MAINTENANCE OF THE COAL SAMPLE BANK AND DATABASE

Final Technical Report

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ABSTRACT

This project generated and distributed coal samples and accompanying analytical data for use in research by DOE contractors and others. All activities specified under the five-year contract (as revised) and a six-month no-cost extension have been completed.

Eleven DECS samples were collected, processed to a variety of particle sizes, heat-sealed in foil laminate bags under argon, and placed in refrigerated storage. All were analyzed for basic chemical composition, inorganic major and trace element composition including hazardous air pollutant elements, petrographic composition and characteristics, thermoplastic behavior (if applicable), and other properties relevant to research and commercial utilization. Most were also analyzed by NMR, py/gc/ms, and a standardized liquefaction test; trends and relationships observed were evaluated and summarized. Twenty-two DECS samples collected under the previous contract received further processing, and most of these were subjected to organic geochemical and standardized liquefaction tests as well. Selected DECS samples were monitored annually to evaluate the effectiveness of foil laminate bags for preserving samples in long-term storage.

In addition to the 33 DECS samples, 23 PSOC samples collected under previous contracts and purged with argon before storage were also maintained and distributed, for a total of 56 samples covered by the contract. During the 5.5 years, 570 samples in 1,586 containers, 2,109 data printouts, and individual data items from 34,208 samples were distributed. All DECS samples are now available for distribution at minus 6 mm (-1/4 inch), minus 0.85 mm (- 20 mesh U.S.), and minus 0.25 mm (- 60 mesh U.S.).

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EXECUTIVE SUMMARY

Maintenance of the Coal Sample Bank and Database

Final Technical Report 9/28/1993 - 3/30/1999

The mission of the DOE Coal Sample Bank and Database is to provide a variety of well-characterized, high-quality coal samples for public and private coal research. Eleven coal samples collected under the current contract and 45 from previous contracts, along with analytical data, are distributed on a continuing basis to DOE contractors and others performing coal research.

Additional analyses of liquefaction behavior and organic geochemical characteristics revealed through py/gc/ms and NMR studies were performed under the contract. The samples are stored to minimize deterioration, and 10 samples were analyzed annually to monitor the effectiveness of the storage methods. Foil laminate bags purged with argon gas and stored under refrigeration were shown to perform well in preserving the properties of the coal samples.

This report reflects the level of effort described in the revised work statement submitted to DOE on September 5, 1996, setting out a reduction in effort following a cut in the level of funding of the project.

INTRODUCTION

This five and one-half year project was performed to ensure the availability of well-characterized, high-quality coal samples for public and private coal research. It continued support of the DOE Coal Sample Bank and Database at The Pennsylvania State University, an effort which followed projects funded first by the Office of Coal Research, then the Energy Research and Development Administration, and several successive contracts with the Department of Energy. No further funding is planned by DOE.

Eleven coal samples in the DECS- series have been collected, processed, packaged, and extensively analyzed under the contract, and a resulting database is being maintained. These samples and data, as well as 22 DECS samples and 23 PSOC samples collected under previous contracts, were distributed on an ongoing basis to DOE contractors and others performing coal research.

Samples were chosen to maintain a sample bank of 56 coals representing the major U.S. coal fields and a variety of coal ranks and compositions. In addition to standard analyses, liquefaction tests and organic geochemical analyses (NMR, py/gc/ms) have been performed. The DECS samples employ advanced storage techniques (foil laminate bags purged with argon, heat-sealed and refrigerated) to minimize deterioration; ten are monitored annually by proximate, sulfur forms, calorific value, and gaseous oxygen analysis to evaluate their condition. In the fourth year, additional monitoring was performed to evaluate the influence of various storage methods. The monitoring program showed that foil laminate bags continue to preserve the samples well.

RESULTS AND DISCUSSION

Task 1. The Coal Sample Bank

Task 1A. Initiation of Sample Bank Activities

This contract continued support of a previous sample bank and database at Penn State, so activities commenced immediately. Coal samples and data were already located at Penn State; the inventory and procedures for storage, selection, retrieval and distribution were in place and fully functional. Samples and data were available for distribution from the first day of the contract.

Task 1B. Storage and Inventory of Samples

All samples supported by the contract are stored in containers purged with argon before sealing; container locations are tracked by a computer inventory program. PSOC-series samples are stored in drums or buckets at the Coal Sample Bank building, or in cans in the Coal and Organic Petrology Laboratories. All DECS-series samples are stored in foil laminate bags; the methods by which they are processed and packaged are discussed under Task 1D.

Refrigerated Storage for all DECS samples

During the previous contract, a 4.25 cubic meter (150 cubic foot) refrigerator had been acquired to store the candidates (DECS-15, -16 and 17) for the special dispersed catalyst liquefaction sample. The refrigerator was also used to store part of the set of 300g foil laminate bags from each successive sample DECS-18 through -22 collected later in that contract. As planned, four months after the inception of the subject contract a larger refrigerated storage facility became available. All containers of all DECS samples were moved to this 164 cubic meter (5,780 cubic foot) refrigerated room. All samples collected under the current contract have been stored under refrigeration for their entire history. The retardation of coal deterioration at lowered temperatures has been reported by Beier (1983), Dutcher et al. (1985), Wu et al. (1988), Huggins and Huffman (1989), and Davidson (1990).

Computerized Inventory Tracking

At the completion of processing of each DECS sample, data (bag number, weight, mesh size, storage location, etc.) for each foil laminate bag are entered in a computerized inventory program. When an order for samples is received, the program is queried and the locations, weights and particle sizes of the available bags are displayed or printed. After the bags desired have been removed from the physical inventory, the program is used to transfer their entries to a separate transactions file, and data identifying the recipient are added and stored there as well. Summaries of samples distributed and their recipients may be created from the transactions file.

The program used under the contract stores its files in the format of a commercial data management package, so both the main file and the transactions file can be examined and manipulated with a wide range of commands if the inventory program does not provide the functions required. This is also the format of the Coal Database, so although the inventory and the Database are normally completely separate, they can be merged if needed for specific tasks.

Use of these programs after December 31, 1999, will be curtailed and will be terminated before June 1, 2000, because of year 2000 compliance problems and limited usage of the operating system under which they run. Like the Penn State Coal Database (see Task 2A), after the completion of the subject contract the data files were transferred to personal computers for continued use.

Task 1C. Monitoring of Sample Condition after Storage

The final report for the previous contract (Davis and Glick, 1993) detailed the studies of deterioration of coal samples in conventional containers, and subsequent testing and adoption of foil multilaminate bags for storage of all DECS samples. These bags were suggested for coal sample storage durations of one month by Sharp (1986). Under the previous contract, their success in preserving samples for up to 3 years was demonstrated. In the subject contract, monitoring was continued in order to examine preservation over a longer term (up to 9 years for the earliest DECS samples) for samples with a variety of sulfur contents, calorific values, and thermoplastic behavior. Processing and sealing of DECS samples under argon in foil multilaminate bags is described under Task 1D. PSOC samples were not tested, as extensive analyses had been performed under the previous contract and the storage containers used for PSOC samples have been superseded.

DECS samples were tested by a variety of methods as described below. Appendix A presents the results of up to nine years of monitoring which was instituted with initial analyses of the first DECS samples in 1990. Under the previous contract and the first year of the subject contract, all DECS samples were monitored each year. Following funding reductions, the number was reduced to 10 samples per year, selected to represent groups of samples based on rank, sulfur content, and thermoplastic behavior. In some annual monitoring programs, additional samples were analyzed for specific research goals.

Table 1 shows ASTM repeatability and reproducibility values for analyses used in monitoring. See the appropriate ASTM standard (ASTM, 1998) for details on application of the values shown. In general, it is the reproducibility values which are appropriate for evaluating results in this study, because over a period of several years, equipment and operators are likely to change, even though the same laboratory continued to provide each specific analysis through the entire study.

Table 1. ASTM repeatability and reproducibility values

ASTM Procedure	Repeatability	Reproducibility
Moisture, D3173-87		
coals < 5% moisture	0.2	0.3
coals > 5% moisture	0.3	0.5
Volatile Matter D3175-89a, %		
anthracite	0.3	0.6
semianthracite and bituminous	0.5	1.0
subbituminous	0.7	1.4
lignite	1.0	2.0
Ash, D3174-97, %	0.22	0.32
Total Sulfur, D4239-97 method C (IR), %	$0.02 + 0.03\bar{x}$	$0.02 + 0.09\bar{x}$
Calorific Value (dry basis), D2015-96		
bituminous	39 cal/g (69 Btu/lb)	60 cal/g (107 Btu/lb)
subbituminous and lignite	33 cal/g (59 Btu/lb)	78 cal/g (140 Btu/lb)
Forms of Sulfur, D2492-90		
Sulfate, %	0.02	0.04
Pyritic, %	$0.08 + 0.09\bar{x}$	$0.15 + 0.27\bar{x}$
Gieseler Plastometer, D2639-90		
Temperature points, °C	5	not specified
Fluidity, ddpm	$0.1\bar{x}$	not specified
Carbon, D3178-89, %	0.3	not specified
Oxygen, D3176-89, %	not specified	not specified

Proximate Analysis

Short proximate (moisture and ash) analyses were performed in each case. The use of foil laminate bags for coal samples had initially been demonstrated to preserve moisture and calorific value in subbituminous coals for storage times of one month (Sharp, 1986). Appendix A shows that moisture levels are preserved well for the length of the study; in particular, see

samples DECS-1, -8, -10, and -11, the low-rank, high-moisture samples which have been monitored over a period of at least eight years. Although the variation in readings is slightly beyond ASTM reproducibility limits, there is no trend of moisture loss.

Ash yield was not investigated as an indicator of preservation, but does serve as an indicator of the representative splitting which was performed, and would be needed if calculations for an ash-free or mineral-matter-free basis of expression were performed.

Volatile matter was not monitored each year but final values after storage are available for selected samples and can be compared to initial values (Table 2).

Table 2. Changes in volatile matter, carbon and oxygen after storage in foil laminate bags.

DECS	years in storage	Volatile Matter, % dry coal		Carbon, % dry coal		Oxygen (by difference), % dry coal	
		initial	final	initial	final	initial	final
1	9.1	47.40	49.57	62.53	62.79	14.69	16.87
2	8.9	38.14	37.39	65.49	64.90	8.16	8.89
3	8.6	27.19	27.29	82.68	83.24	4.09	4.14
5	8.4	40.33	40.56	72.70	72.47	12.11	12.36
8	8.4	45.23	43.80	64.14	65.52	15.93	16.65
10	8.2	41.67	46.78	68.37	67.41	13.30	13.48
11	8.1	56.08	54.41	66.15	65.93	18.62	21.45
12	8.6	36.02	36.48	74.78	73.97	7.51	8.01
14	8.1	32.59	33.10	76.24	76.55	5.25	4.98
17	7.6	46.75	47.61	76.25	75.81	9.65	10.16
18	7.3	41.18	40.53	69.39	69.83	7.80	8.69
19	6.6	18.31	18.08	85.74	85.30	3.16	3.04
21	5.8	4.51	4.31	80.26	84.05	3.82	1.96
23	3.6	39.42	40.57	74.21	73.70	6.03	6.09
24	3.0	40.83	42.78	66.05	66.85	9.30	8.03
25	4.5	41.98	42.51	65.76	65.19	16.13	21.00
29	3.6	34.30	34.33	81.08	81.13	5.31	5.59
30	3.6	30.13	30.40	84.41	83.61	4.25	5.02
33	3.6	43.06	43.57	69.51	69.05	8.43	8.89

Sulfur Forms

Sulfur forms analyses were conducted in order to monitor the oxidation of sulfides (pyritic sulfur) to sulfates. This is a sensitive indicator of deterioration of coal samples in storage (Huffman et al., 1985); poorly protected high-sulfide samples can experience oxidation of half of their pyritic sulfur to sulfates over a period of several years (Davis and Glick, 1993). Starting with 0.00 or 0.01 percent sulfate sulfur in the coal, they may reach 1.0 to 2.0 percent after 5 years. Stored under argon in foil laminate bags, most samples show no trend of increase, and only random changes within a 0.06 percent range. Figure 1 shows linear regression trends for the 12 samples stored and analyzed at least 4 times over a period of at least 5 years. All but two of these samples yield a regression line which does not differ from 0.00 % by more than the 0.04% ASTM reproducibility limit for at least 10 years. DECS-15 is within 0.04% of its lowest measured value (0.02%) for that time period. The only outlier is DECS-18, a high pyritic sulfur coal from the Interior Coal Province. After 4 years of 0.04% sulfate sulfur or less, its final two monitoring analyses (Appendix A) yielded levels above 0.10%, causing the steep slope of the regression line.

Figure 1. Change in sulfate sulfur after storage in foil laminate bags (linear regression lines). Numeric labels indicate DECS sample numbers.

Calorific Value

Calorific value is a useful indicator of deterioration, particularly for those samples which do not exhibit fluid behavior or high pyritic sulfur levels. Poorly protected samples may lose 100 Btu/lb on a dry basis (the ASTM reproducibility limit) per year (Davis and Glick, 1993). Figure 2 shows the succession of calorific value analyses for 12 samples measured over at least 7 years.

Figure 2. Change in calorific value after storage in foil laminate bags. Numeric labels represent DECS sample numbers.

Gieseler Plastometry

Thermoplastic behavior as measured by the Gieseler plastometer is another sensitive indicator of deterioration, but can only be used for those bituminous coal samples which exhibit fluidity upon heating. Davidson (1990) notes the agreement between many researchers on the sensitivity of this technique. The analysis provides an initial and final temperature between which fluidity occurs, and from which a fluid temperature range can be calculated, as well as a maximum amount of fluidity. Both fluid temperature range and the maximum fluidity decrease as coal deteriorates in storage, but the former is a more stable indicator and was used in this

study. Poorly protected samples vary in their loss of fluid temperature range, but it is typical for half of the range to be lost in two to three years (Davis and Glick, 1993). Figure 3 includes all DECS samples monitored by Gieseler plastometry over at least 7 years. New data for PSOC-1536, the medium volatile bituminous sample used in the preliminary study under the previous contract, are also included. The figure shows that storage under argon in foil laminate bags preserves fluid temperature range well for most samples.

Figure 3. Change in Gieseler fluid range after storage in foil laminate bags. Numeric labels represent DECS sample numbers.

Gaseous Oxygen

A polarographic analyzer was used to measure gaseous oxygen within the foil laminate bags just prior to their being opened for analysis. These results are shown in Appendix A. Nearly every result showed oxygen to be below 0.10 %, so no trends could be discerned.

Ultimate Analysis

Ultimate analysis was not used routinely but initial (as part of basic analysis) and final data are available for 19 samples. Table 2 shows the change in carbon and oxygen with time in storage. Relationships between C, O, and the other indicators described above were investigated, however, the efficiency of foil laminate bag storage in preserving these indicators hindered observation of such relationships. Variability in oxygen values, caused by accumulation of errors in its calculation by difference from other values in the ultimate analysis, also contributes

to the difficulties. Figures 4 and 5 illustrate that changes in C and O may be positive or negative, and tend to center near zero change, even after several years in storage.

Among the stronger relationships is that between change in carbon and change in calorific value. Figure 6 shows that samples which lost calorific value during their years in storage tended to also lose carbon, and those which gained calorific value also tended to gain carbon.

Figure 6. Change in calorific value with change in carbon for DECS samples monitored.

Task 1D. Collection and Processing of Replacement Samples

Samples were collected to replace PSOC samples from earlier contracts. The goal in each case was to collect a sample which represented the entire thickness of the seam. Whenever feasible this was achieved by collection of a channel sample of the full seam. For particularly thick seams, lack of access to the entire seam, coupled with the quantity per unit thickness required to achieve a representative sample, made a channel sample inappropriate. In these cases a run-of-mine sample (DECS-26) or drill cutting sample (DECS-27) was collected. Collection was undertaken from active sections of mines in order to obtain fresh, recently exposed coal. Each

sample was collected by Penn State personnel in order to ensure consistent methods for collection and immediate efforts to minimize deterioration.

Bulk samples of at least 180 kg (400 lb) were placed in steel drums outfitted with high-density lid gaskets and valved inlet and outlet ports as shown in Figure 7. This method was a modification of that used for the Illinois Basin Coal Sample Program (Harvey and Kruse, 1988; Kruse, 1989). The valve bodies were machined so that the valve body outside the drum lid and the O-ring sealing fixture inside the lid held the sheet metal of the drum lid securely between them. Two such assemblies (inlet and outlet ports) were fitted to holes in the drum lid. The inlet port had a stainless steel tube extending through the coal to the bottom of the drum for argon introduction. The outlet port provided a valved hole for the air to escape at the opposite end of the container from the argon introduction tube. During purging, argon flowed from the tube at the bottom of the drum up through the coal sample, displacing the lighter air and expelling it at the outlet port. The valves were closed to capture a slight positive pressure of argon inside the drum, and this pressure was monitored periodically while the drums were in the contractor's possession in the field to determine whether additional argon was needed to maintain positive pressure and prevent infiltration of air. This storage method was used only until the samples were returned to Penn State and processing began.

Where large blocks of coal were available for collection at the mine, a number of these were also obtained and sealed in foil laminate bags purged with argon. Such blocks will not match perfectly with the analysis of the bulk sample because of the natural heterogeneity of coal seams, but they are required for certain research. There has been a significant demand for these blocks.

Samples and Sample Types Collected

The contract had been intended to replace the 34 remaining PSOC samples funded by DOE, but reductions in funding lead to only 11 new samples being collected. In combination with the 22 existing DECS samples, the 11 were selected to achieve a balance of ranks, geographic representation, geologic age and characteristics, organic components, and inorganic composition, as well as correspondence to the Argonne Premium Coal Sample series (Table 3). After approval by DOE, the samples described below were collected.

DECS-24 is a whole-seam channel sample of the hvCb Illinois #6 seam collected from an underground mine in Macoupin County, Illinois on June 2, 1994. This sample is comparable to that used for the concurrent HRI liquefaction contract, so expected demand was high and a large sample (270 kg) was therefore collected. A large quantity of associated blocks of coal, to be kept separate from the channel sample, was also collected. These were intended to be used in particular for Task IG and contract DE-FG22-93PC93223, Surface Properties of Photooxidized Bituminous Coals. Processing of this sample began on June 13, 1994, at Penn State.

Figure 7. Apparatus for inert gas purging of samples stored temporarily in 113 liter (30 gallon) steel drums (from Davis and Glick, 1993).

Table 3. Correspondence of Argonne Premium Coal Samples to DECS samples (Smith and Smoot, 1988; Vorres, 1989)

Argonne Sample	Coal Seam	State	DECS sample from same seam and mine	DECS sample from same seam, nearby mine
APCS-1	Upper Freeport	PA		
APCS-2	Wyodak-Anderson	WY	DECS-8	DECS-26
APCS-3	Illinois #6	IL	DECS-2	DECS-24
APCS-4	Pittsburgh (#8)	PA	DECS-12	DECS-23
APCS-5	Pocahontas #3	VA		DECS-19
APCS-6	Blind Canyon	UT	DECS-6, -16, -17	
APCS-7	Lewiston-Stockton	WV		DECS-32
APCS-8	Beulah-Zap	ND	DECS-11	

DECS-25 is a whole-seam channel sample of the Pust seam (lignite) in Richland County, Montana, collected on June 6, 1994. Because of the nature of the fresh exposures of coal, channel samples were collected separately from the upper and lower benches in the surface mine and combined based on the relative thicknesses of the two benches. Separate block samples were also collected.

DECS-26 is a run-of-mine sample of the subB Wyodak seam in Campbell County, Wyoming. This sample corresponds to the coal concurrently used for an HRI liquefaction project. It was collected from a surface mine on June 9, 1994, in multiple cuts from an automatic sampler on an overland conveyor belt system. A large sample was taken because demand is expected to be high for HRI samples and for Wyodak samples. Separate block samples were also collected.

DECS-27 is a whole-seam auger drill cutting sample of the subA Deadman (D-31) seam in Sweetwater County, Wyoming. It was collected from a surface mine on June 10, 1994, as a composite of material from 10 separate drill holes within a 10 meter diameter area. Blocks directly related to the sample were unavailable because of comminution of the exposed coal surface.

DECS-28 is a whole-seam channel sample of the hvCb Green seam from a surface mine in Navajo County, Arizona. It was collected June 13, 1994, and separate blocks were also taken.

DECS-29 is a whole-seam channel sample of the hvAb Upper Banner #3 seam collected from a surface mine in Dickenson County, Virginia, on June 19, 1995. At this site the Upper Banner is split into four separate seams, numbered 1 through 4 from bottom to top; they are exposed in separate pits in the mine. This channel sample was collected from the #3 split; separate block samples were also collected. It was later determined that the coal was somewhat oxidized prior to collection. Initial processing of this sample was accomplished on June 28.

DECS-30 is a whole-seam channel sample of the mvb Splash Dam seam from Buchanan County, Virginia. The sample was collected on June 20, 1995, from an underground mine; the coal had been exposed less than two days prior to collection. Separate block samples were also collected. Initial processing was performed on June 29.

DECS-31 is a whole-seam channel sample of the Pond Creek seam collected on June 21, 1995, from an underground mine in Pike County, Kentucky. The coal had been exposed less than two days; block samples were also collected. Initial processing was performed on June 27.

DECS-32 is a whole-seam channel sample of the Stockton-Lewiston seam collected on June 23, 1995, from an underground mine in Kanawha County, West Virginia. The coal had been exposed approximately 20 hours prior to collection of the sample. Separate block samples were also collected. Initial processing was accomplished on June 26.

DECS-33 is a whole-seam channel sample of the Ohio #4A seam collected from an underground mine in Meigs County, Ohio, on July 25, 1995. The coal had been exposed less than two days prior to collection. Initial processing of this sample was accomplished on July 27.

Sample Processing and Packaging

The procedures for processing of samples were similar to those developed under the previous contract (Davis and Glick, 1993) and the following discussion is drawn from that final report, incorporating changes made during the current contract. The method creates representative subsamples at three particle sizes, in foil laminate bags of appropriate size. The steel drums packed at the mine are weighed and opened. Large pieces are broken with a hammer and the entire sample is briefly air-dried if required to avoid clogging the crushing equipment. The entire sample is crushed in a hammer mill with no plate installed, to yield nominal minus 25 mm (-1") particles. The general scheme, which requires some adjustment for individual samples based on total amount collected, is shown in Figure 8. These adjustments vary the fraction of coal crushed to minus 0.85 mm (-20 mesh) in order to obtain the constant quantity (75 kg, 165 lbs) needed for the final splits into 256 small bags.

The coal destined for the 256 bags is riffled into 8 splits, each of which is crushed to minus 0.85 mm (-20 mesh). Each split is then riffled into four, producing 32 splits of approximately 2.3 kg (5.0 lb), which are sealed under argon in foil laminate bags. Together with all splitting of minus 6 mm material, this constitutes the initial phase of processing, concluding with all samples sealed in foil laminate bags.

Figure 8. Typical crushing and splitting steps for a DECS sample.

For the second phase, an 8-tube rotary divider is used to divide each of the 32 2.3 kg splits at minus 0.85 mm into 8 final subsamples of nominally 300 g (2/3 lb) each. Each subsample is placed in a polyethylene bag; the bag's top is folded over once and it is placed in a labeled and

numbered 19 x 24 cm foil laminate bag. The inner unsealed bag prevents the sealing area of the foil bag, and the sealer apparatus, from being contaminated by coal particles. The bags are then placed in the chamber of a sealer which is programmed to evacuate the chamber (including the bag), introduce argon to near atmospheric pressure, and heat-seal the top of the foil bag. As the bags are removed from the sealer their weights are recorded and these are then entered in the computerized inventory. Finally, eight to 24 of the 300 g bags, sealed or unsealed depending upon timing, are further processed to minus 0.25 mm and split once more to produce 75 g splits. These are placed in polyethylene bags and sealed in 14 x 24 cm foil bags as described above.

Under the previous contract, 75 g bags of minus 0.25 mm samples had not been produced as part of the initial processing effort. With the approval of DOE, -0.85 mm portions of each of samples DECS-1 through -22 were pulverized to -0.25 mm, subsampled and sealed to make similar bags. All 33 DECS samples are now available at -6 mm (-1/4"), -0.85 mm (-20 mesh U.S.) and -0.25 mm (-60 mesh U.S.).

Task 1E. Basic Characterization of Coal Samples

All samples collected were subjected to characterization using the following compositional analyses and tests:

- Proximate Analysis
- Ultimate Analysis
- Sulfur Forms Analysis
- Calorific Value Determination
- Equilibrium Moisture Determination
- Maceral Analysis
- Vitrinite Reflectance Analysis
- Ash Fusion Temperature Determination
- Free-swelling Index Determination
- Hardgrove Grindability Index Determination
- Gieseler Plasticity Determination (for samples of bituminous rank)
- Carbon Dioxide Content
- Chlorine Content
- Major Inorganic Elements Analysis
- Trace Inorganic Elements Analysis including Hazardous Air Pollutant Elements

In addition, results of many of the above analyses were further calculated to several different bases of expression. Assignment of coal rank was performed. Information on location and collection of the sample, its field description, and related geologic information were kept associated with the analytical information. Example bivariate plots of data determined in this Task are presented in Figures 9, 10 and 11; these include data for samples collected and characterized under the previous contract in order to represent the complete set of 33 samples in the DECS series. See Task 2, The Coal Database, for further information concerning the treatment and distribution of these data under the contract.

Non-routine characterization of the coal samples constituted a major part of the contract. See Tasks 1F and 1H for results of liquefaction, nuclear magnetic resonance and pyrolysis / gas chromatography / mass spectrometry.

Determinations of eight hazardous air pollutant elements were performed on 22 DECS samples from the previous contract as well as the 11 collected under the current contract. Results are shown in Table 4.

Figure 9. Vitrinite reflectance vs. carbon (numeric labels are DECS sample numbers).

Figure 10. Vitrinite reflectance vs. calorific value (numeric labels are DECS sample numbers).

Figure 11. Vitrinite reflectance vs. volatile matter (numeric labels are DECS sample numbers).

Table 4. Hazardous Air Pollutant Element Analyses of DECS samples, as ppm dry coal.

