notes regarding the core. Core descriptions will provide useful information in conjunction with Appendix A (taken from U.S. Geological Survey Bulletin 1823) details below. Precise core descriptions are critical and provide a useful when tying geochemical data back into coal sediment system assessments.
4. Allow air circulation to dry the coal core in place. This may require the use of a fan or air handling system such as a laboratory hood. Core box lids can be partially propped

over the open core to keep debris from falling in. However, air circulation should not be interfered with. It may take days to even weeks for coal core to dry completely and assure biological processes are not progressing. In humid environments, dehydration equipment and additional airflow may be needed to complete this step.

5. Once core is dry, mark depths along the outside of the core collection bags using a permanent marker. Double check depth of segments and cross reference notes from the drilling operation and core log. Mark one foot intervals for the entire collected core.
6. You will want to collect a coal sample at a minimum of every foot through the entire coal segment as well as sampling the roof and floor external to the coal seam itself (grid sampling). Bias the first coal sample (top of the coal seam) to be collected within the upper most foot of the coal seam represented by the collected core. For coal seams with abrupt contacts to the roof, six inches from the upper boundary has shown to be a reliable starting point. For gradational or in obvious contacts, it is better to sample in what appears to be the upper most inch or two of coal and work down core from there.
7. The bottom of the coal seam(s) should be biased in the same way the top coal was selected. This may alter the grid spacing for the lowest coal seam sample, but it is of utmost importance to collect a sample within the lowest one foot interval. Follow the procedures for abrupt vs gradational contacts in step 5 above.
8. Once the location of the initial coal sample has been selected, mark a grid every foot above and below the initial sample to assemble a grid of the entire core. Tape or paper tabs with location of each sample are useful for reference. Photograph the marked grid and all core prior to sampling.
9. Take a sample at each grid location and put into a sealed sample bag, correctly labeled and photographed:
    a. For whole core, remove a one inch thick segment from each location, but leave half of the core width in place. This allows reference in the future via handheld XRF methods, etc… and/or secondary/verification sampling.
    b. For split core, remove a one inch thick segment from each location. Due to sample size requirements of geochemical procedures, you will

not be able to leave material for each inch collected. Sample the entire one inch segment and put into labeled and photographed sealed sample bags.

10. Allow sealed sample bags to sit for 24-48 hours prior to next analysis steps. This will verify that all moisture has been removed. Should condensation occur within a sample bag, open the bag and allow it dry for completely before moving into next steps.

11. Once all samples are sealed and ready for geochemical measurement, follow analysis methods for TGA or furnace ashing and geochemical analysis by ICP-OES & ICP-MS.

Section S2

Table S1. Prioritization of data and information collected from geologic samples

Category	Fields	Level of Importance	Suggested / Example Responses
Sample Identification	**Unique ID/Sample ID**	**critical**	
	Project ID	if known	
	Lab ID	if known	
	Field ID	if known	
	Stratigraphic ID (USGS COALQUAL database)	if known	
	API number	if known	
	Other alias	if known	
Sample Description	**Sample material**	**critical**	coal, parting, seam rook rock, seam floor rock
	Sample type-hand sample 1	**critical**	single rock hand sample, bulk rock hand sample (multiple pieces from same coal measure)
	Sample type-hand sample 2	**critical**	in situ, float
	Sample type-underground	**critical**	drill core, underground mine
	Sample type- coal ash	**critical**	fly, bottom, ponded, landfill
	Sample type- aqueous-by-products	**critical**	waste water residue, coal mine drainage, runoff, other
	Sample Thickness [cm]	important	
	Sample location within stratigraphy or coal seam	important	seam, roof, floor, parting
	Coal seam thickness [meters]	important	
	Coal seam name (if different from stratigraphic name)	important	
	Stratigraphic unit association of coal seam	important	Formation, Group, Member, bed
	Geologic age of coal seam (Period or Epoch)	if known	e.g., Pennsylvanian
	Sample status	important	representitive sample exists, sample destoyed (destructive sampling), archieve
	Photos	if known	photo number; file location; point of contact
	Sample description (other relevant info)	important	
Geolocation	**Latitude**	**critical**	
	Longitude	**critical**	
	Depth	**critical**	negative if collected from core
	X	**critical**	e.g. UTM
	Y	**critical**	e.g. UTM
	Z	**critical**	e.g. UTM
	datum	**critical**	
	spheroid	if known	

