

**Geologic processes affecting the quality of the  
Upper Freeport coal bed, west-central Pennsylvania**

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This report has not been reviewed for conformity with USGS editorial standards and stratigraphic nomenclature.

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## ABSTRACT

The origins of organic and inorganic constituents of a coal bed cannot be determined from its bulk composition. Minerals such as quartz, calcite, and pyrite, as well as macerals such as the vitrinite group, can originate from a variety of processes that result from different depositional conditions of peat formation. Subunits (coal-bed facies) of the Upper Freeport coal bed have been mapped over a 120-sq mi area in west-central Pennsylvania. These facies were characterized by a variety of chemical, petrographic, and mineralogical analyses. Facies mapping was based on field description of the bed at mine faces and description of X-ray radiographs of core. Where thickest, the coal bed averages 83 inches and contains eight to ten facies; in other areas, the bed averages about 48 inches and is generally composed of four coal-bed facies.

Each coal-bed facies is characterized by distinctive associations and concentrations of macerals and minerals. Areal isopleth patterns of ash and sulfur data for each coal-bed facies indicate different physical and biochemical conditions during peat formation that affected the concentration and distribution of pre-macerals and minerals. The different conditions inferred were (1) low to absent sediment influx and acid pH conditions that preserved humic tissues and leached mineral matter, (2) low sediment influx and near-neutral pH conditions that were conducive to degradation of plant tissues and formation of calcite and pyrite, and (3) moderate sediment influx and nutrient supply which produced both nonbanded coal and banded coal containing high-ash attrital layers alternating with thick vitrain under near-neutral pH conditions.

The macerals, minerals, and elements can be statistically separated into two major groups which are interpreted to reflect genetic relationships that resulted from the botanical and geochemical conditions during paleopeat formation. In Group I, most minerals and "non-organic" elements are considered to be derived dominantly from plants. In those parts of the bed most influenced by detrital influxes, a mixed source existed for elements and minerals. Where detrital influxes dominated, the coal is poor quality (high ash and thin) and commonly not mined. For example, quartz in the Upper Freeport coal is interpreted to be derived from both authigenic (derived from phytoliths) and detrital sources.

Group II constituents were probably derived from biochemical processes. Sporinite was probably concentrated by degradational processes and micrinite may represent a product of the degradation. In particular, pyrite formed at different times and under different conditions as indicated by trace element contents, petrographic associations, and isotopic data. Calcite also formed under different conditions of bacterial activity as indicated by isotope data; some calcite probably formed from fermentation reactions and other calcite appears to have formed from bacterial sulfate reduction or abiotic reactions.

A geochemical model proposed for the origin of coal-bed facies of the Upper Freeport coal bed is consistent with interpretations of modern peat formation resulting from the interaction of climate, plant types, rainfall, ground water geochemistry, nutrient supply, and sedimentation. This model provides a means to evaluate and predict more precisely the variability of a coal resource's quality.

## **INTRODUCTION**

Knowledge of the physical and chemical properties of coal is becoming increasingly important for the Nation's development of coal as a direct energy source and source of synthetic fuels. Before practical, effective, and predictive coal quality models can be developed, the variations in concentration of constituents, the depositional processes which affect the origins of constituents, and the interrelationships of important quality parameters such as sulfur content, maceral composition, mineralogy, ash content, and element content must be delimited. Identification and quantification of the processes that control the origin of coal quality parameters is a prerequisite to development of models to predict coal quality variability. Such models would aid in the wise use of limited coal resources with specific qualities (such as high-resin or low-sulfur coal beds. Unlike coalbed thicknesses that can be isopached on a regional basis, coal quality changes are more local and modeling geologic controls requires a detailed analytical approach. Therefore, one objective of this study was to develop criteria for establishing models to explain the quality of a bed; these criteria may be related to peat formation processes or diagenetic changes during burial and coalification.