DECS										
#	St	Rank	As	Ba	Cd	Cr	Pb	Hg	Se	Ag
1	TX	subC	3.	133.	<0.2	8.	9.	0.17	<1.0	<0.2
2	IL	hvCb	4.	40.	<0.2	18.	15.	0.05	<1.0	<0.2
3	CO	mvp	<1.	175.	<0.2	2.	5.	0.08	<1.0	<0.2
4	NM	hvCb	<1.	56.	<0.2	3.	6.	<0.02	<1.0	<0.2
5	UT	hvCb	<1.	69.	<0.2	4.	4.	<0.02	<1.0	<0.2
6	UT	hvAb	<1.	68.	<0.2	4.	3.	0.03	<1.0	<0.2
7	WY	hvCb	1.	20.	<0.2	2.	4.	0.02	<1.0	<0.2
8	WY	subC	2.	227.	<0.2	8.	6.	0.03	<1.0	<0.2
9	MT	subB	1.	191.	<0.2	3.	4.	0.04	<1.0	<0.2
10	MT	subB	<1.	91.	<0.2	4.	10.	<0.02	<1.0	<0.2
11	ND	ligA	2.	209.	<0.2	2.	4.	<0.02	<1.0	<0.2
12	PA	hvAb	6.	62.	<0.2	17.	6.	0.11	<1.0	<0.2
13	WV	mvp	18.	106.	0.9	9.	4.	0.08	<1.0	<0.2
14	WV	hvAb	36.	40.	1.9	18.	11.	0.40	<1.0	<0.2
15	UT	hvAb	<1.	49.	<0.2	4.	2.	0.06	<1.0	<0.2
16	UT	hvAb	<1.	54.	<0.2	13.	8.	0.06	<1.0	<0.2
17	UT	hvAb	<1.	51.	<0.2	4.	2.	0.04	<1.0	<0.2
18	KY	hvBb	4.	43.	<0.2	9.	8.	0.09	<1.0	<0.2
19	VA	lvb	12.	157.	0.8	6.	4.	0.08	<1.0	<0.2
20	KY	hvAb	3.	90.	0.8	8.	7.	0.06	<1.0	<0.2
21	PA	an	<1.	19.	<0.2	20.	12.	0.10	<1.0	<0.2
22	PA	hvAb	13.	43.	<0.2	29.	16.	0.60	<1.0	<0.2
23	PA	hvAb	13.	56.	<0.2	13.	6.	0.12	<1.0	<0.2
24	IL	hvCb	2.	48.	<0.3	22.	10.	0.11	4.0	<0.3
25	MT	ligA	2.	520.	<0.3	2.	9.	0.14	3.0	<0.3
26	WY	subB	1.	300.	<0.2	4.	5.	0.12	2.0	<0.2
27	WY	subA	2.	480.	<0.3	9.	13.	0.10	3.0	<0.3
28	AZ	hvCb	1.	310.	<0.2	2.	5.	0.04	2.0	<0.2
29	VA	hvAb	4.	98.	<0.2	6.	7.	0.04	1.0	<0.2
30	VA	mvp	19.	74.	<0.1	6.	4.	0.11	2.0	<0.1
31	KY	hvAb	5.	100.	<0.3	15.	17.	0.04	4.0	<0.3
32	WV	hvAb	5.	160.	<0.5	35.	27.	0.04	5.0	<0.5
33	OH	hvBb	4.	39.	<0.3	16.	<3.	0.09	5.0	<0.3

Task 1F. Liquefaction Testing

Selected DECS coal samples were subjected to a series of organic geochemical tests to provide baseline data for the various coals studied as part of this project. The tests were basically solid-state ^{13}C NMR analyses and pyrolysis/gas chromatography/mass spectrometry, described under Task 1H, and liquefaction (using both tetralin and 1-methylnaphthalene as the solvents). The purpose of this section is to examine the liquefaction results and to develop an explanation for the trends in each data set as a function of coal rank as determined by both dry, ash-free carbon contents and mean-maximum vitrinite reflectance values.

Development of a Standardized Liquefaction Test

A procedure for a standardized liquefaction test and product workup was established; it is described step-by-step in Appendix B. The goal was to maximize the differences in liquefaction behavior and products which might be observed among different coals, rather than to maximize yield from individual coals.

The coal samples were first freeze dried. Tubing-bomb reactor tests were performed in duplicate with 5g coal and 5g 1-methylnaphthalene or tetralin per reactor under 1000 psig H_2 , run in a sand bath at 350°C for 30 min. When the tubing bombs were opened, gas from the first bomb was used to purge the line to the collection container and the gas volume was measured. Gas from the second bomb was collected in a second container and subsequently analyzed by gas chromatography. Results are reported on an ash-free basis. The conversion values calculated were averages of two tubing bomb runs; gas component analysis data result from one tubing bomb run and were adjusted to match the average gas conversion from the two tubing bomb runs. The product workup included percentages of total conversion, volatile hydrocarbons, asphaltenes, preasphaltenes, and ash.

Of the 33 DECS samples available for study, 28 were of high volatile A bituminous or lower rank and were subjected to liquefaction. Those omitted were DECS-3 (mvb), DECS-13 (mvb), DECS-19 (lvb), DECS-21 (an), and DECS-30 (mvb).

In addition, a protocol was developed and splits of samples DECS-23 and -24 were set aside for a planned time study of liquefaction behavior as related to storage conditions, which was to be performed annually in conjunction with the monitoring of sample condition (Task 1C). Annual liquefaction runs were planned for:

- 1) splits remaining sealed in original foil laminate bags, under refrigeration;
 - 2) splits exposed to the laboratory atmosphere, without refrigeration;
- and for samples other than DECS-24,
- 3) splits remaining sealed in original foil laminate bags, without refrigeration.

This study was not completed because of reductions in funding, but the samples remained available at the end of the contract.

Results

The DECS coal samples were subjected to tubing-bomb liquefaction using tetralin and 1-methylnaphthalene. The 28 coal samples examined were all liquefied in tetralin, and nine selected samples were also liquefied with 1-methylnaphthalene in a comparative study. The data for all samples are given in Tables 5 and 6. Table 5 presents the liquefaction in tetralin while Table 6 compares the liquefaction in tetralin with that in 1-methylnaphthalene. The results of this comparison indicated that no significant differences are observed between liquefaction conversions, asphaltene, preasphaltene, oil, and gas contents in replicate situations for the same respective coals. This result indicated that liquefaction data with tetralin as solvent generally provided the equivalent yields as liquefaction with 1-methylnaphthalene and it is this former data set that will be discussed below.

Table 5 provides the data for conversions into the various components. Total liquefaction conversion is plotted as a function of the two rank parameters, %C daf and mean-maximum vitrinite R_o in Figures 12 and 13. There is generally little correlation of conversion with rank, except for a generally decreasing yield in the higher rank samples that is expected. Some low-rank samples have low yields, while others have high yields. This could be related to retrogressive reactions in certain coals, perhaps induced by the higher contents of phenolics. An example of this is DECS-11, the Beulah, North Dakota, lignite known for its high content of phenolics (see NMR and pyrolysis discussions under Task 1H), where a relatively low liquefaction yield is probably due to this effect. On the other hand, the low-rank DECS-1 sample from Texas shows higher yields due to the fact that it is rich in aliphatic moieties (NMR data) and depleted of phenolics (as shown by pyrolysis data).

Yields of asphaltenes, preasphaltenes, and oil (Figures 14-19) also show highly scattered plots as a function of rank and similar explanations can be provided for the lack of direct correlation. The yields of gas (Figures 20 and 21), however, show a correlation of generally decreasing yields with increasing rank, as one might expect.

Table 5. Conversion of DECS samples in a standardized liquefaction test using tetralin (1:1 coal:tetralin, 1000 psig H₂, 350°C, 30 min), with detailed gas composition (average of two runs, except gas components based on one run).

sample			conversion, percent of dry ash-free coal											
number	rank	St	total	asph.	pre-asph.	oil	gas	gas composition						
								c1	c2	c3	c4	c5	c1-c5	other
DECS-1	subC	TX	66.3	12.5	9.2	8.9	35.7	8.5	4.0	1.6			14.1	21.6
DECS-2	hvCb	IL	62.7	9.1	32.7	8.1	12.8	6.5	1.6	1.1			9.2	3.6
DECS-4	hvCb	NM	48.5	6.1	11.7	7.6	23.1	0.5	0.4	0.2			1.1	22.0
DECS-5	hvCb	UT	45.0	6.9	27.2	6.8	4.1	0.5	0.4	0.1			1.0	3.1
DECS-6	hvAb	UT	30.1	7.9	7.7	7.0	7.5	0.5	0.2	0.1			0.8	6.7
DECS-7	hvCb	WY	44.6	8.3	4.9	10.3	21.1	1.1	0.6	0.2			1.9	19.2
DECS-8	subC	WY	60.2	6.6	10.9	11.8	30.9	9.3	4.8	1.2			15.3	15.6
DECS-9	subB	MT	35.0	6.1	9.1	4.2	15.6	0.6	0.4	0.1			1.1	14.5
DECS-10	subB	MT	35.5	7.2	8.6	4.7	15.0	0.7	0.3	0.2			1.2	13.8
DECS-11	ligA	ND	29.5	7.7	4.9	7.8	9.1	2.4	1.1	0.4			3.9	5.2
DECS-12	hvAb	PA	30.6	1.2	14.9	6.7	7.8	2.8	0.9	0.4	0.2	0.2	4.5	3.3
DECS-14	hvAb	WV	44.9	7.4	15.7	7.7	14.1	1.4	0.9	0.2			2.5	11.6
DECS-15	hvAb	UT	43.5	7.8	18.7	8.6	8.4	1.1	0.5	0.1			1.7	6.7
DECS-16	hvAb	UT	51.9	19.2	9.8	13.2	9.7	1.5	0.8	0.3			2.6	7.1
DECS-17	hvAb	UT	54.6	11.4	9.4	15.0	18.8	3.6	1.8	1.1			6.5	12.3
DECS-18	hvBb	KY	31.9	4.6	16.2	7.3	3.8	0.2	0.1	0.1			0.4	3.4
DECS-20	hvAb	KY	29.0	5.9	11.9	6.2	5.0	0.9	0.5	0.2			1.6	3.4
DECS-22	hvAb	PA	42.0	8.2	14.7	8.9	10.2	1.2	0.8	0.2			2.2	8.0
DECS-23	hvAb	PA	64.8	7.2	30.9	8.5	18.2	7.6	1.8	1.5	0.3		11.2	7.0
DECS-24	hvCb	IL	62.5	6.9	35.0	8.8	11.8	6.3	2.7	0.6			9.6	2.2
DECS-25	ligA	MT	53.6	3.9	7.4	6.4	35.9	0.5	0.1				0.6	35.3
DECS-26	subB	WY	54.6	5.3	10.1	6.8	32.4	0.5	0.1				0.6	31.8
DECS-27	subA	WY	48.2	13.9	14.0	7.2	13.1	6.0	1.6	0.5			8.1	5.0
DECS-28*	hvCb	AZ	42.2	10.4	15.0	6.2	10.6	7.1	1.6	0.7			9.4	1.2
DECS-29	hvAb	VA	22.1	3.3	7.7	6.3	4.8	0.6	0.2	0.1			0.9	3.9
DECS-31	hvAb	KY	36.4	15.7	3.2	7.4	10.1	0.5	0.1				0.6	9.5
DECS-32	hvAb	WV	29.8	4.6	16.3	6.6	2.3	0.3	0.1	0.1			0.5	1.8
DECS-33	hvBb	OH	62.8	27.3	20.4	12.2	2.9	0.7	0.4	0.3	0.1		1.5	1.4

* based on one run; second run failed

Table 6. Conversion of DECS samples in a standardized liquefaction test, comparing results from tetralin and 1-methylnaphthalene.

			conversion, percent of dry ash-free coal				
sample	solvent	replicate	total	asph.	preasph.	oil	gas
DECS-1	tetralin	a	65.6	12.4	8.8	9.0	35.4
DECS-1	tetralin	b	66.9	12.6	9.5	8.8	36.0
DECS-1	tetralin	average	66.3	12.5	9.2	8.9	35.7
DECS-1	1-methyl.	a	64.4	11.2	9.4	9.0	34.8
DECS-1	1-methyl.	b	69.0	12.5	9.9	9.4	37.2
DECS-1	1-methyl.	average	66.7	11.9	9.7	9.2	36.0
DECS-2	tetralin	a	63.0	9.0	33.0	8.1	12.9
DECS-2	tetralin	b	62.3	9.2	32.3	8.0	12.8
DECS-2	tetralin	average	62.6	9.1	32.7	8.1	12.9
DECS-2	1-methyl.	a	62.9	9.0	31.5	8.6	13.8
DECS-2	1-methyl.	b	61.9	8.8	32.2	8.1	12.8
DECS-2	1-methyl.	average	62.4	8.9	31.9	8.4	13.3
DECS-8	tetralin	a	62.0	5.6	11.0	10.8	34.6
DECS-8	tetralin	b	58.3	7.7	10.8	12.7	27.1
DECS-8	tetralin	average	60.2	6.7	10.9	11.8	30.9
DECS-8	1-methyl.	a	57.7	9.4	11.0	12.9	24.4
DECS-8	1-methyl.	b	59.3	7.5	11.4	11.0	29.4
DECS-8	1-methyl.	average	58.5	8.5	11.2	12.0	26.9
DECS-12	tetralin	a	23.1	0.1	15.1	6.3	1.6
DECS-12	tetralin	b	38.1	2.2	14.6	7.0	14.3
DECS-12	tetralin	average	30.6	1.2	14.9	6.70	8.0
DECS-12	1-methyl.	a	36.4	1.9	13.4	4.6	16.5
DECS-12	1-methyl.	b	39.1	1.9	16.2	6.6	14.4
DECS-12	1-methyl.	average	37.8	1.9	14.8	5.6	15.5
DECS-24	tetralin	a	62.6	6.8	33.6	9.0	13.2
DECS-24	tetralin	b	62.4	6.9	36.4	8.5	10.6
DECS-24	tetralin	average	62.5	6.9	35.0	8.8	11.9
DECS-24	1-methyl.	a	64.1	7.2	37.1	4.5	15.3
DECS-24	1-methyl.	b	61.1	6.9	35.7	6.1	12.4
DECS-24	1-methyl.	average	62.6	7.1	36.4	5.3	13.9

Table 6. continued

DECS-25	tetralin	a	52.8	3.6	7.7	6.7	34.8
DECS-25	tetralin	b	54.5	4.2	7.2	6.2	36.9
DECS-25	tetralin	average	53.7	3.9	7.5	6.5	35.9
DECS-25	1-methyl.	a	56.1	4.5	4.8	6.2	40.6
DECS-25	1-methyl.	b	55.1	3.9	6.6	6.9	37.6
DECS-25	1-methyl.	average	55.6	4.2	5.7	6.6	39.2
DECS-26	tetralin	a	55.0	4.9	10.7	6.9	32.5
DECS-26	tetralin	b	54.2	5.7	9.5	6.7	32.3
DECS-26	tetralin	average	54.6	5.3	10.1	6.8	32.4
DECS-26	1-methyl.	a	52.6	14.9	9.8	6.8	21.1
DECS-26	1-methyl.	b	53.3	5.5	10.0	6.4	31.4
DECS-26	1-methyl.	average	53.0	10.2	9.9	6.6	26.3
DECS-27	tetralin	a	48.9	15.5	14.7	7.2	11.5
DECS-27	tetralin	b	47.5	12.2	13.3	7.2	14.8
DECS-27	tetralin	average	48.2	13.9	14.0	7.2	13.2
DECS-27	1-methyl.	a	43.0	11.5	10.0	9.5	12.1
DECS-27	1-methyl.	b	44.5	11.1	11.2	8.3	13.9
DECS-27	1-methyl.	average	43.8	11.3	10.6	8.9	13.0
DECS-28	tetralin	a**	42.2	10.4	15.0	6.2	10.6
DECS-28	1-methyl.	a	41.1	12.4	16.5	5.5	6.7
DECS-28	1-methyl.	b	41.9	11.9	15.8	5.6	8.6
DECS-28	1-methyl.	average	41.5	12.2	16.2	5.6	7.7

** second run for DECS-28 in tetralin failed.

Figure 12. Total liquefaction conversion vs. carbon content, percent of dry ash-free coal; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 13. Total liquefaction conversion, percent of dry ash-free coal, vs. vitrinite reflectance; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 14. Asphaltene products vs. carbon content, percent of dry ash-free coal; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 15. Asphaltene products, percent of dry ash-free coal, vs. vitrinite reflectance; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 16. Preasphaltene products vs. carbon content, percent of dry ash-free coal; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 17. Preasphaltene products, percent of dry ash-free coal, vs. vitrinite reflectance; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 18. Oil products vs. carbon content, percent of dry ash-free coal; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 19. Oil products, percent of dry ash-free coal, vs. vitrinite reflectance; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 20. Gas products vs. carbon content, percent of dry ash-free coal; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Figure 21. Gas products, percent of dry ash-free coal, vs. vitrinite reflectance; 28 DECS samples subjected to standardized liquefaction test, 1:1 coal:tetralin, 1000 psig H_2 , 350°C, 30 min (numeric labels are DECS sample numbers).

Task 1G. Investigation of Changes in Surface Chemistry During Storage

The general objective of this task was to measure the changes in functional group concentration as a function of duration and type of storage method using reflectance-mode FT-i.r. and direct oxygen determination using electron optical techniques. Also, microscopic measurements of fluorescence alteration and intensity were to be employed to determine the extent of surface alteration during coal storage.

The Pittsburgh seam (see Task 1D) was selected as one of 8 coals to be studied under this task and a general procedure was established for sample processing. It was decided that both vitrinite concentrates and bulk samples from eight fresh bituminous coals would be used in the experimental program. Vitrinite bands would be handpicked in a nitrogen-filled glovebox in an attempt to limit their exposure to atmospheric oxygen, to drastic changes in temperature and relative humidity, and exposure to direct sunlight. From these samples, base levels of near-surface oxygen chemistry and concentration would be obtained to compare with measurements of fluorescence intensity and alteration. Subsamples of each bulk coal would be stored under argon in foil bags and matching subsamples would be exposed to the atmosphere. Using the same analytical procedures, these samples would be tested for changes in surface chemistry following two periods of storage (4-6 months and 12 months).

A vitrinite concentrate was prepared from the fresh Pittsburgh seam sample (DECS-23). Five 2.0g subsamples of the concentrate were prepared and processed in a nitrogen-filled glovebox, where they were sealed in foil laminate bags before being placed in refrigerated storage. Proximate, ultimate and petrographic analyses were completed, showing that the concentrate is 97 volume % vitrinite. Further base level fluorescence intensity and alteration measurements were completed on both the whole-seam channel and vitrinite concentrate samples. The UMA 300A infrared microscope which was expected to be used for functional group measurement was evaluated using other samples. Coal blocks corresponding to DECS-24 were collected during the third quarter. Further work was suspended in agreement with DOE when funding for the contract was reduced. The work started under this contract was reported in a final report to DOE under Grant No. DE-FG22-93PC93223 (Mitchell and Davis, 1997).

Task 1H. Organic Geochemistry

Selected DECS coal samples were subjected to a series of organic geochemical tests to provide baseline data for the various coals studied as part of this project. In this Task, solid-state ^{13}C NMR analyses and pyrolysis/gas chromatography/mass spectrometry were performed on 21 samples. This section examines the results and develops explanations for the trends in each data set as a function of coal rank as determined by both dry, ash-free carbon contents and mean-maximum vitrinite reflectance values.

Nuclear Magnetic Resonance: CPMAS, DDMAS, and Bloch Decay

Dried powdered samples of coal were placed in the bullet-type rotor of a Chemagnetics, Inc. M-100 NMR spectrometer and analyzed according to the cross-polarization, magic-angle spinning (CPMAS) and dipolar dephasing with magic angle spinning (DDMAS) procedures outlined by Hatcher (1988). Approximately 10,000 transients having a contact time of 1 ms and a cycle time of 1 s were acquired in 0.5K of data, zero-filled to 4K. The chemical shifts were referenced to hexamethylbenzene. For DDMAS, approximately 8000 transients with a cycle time of 1 s were used at each of 10 dephasing times.

Bloch decay experiments were performed as described by Hatcher et al. (1992), principally to verify the spectra obtained by conventional CPMAS. Approximately 2500 transients with a cycle time of 80 s were collected.

Results

Solid-state ^{13}C NMR data for the DECS coals examined in this report are listed in Table 7, and Table 8 shows the dipolar dephasing data for each coal sample. Figures 22-63 show the sets of individual NMR spectra obtained first (in odd numbered figures) by the technique of cross polarization with magic-angle spinning (CPMAS) and then (in even numbered figures) by simple Bloch decay with magic angle-spinning. While the data for Bloch decay spectra suffer from poor signal-to-noise, the carbon aromaticities calculated for most samples match within 10-15% of that calculated by the CPMAS method. Because the spectral quality for the CPMAS data are so much better than those of the Bloch decay NMR spectra, only the CPMAS data will be discussed here. Thus, from the spectra, data for carbon aromaticities, aromatic + carbonyl + carboxyl relative to total carbon, phenolic/total carbon, carboxyl + carbonyl/total carbon, and oxygenated aliphatic carbons/total carbons are calculated (Table 7). Dipolar dephasing provides a measure of the protonated aromatic contents and the proportions of methyl and quaternary carbons as a proportion of the aliphatic carbons (Table 8).

Plots of carbon aromaticity with rank parameters (Figures 64 and 65) show excellent and expected trends. DECS-1 and DECS-17 deviate significantly from the trend. This can be explained by the fact that the former is a more sapropelic coal with high liptinite content and the latter is a resin-rich coal. The liptinitic maceral content of these coals lowers the aromaticity due to the fact that the liptinites are generally aliphatic-rich. The other parameters measured from NMR data also show general correlations with rank (Figures 67-73), with DECS-1 and DECS-17 being deviants in most correlations. Perhaps the most interesting parameter, phenolics/total carbon, shows a decreasing trend with rank, except for DECS-1. This sample showed the highest liquefaction yield for low-rank coals, due largely to the fact that the reduced phenolic content limited retrogressive reactions. The DECS-11 sample, however, showed higher phenolic contents and attendant low liquefaction yields.

Table 7. Structural parameters of DECS coals determined by CPMAS measurements

sample				carbon aromaticity	(aromatic + carbonyl + carboxyl) / total carbons	phenolics/ total carbons	(carboxyl+ carbonyl)/ total carbons	oxygenated aliphatic carbons / total carbons
DECS-	seam	rank	St					
1	Bottom	subC	TX	0.45	0.52	0.14	0.07	0.050
2	Illinois #6	hvCb	IL	0.64	0.73	0.19	0.09	0.040
8	Smith-Roland	subC	WY	0.51	0.62	0.21	0.11	0.050
9	Dietz	subB	MT	0.59	0.68	0.20	0.09	0.030
11	Beulah	ligA	ND	0.60	0.71	0.20	0.11	0.020
12	Pittsburgh	hvAb	PA	0.69	0.76	0.16	0.07	0.023
13	Sewell	mvb	WV	0.79	0.80	0.14	0.01	0.010
17	Blind Canyon	hvAb	UT	0.54	0.60	0.18	0.06	0.040
18	Kentucky #9	hvBb	KY	0.63	0.66	0.15	0.03	0.020
19	Pocahontas #3	lvb	VA	0.80	0.81	0.13	0.01	0.010
23	Pittsburgh	hvAb	PA	0.67	0.75	0.17	0.08	0.024
24	Illinois #6	hvCb	IL	0.65	0.72	0.20	0.07	0.017
25	Pust	ligA	MT	0.60	0.72	0.21	0.12	0.037
26	Wyodak	subB	WY	0.56	0.68	0.20	0.12	0.022
27	Deadman	subA	WY	0.63	0.75	0.20	0.12	0.020
28	Green	hvCb	AZ	0.57	0.63	0.18	0.07	0.020
29	U. Banner #3	hvAb	VA	0.72	0.74	0.11	0.02	0.007
30	Splash Dam	mvb	VA	0.76	0.78	0.11	0.02	0.002
31	Pond Creek	hvAb	KY	0.70	0.72	0.13	0.02	0.009
32	Stockton-Lew.	hvAb	WV	0.73	0.75	0.15	0.02	0.002
33	Ohio #4A	hvBb	OH	0.75	0.80	0.15	0.05	0.019

Definitions:

carbon aromaticity*

(aromatic + carbonyl + carboxyl) / total carbons

phenolics* / total carbons

(carboxyl + carbonyl) / total carbons

oxygenated aliphatic carbons / total carbons

$fa' = I_{100-165 \text{ ppm}} / I_{\text{total}}$

$fa = I_{100-220 \text{ ppm}} / I_{\text{total}}$

$fp = I_{140-165 \text{ ppm}} / I_{\text{total}}$

$fc = I_{165-220 \text{ ppm}} / I_{\text{total}}$

$fo = I_{60-90 \text{ ppm}} / I_{\text{total}}$

where:

I = area within the indicated chemical shift ranges in a CPMAS spectrum

$I_{\text{total}} = 1 - 220 \text{ ppm}$

* corrected for contributions from spinning sidebands of aromatic carbons

Table 8. Structural Parameters of DECS coals determined by DDMAS measurements

sample				aromatic protonated C	mobile CH ₃ and quaternary aliphatic C
number	seam	rank	St		
DECS-1	Bottom	subC	TX	0.30	0.15
DECS-2	Illinois #6	hvCb	IL	0.55	0.48
DECS-8	Smith-Roland	subC	WY	0.28	0.35
DECS-9	Dietz	subB	MT	0.34	0.19
DECS-11	Beulah	ligA	ND	0.45	0.22
DECS-12	Pittsburgh	hvAb	PA	0.49	0.29
DECS-13	Sewell	mvb	WV	0.37	0.19
DECS-17	Blind Canyon	hvAb	UT	0.40	0.14
DECS-18	Kentucky #9	hvBb	KY	0.20	0.34
DECS-19	Pocahontas #3	lvb	VA	0.25	0.34
DECS-23	Pittsburgh	hvAb	PA	0.39	0.58
DECS-24	Illinois #6	hvCb	IL	0.15	0.39
DECS-25	Pust	ligA	MT	0.43	0.14
DECS-26	Wyodak	subB	WY	0.56	0.15
DECS-27	Deadman	subA	WY	0.37	0.16
DECS-28	Green	hvCb	AZ	0.25	0.35
DECS-29	Upper Banner #3	hvAb	VA	0.29	0.49
DECS-30	Splash Dam	mvb	VA	0.21	0.72
DECS-31	Pond Creek	hvAb	KY	0.27	0.25
DECS-32	Stockton-Lewiston	hvAb	WV	0.19	0.53
DECS-33	Ohio #4A	hvBb	OH	0.17	0.65

Figure 22. CPMAS NMR spectrum of DECS-1, subC Bottom seam, TX.

Figure 23. Bloch decay NMR spectrum of DECS-1, subC Bottom seam, TX.

Figure 24. CPMAS NMR spectrum of DECS-2, hvCb Illinois #6 seam, IL.

Figure 25. Bloch decay NMR spectrum of DECS-2, hvCb Illinois #6 seam, IL.

Figure 26. CPMAS NMR spectrum of DECS-8, subC Smith-Roland (“Wyodak”) seam, WY.

Figure 27. Bloch decay NMR spectrum of DECS-8, subC Smith-Roland (“Wyodak”) seam, WY.

Figure 28. CPMAS NMR spectrum of DECS-9, subB Dietz seam, MT.

Figure 29. Bloch decay NMR spectrum of DECS-9, subB Dietz seam, MT.

Figure 30. CPMAS NMR spectrum of DECS-11, ligA Beulah seam, ND.

Figure 31. Bloch decay NMR spectrum of DECS-11, ligA Beulah seam, ND.

Figure 32. CPMAS NMR spectrum of DECS-12, hvAb Pittsburgh seam, PA.

Figure 33. Bloch decay NMR spectrum of DECS-12, hvAb Pittsburgh seam, PA.

Figure 34. CPMAS NMR spectrum of DECS-13, mvb Sewell seam, WV.

Figure 35. Bloch decay NMR spectrum of DECS-13, mvb Sewell seam, WV.

Figure 36. CPMAS NMR spectrum of DECS-17, hvAb Blind Canyon seam, UT.

Figure 37. Bloch decay NMR spectrum of DECS-17, hvAb Blind Canyon seam, UT.

Figure 38. CPMAS NMR spectrum of DECS-18, hvBb Kentucky #9 seam, KY.