Category	Fields	Level of Importance	Suggested / Example Responses
Geolocation cont'd	projection	if known	
	township	if known	
	range	if known	
	City (nearest)	if known	
	County	if known	
	State	if known	
	Country	if known	
	Sedimentary basin	if known	
	Coal field	if known	Enter name of coal field. Refer to USGS Open File Report 2012-2015
Site Characteristics	**Unique site ID**	**critical**	name
	Company, Owner, Operator	**critical**	name
	Physical setting or environment	important	e.g., collected from roadcut along Hwy 99
	Development status 1	important	public property, private property
	Development status 2	if known	commercial, residential
	Lithology of rock contacting upper coal seam	important	e.g., sandstone
	Lithology of rock contacting lower coal seam	important	e.g., shale
	Clay present (observed) in coal seam / core	important	yes, no
	Depth of coal seam from surface, overburden [meters]	important	
	Proximity to igneous/metamorphic rock nearby [kilometers]	if known	
	Outcrop / core condition	if known	fresh, weathered
	Local geologic structure	if known	antiform, anticline, synform, syncline, monocline
	Faults observed in outcrop/core	if known	yes, no
	Proximity to nearby fault (if observed) [kilometers]	if known	
	Proximal fault type (if present)	if known	normal, reverse, strike slip, vertical, unknown
	Coal cleat observed	if known	yes, no
	Most likely mechanism of REE concentration	if known	volcanic ash-fall, meteoric enrichment, hydrothermal enrichment, other, unknown
	Tonnage and grades of commodity oxides (mine site)	if known	
	Key comments (any comments relevant to day of sample collection)	important	
	Picture/Photo	if known	e.g., file number or URL for download
Collection Information	**Project ID / Lab ID**	**critical**	
	Name of sample collector	**critical**	name
	Date Collected	**critical**	YYYYMMDD
	Date Catalogued	important	YYYYMMDD
	Date Analyzed	important	YYYYMMDD
	Date Analyses Published	if known	YYYYMMDD
	Date uploaded to EDX	if known	YYYYMMDD

Category	Fields	Level of Importance	Suggested / Example Responses
Other Metadata	**Contact info - principle investigator / project coordinator**	**critical**	name, email, phone
	Contact info - lab	**critical**	name, email, phone
	Contact info - sample collector	important	name, email, phone
	contact info - sample curator	important	name, email, phone
	Link or source to other data or studies associated with samples	important	
	Data uploaded to Energy Data Exchange?	important	yes, no
Chemical Analysis	**Sample ID**	**critical**	
	Lab ID (of the sample; if different from Sample ID)	**critical**	
	Laboratory where analyses completed	**critical**	
	Analysis technique	**critical**	XRF, ICP-MS, INAA
	Sample preperation method	**critical**	
	Whole rock or ash yield?	**critical**	Whole sample, ash
	Coal rank	if known	lignite, sub-bituminous, bituminous, anthracite
	Alteration	important	indicate type
	REE-bearing minerals identified in the coal	if known	indicate type
	Other significant minerology	if known	
	Elements [ppm]	**critical**	Li, Be, B, F, Na, Mg, Al, Si, P, Cl, K, Ca, Sc, Ti, V, Cr, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Rb, Sr, Zr, Nb, Mo, Ag, Cd, In, Sn, Sb, Cs, Ba
	Lanthanides [ppm]	**critical**	La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Y, Ho, Er, Tm, Yb, Lu
	Other metals [ppm]	important	Hf, Ta, W, Hg, Tl, Pb, Bi
	Actinides [ppm]	important	U, Th
	Total REE concentration (whole rock) [ppm]	**critical**	
	Total REE + Y concentration (whole rock) [ppm]	**critical**	
	Total REE concentration (ashed)	**critical**	
	Total REE + Y concentration (ashed)	**critical**	
	Oxides [ppm]	important	Al_2O_3, SiO_2, CaO, K_2O, TiO_2, Fe_2O_3, MgO, Na_2O, MnO, P_2O_5
	Radiometric age [Ma]	important	
	Sulfur [wt %]		
	Moisture content [wt %]	important	
	Volatile matter content [wt %]	important	
	Fixed carbon content [wt %]	important	
	Ash yield [Dry, wt %]	important	
	Carbon [%]	important	
	Hydrogen [%]	important	
	Sulfur [%]	important	
	Oxygen [%]	important	
	Nitrogen [%]	important	
	Vitrinite Reflectance [%Ro]	if known	