The study reported here represents a major cooperative effort by the U.S. Environmental Protection Agency and the U.S. Geological Survey (USGS) to determine the geologic factors that govern the variation of more than 100 coal quality parameters in the Upper Freeport coal bed in west-central Pennsylvania (fig. 1). Initially, the study involved describing, sampling, and analyzing the coal to evaluate its "contaminant" content at 21 locations within the Homer City, Pa., dedicated reserves; a total of 75 coal-bed facies samples were studied. Since the initial study, an additional 72 locations consisting of cores and underground sites were visually described or described from X-ray radiographs; 39 of these additional locations were sampled for compositional analyses. A total of 351 coal-bed facies samples of coal and rock were analyzed from both studies. Compositional analyses included determination of elemental, maceral, and mineral contents by using instrumental and wet chemical analytical techniques, modal petrographic analyses, and X-ray diffraction of low temperature ash as described in Cecil and others (1981). Other specific studies of selected minerals involving specialized or novel approaches grew out of the initial evaluation of the bulk compositional data. These specialized studies included optical and scanning electron microscopy, electron microprobe analyses, isotope analyses, Mossbauer spectroscopy, and spectral cathodoluminescence microscopy.

## **ACKNOWLEDGMENTS**

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## **COAL QUALITY**

Coal quality is defined here as any and all compositional and physical properties of coal, the more noteworthy of which affect a particular use.

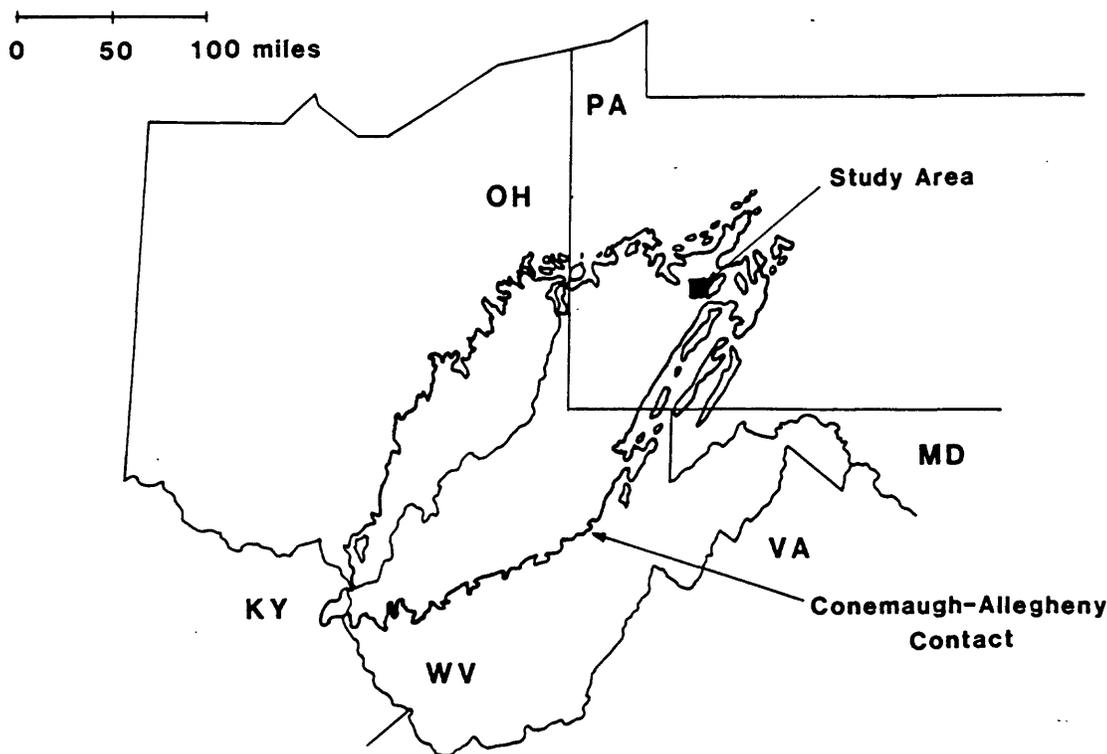
Different uses of coal require different quality parameters. For example, high amounts of pyrite and other ash-forming minerals in coal are undesirable in coking and combustion, but may be beneficial in certain liquefaction reactions. Coal quality parameters are not limited to certain element or mineral contents but also include maceral contents and degree of coalification. The degree of coalification (governed primarily by the rise of temperature and the effective heating time and retarded by the effects of pressure, (Teichmuller and Teichmuller, 1982)) and the mineral-free composition (primarily the chemical composition of macerals) of a coal directly affect the parameters used to determine rank. Like certain minerals, certain maceral contents or ratios are more desirable for some uses than for others. Quality therefore, encompasses all aspects of coal composition and as uses of coal become more diverse, coal quality parameters will become more important and must be accurately defined. In some cases, certain quality parameters may be desirable whereas in other cases, these same parameters may cause problems in the use of the coal. In other cases, for example, physical "deep-cleaning" of coal may produce a product with minimum sulfur content but may also alter the ratio of reactive to inert macerals, which, in turn, may alter combustion characteristics.