Figure 39. Bloch decay NMR spectrum of DECS-18, hvBb Kentucky #9 seam, KY.

Figure 40. CPMAS NMR spectrum of DECS-19, lvb Pocahontas #3 seam, VA.

Figure 41. Bloch decay NMR spectrum of DECS-19, lvb Pocahontas #3 seam, VA.

Figure 42. CPMAS NMR spectrum of DECS-23, hvAb Pittsburgh seam, PA.

Figure 43. Bloch decay NMR spectrum of DECS-23, hvAb Pittsburgh seam, PA.

Figure 44. CPMAS NMR spectrum of DECS-24, hvCb Illinois #6 seam, IL.

Figure 45. Bloch decay NMR spectrum of DECS-24, hvCb Illinois #6 seam, IL.

Figure 46. CPMAS NMR spectrum of DECS-25, ligA Pust seam, MT.

Figure 47. Bloch decay NMR spectrum of DECS-25, ligA Pust seam, MT.

Figure 48. CPMAS NMR spectrum of DECS-26, subB Wyodak seam, WY.

Figure 49. Bloch decay NMR spectrum of DECS-26, subB Wyodak seam, WY.

Figure 50. CPMAS NMR spectrum of DECS-27, subA Deadman seam, WY.

Figure 51. Bloch decay NMR spectrum of DECS-27, subA Deadman seam, WY.

Figure 52. CPMAS NMR spectrum of DECS-28, hvCb Green seam, AZ.

Figure 53. Bloch decay NMR spectrum of DECS-28, hvCb Green seam, AZ.

Figure 54. CPMAS NMR spectrum of DECS-29, hvAb Upper Banner seam, VA.

Figure 55. Bloch decay NMR spectrum of DECS-29, hvAb Upper Banner seam, VA.

Figure 56. CPMAS NMR spectrum of DECS-30, mvb Splash Dam seam, VA.

Figure 57. Bloch decay NMR spectrum of DECS-30, mvb Splash Dam seam, VA.

Figure 58. CPMAS NMR spectrum of DECS-31, hvAb Pond Creek seam, KY.

Figure 59. Bloch decay NMR spectrum of DECS-31, hvAb Pond Creek seam, KY.

Figure 60. CPMAS NMR spectrum of DECS-32, hvAb Stockton-Lewiston seam, WV.

Figure 61. Bloch decay NMR spectrum of DECS-32, hvAb Stockton-Lewiston seam, WV.

Figure 62. CPMAS NMR spectrum of DECS-33, hvBb Ohio #4 seam, OH.

Figure 63. Bloch decay NMR spectrum of DECS-33, hvBb Ohio #4 seam, OH.

Figure 64. Carbon aromaticity vs. carbon content of dry ash-free coal for 21 DECS samples.

Figure 65. Carbon aromaticity vs. vitrinite reflectance for 21 DECS samples.

Figure 66. Aromatic + carbonyl + carboxyl fraction of total carbons vs. carbon content of dry ash-free coal for 21 DECS samples.

Figure 67. Aromatic + carbonyl + carboxyl fraction of total carbons vs. vitritine reflectance of dry ash-free coal for 21 DECS samples.

Figure 68. Phenolic fraction of total carbons vs. carbon content of dry ash-free coal for 21 DECS samples.

Figure 69. Phenolic fraction of total carbons vs. vitrinite reflectance of dry ash-free coal for 21 DECS samples.

Figure 70. Carboxyl + carbonyl fraction of total carbons vs. carbon content of dry ash-free coal for 21 DECS samples

Figure 71. Carboxyl + carbonyl fraction of total carbons vs. vitrinite reflectance of dry ash-free coal for 21 DECS samples.

Figure 72. Oxygenated aliphatic fraction of total carbons vs. carbon content of dry ash-free coal for 21 DECS samples.

Figure 73. Oxygenated aliphatic fraction of total carbons vs. vitrinite reflectance of dry ash-free coal for 21 DECS samples.

Figure 74. Aromatic protonated fraction of total carbons vs. carbon content of dry ash-free coal for 21 DECS samples

Figure 75. Aromatic protonated fraction of total carbons vs. vitrinite reflectance of dry ash-free coal for 21 DECS samples.

Figure 76. Mobile CH₃ + quaternary aliphatic fraction of total carbons vs. carbon content of dry ash-free coal for 21 DECS samples.

Figure 77. Mobile CH₃ + quaternary aliphatic fraction of total carbons vs. vitrinite reflectance of dry ash-free coal for 21 DECS samples.

Pyrolysis - Gas Chromatography - Mass Spectrometry

Pyrolysis/gas chromatography/mass spectrometry (py/gc/ms) is a technique that produces volatile thermal degradation products from coal and the products can be identified from their mass spectra after being separated by gas chromatography. Py/gc/ms is performed using a Varian 2700 gas chromatograph and a DuPont 21-490B mass spectrometer equipped with a Chemical Data Systems Pyroprobe 1000 according to the methods outlined by Hatcher et al. (1988). The pyroprobe pyrolyzes samples at any fixed heating rate ranging from 10 to 20,000°C/s to a desired final temperature (maximum of 1400°C), and holds at the final temperature for a given time (0.01 - 99.99 s). In this project a flash pyrolysis temperature of 610°C is employed. Lower temperatures would partially pyrolyze the sample in the probe, whereas higher temperatures produce smaller fragments of low molecular weight which would provide little structural detail and obscure the information on the exact structural features present in the sample. A heating rate of 10°C/ms is used because relatively rapid heating minimizes the potential for secondary reactions, enhancing the detection of pyrolysis fragments characteristic of the original macromolecular, insoluble nature of the coal. The time of pyrolysis is 10 s to ensure complete expulsion of the volatile pyrolyzates from the capillary tube into the gas chromatograph - mass spectrometer.

It is important to carefully prepare the finely powdered sample and properly select the sample weight to minimize the effects of thermal gradients in the sample and to ensure that the representative sample is completely pyrolyzed. A sample weight of about 0.3 mg for lignites and subbituminous coals and 0.5 mg for higher ranks is used. Samples are weighed in a microbalance and loaded into a quartz capillary tube as evenly as possible to minimize thermal gradients. The quartz tube is placed inside the platinum heating coil of the pyroprobe; this assembly is then inserted into the injection port (temperature maintained at 280°C) of a Varian 2700 gas chromatograph and the sample is pyrolyzed. The pyrolyzate is cryotrapped with liquid nitrogen prior to being subjected to gas chromatography on a J&W DB-17 capillary column (25 m in length, 0.25 mm in diameter, made of 50% phenyl methyl silicone). The chromatograph temperature is programmed from 30°C (0 min) to 280°C (20 min) at a rate of 4°C/min. The effluent was swept into the source of a DuPont 21-490B mass spectrometer fitted with a Teknivent Vector/One data system for detection and compound identification. Compounds are identified by a combination of methods including comparison of mass spectra to the NBS/Wiley library and other published mass spectra and to authentic standards. This py/gc/ms technique has been found to be very reproducible for repetitive analysis of the same sample.

Results

Pyrograms produced from each of the DECS samples are shown in Figures 78-98. From these traces, peaks can be identified and grouped into compound classes (e.g., n-alkanes-group 1, phenols-group 2, and non-oxygenated aromatic hydrocarbons-group 3). The yields of each group (peak areas) normalized to the total areas of all peaks are shown in Table 9. Often, many peaks remain unidentified and these are also tabulated. One usually normalizes the summed areas of compound classes relative to the total area of identified peaks and these data are shown in Table 10. The inability to identify peaks is usually not due to the lack of spectral recognition but rather

to the fact that so many peaks are overlapping in certain regions of the chromatograms that it is difficult to make a positive identification. Often, co-elution of peaks renders quantitative measurements difficult.

As one progresses from low-rank coals to the higher rank samples, a transition is observed as the highly phenolic (in most instances) content of the low rank samples gives way to the non-oxygenated aromatic-dominated coals. This trend is generally observed by plotting the yields of non-oxygenated aromatics with rank in Figures 99 and 100. Samples DECS-29, 30, and 13 do not appear to follow this trend. Examination of the pyrograms reveals that these samples contain n-alkanes in overabundance for their high rank. This could be indicative that oil or petroleum hydrocarbons may have migrated into the samples. This coupled with the fact that high rank coals usually do not produce significant amounts of pyrolysis products explains the low yield of non-oxygenated aromatic products. If one examines the correlation in Figure 100 ignoring the data for these samples, then an excellent trend is observed.

Plots of the yields of n-alkanes and alkenes (Figures 101 and 102) show no correlation with rank. If one ignores the aforementioned samples DECS-13, 29 and 30, then a better correlation with Ro is observed in Figure 102.

The best correlations are observed between phenolic contents and rank (Figures 103 and 104), especially if one ignores DECS-1, which is dominated by an homologous series of n-alkanes and alkenes as would be found for liptinitic macerals. The high yields of alkanes and alkenes reduces the phenolic content for this sample. The diminishing yields of phenolic pyrolysis products as rank increases is consistent with the known diminution of phenolics. The NMR data also showed a similar trend. Thus the py/gc/ms data are very well in tune with the NMR data for this series of coals.

The data presented in this final report indicate that there are some correlations among the data sets which could be examined in greater detail. The project goals for this part of the work were to provide the analytical results, a goal completed and demonstrated by the large amounts of data that were obtained. Preliminary correlations among the data sets gave indications that more information is available upon closer examination. The highlighted trends show typical behavior expected for most coals. A number of the outliers from the trends shown can be explained based on the maceral compositions or other known properties of the various coals. Further investigation of the data could be performed under a subsequent contract.

Figure 78. Total ion chromatogram of pyrolyzates from DECS-1, subC Bottom seam, TX.

Figure 79. Total ion chromatogram of pyrolyzates from DECS-2, hvCb Illinois #6 seam, IL.

Figure 80. Total ion chromatogram of pyrolyzates from DECS-8, subC Smith-Roland ("Wyodak") seam, WY.

Figure 81. Total ion chromatogram of pyrolyzates from DECS-9, subB Dietz seam, MT.

Figure 82. Total ion chromatogram of pyrolyzates from DECS-11, ligA Beulah seam, ND.

Figure 83. Total ion chromatogram of pyrolyzates from DECS-12, hvAb Pittsburgh seam, PA.

Figure 84. Total ion chromatogram of pyrolyzates from DECS-13, mvb Sewell seam, WV.

Figure 85. Total ion chromatogram of pyrolyzates from DECS-17, hvAb Blind Canyon seam, UT.

Figure 86. Total ion chromatogram of pyrolyzates from DECS-18, hvBb Kentucky #9 seam, KY.

Figure 87. Total ion chromatogram of pyrolyzates from DECS-19, lvb Pocahontas #3 seam, VA.

Figure 88. Total ion chromatogram of pyrolyzates from DECS-23, hvAb Pittsburgh seam, PA.

Figure 89. Total ion chromatogram of pyrolyzates from DECS-24, hvCb Illinois #6 seam, IL.

Figure 90. Total ion chromatogram of pyrolyzates from DECS-25, ligA Pust seam, MT.

Figure 91. Total ion chromatogram of pyrolyzates from DECS-26, subB Wyodak seam, WY.

Figure 92. Total ion chromatogram of pyrolyzates from DECS-27, subA Deadman seam, WY.

Figure 93. Total ion chromatogram of pyrolyzates from DECS-28, hvCb Green seam, AZ.

Figure 94. Total ion chromatogram of pyrolyzates from DECS-29, hvAb U. Banner #3 seam, VA.

Figure 95. Total ion chromatogram of pyrolyzates from DECS-30, mvb Splash Dam seam, VA.

Figure 96. Total ion chromatogram of pyrolyzates from DECS-31, hvAb Pond Creek seam, KY.

Figure 97. Total ion chromatogram of pyrolyzates from DECS-32, hvAb Stockton-Lewiston seam, WV.

Figure 98. Total ion chromatogram of pyrolyzates from DECS-33, hvBb Ohio #4A seam, OH.

Table 9. Structural parameters determined by py/gc/ms, flash pyrolysis temperature of 610°C, heating rate 10°C/ms, pyrolysis time 10 s (percent of total gc-amenable products).

sample				n-alkanes and alkenes	phenols	non-oxygenated aromatic hydrocarbons	unident- ified
number	seam	rank	state				
DECS-1	Bottom	subC	TX	39.2	8.3	37.1	15.4
DECS-2	Illinois #6	hvCb	IL	26.7	21.5	35.6	16.2
DECS-8	Smith-Roland	subC	WY	27.2	15.6	14.3	42.9
DECS-9	Dietz	subB	MT	34.9	17.3	6.7	41.1
DECS-11	Beulah	ligA	ND	37.3	32.8	12.9	17.0
DECS-12	Pittsburgh	hvAb	PA	18.1*	31.3*	51.2*	
DECS-13	Sewell	mvp	WV	32.2	16.8	19.5	31.5
DECS-17	Blind Canyon	hvAb	UT	24.3	5.4	5.5	64.8
DECS-18	Kentucky #9	hvBb	KY	41.5	22.3	7.6	28.6
DECS-19	Pocahontas #3	lvb	VA	4.4	3.0	37.1	55.5
DECS-23	Pittsburgh	hvAb	PA	37.1	15.8	36.8	10.3
DECS-24	Illinois #6	hvCb	IL	27.4	27.5	27.8	17.4
DECS-25	Pust	ligA	MT	19.9	8.8	1.6	69.7
DECS-26	Wyodak	subB	WY	34.8	26.6	27.2	11.4
DECS-27	Deadman	subA	WY	29.4	11.6	8.5	50.5
DECS-28	Green	hvCb	AZ	36.5	25.6	27.2	10.6
DECS-29	Upper Banner #3	hvAb	VA	21.8	3.5	10.7	64.0
DECS-30	Splash Dam	mvp	VA	28.0	3.6	4.3	64.1
DECS-31	Pond Creek	hvAb	KY	17.9	15.4	4.5	62.2
DECS-32	Stockton-Lewiston	hvAb	WV	15.3	20.1	10.3	53.5
DECS-33	Ohio #4A	hvBb	OH	32.2	19.1	34.7	14.0

* as percent of identified products

Table 10. Structural parameters determined by py/gc/ms, flash pyrolysis temperature of 610°C, heating rate 10°C/ms, pyrolysis time 10 s (percent of identified products).

sample				n-alkanes and alkenes	phenols	non-oxygenated aromatic hydrocarbons
number	seam	rank	state			
DECS-1	Bottom	subC	TX	46.3	9.8	43.9
DECS-2	Illinois #6	hvCb	IL	31.9	25.6	42.5
DECS-8	Smith-Roland	subC	WY	47.6	27.4	25.0
DECS-9	Dietz	subB	MT	59.3	29.4	11.3
DECS-11	Beulah	ligA	ND	44.9	39.6	15.5
DECS-12	Pittsburgh	hvAb	PA	18.1	31.3	51.2
DECS-13	Sewell	mvp	WV	47.0	24.5	28.5
DECS-17	Blind Canyon	hvAb	UT	69.1	15.3	15.6
DECS-18	Kentucky #9	hvBb	KY	58.2	31.2	10.6
DECS-19	Pocahontas #3	lvb	VA	9.88	6.74	83.3
DECS-23	Pittsburgh	hvAb	PA	43.6	17.6	41.0
DECS-24	Illinois #6	hvCb	IL	33.1	33.3	33.6
DECS-25	Pust	ligA	MT	65.7	29.0	5.3
DECS-26	Wyodak	subB	WY	39.3	30.0	30.7
DECS-27	Deadman	subA	WY	59.4	23.4	17.2
DECS-28	Green	hvCb	AZ	40.9	28.7	30.4
DECS-29	Upper Banner #3	hvAb	VA	60.6	9.7	29.7
DECS-30	Splash Dam	mvp	VA	78.0	10.0	12.0
DECS-31	Pond Creek	hvAb	KY	47.4	11.9	40.7
DECS-32	Stockton-Lewiston	hvAb	WV	32.9	22.2	44.9
DECS-33	Ohio #4A	hvBb	OH	37.5	22.2	40.3

Figure 99. Non-oxygenated aromatic hydrocarbon fraction of identified products vs. carbon content for 21 DECS coals.

Figure 100. Non-oxygenated aromatic hydrocarbon fraction of identified products vs. vitritine reflectance for 21 DECS coals.

Figure 101. n-Alkanes + alkenes fraction of identified products vs. carbon content for 21 DECS coals.

Figure 102. n-Alkanes + alkenes fraction of identified products vs. vitrinite reflectance for 21 DECS coals.

Figure 103. Phenolic fraction of identified products vs. carbon content for 21 DECS coals.

Figure 104. Phenolic fraction of identified products vs. vitrinite reflectance for 21 DECS coals.

Task 11. Distribution of Coal Samples to Users

Distribution of samples took place under the conditions of the contract. Up to 1 kg (2.2 lbs) each of up to 15 samples per year per requestor were distributed to DOE contractors and grantees at no charge to the recipient. Samples were distributed for a wide variety of proposed uses, as summarized for approximately 4 years of the contract in Table 11. Appendix C lists the agencies receiving samples and/or data during the five-year contract and the following six-month extension period. Numbers in parentheses enumerate separate requests from the same agency. In total, 502 requests were received; most were for more than one sample or data printout.

Table 11. Sample distribution by category of recipient's use, 9/29/93 to 8/15/97.

Category	number of samples	percentage of samples	number of containers	percentage of containers
Liquefaction	147	26	360	39
Combustion	88	16	194	21
Physical cleaning	21	4	43	5
Biological cleaning	23	4	33	4
Characterization	80	14	86	9
Education and outreach	7	1	7	1
Pyrolysis and gasification	14	3	14	2
Geology	100	18	100	11
Health and medical	60	11	60	6
Carbon products	16	3	29	2
TOTAL	556	100 %	917	100 %

A record of distribution of samples and data is shown in Table 12. For record-keeping under the contract, and this Table, a "sample" is any amount of one coal sample provided to one requestor at one time. Thus one 5 kg foil laminate bag of DECS-12 sent out is one "sample," but one 300 g bag each of DECS-1 and -2 sent every year for four years is 8 "samples." Special sample DECS-17 is excluded in accord with the method used under the previous contract, but is added in a consistent manner in the final line of the table. At least 502 DECS and PSOC samples in 1586 containers were distributed during the contract. Numbers of samples distributed from various coal sample banks have been discussed by Vorres et al. (1994)

Table 12. Samples and data distributed 9/29/93 to 3/30/99 (5.5 years)

Quarter ending	DOE samples (excluding DECS-17)			Other PSOC samples			Total samples	Total containers	Print-outs	Special data requests		Total requests
	Total	to DOE contractor	to others	Total	to DOE contractor	to others				#	limited information on # samples	
12/93	25	19	6	3	1	2	28	42	42	11	2229	23
3/94	8	5	3	4	1	3	12	25	25	4	543	18
6/94	16	13	3	30	0	30	46	56	157	7	422	23
9/94	36	26	10	32	6	26	68	155	104	8	1268	31
12/94	19	19	0	1	0	1	20	26	66	5	215	16
3/95	25	14	11	12	5	7	37	68	150	19	2530	38
6/95	94	30	64	16	1	15	110	125	60	10	449	29
9/95	20	10	10	1	1	0	21	47	41	3	790	21
12/95	13	6	7	2	0	2	15	31	48	5	235	15
3/96	16	14	2	3	2	1	19	28	136	8	325	19
6/96	31	22	9	34	3	31	65	103	84	16	3826	30
9/96	24	17	7	2	0	2	26	48	41	10	2018	17
12/96	18	17	1	9	4	5	27	49	139	17	3289	27
3/97	25	14	11	6	4	2	31	34	177	10	2117	21
6/97	15	11	4	27	3	24	42	88	66	17	1765	23
9/97	27	15	12	106	95	11	133	143	291	15	4002	20
12/97	39	26	13	2	1	1	41	50	160	6	102	17
3/98	9	9	0	2	0	2	11	18	139	121	2549	34
6/98	19	10	9	0	0	0	19	47	90	20	416	30
9/98	29	10	19	16	0	16	45	85	101	4	1237	11
12/98	21	3	18	2	0	2	23	56	16	7	2507	19
3/99	25	2	23	0	0	0	25	29	18	30	1374	20
TOTAL	554	312	242	307	127	181	836	1351	2109	353	34208	502
TOTAL including DECS-17*	570	328	242	307	127	181	852	1586	2109	353	34208	502

*including 225 bags of DECS-17 (16 requests)

Task 2. The Coal Database

Task 2A. Programming

Computer programming for the Coal Database was performed for three distinct computer platforms. First, in conjunction with the existing Watfile interactive database system running under VM/CMS on the Penn State mainframe, a program was completed to create printed reports in standard formats of four pages per sample or a condensed printout of one page per sample. Written in REXX, it read the Watfile database and created output in the Waterloo Script markup language for a mainframe-attached printer. This program was used throughout the contract to provide data printouts of DECS and PSOC samples. Other REXX programs were written to perform calculations of analytical data to a variety of bases of expression, and to provide other ancillary services for the Coal Database.

Late in the contract, support for the mainframe-attached printing system was discontinued, and discontinuation of the VM/CMS operating system was announced. The database structure was recreated in Microsoft Access 97 under the Windows 95 operating system, and the data were put in place. This system was in operation for queries and summaries of the database at the end of the contract. A format for printed reports, to replicate those from the earlier system, was under development at the end of the contract. The computerized inventory of sample containers was also transferred to Access 97, providing the possibility for linking it with the Coal Database if required.

During the contract, use of the world wide web on the Internet became widespread. Web pages were written describing the DOE Coal Sample Bank and Database and placed on a web server at <http://www.ems.psu.edu/COPL/doesb.htm> for access by the public. Penn State's College of Earth and Mineral Sciences provided programming services in CGI and Perl to create a searchable subset of the Database, including all 33 DECS samples, on the web. The URL during the contract was <http://www.ems.psu.edu/COPL/coal.html> but the pages were expected to be moved to the <http://www.energyinstitute.psu.edu/> site during 1999.

Task 2B. Data Entry

Data for the 11 DECS samples collected under the contract were entered in the Coal Database as they became available from the analysts. Hazardous air pollutant trace element data for the 22 earlier DECS samples were also entered late in the contract.

Task 2C. Distribution of Data to Users

Data were distributed in a variety of formats. Standard four-page or one-page per sample data printouts were distributed individually in response to specific requests, alone or in conjunction with coal samples. A complete set of four-page per sample printouts for the 33 DECS samples was compiled and distributed to DOE contractors and grantees on request. Numbers of printouts distributed each quarter are shown in Table 12 (see Task 1I, above). Four-page printouts for the 11 DECS samples collected and analyzed under the contract are presented in Appendix D.

The Database may be interactively queried to identify samples matching requestor's criteria. When a list of samples has been produced, a custom-formatted table of data may be created and printed, or the list of samples may be used to specify that a one-page or five-page data printout be produced for each sample. Subsets of the Database or formatted tables may also be transmitted in electronic form. Custom formatted reports or subsets and the number of sample records they contained are counted in Table 12 under "Special Data Requests"

The searchable data subset on the world wide web also delivered data to users in several formats (Table 13). A search performed through this system results in a table of samples meeting the criteria specified, and displaying several data fields. Each sample number in the table is a link to a more detailed page for that sample. In addition, there were many accesses of the brief table of DOE Coal Database data on the web site which are not counted here. This table was part of a printed brochure which was created and widely distributed during the contract to described the Coal Sample Bank and Database. Its contents are shown in Appendix E.

Table 13. Data delivered to users via the world wide web site

year	month	search result screens presented	individual DECS screens	individual PSOC screens
1998	1	39	1	6
	2	132	10	110
	3	69	8	71
	4	70	64	1082
	5	18	0	9
	6	51	30	575
	7	14	18	248
	8	24	108	1041
	9	17	15	245
	10	76	1	30
	11	63	3	82
	12	13	41	109
1999	1	62	33	332
	2	109	77	916
	3	64	12	219
Total		821	421	5075

CONCLUSIONS

The coal samples and data supported under this contract were used on an ongoing basis by a wide variety of DOE contractors and others performing coal research. Sample collection, processing, analysis, monitoring, and distribution have been completed as specified in the revised contract.

Thirty-three DECS samples are stored in argon under refrigeration in multilaminate bags. The succession of annual monitoring programs under this and the previous contract have demonstrated that this protocol preserves sample properties (thermoplastic behavior, sulfur forms, and calorific value) well over the evaluation period of up to nine years for some samples. These bags are inexpensive and can be employed with a minimum investment in supporting equipment, and should therefore be considered by researchers using coal samples over short or long time periods. Some samples did exhibit small degrees of deterioration; continued study to determine whether these are trends or random variation, and whether any trends might accelerate over longer time periods, would be valuable to coal researchers.

The DECS samples provide a well characterized set with a variety of properties suitable for laboratory research. A further benefit was their availability for immediate distribution at a variety of particle sizes and package sizes, all stored in the same manner: 2.3 kg of minus 6.4 mm (-1/4 inch) coal, 300 g of minus 0.85 mm (-20 mesh U.S.) coal, and 75 g of minus 0.25 mm (-60 mesh U.S.) coal.

Analytical data for these samples were obtained in a consistent manner and were widely distributed. A searchable data set was created on a world wide web site to provide data more efficiently to all interested parties.

