DOE/PC/93051--T10

MAINTENANCE OF THE COAL SAMPLE BANK AND DATABASE

Quarterly Technical Progress Report

Contract Number DE-AC22-93PC93051

The Pennsylvania State University
Coal and Organic Petrology Laboratories

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AUG 26 1996
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Reporting Period: 10/01/95 - 12/31/95

Report Date: 3/22/96

Contract Date: 9/28/93

Anticipated Completion Date: 9/28/98

Government Award: \$156,000. for current contract year

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Quarterly Technical Progress Report: 10/01/95 - 12/31/95

Objectives:

This five year project is intended to ensure the availability of well-characterized, high-quality coal samples for public and private coal research. It continues support of the DOE Coal Sample Bank and Database at The Pennsylvania State University. Eleven coal samples will be collected, processed, packaged, and analyzed, and a resulting database will be maintained. These samples and data, as well as 45 samples collected under previous contracts, will be distributed to DOE contractors and others performing coal research.

Samples will be 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 will be performed. The samples will be stored to minimize deterioration, and 10 samples will be monitored annually by proximate, sulfur forms, and gaseous oxygen analysis to evaluate their condition.

This report reflects the level of effort described in the revised work statement submitted to DOE on February 2, 1996, setting out a reduction in effort following a cut in the level of funding of the project.

Summary of Technical Progress

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 under refrigeration in foil laminate bags.

During the quarter, samples were distributed and inventory records were updated. Individual containers of splits of samples collected in recent quarters were added to the inventory records. Storage and inventory of sample containers is expected to continue routinely through the next quarter.

Task 1C. Monitoring of Sample Quality

It was planned that one 300 g (2/3 lb) bag of each DECS sample would be analyzed annually to monitor sample condition. This Task has been reduced in scope, to 10 samples per year, because of reduction in funding. The third annual monitoring program was begun at the end of the quarter. Two of the 10 samples were analyzed; both showed excellent preservation of their original properties.

The third annual monitoring program is scheduled for completion and reporting in the next quarter.

Effort in the related study of liquefaction behavior (under Task 1F) over time has also been reduced.

Task 1D. Collection and Processing of Replacement Samples

Collection of 11 samples, as described in the Revised Statement of Work (Feb. 2, 1996) has been completed. During the quarter, standard processing of the last of these samples was completed.

Processing of earlier DECS samples to minus 60 mesh (-0.25 mm) will continue in succeeding quarters.

Task 1E. Basic Characterization of Coal Samples

All basic characterization of samples planned for collection under the contract has been completed.

Task 1F. Liquefaction Testing

In this Task, appropriate samples will be subjected to a standardized liquefaction test using tetralin and subsequent product workup.

Product workup was completed on four samples collected during the contract, as shown in Table 1.

Table 1. Conversion of DECS samples in a standardized liquefaction test using tetralin, with detailed gas composition (average of two runs, except gas components based on one run; see Task 1F).

sample	conversion, percent of dry ash-free coal											
	total	asph.	pre-asph.	oil	gas							
					total	c1	c2	c3	c4	c5	c1-c5	other
DECS-25	53.6	3.9	7.4	6.4	35.9	0.5	0.1				0.6	35.3
DECS-26	54.6	5.3	10.1	6.8	32.4	0.5	0.1				0.6	31.8
DECS-29	22.1	3.3	7.7	6.3	4.8	0.6	0.2	0.1			0.9	3.9
DECS-33	62.8	27.3	20.4	12.2	2.9	0.7	0.4	0.3	0.1		1.5	1.4

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

This Task has been discontinued.

Task 1H. Organic Geochemistry

Pyrolysis - Gas Chromatography - Mass Spectrometry

Tables 2 and 3 summarize the composition of the pyrolysis products by type of compound for several samples collected during the contract. Table 2 shows results as percent of gc-amenable products; Table 3 normalizes these results to percent of

identified products. In each table, results are preliminary; more peaks may be identified in the future. The Appendix shows the total ion chromatograms of the pyrolyzates produced from these samples.