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APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-1 unnamed seam		lig		Ro max= 0.35		
FOIL BAG	original analysis	22 of 256	93 of 256	113 of 256	109 of 256	62 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note						
date sealed		8/ 14/ 90	8/ 14/ 90	8/ 14/ 90	8/ 14/ 90	8/ 14/ 90
date analyzed	4/ 17/ 90	1/ 25/ 91	10/ 01/ 92	6/ 14/ 93	3/ 23/ 94	3/ 17/ 99
PROXIMATE						
% moisture	30.0	28.2	29.0	29.3	29.6	29.8
% ash (dry basis)	15.8	16.2	15.2	16.4	16.4	15.9
SULFUR FORMS (dry %)						
total sulfur	0.99	1.03	0.97	1.07	1.08	1.10
sulfate	0.01	0.06	0.00	0.00	0.00	0.01
pyritic	0.11	0.13	0.11	0.13	0.11	0.23
organic	0.86	0.85	0.86	0.94	0.96	0.86
CALORIFIC VALUE (dry)						
Btu/lb	10956	10791	11023	10912	10941	11009
GASEOUS OXYGEN						
% in bag atmosphere					0.00	Not
date analyzed					3/08/94	determined

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS-2	Illinois #6 seam				hvCb				Ro max= 0.52 %	
FOIL BAG	original analysis	21 of 256	100 of 256	109 of 256	114 of 256 115 of 256	136 of 256	138 of 256	152 of 256	155 of 256	154 of 1256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note										
date sealed		8/ 06/ 90	8/ 06/ 90	8/ 06/ 90	8/ 06/ 90	8/ 06/ 90	8/ 06/ 90	8/ 06/ 90	8/ 06/ 90	8/ 06/ 90
date analyzed	2/ 28/ 90	1/ 25/ 91	11/ 27/ 92	6/ 14/ 93	3/ 23/ 94	5/ 23/ 95	2/ 13/ 96	7/ 31/ 97	7/ 28/ 98	3/ 12/ 99
PROXIMATE										
% moisture	10.4	10.3	10.1	9.8	9.6	10.2	10.0	10.2	9.9	10.2
% ash (dry basis)	16.2	16.1	16.2	15.9	16.1	15.9	16.0	16.1	16.3	15.9
SULFUR FORMS (dry %)										
total sulfur	4.51	4.33	4.54	4.50	4.64	4.62	4.59	4.63	4.78	4.67
sulfate	0.01	0.06	0.01	0.03	0.01	0.04	0.01	0.07	0.03	0.01
pyritic	2.27	2.27	2.31	2.06	1.92	2.06	2.27	2.35	2.46	2.57
organic	2.24	2.00	2.22	2.41	2.72	2.51	2.30	2.21	2.29	2.10
CALORIFIC VALUE (dry)										
Btu/lb	11880	11740	11814	11787	11895	11833	11813	11794	11752	11802
GIESELER FLUIDITY										
maximum fluidity, ddpm	8	9	10	7	8	11	9	6	12	
fluid range, °C	47	58	61	55	63	64	58	57	54	Not
date analyzed	2/ 08/ 90	2/ 11/ 91	2/ 02/ 93	7/ 19/ 93	3/ 07/ 94	5/ 09/ 95	1/ 23/ 96	7/ 22/ 97	7/ 02/ 98	determined
FREE SWELLING INDEX	3.5				3.5	3.5	2.5	3	5	
GASEOUS OXYGEN									(a)	
% in bag atmosphere					0.12	0.00	0.17	0.08	0.00	Not
date analyzed					3/ 08/ 94	5/ 09/ 95	1/ 18/ 96	7/ 21/ 97	7/01/ 98	determined

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-3	Coal Basin M seam	mvb		Ro max=1.28		
FOIL BAG	original analysis	5 of 256	13 of 256	31 of 256	15 of 256	20 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note						
date sealed		8/ 24/ 90	8/ 24/ 90	8/ 24/ 90	8/ 24/ 90	8/ 24/ 90
date analyzed	8/ 23/ 90	1/ 25/ 91	11/ 27/ 92	6/ 14/ 93	3/ 23/ 94	3/ 16/ 99
PROXIMATE						
% moisture	1.10	0.87	0.82	0.72	1.01	1.02
% ash (dry basis)	5.37	5.24	5.26	5.52	5.22	5.15
SULFUR FORMS (dry %)						
total sulfur	0.65	0.65	0.67	0.64	0.64	0.65
sulfate	0.01	0.05	0.01	0.05	0.01	0.00
pyritic	0.10	0.08	0.05	0.05	0.07	0.20
organic	0.54	0.52	0.61	0.55	0.56	0.44
CALORIFIC VALUE (dry)						
Btu/lb	14889	14907	14797	14828	14956	15023
GIESELER FLUIDITY						
maximum fluidity, ddpm	9774	17 (a)	383 (b)	234	1354	Not determined
fluid range, °C	100	79	94	94	111	
date analyzed	7/ 11/ 90	11/ 06/ 91	11/ 27/ 92	7/ 20/ 93	3/ 08/ 94	
FREE SWELLING INDEX	9				9	
GASEOUS OXYGEN						
% in bag atmosphere					0.05	Not determined
date analyzed					3/ 08/ 94	

(a) erratic behavior during testing (3 runs performed)

(b) erratic behavior during testing (6 runs performed)

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS-4	Blue seam	hvCb	Ro max= 0.51	
FOIL BAG	original analysis	6 of 256	16 of 256	11 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh
note				
date sealed		9/ 27/ 90	9/ 27/ 90	9/ 27/ 90
date analyzed	10/ 29/ 90	11/ 27/ 92	6/ 03/ 93	3/ 23/ 94
PROXIMATE				
% moisture	15.1	15.0	14.8	15.2
% ash (dry basis)	6.2	6.2	6.2	6.0
SULFUR FORMS (dry %)				
total sulfur	0.46	0.57	0.54	0.54
sulfate	0.02	0.00	0.00	0.01
pyritic	0.04	0.04	0.04	0.04
organic	0.41	0.52	0.50	0.50
CALORIFIC VALUE (dry)				
Btu/lb	13000	12919	12964	13053
GIESELER FLUIDITY				
maximum fluidity, ddpm	0	0	0	discon-
fluid range, °C	0	0	0	tinued
date analyzed	2/ 12/ 91	2/ 02/ 93	7/ 21/ 93	
FREE SWELLING INDEX	0.5			
GASEOUS OXYGEN				
% in bag atmosphere				0.00
date analyzed				3/ 08/ 94

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-5 Hiawatha seam		hvCb		Ro max= 0.59	
FOIL BAG	original analysis	11 of 256	32 of 256	14 of 256	18 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh
note					
date sealed		9/ 07/ 90	9/ 07/ 90	9/ 07/ 90	9/ 07/ 90
date analyzed	10/ 29/ 90	10/ 02/ 92	6/ 14/ 93	3/ 23/ 94	3/ 17/ 99
PROXIMATE					
% moisture	7.5	7.3	7.1	7.2	7.4
% ash (dry basis)	8.5	8.7	8.7	8.7	8.6
SULFUR FORMS (dry %)					
total sulfur	0.56	0.63	0.67	0.64	0.64
sulfate	0.01	0.01	0.01	0.00	0.01
pyritic	0.27	0.26	0.24	0.24	0.36
organic	0.28	0.35	0.42	0.40	0.27
CALORIFIC VALUE (dry)					
Btu/lb	12760	12681	12723	12784	12833
GASEOUS OXYGEN					
% in bag atmosphere				0.00	Not
date analyzed				3/ 08/ 94	determined

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS- 6		Blind Canyon seam		hvAb	Ro max= 0.66	
FOIL BAG	original analysis	12 of 256	107 of 256	125 of 256	128 of 256	
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	
note						
date sealed		7/ 19/ 90	7/ 19/ 90	7/ 19/ 90	7/ 19/ 90	
date analyzed	8/ 23/ 90	1/ 25/ 91	10/ 21/ 92	6/ 23/ 93	3/ 23/ 94	
PROXIMATE						
% moisture	4.73	4.35	4.06	4.45	4.42	
% ash (dry basis)	5.84	5.96	5.92	6.00	6.04	
SULFUR FORMS (dry %)						
total sulfur	0.40	0.43	0.35	0.43	0.42	
sulfate	0.01	0.03	0.00	0.01	0.02	
pyritic	0.02	0.02	0.02	0.02	0.02	
organic	0.37	0.38	0.33	0.40	0.40	
CALORIFIC VALUE (dry)						
Btu/lb	13923	13828	13814	13874	13920	
GIESELER FLUIDITY						
maximum fluidity, ddpm	3	0	discontinued			
fluid range, °C	38	0				
date analyzed	2/ 14/ 91	11/ 04/ 91				
GASEOUS OXYGEN						
% in bag atmosphere					0.06	
date analyzed					3/ 08/ 94	

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS- 7	Adaville #1 seam	hvCb		Ro max= 0.45
FOIL BAG	original analysis	21 of 256	26 of 256	28 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh
note				
date sealed		12/ 10/ 90	12/ 10/ 90	12/ 10/ 90
date analyzed	1/ 16/ 91	10/ 15 /92	6/ 03/ 93	3/ 23/ 94
PROXIMATE				
% moisture	17.3	16.8	17.0	17.1
% ash (dry basis)	4.2	4.3	4.3	4.2
SULFUR FORMS (dry %)				
total sulfur	0.98	0.99	1.04	1.03
sulfate	0.01	0.01	0.01	0.00
pyritic	0.10	0.08	0.08	0.08
organic	0.87	0.90	0.94	0.94
CALORIFIC VALUE (dry)				
Btu/lb	13068	12898	12947	12988
GASEOUS OXYGEN				
% in bag atmosphere				0.08
date analyzed				3/ 08/ 94

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS-8	Smith-Roland seam			subC			Ro max= 0.37 %		
FOIL BAG	original analysis	27 of 256	127 of 256	138 of 256	144 of 256	159 of 256	65 of 256	71 of 256	72 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note									
date sealed		10/ 22/ 90	10/ 22/ 90	10/ 22/ 90	10/ 22/ 90	10/ 22/ 96	10/ 22/ 90	10/ 22/ 90	10/ 22/ 90
date analyzed	10/ 30/ 90	10/ 21/ 92	6/ 03/ 93	3/ 23/ 94	5/ 09/ 95	2/ 13/ 96	8/ 01/ 97	7/ 28/ 98	3/ 17/ 99
PROXIMATE									
% moisture	28.4	28.3	28.6	28.1	28.6	28.7	28.6	28.9	28.7
% ash (dry basis)	13.8	12.8	13.1	13.0	13.6	13.0	13.1	13.0	12.9
SULFUR FORMS (dry %)									
total sulfur	0.73	0.77	0.81	0.95	0.87	0.80	0.78	0.82	0.79
sulfate	0.02	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.01
pyritic	0.28	0.20	0.22	0.22	0.27	0.25	0.31	0.31	0.29
organic	0.43	0.56	0.58	0.72	0.58	0.54	0.47	0.50	0.48
CALORIFIC VALUE (dry)						(a)			Not
Btu/lb	11168	11275	11287	11244	11210	11263	11223	11215	determined
GASEOUS OXYGEN								(b)	
% in bag atmosphere				0.08	0.14	0.28	0.13	0.00	Not
date analyzed				3/ 08/ 94	5/ 09/ 95	1/ 18/ 96	7/ 21/ 97	7/ 02/ 98	determined

(a) result from repeat analysis 4/29/96, change from Quarterly Technical Progress Report dated 4/25/96.

(b) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS- 9 Dietz seam subB Ro max= 0.38				
FOIL BAG	original analysis	of 256	of 256	of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh
note				
date sealed		1/ 10/ 91	1/ 10/ 91	1/ 10/ 91
date analyzed	1/ 18/ 91	10/ 21/ 92	6/ 03/ 93	3/ 23/ 94
PROXIMATE				
% moisture	24.7	23.8	24.8	24.6
% ash (dry basis)	6.4	6.7	6.5	6.3
SULFUR FORMS (dry %)				
total sulfur	0.41	0.42	0.44	0.42
sulfate	0.02	0.03	0.03	0.01
pyritic	0.08	0.06	0.05	0.05
organic	0.31	0.33	0.35	0.36
CALORIFIC VALUE (dry)				
Btu/lb	12330	12230	12401	12313
GASEOUS OXYGEN				
% in bag atmosphere				0.03
date analyzed				3/ 08/ 94

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS- 10		Rosebud seam		subB		Ro max= 0.42	
FOIL BAG	original analysis	8 of 256	27 of 256	10 of 256	28 of 256		
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh		
note							
date sealed		1/ 18/ 91	1/ 18/ 91	1/ 18/ 91	1/ 18/ 91		
date analyzed	1/ 28/ 91	10/ 15/ 92	6/ 04/ 93	3/ 23/ 94	3/ 17/ 99		
PROXIMATE							
% moisture	21.6	21.1	22.4	22.3	22.6		
% ash (dry basis)	12.6	13.0	13.1	13.3	13.2		
SULFUR FORMS (dry %)							
total sulfur	1.16	1.14	1.33	1.26	1.15		
sulfate	0.02	0.02	0.02	0.01	0.01		
pyritic	0.68	0.69	0.61	0.59	0.85		
organic	0.47	0.43	0.70	0.67	0.29		
CALORIFIC VALUE (dry)							
Btu/lb	11536	11383	11472	11443	11524		
GASEOUS OXYGEN							
% in bag atmosphere				0.00	Not		
date analyzed				3/ 08/ 94	determined		

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS- 11 Beulah seam		ligA		Ro max= 0.35	
FOIL BAG	original analysis	27 of 256	119 of 256	94 of 256	126 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh
note					
date sealed		1/ 25/ 91	1/ 25/ 91	1/ 25/ 91	1/ 25/ 91
date analyzed	2/ 06/ 91	10/ 21/ 92	6/ 04/ 93	3/ 23/ 94	3/ 22/ 99
PROXIMATE					
% moisture	33.4	32.5	32.9	33.1	33.8
% ash (dry basis)	9.6	10.4	9.5	9.8	9.3
SULFUR FORMS (dry %)					
total sulfur	0.74	0.74	0.74	0.57	0.80
sulfate	0.03	0.04	0.03	0.02	0.04
pyritic	0.31	0.24	0.22	0.25	0.36
organic	0.39	0.46	0.49	0.31	0.41
CALORIFIC VALUE (dry)					
Btu/lb	11062	10863	11012	10863	11040
GASEOUS OXYGEN					
% in bag atmosphere				0.00	Not
date analyzed				3/ 08/ 94	determined

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS- 12	Pittsburgh seam	hvAb			Ro max= 0.87 %					
FOIL BAG	original analysis	86 of 256	117 of 256	120 of 256	132 of 256	142 of 256	155 of 256	173 of 256	62 of 256	63 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note										
date sealed		7/ 30/ 90	7/ 30/ 90	7/ 30/ 90	7/ 30/ 90	7/ 30/ 90	7/ 30/ 90	7/ 30/ 90	7/ 30/ 90	7/ 30/ 90
date analyzed	8/ 23/ 90	7/ 31/ 91	10/ 23/ 92	6/ 04/ 93	3/ 23/ 94	5/ 23/ 95	2/ 13/ 96	7/ 30/ 97	7/ 29/ 98	3/ 17/ 99
PROXIMATE										
% moisture	2.40	2.47	2.99	1.98	2.35	2.46	2.23	2.41	2.31	2.39
% ash (dry basis)	10.25	11.05	10.35	9.52	9.86	9.69	9.34	10.12	10.8	10.6
SULFUR FORMS (dry %)										
total sulfur	1.12	1.18	1.16	1.17	1.16	1.16	1.16	1.26	1.19	1.15
sulfate	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.00	0.01	0.00
pyritic	0.38	0.29	0.17	0.35	0.35	0.39	0.40	0.53	0.46	0.46
organic	0.73	0.88	0.98	0.82	0.81	0.76	0.74	0.73	0.73	0.68
CALORIFIC VALUE (dry)										
Btu/lb	13532	13337	13471	13563	13534	13603	13646	13481	13397	13389
GIESELER FLUIDITY					(a)					
maximum fluidity, ddpm	20002	6458	4309	2173	7866	6986	17800	20489	9152	Not determined
fluid range, °C	90	90	75	80	86	83	87	89	81	
date analyzed	7/ 27/ 90	7/ 24/ 91	10/27/92	7/ 21/ 92	3/ 09/ 94	5/ 10/ 95	1/ 24/ 96	7/ 18/ 97	7/ 03/ 98	
FREE SWELLING INDEX	7.5				8	8	8	9	8.5	
GASEOUS OXYGEN									(b)	
% in bag atmosphere					0.01	0.04	0.00	0.04	0.00	Not determined
date analyzed					3/ 08/ 94	5/ 10/ 95	1/ 18/ 96	7/ 18/ 97	7/ 02/ 98	

(a) based on two of three runs which agreed within ASTM limits

(b) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS- 13	Sewell seam	mvb	Ro max= 1.35	
FOIL BAG	original analysis	7 of 256	23 of 256	17 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh
note				
date sealed		2/ 05/ 91	2/ 05/ 91	2/ 05/ 91
date analyzed	2/ 18/ 91	12/ 07/ 92	6/ 04/ 93	3/ 25/ 94
PROXIMATE				
% moisture	1.5	1.8	1.5	1.8
% ash (dry basis)	4.2	4.3	4.6	4.7
SULFUR FORMS (dry %)				
total sulfur	0.62	0.62	0.65	0.67
sulfate	0.01	0.00	0.00	0.01
pyritic	0.07	0.07	0.08	0.09
organic	0.54	0.55	0.56	0.57
CALORIFIC VALUE (dry)				
Btu/lb	14871	14827	14830	14884
GIESELER FLUIDITY				
maximum fluidity, ddpm	909	1294	915	1676
fluid range, °C	89	90	86	86
date analyzed	2/ 18/ 91	2/ 03/ 93	7/ 23/ 93	3/ 10/ 94
FREE SWELLING INDEX	8			8.5
GASEOUS OXYGEN				
% in bag atmosphere				0.00
date analyzed				3/ 08/ 94

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DECS- 14		Upper Kittanning seam			hvAb			Ro max= 1.07 %	
FOIL BAG	original analysis	6 of 256	20 of 256	11 of 256	16 of 256	23 of 256	24 of 256	25 of 256	26 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note									
date sealed	2/ 08/ 91	2/ 08/ 91	2/ 08/ 91	2/ 08/ 91	2/ 08/ 91	2/ 08/ 91	2/ 08/ 91	2/ 08/ 91	2/ 08/ 91
date analyzed	2/ 15/ 91	11/ 27/ 92	6/ 15/ 93	3/ 24/ 94	5/ 23/ 95	2/ 13/ 96	7/ 31/ 97	7/ 28/ 98	3/ 16/ 99
PROXIMATE									
% moisture	1.5	1.7	1.4	1.8	1.7	1.6	1.7	1.6	1.7
% ash (dry basis)	10.5	10.3	10.6	10.5	10.7	10.3	10.8	10.4	10.4
SULFUR FORMS (dry %)									
total sulfur	1.80	1.71	1.80	1.79	1.86	1.90	1.96	1.89	1.87
sulfate	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.00
pyritic	0.94	0.08	1.02	1.01	1.03	1.15	1.25	1.14	1.24
organic	0.85	1.62	0.78	0.77	0.82	0.74	0.71	0.75	0.63
CALORIFIC VALUE (dry)									
Btu/lb	13678	13723	13701	13803	13602	13739	13621	13760	13800
GIESELER FLUIDITY									
maximum fluidity, ddpm	29930	27625	23619	29836	29945	29953	28578	29814	Not determined
fluid range, °C	109	108	104	108	110	108	108	110	
date analyzed	2/ 19/ 91	2/ 04/ 93	7/ 23/ 93	3/ 10/ 94	5/ 16/ 95	1/ 24/ 96	7/ 23/ 97	7/ 03/ 98	
FREE SWELLING INDEX	8			7.5	8	7.5	9.0	8.5	
GASEOUS OXYGEN					(a)			(a)	Not determined
% in bag atmosphere				0.04	0	0.08	0.06	0.00	
date analyzed				3/ 08/ 94	5/ 15/ 95	1/ 18/ 96	7/ 22/ 97	7/ 02/ 98	

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-15		Lower Sunnyside seam			hvAb		Ro max= 0.80 %	
FOIL BAG	original analysis	3 of 256	6 of 256	5 of 256	8 of 256	10 of 256	11 of 256	14 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note								
date sealed	7/ 05/ 91	10/ 15/ 92	10/ 15/ 92	10/ 15/ 92	10/ 15/ 92	10/ 15/ 92	10/ 15/ 92	10/ 15/ 98
date analyzed	7/ 05/ 91	11/ 27/ 92	6/ 15/ 93	3/ 24/ 94	5/ 23/ 95	2/ 13/ 96	7/ 31/ 97	7/ 28/ 98
PROXIMATE								
% moisture	2.9	2.9	2.6	3.1	3.0	3.0	3.2	3.0
% ash (dry basis)	10.0	10.1	9.8	9.8	10.0	10.1	10.4	10.1
SULFUR FORMS (dry %)								
total sulfur	1.65	1.75	1.62	1.64	1.66	1.58	1.65	1.63
sulfate	0.05	0.03	0.02	0.02	0.02	0.05	0.05	0.07
pyritic	0.61	0.94	0.69	0.76	0.70	0.77	0.76	0.77
organic	0.99	0.78	0.91	0.87	0.94	0.76	0.83	0.79
CALORIFIC VALUE (dry)								
Btu/lb	13429	13275	13396	13553	13415	13295	13180	13334
GIESELER FLUIDITY								
maximum fluidity, ddpm	959	258	170	215	246	60	68	78
fluid range, °C	76	75	69	70	72	63	66	68
date analyzed	6/ 13/ 91	2/ 05/ 93	7/ 26/ 93	3/ 11/ 94	5/ 11/ 95	1/ 25/ 96	7/ 23/ 97	7/ 06/ 98
FREE SWELLING INDEX	4.5			4	4.5	3.5	5.5	5.5
GASEOUS OXYGEN					(a)			(a)
% in bag atmosphere				0.04	0	0.18	0.01	0.00
date analyzed				3/ 08/ 94	5/ 11/ 95	1/ 18/ 96	7/ 22/ 97	7/ 05/ 98

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS- 16 Blind Canyon seam		hvAb		Ro max= 0.64	
FOIL BAG	original analysis	7 of 256	36 of 256	11 of 256	
particle size stored		-20 mesh	-20 mesh	-20 mesh	
note					
date sealed		8/ 25/ 92	8/ 25/ 92	8/ 25/ 92	
date analyzed	7/ 05/ 91	11/ 27/ 92	6/ 15/ 93	3/ 24/ 94	
PROXIMATE					
% moisture	5.4	4.9	5.0	5.4	
% ash (dry basis)	13.9	15.2	15.7	15.3	
SULFUR FORMS (dry %)					
total sulfur	0.47	0.48	0.46	0.49	
sulfate	0.02	0.05	0.01	0.01	
pyritic	0.06	0.07	0.06	0.06	
organic	0.38	0.37	0.39	0.42	
CALORIFIC VALUE (dry)					
Btu/lb	12580	12253	12297	12418	
GIESELER FLUIDITY					
maximum fluidity, ddpm	6	3	2	2	
fluid range, °C	42	42	41	42	
date analyzed	6/ 14/ 91	2/ 08/ 93	7/ 26/ 93	3/ 15/ 94	
FREE SWELLING INDEX	2			2	
GASEOUS OXYGEN					
% in bag atmosphere				0.02	
date analyzed				3/ 08/ 94	

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-17		REFRIGERATED, -20 MESH		Blind Canyon seam		hvAb		Ro max=0.59 %	
FOIL BAG	original analysis	204 of 256	205 of 256	17 of 256	10 of 256	11 of 256	12 of 256	13 of 256	14 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note									
date sealed		12/ 04/ 91	12/ 04/ 91	12/ 04/ 91	12/ 04/ 91	12/ 04/ 91	12/ 04/ 91	12/ 04/ 91	12/ 04/ 91
date analyzed	8/ 27/ 91	4/ 16/ 93	6/ 15/ 93	4/ 26/ 94	5/ 23/ 95	2/ 13/ 96	7/ 31/ 97	7/ 28/ 98	3/ 16/ 99
PROXIMATE									
% moisture	3.7	3.9	3.8	3.9	4.1	4.0	4.1	4.0	4.1
% ash (dry basis)	6.6	6.6	6.7	6.4	6.5	6.7	6.7	6.4	6.6
SULFUR FORMS (dry %)									
total sulfur	0.44	0.43	0.42	0.47	0.44	0.43	0.43	0.44	0.43
sulfate	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.01
pyritic	0.02	0.03	0.05	0.04	0.04	0.04	0.06	0.06	0.07
organic	0.41	0.39	0.36	0.43	0.39	0.38	0.37	0.37	0.35
CALORIFIC VALUE (dry)									
Btu/lb	13826	13869	13904	13926	13745	13942	13861	13872	13897
GIESELER FLUIDITY									
maximum fluidity, ddpm	5	4	2	2	2	2	3	3	Not determined
fluid range, °C	55	52	47	44	48	46	48	43	
date analyzed	8/ 16/ 91	10/ 28/ 92	7/ 27/ 93	4/ 20/ 94	5/ 16/ 95	1/ 26/ 96	7/ 24/ 97	7/ 07/ 98	
FREE SWELLING INDEX	2			2	2.5	1.5	2	4.5	
GASEOUS OXYGEN					(a)			(a)	Not determined
% in bag atmosphere				0.00	0	0.10	0.00	0.00	
date analyzed				4/ 20/ 94	5/ 16/ 95	1/ 18/ 96	7/ 22/ 97	7/ 06/ 98	

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-18		Kentucky #9 seam		hvBb	Ro max= 0.56		
FOIL BAG	original analysis	3 of 256	2 of 256	5 of 256	8 of 256	15 of 256	20 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh	-20 mesh
note							
date sealed		10/ 09/ 92	10/ 09/ 92	10/ 09/ 92	10/ 09/ 92	10/ 09/ 92	10/ 09/ 92
date analyzed	11/ 22/ 91	6/ 18/ 93	4/ 26/ 94	5/ 25/ 95	2/ 13/ 96	7/ 28/ 98	3/ 16/ 99
PROXIMATE							
% moisture	6.8	7.3	7.4	7.4	7.1	7.5	7.7
% ash (dry basis)	12.3	11.3	11.8	11.7	11.7	12.2	11.9
SULFUR FORMS (dry %)							
total sulfur	4.21	3.91	3.97	4.02	4.05	4.16	3.76
sulfate	0.01	0.04	0.04	0.03	0.01	0.13	0.21
pyritic	2.37	1.78	1.99	1.71	2.03	1.91	2.02
organic	1.83	2.10	1.94	2.27	2.01	2.13	1.54
CALORIFIC VALUE (dry)							
Btu/lb	12687	12763	12794	12723	12818	12688	12615
GIESELER FLUIDITY							
maximum fluidity, ddpm	527	409	159	677	513	421	Not determined
fluid range, °C	80	74	73	90	82	70	
date analyzed	2/ 11/ 93	7/ 29/ 93	4/ 11/ 94	5/ 12/ 95	1/ 25/ 96	7/ 07/ 98	
FREE SWELLING INDEX	2		3	4	3.5	6	
GASEOUS OXYGEN				(a)		(a)	
% in bag atmosphere			0.21	0	0.09	0.00	Not determined
date analyzed			3/ 29/ 94	5/ 12/ 95	1/ 18/ 96	7/ 06/ 98	

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-19	Pocahontas #3 seam	lvb	Ro max=1.71	
FOIL BAG	original analysis	10 of 256	9 of 256	27 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh
note				
date sealed		7/ 14/ 92	7/ 14/ 92	7/ 14/ 92
date analyzed	8/ 21/ 92	6/ 18/ 93	4/ 26/ 94	3/ 16/ 99
PROXIMATE				
% moisture	1.0	0.8	0.8	0.9
% ash (dry basis)	4.6	5.5	5.4	5.5
SULFUR FORMS (dry %)				
total sulfur	0.74	0.78	0.77	0.76
sulfate	0.00	0.00	0.01	0.00
pyritic	0.21	0.24	0.26	0.33
organic	0.52	0.53	0.50	0.42
CALORIFIC VALUE (dry)				
Btu/lb	15006	14790	14867	14854
GIESELER FLUIDITY				
maximum fluidity, ddpm	17	9	13	Not determined
fluid range, °C	50	52	53	
date analyzed	1/ 22/ 93	7/ 30/ 93	4/ 18/ 94	
FREE SWELLING INDEX	6		7.5	
GASEOUS OXYGEN				
% in bag atmosphere			0.08	Not determined
date analyzed			4/ 18/ 94	

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DECS-20	Elkhorn #3 seam	hvAb	Ro max= 0.87
FOIL BAG	original analysis	16 of 256	5 of 256
particle size stored		-20 mesh	-20 mesh
note			
date sealed		7/ 15/ 92	7/ 15/ 92
date analyzed	8/ 21/ 92	6/ 18/ 93	4/ 26/ 94
PROXIMATE			
% moisture	2.8	2.7	2.8
% ash (dry basis)	5.5	5.2	5.1
SULFUR FORMS (dry %)			
total sulfur	0.97	0.96	1.01
sulfate	0.00	0.00	0.02
pyritic	0.21	0.17	0.21
organic	0.75	0.78	0.78
CALORIFIC VALUE (dry)			
Btu/lb	14244	14204	14277
GIESELER FLUIDITY			
maximum fluidity, ddpm	1612	1149	1206
fluid range, °C	66	66	69
date analyzed	1/ 19/ 93	7/ 30/ 93	4/ 18/ 94
FREE SWELLING INDEX	4		4
GASEOUS OXYGEN			
% in bag atmosphere			0.00
date analyzed			4/18/94

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-21 Lykens Valley #2 seam an Ro max= 5.19			
FOIL BAG	original analysis	6 of 256	25 of 256
particle size stored		-20 mesh	-20 mesh
note			
date sealed		4/ 09/ 93	4/ 09/ 93
date analyzed	5/ 03/ 93	4/ 26/ 94	3/ 16/ 99
PROXIMATE			
% moisture	4.0	4.2	4.0
% ash (dry basis)	10.7	11.5	10.9
SULFUR FORMS (dry %)			
total sulfur	0.50	0.51	0.47
sulfate	0.00	0.01	0.01
pyritic	0.60	0.08	0.12
organic	0.43	0.42	0.34
CALORIFIC VALUE (dry)			
Btu/lb	13284	13336	13356
GASEOUS OXYGEN			
% in bag atmosphere		0.03	Not
date analyzed		4/ 19/ 94	determined

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS-22 Upper Kittanning seam hvAb Ro max= 0.77		
FOIL BAG	original analysis	3 of 256
particle size stored		-20 mesh
note		
date sealed		6/ 18/ 93
date analyzed	6/ 25/ 93	4/ 22/ 94
PROXIMATE		
% moisture	0.9	0.9
% ash (dry basis)	23.1	22.8
SULFUR FORMS (dry %)		
total sulfur	1.71	1.61
sulfate	0.03	0.03
pyritic	1.15	1.12
organic	0.53	0.47
CALORIFIC VALUE (dry)		
Btu/lb	11786	11837
GIESELER FLUIDITY		
maximum fluidity, ddpm	11719	8991
fluid range, °C	66	60
date analyzed	6/ 23/ 93	4/ 20/ 94
FREE SWELLING INDEX	1	1
GASEOUS OXYGEN		
% in bag atmosphere		0.04
date analyzed		4/ 19/ 94

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-23		Pittsburgh seam	hvAb	Ro max= 0.73 %	
FOIL BAG	original analysis	17 of 256	18 of 256	19 of 256	16 of 256
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh
note					
date sealed		2/ 11/ 94	2/ 11/ 94	2/ 11/ 94	2/ 11/ 94
date analyzed	2/ 21/ 94	2/ 08/ 95	11/ 30/ 95	7/ 30/ 97	7/ 28/ 98
PROXIMATE					
% moisture	2.00	2.03	2.09	2.13	2.12
% ash (dry basis)	9.44	9.64	9.67	9.61	9.60
SULFUR FORMS (dry %)					
total sulfur	3.87	3.79	3.66	3.89	4.09
sulfate	0.01	0.01	0.00	0.00	0.01
pyritic	2.23	2.42	2.45	2.73	2.72
organic	1.63	1.36	1.20	1.16	1.36
CALORIFIC VALUE (dry)					
Btu/lb	13614	13553	13565	13487	13628
GIESELER FLUIDITY					
maximum fluidity, ddpm	30000	30000	30000	30002	30000
fluid range, °C	97	106	100	104	101
date analyzed	2/ 07/ 94	1/ 23/ 95	11/ 28/ 95	7/ 15/ 97	7/ 09/ 98
FREE SWELLING INDEX	7.5	7	7.5	9	7
GASEOUS OXYGEN		(a)			(a)
% in bag atmosphere		0	not	0.00	0.00
date analyzed		5/ 16/ 95	determined	7/ 15/ 97	7/ 06/ 98

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS-24	Illinois #6 seam	hvBb	Ro max= 0.49 %		
FOIL BAG	original analysis	105 of 328	106 of 328	107 of 328	133 of 328
particle size stored		-20 mesh	-20 mesh	-20 mesh	-20 mesh
note					
date sealed		7/ 19/ 94	7/ 19/ 94	7/ 19/ 94	7/ 19/ 94
date analyzed	9/ 07/ 94	2/ 08/ 95	11/ 29/ 95	7/ 30/ 97	7/ 28/ 98
PROXIMATE					
% moisture	13.2	13.4	13.4	13.4	13.4
% ash (dry basis)	13.4	13.5	13.6	13.5	13.4
SULFUR FORMS (dry %)					
total sulfur	5.53	5.92	5.76	5.75	5.87
sulfate	0.25	0.01	0.01	0.06	0.01
pyritic	2.64	2.86	2.77	2.96	2.99
organic	2.64	3.05	2.98	2.73	2.88
CALORIFIC VALUE (dry)					
Btu/lb	12162	12074	12242	12203	12300
GIESELER FLUIDITY					
maximum fluidity, ddpm	49	55	53	54	56
fluid range, °C	78	82	82	74	76
date analyzed	6/ 14/ 94	1/ 24/ 95	11/ 29/ 95	7/ 16/ 97	7/ 09/ 98
FREE SWELLING INDEX	3	3.5	3.5	6	5.5
GASEOUS OXYGEN		(a)			(a)
% in bag atmosphere		0	not	0.00	0.00
date analyzed		5/ 16/ 95	determined	7/ 15/ 97	7/ 06/ 98

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-25	Pust seam	ligA	Ro max= 0.23 %
FOIL BAG	original analysis	62 of 280	
particle size stored		-20 mesh	
note			
date sealed		7/ 25/ 94	
date analyzed	9/ 07/ 94	3/ 17/ 94	
PROXIMATE			
% moisture	34.9	35.9	
% ash (dry basis)	11.9	11.0	
SULFUR FORMS (dry %)			
total sulfur	0.72	0.80	
sulfate	0.05	0.03	
pyritic	0.31	0.47	
organic	0.35	0.29	
CALORIFIC VALUE (dry)			
Btu/lb	10947	10938	
GASEOUS OXYGEN			
% in bag atmosphere	Not		
date analyzed	determined		

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS-29 Upper Banner No. 3 seam		hvAb	Ro max= 1.00 %
FOIL BAG	original analysis	37 of 328	35 of 328
particle size stored		-20 mesh	-20 mesh
note			
date sealed		7/ 10/ 95	7/ 10/ 95
date analyzed	8/ 10/ 95	7/ 28/ 98	3/ 17/ 99
PROXIMATE			
% moisture	2.4	2.3	2.3
% ash (dry basis)	6.4	6.4	6.5
SULFUR FORMS (dry %)			
total sulfur	0.59	0.59	0.56
sulfate	0.01	0.01	0.01
pyritic	0.09	0.17	0.20
organic	0.50	0.41	0.35
CALORIFIC VALUE (dry)			
Btu/lb	14543	14521	14492
GIESELER FLUIDITY			
maximum fluidity, ddpm	8942	10538	
fluid range, °C	90	84	Not
date analyzed	6/ 29/ 95	7/ 10/ 98	determined
FREE SWELLING INDEX	8	8.5	
GASEOUS OXYGEN		(a)	
% in bag atmosphere		0.00	Not
date analyzed		7/ 06/ 98	determined

(a) less than usual accuracy but definitely no significant oxygen

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-30	Splash Dam seam	mvb	Ro max= 1.16 %	
FOIL BAG	original analysis	35 of 280	37 of 280	
particle size stored		-20 mesh	-20 mesh	
note				
date sealed		7/ 11/ 95	7/ 11/ 95	
date analyzed	8/ 15/ 95	8/ 01/ 97	3/ 17/ 99	
PROXIMATE				
% moisture	2.06	1.59	1.53	
% ash (dry basis)	3.89	3.99	4.01	
SULFUR FORMS (dry %)				
total sulfur	0.79	0.80	0.78	
sulfate	0.00	0.00	0.01	
pyritic	0.14	0.20	0.25	
organic	0.65	0.60	0.53	
CALORIFIC VALUE (dry)				
Btu/lb	15060	14967	15018	
GIESELER FLUIDITY				
maximum fluidity, ddpm	28188	19182		
fluid range, °C	117	110		
date analyzed	6/ 30/ 95	7/ 31/ 97		Not determined
FREE SWELLING INDEX	8	9		
GASEOUS OXYGEN				
% in bag atmosphere		0.00		Not determined
date analyzed		7/ 25/ 97		

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-31	Pond Creek seam	hvAb	Ro max= 0.99 %	
FOIL BAG	original analysis	35 of 280		
particle size stored		-20 mesh		
note				
date sealed		7/ 12/ 95		
date analyzed	8/ 14/ 95	8/ 01/ 97		
PROXIMATE				
% moisture	2.32	1.94		
% ash (dry basis)	10.89	11.46		
SULFUR FORMS (dry %)				
total sulfur	0.60	0.63		
sulfate	0.01	0.01		
pyritic	0.11	0.17		
organic	0.49	0.46		
CALORIFIC VALUE (dry)				
Btu/lb	13689	13467		
GIESELER FLUIDITY				
maximum fluidity, ddpm	3634	3472		
fluid range, °C	79	74		
date analyzed	6/ 28/ 95	7/ 28/ 97		
FREE SWELLING INDEX	8	9		
GASEOUS OXYGEN				
% in bag atmosphere		0.00		
date analyzed		7/ 28/ 97		

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

DECS-32 Stockton-Lewiston seam		hvAb	Ro max= 1.16 %
FOIL BAG	original analysis	35 of 280	
particle size stored		-20 mesh	
note			
date sealed		7/ 13/ 95	
date analyzed	8/ 14/ 95	8/ 01/ 95	
PROXIMATE			
% moisture	2.64	2.42	
% ash (dry basis)	20.30	20.88	
SULFUR FORMS (dry %)			
total sulfur	0.73	0.73	
sulfate	0.01	0.00	
pyritic	0.10	0.17	
organic	0.62	0.55	
CALORIFIC VALUE (dry)			
Btu/lb	11853	11685	
GIESELER FLUIDITY			
maximum fluidity, ddpm	450	472	
fluid range, °C	67	64	
date analyzed	6/ 27/ 95	7/ 29/ 97	
FREE SWELLING INDEX	5	5.5	
GASEOUS OXYGEN			
% in bag atmosphere		0.00	
date analyzed		7/ 28/ 97	

APPENDIX A. Monitoring of DECS Coals to Evaluate Sample Condition after Storage

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DECS-33	Ohio #4A seam	hvBb	Ro max= 0.51 %	
FOIL BAG	original analysis	35 of 280	57 of 280	
particle size stored		-20 mesh	-20 mesh	
note				
date sealed		8/ 02/ 95	8/ 02/ 95	
date analyzed	8/ 16/ 95	8/ 01/ 97	3/ 17/ 99	
PROXIMATE				
% moisture	5.97	5.86	5.95	
% ash (dry basis)	12.0	12.0	12.0	
SULFUR FORMS (dry %)				
total sulfur	3.74	3.76	4.18	
sulfate	0.01	0.01	0.10	
pyritic	1.41	1.84	1.81	
organic	2.32	1.92	2.27	
CALORIFIC VALUE (dry)				
Btu/lb	12617	12662	12569	
GIESELER FLUIDITY				
maximum fluidity, ddpm	86	116		
fluid range, °C	75	66		
date analyzed	7/ 28/ 95	7/ 30/ 97	Not determined	
FREE SWELLING INDEX	4	5		
GASEOUS OXYGEN				
% in bag atmosphere		0.00		
date analyzed		7/ 28/ 97	Not determined	

APPENDIX B. Procedures for Standardized Liquefaction Test of DECS Samples including Extraction and Gas Analysis

MATERIALS

Solvents (HPLC grade)

Tetrahydrofuran (THF)
Hexane
Toluene
1-methylnaphthalene 98%
1,2,3,4-tetrahydronaphthalene 99% (tetralin)

Equipment

Buchi RE111 Rotovapor
Omega XA-100 balance
Napco #5831 vacuum oven
sand bath reactor
stir plate

Reactor Vessels

4 tubing bomb reactors with 2000 psi pressure gauges and Swagelok fittings
approximately 24 ml capacity

Glassware and other supplies

(NOTE: all glassware is baked at 450°C prior to use; all other supplies are rinsed with THF)

250 ml beakers
250 ml round bottom flasks
400 ml round bottom flasks
Soxhlet apparatus (for extractions)
Whatman glass microfibre filters (GF/C)
Whatman glass microfibre extraction thimbles (GF; 30x100mm)
boiling chips (cleaned with THF)
compressed nitrogen
gas-tight syringe
gas bulbs
metal spatula
magnetic stirrer
Petri dish

LIQUEFACTION

For each complete standardized liquefaction analysis, perform the following procedure for two tubing-bomb reactors using tetralin and two tubing-bomb reactors using 1-methylnaphthalene.

Ensure that baking of glassware and rinsing of other supplies has been performed.

All items which come in contact with sample or resulting products must be weighed to 0.0001 g before and after contact so that sample loss may be calculated.

Weigh out 5 grams of freeze-dried coal and 5 grams of tetralin (or 1-methylnaphthalene) and place both into the tubing bomb reactor.

Screw the end caps of the reactor on very tightly.

Fill and then purge the reactor with nitrogen up to 1000 psi (repeat 3 times).

Fill the reactor with hydrogen up to 1000 psi and then purge very slowly (over a period of 5 min.). Repeat 3 times. After the third fill, close the valve on the reactor, leaving it pressurized with hydrogen.

Submerge the reactor in water to check for leaks.

Place the reactor in a secure place where it is in a stable position. Observe the pressure reading on the gauge. If the pressure remains stable for 10 minutes you may assume no significant leaks exist.

Place the reactor into the sand bath which has been set at 350° C. The temperature of the sand bath will decrease rapidly after introducing the reactor. Wait until the temperature reaches 350°C and then begin timing the length of the run (30 minutes).

After 30 min remove the reactor from the sand bath and submerge it in water to cool the reactor.

At this point remember to keep the valve on the reactor closed and to store it in a secure place if it must be stored temporarily.

GAS ANALYSIS

Measuring the volume of gas

Attach a Swagelok purge valve with a 15 cm length of tubing onto the reactor, making sure that the valve on the reactor remains closed.

Onto the other end of the tubing, attach a flow-through gas bulb.

Onto the other end of the gas bulb attach a 1-meter length of tubing, so that the sequence is: reactor, Swagelok purge valve, tubing, gas bulb (for trapping gas), and a longer piece of tubing (1 meter).

Place the end of the longer piece of tubing into an inverted graduated cylinder filled with water. (For these reactions, gas production has been from 1-2 liters, so a 2 liter graduated cylinder is suggested.)

Make sure that the valves on the flow-through gas bulb are open.

Slowly open the valve on the reactor. Water should begin to evacuate from the inverted graduated cylinder as the gas displaces it.

When all the gas has left the reactor, close both valves on the flow-through gas bulb (trapping a sample of gas in the bulb).

Close the valve on the reactor.

From the inverted graduated cylinder, read the volume of gas that was in the reactor and record the data.

Take a gas-tight syringe and sample 1ml of the gas from the bulb. Inject the sample into the gas chromatograph.

The gas chromatograph is then run to analyze for CO₂ and C1, C2, C3 and C4 compounds.

After injection of the gaseous sample and the completion of the run, an external gaseous standard must be injected for a separate run (this will allow for the quantification of the sample injection).

Soxhlet extraction

Open the reactor.

Rinse the contents of the reactor into an extraction thimble (place the thimble in a 250 ml beaker) using no more than 200ml of toluene. The products will be adhered to the sides of the reactor and in the caps; scraping with the metal spatula will be necessary. Be careful not to spill any sample; this is where the greatest chance for error lies.

Take a 250ml round bottom flask, add boiling chips, and then attach to the Soxhlet apparatus.

Place the extraction thimble into the Soxhlet and then pour the contents of the beaker into the thimble. With more toluene, rinse the beaker into the thimble. Make sure that all of the sample is in the thimble and not lying in the bottom of the Soxhlet.

After all of the sample has been washed into the extraction thimble, add enough toluene to the round bottom flask to bring the total amount of toluene up to approximately 200ml (this includes the amount of toluene that is also in the Soxhlet).

Using tubing, connect the tank of compressed nitrogen to the condensing tower on the Soxhlet.

Turn on the nitrogen to the point where there is a light flow of gas going through the Soxhlet.

Turn on the water to the condensing tower.

Turn on the heating mantle and bring the toluene in the 250ml flask to a moderate boil.

At this point the toluene should start to cycle through the Soxhlet extractor.

Continue the extraction until the toluene in the Soxhlet has become colorless again. This takes approximately 48 h.

During this time it may be necessary to add more toluene to maintain a volume of 200ml.

After the extraction is complete, turn off the mantle and allow the solution to cool to room temperature.

Keeping the round bottom flask attached to the Soxhlet, tilt the assembly until the toluene in the Soxhlet pours into the 250ml round bottom flask.

After this is done, separate the 250ml round bottom flask from the Soxhlet and set the 250ml round bottom flask aside temporarily (these instructions resume below).

Take another 250ml round bottom flask, containing boiling chips, and fill it with approximately 200ml of THF.

Attach the 250ml round bottom flask to the Soxhlet.

Turn on the heating mantle and bring the THF to a moderate boil. The THF should start to cycle through the Soxhlet (remember, both the water and nitrogen should still be on).

This extraction should also take approximately 48 h. However, continue until the THF in the Soxhlet has become colorless again.

After the THF extraction is under way, return to the 250ml round bottom flask containing the toluene and toluene extractable material.

Transfer the contents of the 250ml round bottom flask into a 400ml round bottom flask. Be sure to rinse the 250ml round bottom flask (using toluene) into the 400ml round bottom flask at least 3 times.

Rotovaporate the 400ml round bottom flask, which will remove most of the toluene. (However, there will be some left, as well as some liquid product from the extraction).

After rotary evaporation, add approximately 400ml of hexane to the 400ml round bottom flask.

Add a magnetic stirrer to the 400ml round bottom flask.

Stir the contents of the 400ml round bottom flask for exactly 1 h.

After stirring, cover the 400ml round bottom flask and let it sit overnight.

The next day, filter the contents of the 400ml round bottom flask through the Whatman GF/C glass microfibre filters. Be sure to rinse the contents of the 400ml round bottom flask into the filter using hexane; rinse at least 3 times.

Transfer the filter paper, boiling chips, magnetic stirrer, and hexane- insoluble matter into a Petri dish (you may wish to rinse off the stirrer and remove it from the Petri dish before placing the dish in the vacuum drying oven).

Rotovaporate the hexane solubles (the solution not caught in the filter) to remove hexane. (This will remove most of the hexane; however, there will be some hexane as well as some liquid product from the extraction left in the round bottom flask).

Place both the Petri dish and the round bottom flask into the vacuum drying oven at 150° C for 2 h.

After drying, weigh the samples. The sample in the Petri dish is the asphaltene fraction. The sample in the round bottom flask is the oil fraction.

Return to the THF extraction:

Once the THF in the Soxhlet is colorless turn off the mantle and let cool to room temperature.

After cooling, turn off the nitrogen and the water.

Keeping the round bottom flask attached to the Soxhlet, tilt the assembly until the THF in the Soxhlet pours into the 250ml round bottom flask.

Wash all of the contents of the 250ml round bottom flask into a 400ml round bottom flask using THF.

Rinse the 250ml round bottom flask into the 400ml round bottom flask using THF at least 3 times.

Rotovaporate the 400ml round bottom flask (this will remove most of the THF; however, some THF and a liquid product from the extraction will be left.

Place the 400ml round bottom flask in the vacuum drying oven at 150° C for 2 h.

After drying, weigh the product in the 400ml round bottom flask. This is the preasphaltene fraction.

Remove the extraction thimble from the Soxhlet and place in the vacuum drying oven.

After drying, weigh the product in the thimble. This is the insoluble fraction.

Calculation of Product Distribution and Conversion

Apply the calculated sample weight losses from the before-contact and after-contact weighing of glassware and supplies to the appropriate steps in conversion calculation procedures.

insoluble residue weight = (wt. of thimble + wt. of sample remaining in thimble after all extractions are completed) - wt. of thimble (clean)

preasphaltenes weight = wt. of 250ml round bottom flask (containing boiling chips and dried extract) - (wt of 250ml round bottom flask (clean) + wt. of boiling chips (clean))

asphaltenes weight = wt. of Petri dish (containing boiling chips, dried extract, filter paper, and stirrer) - (wt. of petri dish (clean) + wt. of boiling chips (clean) + wt. of filter paper (clean) + wt. of stirrer (clean))

oil fraction weight = wt. of 500ml flat bottom flask (containing dried extract) - wt. of 500ml flat bottom flask (clean)

gas fraction (recovered using GC) weight = wt. of (CO₂ + C1 + C2 + C3 + C4)

weight of total recovered material = (wt. of insoluble residue + wt. of preasphaltenes + wt. of asphaltenes + wt. of oil fraction + wt. of gas fraction)

Conversion % for specific fraction = wt. of fraction x 100 % / wt. of original sample (before liquefaction)

Conversion % (total) = (wt. of preasphaltenes + wt. of asphaltenes + wt. of oil fraction + wt. of gas fraction) x 100 % / wt. of original sample (before liquefaction)

The procedures used were presented in the Quarterly Technical Progress Report for January through March, 1994. The calculations listed therein were on a raw (ash-containing) basis, and the gas fraction and total recovered material weights were incorrect; correct explanations for values on an ash-free basis (which will be used henceforth) are as follows:

gas fraction weight by difference = initial sample weight - (weights of insoluble residue + preasphaltenes + asphaltenes + oil fraction)

conversion % for specific fraction, ash-free basis = $\frac{\text{wt. of fraction}}{\text{initial weight} * (1 - (\text{ash\%} / 100\%))}$

conversion % (total, ash-free basis) = $\frac{\text{initial weight} - \text{insoluble residue weight}}{\text{initial weight} * (1 - (\text{ash\%} / 100\%))}$

APPENDIX C. Agencies Supplied with Coal Samples and/or Data 9/29/93 to 3/30/99

The numbers in parentheses represent multiple requests which were separately processed.

ABB Combustion Engineering
Action Mining, Inc.
Advanced Fuel Research (3)
American Colloid Company (3)
Amoco
APTI Geoscience Operations
ARCO Oil and Gas Company
Arctech, Inc. (3)
Argonne National Laboratory (2)
Arizona State University, Chemistry Department
Auburn University, Chemical Engineering Department (3)
Babcock and Wilcox, Alliance Research Center
Battelle Memorial Institute
Bell Laboratories
Brigham Young University, Chemical Engineering Department (2)
Brown University, Division of Engineering (5)
Buckeye Industrial Mining Company (4)
Burgueno, Mrs. M.
Cal Tech University
Calcott Consulting (Australia)
Calgon Carbon (2)
Carbon Sales, Inc. (3)
Centenary College, Chemistry Department
Central Research Institute for Electric Power, Biosciences Department, Japan
Centre Lime & Stone Company
Chevron Petroleum Technology Company (2)
City College of New York, Chemical Engineering Department
Clark Atlanta University, Chemistry Department (3)
Coal Education Development and Resources (CEDAR) Program of Eastern Kentucky
Coal Technology Corporation (6)
Colorado School of Mines
Colorado Geological Survey
Colorado State University, Natural Resource Ecology Laboratory
Columbia University, Geology Department
Cominco, Inc. (Canada)
Consol Pennsylvania Coal Company
CSIRO Division of Energy Technology (Australia) (2)
E.I. Dupont de Nemours and Company, Central Research and Development
East Fairfield Coal Company
Eco-Systems

EER

Emission Monitoring, Inc.

Exergetic Systems (2)

Exportech, Inc.

Exxon Production Research Company (5)

Exxon Research and Engineering Center

Foster-Wheeler Development Corp. (3)

Geological Survey of Denmark

Geological Survey of Canada

GeoMet, Inc.

Giant Foods

Global Import/ Export of Charleston (2)

Goldman-Sachs

Hazen Research

Hokkaido University, Faculty of Engineering (Japan) (2)

Illinois State Geological Survey (5)

Imperial College, Chemical Engineering Department (United Kingdom)

Indiana Geological Survey (3)

Instituto Nacional del Carbon (Spain)

Internal Revenue Service (3)

International Committee on Coal and Organic Petrology

KAIST, Department of Chemical Engineering (S. Korea) (3)

Kelastec, Inc. (2)

Kentucky Geological Survey

Keystone Filler Co.

Lamar University, Chemical Engineering Department

Larsen, Mr. David

Law Environmental

Levine, Jeffrey R., Consulting Geologist

Little Bear Laboratories, Montana (3)

Marshall University, Chemistry Department

Michigan Tech University, Metals and Materials Engineering Research

Mineral Labs, Inc.

Monash University, Chemistry Department (Australia) (4)

National Institutes of Occupational Safety and Health (4)

National Mining Association (2)

National Institute of Standards and Technology

New York University Medical Center, Nelson Institute of Environmental Medicine (2)

Nittany Geosciences, Inc.