Table 2. Structural parameters determined by py/gc/ms (percent of total gc-amenable products). Results of preliminary identification of peaks.

sample	seam	rank	n-alkanes and alkenes	phenols	non-oxygenated aromatic hydrocarbons	unident- ified
DECS-25	Pust	ligA	19.9	8.8	1.61	69.7
DECS-27	Deadman	subA	29.4	11.6	8.5	50.5
DECS-29	Upper Banner #3	hvAb	21.8	3.5	10.7	64.0
DECS-30	Splash Dam	mvb	28.0	3.6	4.3	64.1
DECS-31	Pond Creek	hvAb	17.9	15.4	4.5	62.2
DECS-32	Stockton-Lewiston	hvAb	15.3	20.1	10.3	53.5

Table 3. Structural parameters determined by py/gc/ms (percent of identified products). Results of preliminary identification of peaks.

sample	seam	rank	n-alkanes and alkenes	phenols	non-oxygenated aromatic hydrocarbons
DECS-25	Pust	lig	65.7	29.0	5.3
DECS-27	Deadman	subA	59.4	23.4	17.2
DECS-29	Upper Banner #3	hvAb	60.6	9.7	29.7
DECS-30	Splash Dam	mvb	78.0	10.0	12.0
DECS-31	Pond Creek	hvAb	47.4	11.9	40.7
DECS-32	Stockton-Lewiston	hvAb	32.9	22.2	44.9

Task 1I. Distribution of Coal Samples to Users

During the period 10/01/95 - 12/31/95 a total of 15 samples (13 DOE Sample Bank samples and 2 other Penn State samples) of various sizes in 31 containers were distributed. In addition, 16 30g bags of special sample DECS-17 were distributed. See Task 2C for a list of sample and data recipients. This task will continue in the same manner through the next quarter.

Task 2A. Programming

No significant programming was undertaken during the quarter.

Task 2B. Data Entry

Entry of basic characterization data for the 11 samples collected under the contract has been completed.

Task 2C. Distribution of Data to Users

During the quarter a total of 48 data printouts were distributed. In addition, 5 special data requests were filled by database searches and printed output or creation of a data disk, resulting in distribution of limited information on 235 samples. Preliminary requests for Sample Bank and Database information have been filled. This task will continue in the same manner through the next quarter.

Organizations supplied with coal samples and/or data include:

Indiana Geological Survey
Little Bear Laboratories
Nittany Geosciences, Inc.
Pennsylvania Department of Environmental Protection
Pennsylvania State University, Chemical Engineering Department
Pennsylvania State University, Geosciences Department
Pennsylvania State University, Office of Physical Plant, Steam Plant
Pennsylvania State University, Polymer Science Department
Pennsylvania State University, Mineral Processing Department
Pennsylvania State University, Fuel Science Department (2)
Southern Illinois University, Geology Department
University of Utah, Chemical and Fuels Engineering Department
West Virginia University, Chemical Engineering Department (2)

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

APPENDIX. Total ion chromatograms of pyrolyzates

Figure 1. Total ion chromatogram of pyrolyzates from DECS-25, ligA Pust seam, MT.

Figure 2. Total ion chromatogram of pyrolyzates from DECS-27, subA Deadman seam, WY.

APPENDIX. Total ion chromatograms of pyrolyzates

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

Figure 4. Total ion chromatogram of pyrolyzates from DECS-30, mvb Splash Dam seam, VA.

APPENDIX. Total ion chromatograms of pyrolyzates

Figure 7. Total ion chromatogram of pyrolyzates from DECS-31, hvAb Pond Creek seam, KY.

Figure 8. Total ion chromatogram of pyrolyzates from DECS-32, hvAb Stockton-Lewiston seam, WV

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