North Carolina A & T State University, Mechanical Engineering Department (2)

Northeastern University, Mechanical Engineering Department (6)

Oak Ridge National Laboratory (2)

Oklahoma Geological Survey

Original Fuels Co. (2)

Pennsylvania Bureau of Mining and Reclamation
 Pennsylvania Department of Environmental Protection
 Pennsylvania Department of Environmental Resources, Hawk Run Field Office
 Pennsylvania Geological Survey
 Pennsylvania Power and Light Company
 Pennsylvania State University, Chemical Engineering Department (2)
 Pennsylvania State University, Coal and Organic Petrology Laboratories (3)
 Pennsylvania State University, Energy and Fuels Research Center (10)
 Pennsylvania State University, Energy and Geo-Environmental Engineering Dept. (4)
 Pennsylvania State University, The Energy Institute (12)
 Pennsylvania State University, Fuel Science Program (78)
 Pennsylvania State University, Geosciences Department (15)
 Pennsylvania State University, Materials Research Laboratory
 Pennsylvania State University, Mineral Processing Program (14)
 Pennsylvania State University, Mining Engineering Program (5)
 Pennsylvania State University, Office of Physical Plant, Steam Plant
 Pennsylvania State University, Polymer Science Program (13)
 Pickands-Mather Coal Company (2)
 PSI Technology Co.
 Ralph Gray Services
 Reaction Engineering
 Rice University, Chemistry Department
 Rocky Mountain Institute (3)
 RTC Consultants
 Rust College, Division of Science and Mathematics (2)
 Salem Tool, Inc.
 Sandia National Laboratory (3)
 Seoul National University, Civil, Urban & Geosystem Engineering Department (S. Korea)
 SGI International, Development Center
 Shell Exploration and Production Technology Company (6)
 Shell (5)
 Silogran Trading Ltd. (Switzerland)
 Southern Illinois University, Geology Department (5)
 Southern Illinois University, Mining Engineering Department
 Southern Illinois University, Mechanical Engineering Department
 Southern Illinois University
 SRI International (3)
 SRI International, Molecular Physics Department
 Stanford University, Geosciences Department
 Tata, Inc.
 TDA Research
 Technical University of Denmark, Lab. of Heating and Air Conditioning (Denmark)
 Technology Management Associates International
 TIMCAL (Switzerland) (2)

Tri-Valley Research Company (2)
 Truman, Mr. James
 Tuskegee Institute
 U.S. Geological Survey (13)
 U.S. Department of Energy, Federal Energy Technology Center (4)
 U.S. Department of Energy, Pittsburgh Energy Technology Center (5)
 U.S. Environmental Protection Agency
 U.S. Office of Surface Mining
 Universidade do Porto (Portugal) (2)
 Università degli studi di Napoli Federico II, Chemical Engineering Department (Italy)
 Université Pierre et Marie Curie, Lab. Géochimie et Métallurgie (France)
 University of Alabama at Birmingham, Geology Department (2)
 University of British Columbia, Earth and Ocean Sciences Department (Canada)
 University of British Columbia, Pathology Department (Canada)
 University of California at Davis, Chemical Eng. & Materials Science Dept.
 University of Cincinnati, Chemical Engineering Department (2)
 University of Cincinnati, Civil and Environmental Engineering Department (8)
 University of Cincinnati, Engineering Research Division (2)
 University of Delaware, Chemical Engineering Department (15)
 University of Kentucky, Center for Applied Energy Research
 University of Kentucky, Consortium for Fossil Fuel Liquefaction Science (2)
 University of Maryland
 University of Maryland of the Eastern Shore, Natural Sciences Department
 University of Mississippi
 University of Mississippi, Chemical Engineering Department (3)
 University of Newcastle, Chemical Engineering Department (Australia) (2)
 University of North Dakota, Energy and Environmental Research Center
 University of Oklahoma
 University of Oklahoma, Chemical Engineering and Materials Science Department
 University of Oklahoma, School of Geology and Geophysics (2)
 University of Pittsburgh, Chemical Engineering Department (3)
 University of South Carolina, Biology Department (2)
 University of Southern California, Chemical Engineering Department
 University of Tennessee, Geology Department (2)
 University of Tennessee at Knoxville, Geological Science Department
 University of Texas of the Permian Basin, Chemistry Faculty (2)
 University of Utah (2)
 University of Utah, Center for Microanalysis (2)
 University of Utah, Chemical and Fuels Engineering Department (2)
 University of Utah, Chemistry Department (6)
 University of Wyoming, Department of Chemical and Petroleum Engineering (2)
 Unocal Science and Technology Division (4)
 Utah Geological Survey (3)
 Viking Systems

Virginia Division of Mineral Resources (2)
Washington and Jefferson College, Chemistry Department
West Virginia University, Chemical Engineering Department (10)
West Virginia University, Geology Department (2)
West Virginia University, Physics Department (2)
Western Research Institute
WPSX Television
Wyoming State Geological Survey

APPENDIX D. Coal Database Printouts of DECS Samples

The Penn State Coal Sample Bank and Database**Sample DECS-23****Pittsburgh Seam
Washington County, PA****hvAb rank**page 1 of 4
printed 8/24/95
sampled 2/02/94**SAMPLE LOCATION**

Washington County, Pennsylvania, USA
 West Finley Township near West Finley, Pennsylvania
 Eastern Coal Province
 Appalachian Region
 Main Bituminous
 Wind Ridge (7.5') Topographic Quadrangle
 Latitude 39° 58' 48" North, Longitude 80° 27' 36" West

SAMPLE HISTORY

Whole-Seam Channel Sample collected February 2, 1994 by Penn State
 Mining method: underground
 4" rider & 4" parting above main seam not sampled

Coal Sample Bank reserve: 202 kg (446 lbs)

SAMPLE INFORMATION

Pennsylvanian
 Monongahela Group

Seam thickness at sample location: 216 cm (7 ft 1 in.)
 Sample thickness: 216 cm (7 ft 1 in.)

Seam profile:

ROOF	gray mudstone
20 cm	bright clarain, shale lenses
5 cm	parting not sampled
46 cm	clarain with shale, pyrite
51 cm	clarain; 1" high vitrain layer
8 cm	clarain; partings not sampled
86 cm	clarain with vitrain, shale
FLOOR	gray mudstone

The Penn State Coal Sample Bank and Database

Sample DECS-23

Pittsburgh Seam
Washington County, PA

hvAb rank

page 2 of 4
printed 8/24/95
sampled 2/02/94

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	2.00			
% Ash	9.25	9.44		
% Vol. Matter	38.63	39.42	43.53	42.33
% Fixed Carbon	50.12	51.14	56.47	57.67

SULFUR FORMS

	dry	daf
% Pyritic	2.23	2.46
% Sulfate	0.01	0.01
% Organic	1.63	1.80
% Total	3.87	4.27

MOISTURE

% as received	2.00
% equilibrium	2.50

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	9.25	9.44		(12.32%MM)
% Carbon	72.72	74.21	81.95	84.64
% Hydrogen	5.00*	5.10	5.63	5.82
% Nitrogen	1.32	1.35	1.49	1.54
% Total Sulfur	3.79	3.87	4.27	
% Oxygen (diff.)	5.91*	6.03	6.66	8.00

* excluding H and O in moisture

Dry % Chlorine = 0.10 Dry % Carbon dioxide = 0.12

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(11.77% MM)
% Carbon	74.18	84.07
% Hydrogen	5.02	5.69
% Nitrogen	1.35	1.53
% Organic Sulfur	1.63	1.85
% Oxygen (diff.)	6.06	6.86
% Mineral Matter	11.77	
(incl. 4.17% FeS ₂)		

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	31.664	13614	31.031	13342	30.873	13274
MM-free (Parr)	35.602	15307	34.792	14959	34.590	14872
MM-free (mod. Parr)	35.569	15293	34.764	14947	34.564	14861
Net, dmmf Btu/lb	34.322	14757				

Mott-Spooner difference = 26 Btu/lb

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.825	0.813
Atomic O/C	0.071	0.061

The Penn State Coal Sample Bank and Database

Sample DECS-23

Pittsburgh Seam
Washington County, PA

hvAb rank

page 3 of 4
printed 8/24/95
sampled 2/02/94

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	hvAb	Reflectance Rank	hvAb
(as rec'd moist.)	hvAb		

MACERAL COMPOSITION (blue + white light, volume %)

	mineral- free	mineral- containing
Vitrinite	79.4	74.3
TOTAL VITRINITE	79.4	74.3
Fusinite	1.7	1.6
Semifusinite	8.5	8.0
Macrinite	0.0	0.0
Micrinite	3.0	2.8
Sclerotinite	0.0	0.0
Inertodetrinite	0.5	0.5
TOTAL INERTINITE	13.7	12.9
Sporinite	5.2	4.9
Resinite	0.2	0.2
Alginite	0.0	0.0
Cutinite	0.6	0.6
Liptodetrinite	0.9	0.8
Exudatinite		
Bituminite		
Fluorinite		
TOTAL LIPTINITE	6.9	6.5
Mineral matter (Parr, volume %)		6.34

REFLECTANCE DATA

Vitrinite:	Mean-max R_0 : 0.73%			
Vtypes:	V 5	V 6	V 7	V 8
percent:	1.0	20.0	73.0	6.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	7.5	Gieseler Coal Plastometer:	
		Initial softening	373°C
Hardgrove grindability index	56.8	Maximum fluidity	428°C
Vickers' microhardness index	n.d.	Solidification	470°C
Washability data not available		Fluid temp. range	97°C
		Maximum fluidity	30000 ddpm

The Penn State Coal Sample Bank and Database

Pittsburgh Seam
Washington County, PA

hvAb rank

Sample DECS-23

page 4 of 4
printed 8/24/95
sampled 2/02/94

INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements		
	oxide % of HTA		element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	36.3	Si	1.6	Ag		< 0.2
Al ₂ O ₃	17.6	Al	0.9	As		13
TiO ₂	0.76	Ti	0.04	Ba	537	51
Fe ₂ O ₃	36.7	Fe	2.4	Be	11	1
MgO	0.62	Mg	0.04	Bi		
CaO	3.03	Ca	0.20	Cd		< 0.2
Na ₂ O	0.33	Na	0.02	Ce		
K ₂ O	1.41	K	0.11	Cl		1000
P ₂ O ₅	0.59	P	0.024	Co		
SO ₃	1.70			Cr	115	11
				Cu	110	10
				Ga		
				Ge		
				Hg		0.12
				La		
				Mn	310	29
				Nb		
				Ni	85	8
				Pb		6
				Rb	32	3
				Sc		
				Se		2
				Sn		
				Sr	930	87
				Th		
				U		
				V	155	15
				Y		
				Yb		
				Zn	100	9
				Zr	160	15

High-temperature ash (HTA)
used for inorganic analysis
= 9.39 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1063°C	1945°F	1382°C	2520°F
Softening	1074°C	1965°F	1404°C	2560°F
Hemispherical	1107°C	2025°F	1416°C	2580°F
Fluid	1152°C	2105°F	1424°C	2595°F

The Penn State Coal Sample Bank and Database**Sample DECS-24****Illinois #6 Seam (Herrin Seam)**
Macoupin County, IL**hVcb rank**page 1 of 4
printed 8/24/95
sampled 6/02/94**SAMPLE LOCATION**Macoupin County, Illinois, USA
Virden Township near Virden, Illinois
Interior Coal Province
Eastern RegionFarmersville (7.5') Topographic Quadrangle
Latitude 39° 29' 06" North, Longitude 89° 44' 40" West**SAMPLE HISTORY**Whole-Seam Channel Sample collected June 2, 1994 by Penn State
Mining method: underground

Coal Sample Bank reserve: 225 kg (497 lbs)

SAMPLE INFORMATION

Pennsylvanian

Kewanee Group

Carbondale Formation

Seam thickness at sample location: 229 cm (7 ft 6 in.)

Sample thickness: 229 cm (7 ft 6 in.)

Seam profile:

ROOF	black shale
99 cm	dull clarain, pyrite partings
58 cm	bright clarain with vitrain
10 cm	dull clarain, partings
61 cm	very dull clarain, pyrite
FLOOR	soft gray clay

The Penn State Coal Sample Bank and Database

Sample DECS-24

Illinois #6 Seam (Herrin Seam)
Macoupin County, IL

hvCb rank

page 2 of 4
printed 8/24/95
sampled 6/02/94

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	13.20			
% Ash	11.62	13.39		
% Vol. Matter	35.44	40.83	47.14	45.51
% Fixed Carbon	39.74	45.78	52.86	54.49

SULFUR FORMS

	dry	daf
% Pyritic	2.64	3.05
% Sulfate	0.25	0.29
% Organic	2.64	3.05
% Total	5.53	6.38

MOISTURE

% as received	13.20
% equilibrium	11.59

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	11.62	13.39		(17.50%MM)
% Carbon	57.33	66.05	76.26	80.06
% Hydrogen	3.98*	4.59	5.30	5.56
% Nitrogen	0.99	1.14	1.32	1.38
% Total Sulfur	4.80	5.53	6.38	
% Oxygen (diff.)	8.07*	9.30	10.74	12.99

* excluding H and O in moisture

Dry % Chlorine = 0.14 Dry % Carbon dioxide = 0.65

ELEMENTAL ANALYSIS

	dry	dmmf(Mod. P)
		(16.44% MM)
% Carbon	65.87	78.83
% Hydrogen	4.47	5.35
% Nitrogen	1.14	1.36
% Organic Sulfur	2.64	3.16
% Oxygen (diff.)	9.44	11.29
% Mineral Matter	16.44	
(incl. 4.94% FeS ₂)		

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	28.287	12162	24.554	10557	25.007	10752
MM-free (Parr)	33.508	14407	28.294	12165	28.915	12432
MM-free (mod. Parr)	33.455	14384	28.305	12170	28.919	12434
Net, dmmf Btu/lb	32.271	13875				

Mott-Spooner difference = 307 Btu/lb

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.835	0.815
Atomic O/C	0.122	0.108

The Penn State Coal Sample Bank and Database

Sample DECS-24

Illinois #6 Seam (Herrin Seam)
Macoupin County, IL

hvCb rank

page 3 of 4
printed 8/24/95
sampled 6/02/94

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	hvCb	Reflectance Rank	hvCb
(as rec'd moist.)	hvCb		

MACERAL COMPOSITION (white light, volume %)

	mineral- free	mineral- containing
Vitrinite	90.2	81.8
TOTAL VITRINITE	90.2	81.8
Fusinite	2.5	2.3
Semifusinite	3.4	3.1
Macrinite	0.0	0.0
Micrinite	0.9	0.8
Sclerotinite	0.0	0.0
Inertodetrinite	0.0	0.0
TOTAL INERTINITE	6.8	6.2
Sporinite	1.7	1.5
Resinite	0.2	0.2
Alginite	0.0	0.0
Cutinite	1.1	1.0
Liptodetrinite	0.0	0.0
TOTAL LIPTINITE	3.0	2.7
Mineral matter (Parr, volume %)		9.28

REFLECTANCE DATA

Vitrinite:	Mean-max R_o : 0.49%			
Vtypes:	V 3	V 4	V 5	V 6
percent:	2.0	57.0	38.0	3.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	3	Gieseler Coal Plastometer:	
Hardgrove grindability index	57.8	Initial softening	366°C
Vickers' microhardness index	n.d.	Maximum fluidity	410°C
Washability data not available		Solidification	444°C
		Fluid temp. range	78°C
		Maximum fluidity	49 ddpm

The Penn State Coal Sample Bank and Database

Sample DECS-24

Illinois #6 Seam (Herrin Seam)
Macoupin County, IL

hvCb rank

page 4 of 4
printed 8/24/95
sampled 6/02/94

INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements		
	oxide % of HTA		element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	41.3	Si	2.6	Ag		< 0.3
Al ₂ O ₃	14.8	Al	1.1	As		2
TiO ₂	0.69	Ti	0.06	Ba	358	49
Fe ₂ O ₃	29.4	Fe	2.8	Be	8.0	1
MgO	0.66	Mg	0.05	Bi		
CaO	5.47	Ca	0.53	Cd		< 0.3
Na ₂ O	1.05	Na	0.11	Ce		
K ₂ O	1.58	K	0.18	Cl		1400
P ₂ O ₅	0.28	P	0.017	Co		
SO ₃	4.50			Cr	165	23
				Cu	95	13
				Ga		
				Ge		
				Hg		0.11
				La		
				Mn	387	53
				Nb		
				Ni	120	16
				Pb		10
				Rb	36	5
				Sc		
				Se		4
				Sn		
				Sr	254	35
				Th		
				U		
				V	195	27
				Y		
				Yb		
				Zn	240	33
				Zr	125	17

High-temperature ash (HTA)
used for inorganic analysis
= 13.68 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1060°C	1940°F	1296°C	2365°F
Softening	1082°C	1980°F	1321°C	2410°F
Hemispherical	1149°C	2100°F	1354°C	2470°F
Fluid	1199°C	2190°F	1382°C	2520°F

The Penn State Coal Sample Bank and Database**Sample DECS-25****Pust Seam**
Richland County, MT**ligA rank**page 1 of 4
printed 8/24/95
sampled 6/06/94**SAMPLE LOCATION**Richland County, Montana, USA
near Savage, Montana
Northern Great Plains Coal Province
Fort Union RegionKnife River Mine (7.5') Topographic Quadrangle
Latitude 47° 28' 25" North, Longitude 104° 26' 35" West**SAMPLE HISTORY**Whole-Seam Channel Sample collected June 6, 1994 by Penn State
Mining method: surface
sampled upper and lower parts 100 meters apart

Coal Sample Bank reserve: 176 kg (388 lbs)

SAMPLE INFORMATION

Paleocene

Fort Union Formation

Seam thickness at sample location: 701 cm (23 ft 0 in.)

Sample thickness: 701 cm (23 ft 0 in.)

Seam profile:

137 cm	dull, brownish
229 cm	dull, pyrite on cleat for 2"
61 cm	parting, not sampled
91 cm	dull
61 cm	dull with shaly layers
122 cm	dull

The Penn State Coal Sample Bank and Database

Sample DECS-25

Pust Seam
Richland County, MT

ligA rank

page 2 of 4
printed 8/24/95
sampled 6/06/94

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	34.91			
% Ash	7.71	11.85		
% Vol. Matter	27.32	41.98	47.62	46.94
% Fixed Carbon	30.05	46.17	52.38	53.06

SULFUR FORMS

	dry	daf
% Pyritic	0.31	0.35
% Sulfate	0.05	0.06
% Organic	0.35	0.40
% Total	0.72	0.82

MOISTURE

% as received	34.91
% equilibrium	34.82

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	7.71	11.85		(13.19%MM)
% Carbon	42.80	65.76	74.60	75.76
% Hydrogen	2.99*	4.60	5.22	5.30
% Nitrogen	0.61	0.94	1.07	1.08
% Total Sulfur	0.47	0.72	0.82	
% Oxygen (diff.)	10.50*	16.13	18.30	17.86
* excluding H and O in moisture				
Dry % Chlorine = 0.04 Dry % Carbon dioxide = 1.38				

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(13.56% MM)
% Carbon	65.38	75.64
% Hydrogen	4.45	5.15
% Nitrogen	0.94	1.09
% Organic Sulfur	0.35	0.40
% Oxygen (diff.)	15.32	17.72
% Mineral Matter (incl. 0.58% FeS ₂)	13.56	

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	25.461	10947	16.572	7125	16.595	7135
MM-free (Parr)	29.233	12569	18.069	7769	18.097	7781
MM-free (mod. Parr)	29.408	12644	18.148	7803	18.176	7815
Net, dmmf Btu/lb	28.261	12151				
Mott-Spooner difference = -374 Btu/lb						

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.840	0.818
Atomic O/C	0.177	0.176

The Penn State Coal Sample Bank and Database

Pust Seam
Richland County, MT

ligA rank

Sample DECS-25

page 3 of 4
printed 8/24/95
sampled 6/06/94

RANK CALCULATIONS

ASTM Rank (equilibrium moist.) ligA
(as rec'd moist.) ligA

MACERAL COMPOSITION (white light, volume %)

	mineral- free	
Textinite	0.0	
Ulminite	42.0	
Humodetrinite	30.9	
Gelinite	0.2	
Corpohuminite	1.2	
TOTAL HUMINITE	74.3	
Fusinite	3.4	
Semifusinite	10.5	
Macrinite	1.4	
Micrinite	0.7	
Sclerotinite	0.6	
Inertodetrinite	5.5	
TOTAL INERTINITE	22.1	
Sporinite	2.0	
Resinite	0.6	
Alginite	0.0	
Suberinite	0.8	
Cutinite	0.2	
Liptodetrinite	0.0	
TOTAL LIPTINITE	3.6	

REFLECTANCE DATA

Huminite: Mean-max R_o : 0.23%

Vtypes: $\frac{V_1}{24.0}$ $\frac{V_2}{68.0}$ $\frac{V_3}{8.0}$
percent:

CAKING AND MECHANICAL PROPERTIES

Free-swelling index 0
Hardgrove grindability index 59.3
Vickers' microhardness index n.d.
Washability data not available

Gieseler Coal Plastometer:

Initial softening n.d.
Maximum fluidity n.d.
Solidification n.d.
Fluid temp. range n.d.
Maximum fluidity n.d.

The Penn State Coal Sample Bank and Database

Sample DECS-25

Pust Seam
Richland County, MT

ligA rank

page 4 of 4
printed 8/24/95
sampled 6/06/94

INORGANIC ELEMENT ANALYSIS

Major Elements			Trace Elements		
	oxide % of HTA	element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	25.7	Si 1.3	Ag		< 0.3
Al ₂ O ₃	16.1	Al 1.0	As		2
TiO ₂	0.58	Ti 0.04	Ba	9225	1031
Fe ₂ O ₃	5.26	Fe 0.41	Be	5.0	
MgO	8.20	Mg 0.55	Bi		
CaO	23.3	Ca 1.9	Cd		< 0.3
Na ₂ O	0.31	Na 0.03	Ce		
K ₂ O	0.28	K 0.03	Cl		400
P ₂ O ₅	0.41	P 0.020	Co		
SO ₃	17.4		Cr	30	3
			Cu	65	7
			Ga		
			Ge		
			Hg		0.14
			La		
			Mn	852	95
			Nb		
			Ni	< 20	< 2
			Pb		9
			Rb	8.0	1
			Sc		
			Se		3
			Sn		
			Sr	3552	397
			Th		
			U		
			V	55	6
			Y		
			Yb		
			Zn	25	3
			Zr	235	26

High-temperature ash (HTA)
used for inorganic analysis
= 11.18 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1243°C	2270°F	1232°C	2250°F
Softening	1249°C	2280°F	1249°C	2280°F
Hemispherical	1254°C	2290°F	1271°C	2320°F
Fluid	1268°C	2315°F	1296°C	2365°F

The Penn State Coal Sample Bank and Database**Sample DECS-26****Wyodak Seam (Wyodak-Anderson)
Campbell County, WY****subB rank**page 1 of 4
printed 8/24/95
sampled 6/09/94**SAMPLE LOCATION**

Campbell County, Wyoming, USA
near Wright, Wyoming
Northern Great Plains Coal Province
Fort Union Region

Reno Reservoir (7.5') Topographic Quadrangle
Latitude 43° 40' 00" North, Longitude 105° 15' 00" West

SAMPLE HISTORY

Whole-Seam Run-of-mine Sample collected June 9, 1994 by Penn State
Mining method: surface
sampled from 38 cuts of automatic sampler

Coal Sample Bank reserve: 281 kg (621 lbs)

SAMPLE INFORMATION

Paleocene

Fort Union Formation
Seam thickness at sample location: 2134 cm (70 ft 0 in.)

The Penn State Coal Sample Bank and Database

Sample DECS-26

Wyodak Seam (Wyodak-Anderson)
Campbell County, WY

subB rank

page 2 of 4
printed 8/24/95
sampled 6/09/94

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	26.30			
% Ash	5.58	7.57		
% Vol. Matter	33.06	44.86	48.53	48.13
% Fixed Carbon	35.06	47.57	51.47	51.87

SULFUR FORMS

	dry	daf
% Pyritic	0.07	0.08
% Sulfate	0.01	0.01
% Organic	0.35	0.38
% Total	0.43	0.47

MOISTURE

% as received	26.30
% equilibrium	26.23

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	5.58	7.57		(8.41%MM)
% Carbon	51.42	69.77	75.48	76.18
% Hydrogen	4.16*	5.65	6.11	6.17
% Nitrogen	0.69	0.94	1.02	1.03
% Total Sulfur	0.32	0.43	0.47	
% Oxygen (diff.)	11.53*	15.64	16.92	16.63
* excluding H and O in moisture				
Dry % Chlorine = 0.0 Dry % Carbon dioxide = 0.12				

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(8.59% MM)
% Carbon	69.74	76.29
% Hydrogen	5.55	6.07
% Nitrogen	0.94	1.03
% Organic Sulfur	0.35	0.38
% Oxygen (diff.)	14.83	16.23
% Mineral Matter (incl. 0.13% FeS ₂)	8.59	

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	28.247	12145	20.819	8951	20.837	8959
MM-free (Parr)	30.787	13237	22.156	9526	22.177	9535
MM-free (mod. Parr)	30.892	13282	22.219	9553	22.240	9562
Net, dmmf Btu/lb	29.559	12709				
Mott-Spooner difference = -477 Btu/lb						

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.973	0.956
Atomic O/C	0.164	0.160

The Penn State Coal Sample Bank and Database

Sample DECS-26

Wyodak Seam (Wyodak-Anderson)
Campbell County, WY

subB rank

page 3 of 4
printed 8/24/95
sampled 6/09/94

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	subB
(as rec'd moist.)	subB

MACERAL COMPOSITION (white light, volume %)

	mineral- free	
Textinite	0.0	
Uminite	41.6	
Humodetrinite	41.1	
Gelinite	1.1	
Corpohuminite	1.9	
TOTAL HUMINITE	85.7	
Fusinite	3.3	
Semifusinite	3.1	
Macrinite	0.3	
Micrinite	0.6	
Sclerotinite	0.1	
Inertodetrinite	2.3	
TOTAL INERTINITE	9.7	
Sporinite	3.6	
Resinite	0.4	
Alginite	0.0	
Suberinite	0.6	
Cutinite	0.0	
Liptodetrinite	0.0	
TOTAL LIPTINITE	4.6	

REFLECTANCE DATA

Huminite: Mean-max R_o : 0.29%

Vtypes:	V 1	V 2	V 3
percent:	2.0	62.0	36.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	0	Gieseler Coal Plastometer:	
Hardgrove grindability index	47.2	Initial softening	n.d.
Vickers' microhardness index	n.d.	Maximum fluidity	n.d.
Washability data not available		Solidification	n.d.
		Fluid temp. range	n.d.
		Maximum fluidity	n.d.

The Penn State Coal Sample Bank and Database

Sample DECS-26

Wyodak Seam (Wyodak-Anderson)
Campbell County, WY

subB rank

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printed 8/24/95
sampled 6/09/94

INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements	
	oxide % of HTA		element % of whole dry coal	ppm HTA	ppm whole dry coal
SiO ₂	31.7	Si	1.0	Ag	< 0.2
Al ₂ O ₃	16.1	Al	0.6	As	1
TiO ₂	1.27	Ti	0.05	Ba	4657
Fe ₂ O ₃	4.84	Fe	0.23	Be	< 2.0
MgO	4.64	Mg	0.19	Bi	< 0.1
CaO	23.5	Ca	1.1	Cd	< 0.2
Na ₂ O	1.80	Na	0.09	Ce	
K ₂ O	0.40	K	0.02	Cl	
P ₂ O ₅	0.89	P	0.026	Co	
SO ₃	12.7			Cr	45
				Cu	135
				Ga	
				Ge	
				Hg	0.12
				La	
				Mn	155
				Nb	
				Ni	35
				Pb	5
				Rb	10
				Sc	
				Se	2
				Sn	
				Sr	2452
				Th	
				U	
				V	160
				Y	
				Yb	
				Zn	85
				Zr	245

High-temperature ash (HTA)
used for inorganic analysis
= 6.68 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1149°C	2100°F	1185°C	2165°F
Softening	1166°C	2130°F	1199°C	2190°F
Hemispherical	1182°C	2160°F	1213°C	2215°F
Fluid	1196°C	2185°F	1235°C	2255°F

The Penn State Coal Sample Bank and Database**Sample DECS-27****Deadman Seam**
Sweetwater County, WY**subA rank**page 1 of 4
printed 8/24/95
sampled 6/10/94**SAMPLE LOCATION**Sweetwater County, Wyoming; USA
near Point of Rocks, Wyoming
Rocky Mountain Coal Province
Green River RegionTwelvemile Well Topographic Quadrangle
Latitude 41° 47' 23" North, Longitude 108° 44' 45" West**SAMPLE HISTORY**Whole-Seam Run-of-mine Sample collected June 10, 1994 by Penn State
Mining method: surface
sampled as 10 3.5" dia. auger drill holes

Coal Sample Bank reserve: 158 kg (350 lbs)

SAMPLE INFORMATION

Paleocene

Fort Union Formation
Seam thickness at sample location: 305 cm (10 ft 0 in.)
Sample thickness: 305 cm (10 ft 0 in.)

The Penn State Coal Sample Bank and Database

Sample DECS-27

Deadman Seam
Sweetwater County, WY

subA rank

page 2 of 4
printed 8/24/95
sampled 6/10/94

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	17.67			
% Ash	11.45	13.91		
% Vol. Matter	29.42	35.73	41.50	40.59
% Fixed Carbon	41.46	50.36	58.50	59.41

SULFUR FORMS

	dry	daf
% Pyritic	0.27	0.31
% Sulfate	0.00	0.00
% Organic	0.44	0.51
% Total	0.72	0.84

MOISTURE

% as received	17.67
% equilibrium	17.10

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	11.45	13.91		(15.42%MM)
% Carbon	55.17	67.01	77.84	79.23
% Hydrogen	3.79*	4.60	5.34	5.44
% Nitrogen	0.91	1.10	1.28	1.30
% Total Sulfur	0.59	0.72	0.84	
% Oxygen (diff.)	10.42*	12.66	14.71	14.04
* excluding H and O in moisture				
Dry % Chlorine = 0.0 Dry % Carbon dioxide = 0.78				

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(15.85% MM)
% Carbon	66.80	79.37
% Hydrogen	4.42	5.26
% Nitrogen	1.10	1.31
% Organic Sulfur	0.44	0.52
% Oxygen (diff.)	11.39	13.54
% Mineral Matter	15.85	
(incl. 0.51% FeS ₂)		

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	27.147	11672	22.351	9610	22.505	9676
MM-free (Parr)	31.996	13757	25.521	10973	25.724	11060
MM-free (mod. Parr)	32.217	13852	25.670	11037	25.875	11125
Net, dmmf Btu/lb	31.041	13346				
Mott-Spooner difference = -1 Btu/lb						

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.825	0.796
Atomic O/C	0.133	0.128

The Penn State Coal Sample Bank and Database

Sample DECS-27

Deadman Seam
Sweetwater County, WY

subA rank

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sampled 6/10/94

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	subA	Reflectance Rank	h _v C _b
(as rec'd moist.)	subA		

MACERAL COMPOSITION (white light, volume %)

	mineral- free	mineral- containing
Vitrinite	81.0	74.4
TOTAL VITRINITE	81.0	74.4
Fusinite	5.1	4.7
Semifusinite	8.9	8.2
Macrinite	0.0	0.0
Micrinite	1.6	1.5
Sclerotinite	0.0	0.0
Inertodetrinite	1.6	1.5
TOTAL INERTINITE	17.2	15.9
Sporinite	0.7	0.6
Resinite	0.5	0.5
Alginite	0.0	0.0
Cutinite	0.4	0.4
Liptodetrinite	0.2	0.2
TOTAL LIPTINITE	1.8	1.7
Mineral matter (Parr, volume %)		8.08

REFLECTANCE DATA

Vitrinite: Mean-max R₀: 0.46%

Vtypes:	V 3	V 4	V 5
percent:	5.0	78.0	17.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	0	Gieseler Coal Plastometer:
		Initial softening
Hardgrove grindability index	57.0	Maximum fluidity
Vickers' microhardness index	n.d.	Solidification
Washability data not available		Fluid temp. range
		Maximum fluidity

The Penn State Coal Sample Bank and Database

Deadman Seam
Sweetwater County, WY

subA rank

Sample DECS-27

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printed 8/24/95
sampled 6/10/94

INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements		
	oxide % of HTA		element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	71.8	Si	4.5	Ag		< 0.3
Al ₂ O ₃	12.4	Al	0.9	As		2
TiO ₂	1.37	Ti	0.11	Ba	3583	477
Fe ₂ O ₃	3.72	Fe	0.35	Be	< 2.0	< 0.3
MgO	0.90	Mg	0.07	Bi		
CaO	2.90	Ca	0.28	Cd		< 0.3
Na ₂ O	3.10	Na	0.30	Ce		
K ₂ O	0.28	K	0.03	Cl		
P ₂ O ₅	0.11	P	0.006	Co		
SO ₃	2.60			Cr	55	7
				Cu	175	23
				Ga		
				Ge		
				Hg		0.10
				La		
				Mn	232	31
				Nb		
				Ni	< 10	< 1
				Pb		13
				Rb	8.0	1
				Sc		
				Se		3
				Sn		
				Sr	761	101
				Th		
				U		
				V	100	13
				Y		
				Yb		
				Zn	35	5
				Zr	545	73

High-temperature ash (HTA)
used for inorganic analysis
= 13.30 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1385°C	2525°F	1360°C	2480°F
Softening	1427°C	2600°F	1404°C	2560°F
Hemispherical	1466°C	2670°F	1438°C	2620°F
Fluid	1488°C	2710°F	1460°C	2660°F

The Penn State Coal Sample Bank and Database

Green Seam
Navajo County, AZ

hvCb rank

Sample DECS-28

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printed 12/07/95
sampled 6/13/94

SAMPLE LOCATION

Navajo County, Arizona, USA
near Kayenta, Arizona
Rocky Mountain Coal Province
San Juan River Region
Black Mesa
Long House Valley Topographic Quadrangle
Latitude 36° 30' 00" North, Longitude 110° 22' 00" West

SAMPLE HISTORY

Whole-Seam Channel Sample collected June 13, 1994 by Penn State
Mining method: surface
Blasted; no description. Resin visible in middle.

Coal Sample Bank reserve: 218 kg (482 lbs)

SAMPLE INFORMATION

Upper Cretaceous
Mesaverde Group
Wepo Formation
Seam thickness at sample location: 366 cm (12 ft 0 in.)
Sample thickness: 366 cm (12 ft 0 in.)

The Penn State Coal Sample Bank and Database

Sample DECS-28

Green Seam
Navajo County, AZ

hvCb rank

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sampled 6/13/94

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	12.21			
% Ash	5.34	6.08		
% Vol. Matter	39.74	45.27	48.20	47.87
% Fixed Carbon	42.71	48.65	51.80	52.13

SULFUR FORMS

	dry	daf
% Pyritic	0.02	0.02
% Sulfate	0.00	0.00
% Organic	0.38	0.40
% Total	0.40	0.43

MOISTURE

% as received	12.21
% equilibrium	13.00

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	5.34	6.08		(6.79%MM)
% Carbon	63.69	72.55	77.25	77.83
% Hydrogen	4.52*	5.15	5.48	5.52
% Nitrogen	1.03	1.17	1.25	1.26
% Total Sulfur	0.35	0.40	0.43	
% Oxygen (diff.)	12.86*	14.65	15.60	15.39
* excluding H and O in moisture				
Dry % Chlorine = 0.0 Dry % Carbon dioxide = 0.16				

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(6.88% MM)
% Carbon	72.51	77.86
% Hydrogen	5.07	5.45
% Nitrogen	1.17	1.26
% Organic Sulfur	0.38	0.41
% Oxygen (diff.)	13.99	15.03
% Mineral Matter	6.88	
(incl. 0.04% FeS ₂)		

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	29.636	12742	26.017	11186	25.784	11086
MM-free (Parr)	31.743	13648	27.622	11876	27.359	11763
MM-free (mod. Parr)	31.822	13682	27.687	11904	27.422	11790
Net, dmmf Btu/lb	30.631	13170				
Mott-Spooner difference = 11 Btu/lb						

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.853	0.840
Atomic O/C	0.148	0.145

The Penn State Coal Sample Bank and Database

Sample DECS-28

Green Seam
Navajo County, AZ

hvCb rank

page 3 of 4
printed 12/07/95
sampled 6/13/94**RANK CALCULATIONS**

ASTM Rank (equilibrium moist.)	hvCb
(as rec'd moist.)	hvCb

MACERAL COMPOSITION (blue + white light, volume %)

	mineral- free	mineral- containing
Vitrinite	78.7	76.0
TOTAL VITRINITE	78.7	76.0
Fusinite	4.8	4.6
Semifusinite	7.1	6.9
Macrinite	0.0	0.0
Micrinite	1.2	1.2
Sclerotinite	0.7	0.7
Inertodetrinite	1.4	1.4
TOTAL INERTINITE	15.2	14.8
Sporinite	1.8	1.7
Resinite	1.5	1.4
Alginite	0.0	0.0
Cutinite	0.7	0.7
Liptodetrinite	0.6	0.6
Exudatinite	1.5	1.4
Bituminite	0.0	0.0
Fluorinite	0.0	0.0
TOTAL LIPTINITE	6.1	5.8
Mineral matter (Parr, volume %)		3.39

REFLECTANCE DATAVitrinite: Mean-max R_o : 0.43%

Vtypes:	V 3	V 4	V 5
percent:	22.0	77.0	1.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	0.5	<u>Gieseler Coal Plastometer:</u>	
		Initial softening	n.d.
Hardgrove grindability index	45.8	Maximum fluidity	n.d.
Vickers' microhardness index	n.d.	Solidification	n.d.
Washability data not available		Fluid temp. range	n.d.
		Maximum fluidity	n.d.

The Penn State Coal Sample Bank and Database

Green Seam
Navajo County, AZ

hvCb rank

Sample DECS-28

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INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements	
	oxide % of HTA		element % of whole dry coal	ppm HTA	ppm whole dry coal
SiO ₂	38.0	Si	1.1	Ag	< 0.2
Al ₂ O ₃	19.7	Al	0.6	As	1
TiO ₂	0.98	Ti	0.03	Ba	6001
Fe ₂ O ₃	5.15	Fe	0.21	Be	< 3.0
MgO	2.35	Mg	0.08	Bi	< 0.2
CaO	15.9	Ca	0.7	Cd	< 0.2
Na ₂ O	4.09	Na	0.18	Ce	
K ₂ O	0.25	K	0.01	Cl	
P ₂ O ₅	0.64	P	0.016	Co	
SO ₃	12.0			Cr	30
High-temperature ash (HTA) used for inorganic analysis = 5.85 % of whole dry coal				Cu	65
				Ga	
				Ge	
				Hg	0.04
				La	
				Mn	77
				Nb	
				Ni	35
				Pb	5
				Rb	7.0
				Sc	
				Se	2
				Sn	
				Sr	4313
				Th	
				U	
				V	90
				Y	
				Yb	
				Zn	25
				Zr	300
					2
					18

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1138°C	2080°F	1216°C	2220°F
Softening	1166°C	2130°F	1238°C	2260°F
Hemispherical	1191°C	2175°F	1263°C	2305°F
Fluid	1216°C	2220°F	1282°C	2340°F

The Penn State Coal Sample Bank and Database**Sample DECS-29****Upper Banner #3 Seam
Dickenson County, VA****hvAb rank**page 1 of 4
printed 12/07/95
sampled 6/19/95**SAMPLE LOCATION**Dickenson County, Virginia, USA
near Carrie, Virginia
Eastern Coal Province
Appalachian RegionDuty (7.5') Topographic Quadrangle
Latitude 37° 02' 03" North, Longitude 82° 11' 10" West**SAMPLE HISTORY**Whole-Seam Channel Sample collected June 19, 1995 by Penn State
Mining method: surface
Mine life expected: 1 years
Sampled 100 meters from crop line - some oxidation

Coal Sample Bank reserve: 189 kg (418 lbs)

SAMPLE INFORMATION

Pennsylvanian

Norton Formation

Seam thickness at sample location: 55 cm (1 ft 10 in.)
Sample thickness: 55 cm (1 ft 10 in.)

Seam profile:

ROOF not present at sample site

The Penn State Coal Sample Bank and Database

Sample DECS-29

Upper Banner #3 Seam
Dickenson County, VA

hvAb rank

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printed 12/07/95
sampled 6/19/95

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	2.44			
% Ash	6.20	6.36		
% Vol. Matter	33.46	34.30	36.63	36.16
% Fixed Carbon	57.89	59.34	63.37	63.84

SULFUR FORMS

	dry	daf
% Pyritic	0.09	0.10
% Sulfate	0.01	0.01
% Organic	0.50	0.53
% Total	0.59	0.63

MOISTURE

% as received	2.44
% equilibrium	2.16

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	6.20	6.36		(7.19%MM)
% Carbon	79.10	81.08	86.59	87.36
% Hydrogen	5.05*	5.18	5.53	5.58
% Nitrogen	1.44	1.48	1.58	1.59
% Total Sulfur	0.58	0.59	0.63	
% Oxygen (diff.)	5.18*	5.31	5.67	5.46
* excluding H and O in moisture				
Dry % Chlorine = 0.0 Dry % Carbon dioxide = 0.63				

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(7.23% MM)
% Carbon	80.91	87.21
% Hydrogen	5.10	5.50
% Nitrogen	1.48	1.60
% Organic Sulfur	0.50	0.54
% Oxygen (diff.)	4.78	5.16
% Mineral Matter (incl. 0.17% FeS ₂)	7.23	

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	33.825	14543	32.999	14188	33.094	14229
MM-free (Parr)	36.371	15638	35.418	15228	35.527	15275
MM-free (mod. Parr)	36.448	15671	35.492	15260	35.602	15307
Net, dmmf Btu/lb	35.243	15153				
Mott-Spooner difference = 15 Btu/lb						

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.767	0.757
Atomic O/C	0.047	0.044

The Penn State Coal Sample Bank and Database

Sample DECS-29

Upper Banner #3 Seam
Dickenson County, VA

hvAb rank

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printed 12/07/95
sampled 6/19/95

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	hvAb	Reflectance Rank	hvAb
(as rec'd moist.)	hvAb		

MACERAL COMPOSITION (blue + white light, volume %)

	mineral- free	mineral- containing
Vitrinite	71.1	68.5
TOTAL VITRINITE	71.1	68.5
Fusinite	3.6	3.4
Semifusinite	8.7	8.4
Macrinite	0.3	0.3
Micrinite	8.4	8.1
Sclerotinite	0.0	0.0
Inertodetrinite	1.0	1.0
TOTAL INERTINITE	22.0	21.2
Sporinite	5.4	5.2
Resinite	0.9	0.9
Alginite	0.0	0.0
Cutinite	0.5	0.5
Liptodetrinite	0.1	0.1
Exudatinite	0.0	0.0
Bituminite	0.0	0.0
Fluorinite	0.0	0.0
TOTAL LIPTINITE	6.9	6.7
Mineral matter (Parr, volume %)		3.60

REFLECTANCE DATA

Vitrinite: Mean-max R_0 : 1.00%

Vtypes:	V 8	V 9	V 10
percent:	1.0	55.0	44.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	8	Gieseler Coal Plastometer:	
Hardgrove grindability index	55.5	Initial softening	397°C
Vickers' microhardness index	n.d.	Maximum fluidity	447°C
Washability data not available		Solidification	487°C
		Fluid temp. range	90°C
		Maximum fluidity	8942 ddpm
		average of 6 runs	

The Penn State Coal Sample Bank and Database

Sample DECS-29

Upper Banner #3 Seam
Dickenson County, VA

hvAb rank

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printed 12/07/95
sampled 6/19/95

INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements		
	oxide % of HTA		element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	48.5	Si	1.4	Ag		< 0.2
Al ₂ O ₃	27.9	Al	0.9	As		4
TiO ₂	0.95	Ti	0.04	Ba	1702	105
Fe ₂ O ₃	10.7	Fe	0.5	Be	25	2
MgO	1.72	Mg	0.06	Bi		
CaO	3.81	Ca	0.17	Cd		< 0.2
Na ₂ O	0.70	Na	0.03	Ce		
K ₂ O	2.53	K	0.13	Cl		
P ₂ O ₅	0.12	P	0.003	Co		
SO ₃	1.60			Cr	120	7
				Cu	240	15
				Ga		
				Ge		
				Hg		0.04
				La		
				Mn	310	19
				Nb		
				Ni	140	9
				Pb		7
				Rb	50	3
				Sc		
				Se		1
				Sn		
				Sr	1353	84
				Th		
				U		
				V	170	11
				Y		
				Yb		
				Zn	110	7
				Zr	240	15

High-temperature ash (HTA)
used for inorganic analysis
= 6.19 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1216°C	2220°F	1438°C	2620°F
Softening	1332°C	2430°F	1468°C	2675°F
Hemispherical	1382°C	2520°F	1482°C	2700°F
Fluid	1427°C	2600°F	1499°C	2730°F

The Penn State Coal Sample Bank and Database**Sample DECS-30****Splash Dam Seam
Buchanan County, VA****mvpb rank**page 1 of 4
printed 12/07/95
sampled 6/20/95**SAMPLE LOCATION**Buchanan County, Virginia, USA
near Harman, Virginia
Eastern Coal Province
Appalachian RegionHarman (7.5') Topographic Quadrangle
Latitude 37° 16' 24" North, Longitude 82° 12' 51" West**SAMPLE HISTORY**Whole-Seam Channel Sample collected June 20, 1995 by Penn State
Mining method: underground

Coal Sample Bank reserve: 191 kg (423 lbs)

SAMPLE INFORMATION

Pennsylvanian

Norton Formation

Seam thickness at sample location: 83 cm (2 ft 9 in.)
Sample thickness: 83 cm (2 ft 9 in.)

Seam profile:

ROOF	black mudstone
13 cm	bright clarain, vit., partings
15 cm	same, 1/4" parting at base
56 cm	bright clarain, thick vitrain
FLOOR	includes occasional 1" coal

The Penn State Coal Sample Bank and Database

Sample DECS-30

Splash Dam Seam
Buchanan County, VA

mvb rank

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printed 12/07/95
sampled 6/20/95

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	2.06			
% Ash	3.81	3.89		
% Vol. Matter	29.51	30.13	31.35	30.94
% Fixed Carbon	64.62	65.98	68.65	69.04

SULFUR FORMS

	dry	daf
% Pyritic	0.14	0.15
% Sulfate	0.00	0.00
% Organic	0.65	0.68
% Total	0.79	0.82

MOISTURE

% as received	2.06
% equilibrium	5.18

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	3.81	3.89		(4.64%MM)
% Carbon	82.67	84.41	87.83	88.51
% Hydrogen	5.04*	5.15	5.36	5.40
% Nitrogen	1.48	1.51	1.57	1.58
% Total Sulfur	0.77	0.79	0.82	
% Oxygen (diff.)	4.16*	4.25	4.42	4.50

* excluding H and O in moisture

Dry % Chlorine = 0.07 Dry % Carbon dioxide = 0.59

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(4.50% MM)
% Carbon	84.25	88.22
% Hydrogen	5.10	5.34
% Nitrogen	1.51	1.58
% Organic Sulfur	0.65	0.68
% Oxygen (diff.)	3.99	4.18
% Mineral Matter	4.50	
(incl. 0.26% FeS ₂)		

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	35.027	15060	34.306	14750	33.213	14280
MM-free (Parr)	36.634	15751	35.843	15411	34.648	14897
MM-free (mod. Parr)	36.657	15761	35.869	15422	34.674	14908
Net, dmmf Btu/lb	35.495	15261				

Mott-Spooner difference = -12 Btu/lb

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.733	0.727
Atomic O/C	0.038	0.036

The Penn State Coal Sample Bank and Database

Sample DECS-30

Splash Dam Seam
Buchanan County, VA

mvb rank

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printed 12/07/95
sampled 6/20/95

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	mvb	Reflectance Rank	mvb
(as rec'd moist.)	mvb		

MACERAL COMPOSITION (white light, volume %)

	mineral- free	mineral- containing
Vitrinite	76.8	75.0
TOTAL VITRINITE	76.8	75.0
Fusinite	3.1	3.0
Semifusinite	10.9	10.7
Macrinite	0.1	0.1
Micrinite	5.0	4.9
Sclerotinite	0.0	0.0
Inertodetrinite	0.5	0.5
TOTAL INERTINITE	19.6	19.2
Sporinite	3.4	3.3
Resinite	0.1	0.1
Alginite	0.0	0.0
Cutinite	0.1	0.1
Liptodetrinite	0.0	0.0
TOTAL LIPTINITE	3.6	3.5
Mineral matter (Parr, volume %)		2.29

REFLECTANCE DATA

Vitrinite: Mean-max R_o : 1.16%

Vtypes: V 10 V 11 V 12
percent: 7.0 72.0 21.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	8	Gieseler Coal Plastometer:
		Initial softening
Hardgrove grindability index	74.7	Maximum fluidity
Vickers' microhardness index	n.d.	Solidification
Washability data not available		Fluid temp. range
		Maximum fluidity

383°C

458°C

500°C

117°C

28188 ddpm

The Penn State Coal Sample Bank and Database

Sample DECS-30

Splash Dam Seam
Buchanan County, VA

mvpb rank

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INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements		
	oxide % of HTA		element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	46.8	Si	0.9	Ag		0.10
Al ₂ O ₃	28.8	Al	0.6	As		19
TiO ₂	1.77	Ti	0.04	Ba	2060	81
Fe ₂ O ₃	13.9	Fe	0.4	Be	20	1
MgO	0.90	Mg	0.02	Bi		
CaO	1.94	Ca	0.05	Cd		0.10
Na ₂ O	2.15	Na	0.06	Ce		
K ₂ O	1.52	K	0.05	Cl		700
P ₂ O ₅	0.52	P	0.009	Co		
SO ₃	0.20			Cr	120	5
				Cu	290	11
				Ga		
				Ge		
				Hg		0.11
				La		
				Mn	387	15
				Nb		
				Ni	140	6
				Pb		4
				Rb	30	1
				Sc		
				Se		2
				Sn		
				Sr	1945	76
				Th		
				U		
				V	230	9
				Y		
				Yb		
				Zn	90	4
				Zr	340	13

High-temperature ash (HTA)
used for inorganic analysis
= 3.91 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1399°C	2550°F	1510°C	2750°F
Softening	1443°C	2630°F	1535°C	2795°F
Hemispherical	1477°C	2690°F	1538°C+	2800°F+
Fluid	1510°C	2750°F	1538°C+	2800°F+

The Penn State Coal Sample Bank and Database**Sample DECS-31****Pond Creek Seam
Pike County, KY****hvAb rank**page 1 of 4
printed 12/07/95
sampled 6/21/95**SAMPLE LOCATION**Pike County, Kentucky, USA
near Kimper, Kentucky
Eastern Coal Province
Appalachian RegionLick Creek (7.5') Topographic Quadrangle
Latitude 37° 29' 00" North, Longitude 82° 15' 21" West**SAMPLE HISTORY**Whole-Seam Channel Sample collected June 21, 1995 by Penn State
Mining method: underground

Coal Sample Bank reserve: 170 kg (375 lbs)

SAMPLE INFORMATION

Pennsylvanian

Breathitt Formation

Seam thickness at sample location: 145 cm (4 ft 9 in.)

Sample thickness: 145 cm (4 ft 9 in.)

Seam profile:

ROOF	gray shale, plant fossils
33 cm	4 cm durain 29 cm dull clarain
10 cm	5 cm fusain, 5 cm dull clarain
33 cm	bright clarain with shale
25 cm	bright clarain
33 cm	clarain with shale stringers
10 cm	durain
FLOOR	gray shale

The Penn State Coal Sample Bank and Database

Sample DECS-31

Pond Creek Seam
Pike County, KY

hvAb rank

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sampled 6/21/95

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	2.32			
% Ash	10.64	10.89		
% Vol. Matter	32.52	33.29	37.36	36.60
% Fixed Carbon	54.52	55.82	62.64	63.40

SULFUR FORMS

	dry	daf
% Pyritic	0.11	0.12
% Sulfate	0.01	0.01
% Organic	0.49	0.55
% Total	0.60	0.67

MOISTURE

% as received	2.32
% equilibrium	2.49

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	10.64	10.89		(12.09%MM)
% Carbon	74.55	76.32	85.65	86.82
% Hydrogen	4.74*	4.85	5.44	5.52
% Nitrogen	1.28	1.31	1.47	1.49
% Total Sulfur	0.59	0.60	0.67	
% Oxygen (diff.)	5.89*	6.03	6.77	6.18

* excluding H and O in moisture

Dry % Chlorine = 0.09 Dry % Carbon dioxide = 0.57

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(12.40% MM)
% Carbon	76.16	86.95
% Hydrogen	4.71	5.38
% Nitrogen	4.71	1.50
% Organic Sulfur	0.49	0.56
% Oxygen (diff.)	4.92	5.62
% Mineral Matter	12.40	
(incl. 0.21% FeS ₂)		

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	31.838	13689	31.099	13371	31.045	13348
MM-free (Parr)	36.139	15538	35.188	15129	35.118	15099
MM-free (mod. Parr)	36.330	15620	35.371	15208	35.302	15178
Net, dmmf Btu/lb	35.136	15107				

Mott-Spooner difference = 103 Btu/lb

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.763	0.743
Atomic O/C	0.053	0.049

The Penn State Coal Sample Bank and Database

Sample DECS-31

Pond Creek Seam
Pike County, KY

hvAb rank

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RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	hvAb	Reflectance Rank	hvAb
(as rec'd moist.)	hvAb		

MACERAL COMPOSITION (blue + white light, volume %)

	mineral-free	mineral-containing
Vitrinite	72.9	68.4
TOTAL VITRINITE	72.9	68.4
Fusinite	5.0	4.7
Semifusinite	7.4	6.9
Macrinite	0.0	0.0
Micrinite	5.2	4.9
Sclerotinite	0.0	0.0
Inertodetrinite	1.4	1.3
TOTAL INERTINITE	19.0	17.8
Sporinite	7.1	6.6
Resinite	0.5	0.5
Alginite	0.0	0.0
Cutinite	0.0	0.0
Liptodetrinite	0.4	0.4
Exudatinite	0.1	0.1
Bituminite	0.0	0.0
Fluorinite	0.0	0.0
TOTAL LIPTINITE	8.1	7.6
Mineral matter (Parr, volume %)		6.22

REFLECTANCE DATA

Vitrinite: Mean-max R_0 : 0.99%

Vtypes:	V 7	V 8	V 9	V 10	V 11
percent:	1.0	12.0	41.0	44.0	2.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index 8

Hardgrove grindability index 54.1

Vickers' microhardness index n.d.

Washability data not available

Gieseler Coal Plastometer:

Initial softening 404°C

Maximum fluidity 446°C

Solidification 483°C

Fluid temp. range 79°C

Maximum fluidity 3634 ddpm

The Penn State Coal Sample Bank and Database

Sample DECS-31

Pond Creek Seam
Pike County, KY

hvAb rank

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INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements		
	oxide % of HTA		element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	52.1	Si	2.6	Ag		< 0.3
Al ₂ O ₃	24.3	Al	1.4	As		5
TiO ₂	1.49	Ti	0.10	Ba	1075	116
Fe ₂ O ₃	15.2	Fe	1.1	Be	20	2
MgO	1.20	Mg	0.08	Bi		
CaO	0.91	Ca	0.07	Cd		< 0.3
Na ₂ O	0.75	Na	0.06	Ce		
K ₂ O	2.97	K	0.27	Cl		900
P ₂ O ₅	0.05	P	0.002	Co		
SO ₃	0.20			Cr	110	12
				Cu	520	56
				Ga		
				Ge		
				Hg		0.04
				La		
				Mn	2168	233
				Nb		
				Ni	140	15
				Pb		17
				Rh	70	8
				Sc		
				Se		4
				Sn		
				Sr	676	73
				Th		
				U		
				V	190	20
				Y		
				Yb		
				Zn	370	40
				Zr	260	28

High-temperature ash (HTA)
used for inorganic analysis
= 10.75 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1343°C	2450°F	1463°C	2665°F
Softening	1396°C	2545°F	1496°C	2725°F
Hemispherical	1435°C	2615°F	1516°C	2760°F
Fluid	1466°C	2670°F	1527°C	2780°F

The Penn State Coal Sample Bank and Database**Sample DECS-32****Stockton - Lewiston Seam (Stockton Seam)**
Kanawha County, WV**hvAb rank**page 1 of 4
printed 12/07/95
sampled 6/23/95**SAMPLE LOCATION**Kanawha County, West Virginia, USA
Cabin Creek Township near Mammoth, West Virginia
Eastern Coal Province
Appalachian RegionMammoth (7.5') Topographic Quadrangle
Latitude 38° 15' 21" North, Longitude 81° 18' 13" West**SAMPLE HISTORY**Whole-Seam Channel Sample collected June 23, 1995 by Penn State
Mining method: underground

Coal Sample Bank reserve: 192 kg (424 lbs)

SAMPLE INFORMATION

Pennsylvanian

Pottsville Group

Kanawha Formation

Seam thickness at sample location: 183 cm (6 ft 0 in.)

Sample thickness: 183 cm (6 ft 0 in.)

Seam profile:

ROOF	gray shale
20 cm	clarain, discontinuous shale
5 cm	hard gray shale included
13 cm	4" dull clarain, 1" vitrain
104 cm	clarain, 1" shale included
15 cm	dull clarain
25 cm	bright clarain

The Penn State Coal Sample Bank and Database

Sample DECS-32

Stockton - Lewiston Seam (Stockton Seam)
Kanawha County, WV

hvAb rank

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printed 12/07/95
sampled 6/23/95

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	2.64			
% Ash	19.76	20.30		
% Vol. Matter	30.74	31.57	39.61	38.18
% Fixed Carbon	46.86	48.12	60.39	61.82

SULFUR FORMS

	dry	daf
% Pyritic	0.10	0.13
% Sulfate	0.01	0.01
% Organic	0.62	0.78
% Total	0.73	0.92

MOISTURE

% as received	2.64
% equilibrium	3.10

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	19.76	20.30		(22.33%MM)
% Carbon	64.60	66.35	83.25	85.42
% Hydrogen	4.38*	4.50	5.65	5.79
% Nitrogen	1.07	1.10	1.38	1.42
% Total Sulfur	0.71	0.73	0.92	
% Oxygen (diff.)	6.83*	7.02	8.81	7.37
* excluding H and O in moisture				
Dry % Chlorine = 0.09 Dry % Carbon dioxide = 0.81				

ELEMENTAL ANALYSIS

	dry	dmmf(Mod. P)
		(22.03% MM)
% Carbon	66.13	85.92
% Hydrogen	4.24	5.51
% Nitrogen	1.10	1.43
% Organic Sulfur	0.62	0.81
% Oxygen (diff.)	4.88	6.34
% Mineral Matter	22.03	
(incl. 0.19% FeS ₂)		

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	27.568	11853	26.840	11540	26.715	11486
MM-free (Parr)	35.383	15213	34.190	14700	33.983	14611
MM-free (mod. Parr)	35.802	15393	34.583	14869	34.371	14778
Net, dmmf Btu/lb	34.541	14851				
Mott-Spooner difference = -19 Btu/lb						

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.815	0.770
Atomic O/C	0.065	0.055

The Penn State Coal Sample Bank and Database

Sample DECS-32

Stockton - Lewiston Seam (Stockton Seam)
Kanawha County, WV

hvAb rank

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printed 12/07/95
sampled 6/23/95

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	hvAb	Reflectance Rank	hvAb
(as rec'd moist.)	hvAb		

MACERAL COMPOSITION (blue + white light, volume %)

	mineral- free	mineral- containing
Vitrinite	67.6	59.4
TOTAL VITRINITE	67.6	59.4
Fusinite	2.8	2.5
Semifusinite	11.2	9.9
Macrinite	0.1	0.1
Micrinite	5.4	4.7
Sclerotinite	0.0	0.0
Inertodetrinite	1.2	1.1
TOTAL INERTINITE	20.7	18.3
Sporinite	8.1	7.1
Resinite	1.4	1.2
Alginite	0.0	0.0
Cutinite	0.7	0.6
Liptodetrinite	1.5	1.3
Exudatinite	0.0	0.0
Bituminite	0.0	0.0
Fluorinite	0.0	0.0
TOTAL LIPTINITE	11.7	10.2
Mineral matter (Parr, volume %)		12.17

REFLECTANCE DATA

Vitrinite: Mean-max R_0 : 0.90%

Vtypes:	V 6	V 7	V 8	V 9	V 10
percent:	1.0	8.0	36.0	53.0	2.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index	5	Gieseler Coal Plastometer:	
Hardgrove grindability index	47.4	Initial softening	406°C
Vickers' microhardness index	n.d.	Maximum fluidity	440°C
Washability data not available		Solidification	473°C
		Fluid temp. range	67°C
		Maximum fluidity	450 ddpm

The Penn State Coal Sample Bank and Database

Sample DECS-32

Stockton - Lewiston Seam (Stockton Seam)
Kanawha County, WV

hvAb rank

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sampled 6/23/95

INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements	
	oxide % of HTA		element % of whole dry coal	ppm HTA	ppm whole dry coal
SiO ₂	51.0	Si	4.8	Ag	< 0.5
Al ₂ O ₃	34.3	Al	3.7	As	5
TiO ₂	1.74	Ti	0.21	Ba	806
Fe ₂ O ₃	3.15	Fe	0.45	Be	10
MgO	1.02	Mg	0.12	Bi	
CaO	1.89	Ca	0.27	Cd	< 0.5
Na ₂ O	0.30	Na	0.05	Ce	
K ₂ O	3.84	K	0.65	Cl	900
P ₂ O ₅	0.40	P	0.035	Co	
SO ₃	0.90			Cr	140
				Cu	110
				Ga	
				Ge	
				Hg	0.04
				La	
				Mn	155
				Nb	
				Ni	120
				Pb	< 27
				Rb	100
				Sc	
				Se	5
				Sn	
				Sr	592
				Th	
				U	
				V	250
				Y	
				Yb	
				Zn	120
				Zr	280

High-temperature ash (HTA)
used for inorganic analysis
= 20.23 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1538°C+	2800°F+	1538°C+	2800°F+
Softening	1538°C+	2800°F+	1538°C+	2800°F+
Hemispherical	1538°C+	2800°F+	1538°C+	2800°F+
Fluid	1538°C+	2800°F+	1538°C+	2800°F+

The Penn State Coal Sample Bank and Database**Sample DECS-33****Ohio #4A Seam (Clarion Seam)**
Meigs County, OH**hvBb rank**page 1 of 4
printed 12/07/95
sampled 7/25/95**SAMPLE LOCATION**Meigs County, Ohio, USA
Columbia Township near Wilkesville, Ohio
Eastern Coal Province
Appalachian RegionVales Mills (7.5') Topographic Quadrangle
Latitude and Longitude not recorded**SAMPLE HISTORY**Whole-Seam Channel Sample collected July 25, 1995 by Penn State
Mining method: underground

Coal Sample Bank reserve: 173 kg (383 lbs)

SAMPLE INFORMATIONPennsylvanian
Allegheny GroupSeam thickness at sample location: 142 cm (4 ft 8 in.)
Sample thickness: 142 cm (4 ft 8 in.)

Seam profile:

ROOF	gray mudstone
58 cm	clarain
8 cm	soft gray mudstone NOT SAMPLED
33 cm	dull clarain
5 cm	hard tan siltstone NOT SAMPLED
38 cm	clarain, occ. pyrite lenses
FLOOR	gray shale

The Penn State Coal Sample Bank and Database

Sample DECS-33

Ohio #4A Seam (Clarion Seam)
Meigs County, OH

hvBb rank

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printed 12/07/95
sampled 7/25/95

PROXIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Moisture	5.97			
% Ash	11.30	12.02		
% Vol. Matter	40.49	43.06	48.94	47.79
% Fixed Carbon	42.24	44.92	51.06	52.21

SULFUR FORMS

	dry	daf
% Pyritic	1.41	1.60
% Sulfate	0.01	0.01
% Organic	2.32	2.64
% Total	3.74	4.25

MOISTURE

% as received	5.97
% equilibrium	5.90

ULTIMATE ANALYSIS

	as rec'd	dry	daf	dmmf(Parr)
% Ash	11.30	12.02		(15.04%MM)
% Carbon	65.36	69.51	79.01	81.81
% Hydrogen	4.80*	5.11	5.81	6.01
% Nitrogen	1.12	1.19	1.35	1.40
% Total Sulfur	3.52	3.74	4.25	
% Oxygen (diff.)	7.93*	8.43	9.58	10.77

* excluding H and O in moisture

Dry % Chlorine = 0.14 Dry % Carbon dioxide = 0.70

ELEMENTAL ANALYSIS

	dry	dmmf(Mod.P)
		(14.32% MM)
% Carbon	69.32	80.90
% Hydrogen	4.98	5.81
% Nitrogen	1.19	1.39
% Organic Sulfur	2.32	2.71
% Oxygen (diff.)	7.87	9.19
% Mineral Matter (incl. 2.64% FeS ₂)	14.32	

CALORIFIC VALUE (Gross)

	dry		as rec'd moist		equil. moist	
	MJ/kg	Btu/lb	MJ/kg	Btu/lb	MJ/kg	Btu/lb
MM-containing	29.345	12617	27.594	11864	27.615	11873
MM-free (Parr)	34.027	14630	31.662	13613	31.689	13625
MM-free (mod. Parr)	34.041	14636	31.692	13626	31.720	13638
Net, dmmf Btu/lb	32.755	14083				

Mott-Spooner difference = -138 Btu/lb

ATOMIC RATIOS (dmmf)

	Parr	mod. Parr
Atomic H/C	0.883	0.863
Atomic O/C	0.099	0.085

The Penn State Coal Sample Bank and Database

Sample DECS-33

Ohio #4A Seam (Clarion Seam)
Meigs County, OH

hvBb rank

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printed 12/07/95
sampled 7/25/95

RANK CALCULATIONS

ASTM Rank (equilibrium moist.)	hvBb	Reflectance Rank	hvCb
(as rec'd moist.)	hvBb		

MACERAL COMPOSITION (blue + white light, volume %)

	mineral- free	mineral- containing
Vitrinite	76.7	70.7
TOTAL VITRINITE	76.7	70.7
Fusinite	3.4	3.1
Semifusinite	4.7	4.4
Macrinite	0.1	0.1
Micrinite	6.1	5.6
Sclerotinite	0.0	0.0
Inertodetrinite	0.7	0.6
TOTAL INERTINITE	15.0	13.8
Sporinite	4.5	4.1
Resinite	1.2	1.1
Alginite	0.0	0.0
Cutinite	0.5	0.5
Liptodetrinite	1.7	1.6
Exudatinite	0.2	0.2
Bituminite	0.1	0.1
Fluorinite	0.1	0.1
TOTAL LIPTINITE	8.3	7.7
Mineral matter (Parr, volume %)		7.86

REFLECTANCE DATA

Vitrinite: Mean-max R_o : 0.51%

Vtypes:	V 4	V 5	V 6
percent:	35.0	63.0	2.0

CAKING AND MECHANICAL PROPERTIES

Free-swelling index 4

Hardgrove grindability index 48.6

Vickers' microhardness index n.d.

Washability data not available

Gieseler Coal Plastometer:

Initial softening 379°C

Maximum fluidity 423°C

Solidification 454°C

Fluid temp. range 75°C

Maximum fluidity 86 ddpm

The Penn State Coal Sample Bank and Database

Sample DECS-33

Ohio #4A Seam (Clarion Seam)
Meigs County, OH

hvBb rank

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printed 12/07/95
sampled 7/25/95

INORGANIC ELEMENT ANALYSIS

Major Elements				Trace Elements		
	oxide % of HTA		element % of whole dry coal		ppm HTA	ppm whole dry coal
SiO ₂	41.5	Si	2.4	Ag		< 0.3
Al ₂ O ₃	22.0	Al	1.4	As		4
TiO ₂	0.97	Ti	0.07	Ba	358	44
Fe ₂ O ₃	19.2	Fe	1.6	Be	15	2
MgO	0.85	Mg	0.06	Bi		
CaO	6.46	Ca	0.56	Cd		< 0.3
Na ₂ O	0.52	Na	0.05	Ce		
K ₂ O	1.70	K	0.17	Cl		1400
P ₂ O ₅	0.07	P	0.004	Co		
SO ₃	5.60			Cr	130	16
				Cu	130	16
				Ga		
				Ge		
				Hg		0.09
				La		
				Mn	310	38
				Nb		
				Ni	75	9
				Pb		3
				Rb	35	4
				Sc		
				Se		5
				Sn		
				Sr	507	62
				Th		
				U		
				V	190	23
				Y		
				Yb		
				Zn	150	18
				Zr	200	25

High-temperature ash (HTA)
used for inorganic analysis
= 12.23 % of whole dry coal

ASH FUSION TEMPERATURES

	Reducing atmosphere		Oxidizing atmosphere	
Initial deformation	1204°C	2200°F	1343°C	2450°F
Softening	1235°C	2255°F	1366°C	2490°F
Hemispherical	1277°C	2330°F	1385°C	2525°F
Fluid	1316°C	2400°F	1396°C	2545°F

APPENDIX E. Coal Sample Bank and Database Brochure

THE DEPARTMENT
OF ENERGY

COAL

SAMPLE BANK

AND

DATABASE

PENNSTATE

March, 1999

<http://www.ems.psu.edu/COPL>

Penn State is maintaining a suite of 56 coals and a corresponding computerized database of analyses for use by DOE contractors and grantees. This includes the 33 well-preserved DECS samples, collected in an ongoing effort begun in 1989, and 23 older PSOC samples. The coals represent a wide spectrum of the major coalfields of the United States and were selected in order to achieve a useful distribution of important coals by rank, geologic province, maceral composition, sulfur content and forms, and ash yield and composition. Due consideration was also given to the prior use of these coals by researchers and to their economic importance. The coals in the DOE Coal Sample Bank are listed at the right. Most were collected as full-seam channel samples (Chan-Seam); however, drill cutting (Drill-Seam), working section of seam (Chan-Work), bench (Chan-Bnch), lithotype (Chan-Lith) and run-of-mine (ROM) samples were also acquired.

Sample Collection and Processing

DECS series samples are the newest and best preserved samples in the collection, and should be chosen when possible for research requiring moderate quantities of sample. They were collected in 180 kg (400 lb.) quantities from recently exposed areas of active mines, where they were placed in 113 L (30 gal.) steel drums with high-density gaskets and purged with argon. As soon as feasible after collection, processing was performed in order to obtain representative subsamples. These were sealed under argon in foil multilaminate bags, which have been shown by annual monitoring to preserve samples very well, and are kept in refrigerated storage (3°C).

DECS samples are available in packages of three nominal sizes:

70 g (3 oz.) at minus 0.20 mm (-60 mesh)
300 g (2/3 lb) at minus 0.85 mm (-20 mesh)
2.3 kg (5 lb) at minus 6 mm (-1/4 inch).

The 300g containers are the ones most often requested by research agencies. Some non-representative blocks of coal, sealed in argon and refrigerated, are also available for certain coals in the Sample Bank.

Older PSOC samples were collected similarly, but 300 g samples were sealed under argon in polyethylene bags which were then sealed in steel cans. Larger quantities were stored in polyethylene buckets or drums.

The Department of Energy Coal Sample Bank

V.M., Sample	Vit. %	VR _o Seam %	ASTM Sample				Ash, S, Btu/lb, C, H,							
dmmt			Rank	Type	State	County	Year	dry	dry	dmmt	dmmt	dmmt		
DECS-1		Bottom	subC	Chan-Seam	TX	Freestone	1989	15.8	0.99	13239	75.9	5.8	55.5	78 0.36
DECS-2		Illinois #6	hvCb	Chan-Seam	IL	Randolph	1989	16.2	4.52	14556	81.8	5.7	43.8	87 0.52
DECS-3		Coal Basin M	mvb	Chan-Seam	CO	Gunnison	1990	5.4	0.65	15831	88.1	5.9	28.2	94 1.28
DECS-4		Blue	hvCb	Chan-Seam	NM	McKinley	1990	6.2	0.46	13951	78.9	5.8	48.1	88 0.51
DECS-5		Hiawatha	hvCb	Chan-Work	UT	Sevier	1990	8.5	0.56	14073	80.4	5.5	43.6	66 0.59
DECS-6		Blind Canyon	hvAb	Chan-Work	UT	Emery	1990	5.8	0.40	14874	81.9	6.3	46.9	69 0.66
DECS-7		Adaville #1	hvCb	Chan-Seam	WY	Lincoln	1990	4.2	0.98	13710	77.8	5.6	47.8	95 0.45
DECS-8		Smith-Roland	subC	ROM	WY	Campbell	1990	13.8	0.73	13148	75.8	5.3	51.8	79 0.37
DECS-9		Dietz	subB	Drill-Seam	MT	Bighorn	1990	6.4	0.41	13251	76.1	5.2	47.1	88 0.38
DECS-10		Rosebud	subB	Chan-Work	MT	Rosebud	1990	12.6	1.16	13378	79.7	4.3	46.9	74 0.42
DECS-11		Beulah	ligA	Chan-Seam	ND	Mercer	1990	9.6	0.74	12350	74.1	4.5	61.6	74 0.35
DECS-12		Pittsburgh	hvAb	Chan-Seam	PA	Greene	1990	10.3	1.12	15259	84.7	5.8	39.4	83 0.87
DECS-13		Sewell	mvb	Chan-Seam	WV	Greenbrier	1990	4.2	0.62	15604	88.8	5.0	25.7	77 1.35
DECS-14		Upper Kittanning	hvAb	Chan-Work	WV	Barbour	1990	10.5	1.80	15503	87.0	5.6	35.4	89 1.07
DECS-15		Lower Sunnyside	hvAb	Chan-Seam	UT	Carbon	1991	10.1	1.67	14967	84.3	5.7	41.3	77 0.80
DECS-16		Blind Canyon	hvAb	Chan-Work	UT	Emery	1991	13.9	0.47	14749	82.4	6.0	47.3	77 0.64
DECS-17*		Blind Canyon	hvAb	Chan-Sect	UT	Emery	1991	6.6	0.44	14897	82.3	6.3	49.7	80 0.59
DECS-18		Kentucky #9	hvBb	Chan-Seam	KY	Union	1991	12.3	4.21	14773	82.2	6.0	45.6	86 0.56
DECS-19		Pocahontas #3	lvb	Chan-Seam	VA	Buchanan	1991	4.6	0.74	15819	90.6	4.9	18.7	89 1.71
DECS-20		Elkhorn #3	hvAb	Chan-Seam	KY	Floyd	1991	5.5	0.97	15173	85.0	5.9	39.2	78 0.87
DECS-21		Lykens Valley #2	an	Chan-Seam	PA	Columbia	1992	11.2	0.50	15122	91.5	4.1	3.9	87 5.19
DECS-22		Upper Kittanning	hvAb	Chan-Lith	PA	Armstrong	1993	23.3	1.71	15827	87.8	6.1	37.8	30 0.77
DECS-23		Pittsburgh	hvAb	Chan-Seam	PA	Washington	1994	9.4	3.87	15307	84.6	5.8	42.3	79 0.73
DECS-24		Illinois #6	hvCb	Chan-Seam	IL	Macoupin	1994	13.4	5.53	14407	80.1	5.6	45.5	90 0.49
DECS-25		Pust	ligA	Chan-Seam	MT	Richland	1994	11.9	0.72	12569	75.8	5.3	46.9	74 0.23
DECS-26		Wyodak	subB	ROM	WY	Campbell	1994	7.6	0.43	13237	76.2	6.2	48.1	86 0.29
DECS-27		Deadman	subA	Drill-Seam	WY	Sweetwater	1994	13.9	0.72	13757	79.2	5.4	40.6	74 0.46
DECS-28		Green	hvCb	Chan-Seam	AZ	Navajo	1994	6.1	0.40	13648	77.8	5.5	47.9	76 0.43
DECS-29		Upper Banner #3	hvAb	Chan-Seam	VA	Dickenson	1995	6.4	0.59	15638	87.4	5.6	36.2	71 1.00
DECS-30		Splash Dam	mvb	Chan-Seam	VA	Buchanan	1995	3.9	0.79	15751	88.5	5.4	30.9	77 1.16
DECS-31		Pond Creek	hvAb	Chan-Seam	KY	Pike	1995	10.9	0.60	15538	86.8	5.5	36.6	73 0.99
DECS-32		Stockton-Lewiston	hvAb	Chan-Seam	WV	Kanawha	1995	20.3	0.73	15213	85.4	5.8	38.2	68 0.90
DECS-33		Ohio #4A	hvBb	Chan-Seam	OH	Meigs	1995	12.0	3.74	14630	81.8	6.0	47.8	77 0.51
PSOC-1442		Darco	ligA	Chan-Seam	TX	Harrison	1985	11.3	0.78	12970	74.9	4.6	75.7	83 0.47
PSOC-1443		unnamed	ligA	Chan-Seam	TX	Titus	1985	21.4	0.74	12878	74.4	5.4	78.2	90 0.44
PSOC-1446		New Mexico #8	hvCb	Chan-Seam	NM	San Juan	1985	20.8	0.85	14142	79.4	5.1	46.4	85 0.59
PSOC-1448		York Canyon	hvAb	Chan-Seam	NM	Colfax	1985	11.4	0.46	15380	85.2	6.1	40.8	85 0.71
PSOC-1468		Buck Mountain	an	ROM	PA	Luzerne	1985	6.8	0.49	14860	96.2	1.4	3.2	86 5.45
PSOC-1470		Pratt	hvBb	Chan-Seam	AL	Walker	1985	20.6	2.50	15031	83.9	5.8	39.6	84 0.89
PSOC-1471		Pee Wee	hvAb	Chan-Seam	TN	Morgan	1985	8.0	1.04	15046	84.0	5.6	39.4	76 0.94
PSOC-1482		Hagel	ligA	Chan-Seam	ND	Oliver	1985	8.5	0.72	12254	72.2	4.6	46.5	88 0.39
PSOC-1486		Big Dirty	subB	Chan-Seam	WA	Lewis	1985	19.4	0.94	13234	75.2	6.1	52.5	90 0.38
PSOC-1490		Brazil Block	hvCb	Chan-Seam	IN	Greene	1985	5.3	0.73	14830	83.4	4.5	39.8	70 0.45
PSOC-1491		Indiana #6	hvCb	Chan-Seam	IN	Sullivan	1985	15.2	2.85	14817	82.4	5.1	43.3	89 0.43
PSOC-1492		Illinois #5	hvCb	Chan-Seam	IL	Perry	1985	10.5	4.35	14490	81.4	5.4	43.6	88 0.62
PSOC-1498		Wadge	hvCb	Chan-Seam	CO	Routt	1985	7.1	0.52	13837	78.2	5.5	44.8	89 0.60
PSOC-1501		Juanita C	hvBb	Chan-Work	CO	Gunnison	1985	5.6	0.64	14465	81.2	5.3	42.7	92 0.73
PSOC-1515		Penna. Semian. C	sa	Chan-Seam	PA	Sullivan	1986	29.2	0.58	15567	91.5	4.1	8.6	91 2.80
PSOC-1516		Lower Kittanning	lvb	Chan-Seam	PA	Somerset	1986	10.3	1.40	15841	90.4	4.8	18.6	90 1.73
PSOC-1517		Ohio #5	hvBb	Chan-Seam	OH	Mahoning	1986	4.8	1.92	15105	84.0	5.5	39.3	87 0.86
PSOC-1521		Lower Hartshorne	lvb	Chan-Seam	AR	Sebastian	1986	11.2	0.80	15510	90.5	4.7	21.1	89 1.61
PSOC-1523		W. Va. #5 Block	hvBb	Chan-Seam	WV	Kanawha	1986	16.1	0.71	15061	85.4	5.5	37.0	62 0.92
PSOC-1532		#4	subC	Chan-Seam	AK	Koy.-Mid. Y.	1987	9.5	0.22	12108	70.6	5.3	58.9	79 0.33
PSOC-1533		#3	ligA	Chan-Work	AK	Koy.-Mid. Y.	1987	8.3	0.16	11665	69.6	5.0	58.4	84 0.35
PSOC-1534		Waterfall	subC	Chan-Work	AK	Kenai-Ck. I.	1987	11.1	0.15	12592	71.7	5.8	49.7	87 0.28
PSOC-1535		Deadfall Syn. #4	subA	Chan-Work	AK	Bar.-Pt. Hp.	1987	3.3	1.46	12586	75.6	4.3	37.5	86 0.73

* distribution limited to DOE dispersed catalyst projects

Analysis

Each of the DOE Sample Bank coals has been subjected to the following analytical procedures: proximate analysis, ultimate analysis, sulfur forms, calorific value, maceral analysis, vitrinite reflectance (VR_o), ash fusion determination, free swelling index, Hardgrove grindability, major inorganic and trace elements, equilibrium moisture, and CO_2 . Gieseler plastometry and a standardized liquefaction test were performed on appropriate samples. NMR and py/gc/ms results were obtained on selected samples.

Sample Availability

Coal samples from the DOE Sample Bank are available to members of the coal research community. Assistance can be given in identifying samples that match specifications or that best suit the research needs of the requestor.

DOE contractors and grantees may receive, at no cost, up to:
 1 kg of -0.85 mm (-20 mesh) coal or
 300 g of -0.25 mm (-60 mesh) coal

Beyond this limit and for larger quantities or special preparation of samples, provision will be at cost to the requestor for preparation, mailing and handling. All requests for more than 2.3 kg (5 lbs.) of a single DECS sample or 4.5 kg (10 lbs.) of a single PSOC sample must be approved by the DOE Project Manager. DECS-17 is limited to 16 30g bags (1 lb.) per year, for DOE dispersed catalyst liquefaction research only.

Penn State currently maintains a Sample Bank that contains over 1000 samples in addition to the DOE Sample Bank of 56 coals. If a DOE contractor's or grantee's needs cannot be met from the 56 coals, then suitable samples can be provided from the larger bank; there is a charge for this service. A booklet describing the entire Penn State Coal Sample Bank and Database is available from the Coal and Organic Petrology Laboratories.

Coal Database, Printouts and Searches

The data that have been assembled by Penn State on the DOE Sample Bank coals have been computerized and are available on request to DOE contractors and grantees. In addition to the analytical data described above, the DOE Coal Database includes details on sample history, location, geology, and seam strata information.

Full (four to five page) or condensed (one-page) printouts of data in 8 1/2 by 11" format can be provided for any sample. The one-page printout is useful for most purposes and contains sample location, geologic information, proximate analysis, equilibrium moisture, calorific value, sulfur forms, ultimate analysis, maceral composition, reflectance data, rank parameters, technologic properties, and physical properties. The full printout includes these data in more detail and calculated to various bases of expression, as well as major inorganic and trace element analyses, ash fusion temperatures, and CO_2 . Liquefaction, NMR, and py/gc/ms results are also available separately for most DECS samples. Data printouts for DOE Sample Bank samples will be provided at no cost to DOE contractors and grantees.

A staff of professionals at Penn State can undertake Database searches to identify samples meeting specified criteria. Simple searches resulting in tables of data or a set of printouts are done at no cost for DOE contractors and grantees. More extensive searches, statistics or electronic transmission of data sets can be performed; a charge may be made for this service.

Investigators can perform their own simple searches on our web site (see below). It includes limited data for all DECS samples and a selected subset of other Penn State samples.

Ordering and Assistance

Request forms, a booklet describing the entire Penn State Coal Sample Bank and Database, and assistance in acquiring samples and data can be obtained from:

Coal and Organic Petrology Laboratories
 The Pennsylvania State University
 105 Academic Projects Building
 University Park, PA 16802-2300
 (814) 865-6543 Fax: (814) 863-7432
<http://www.ems.psu.edu/COPL>

Approval for the provision of larger numbers or quantities of samples must be requested from the Department of Energy Project Manager.