### **GENERAL GEOLOGY**

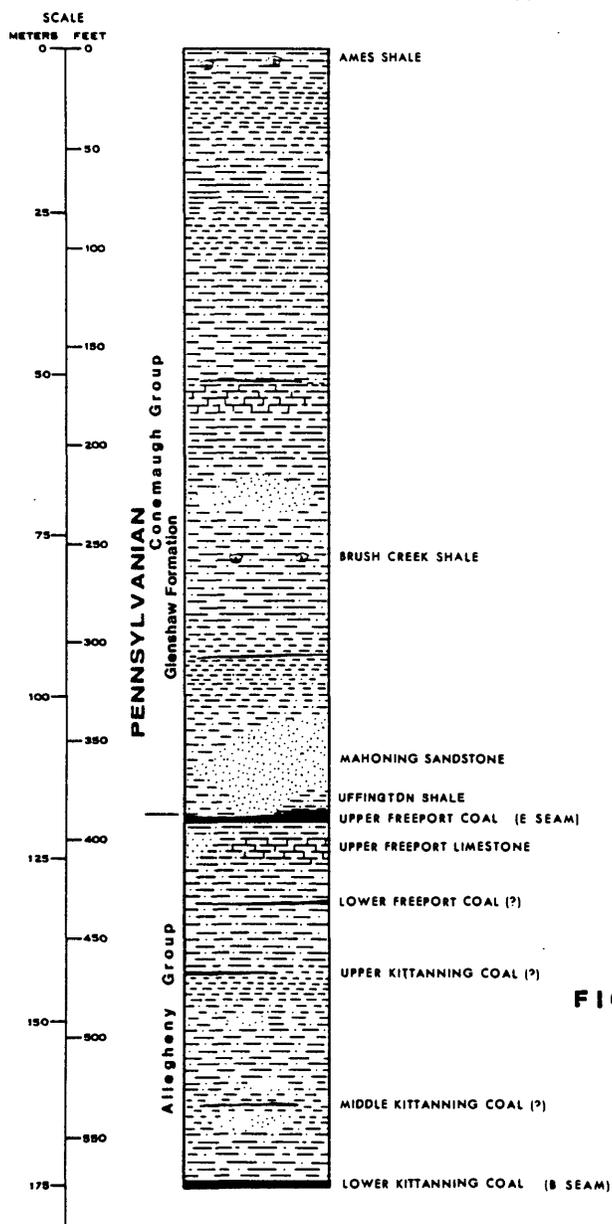
The study area lies between Clarksburg and Homer City, in Indiana County, west-central Pennsylvania (fig. 1) in the southwestward-plunging Elders Ridge and Latrobe synclines which are separated by the Jacksonville anticline. The Latrobe syncline is flanked on the east by the Chestnut Ridge anticline. The major rock units studied are in the upper part of the Allegheny Group and in the lower part of the Glenshaw Formation of the Conemaugh Group, specifically, (1) the Upper Freeport limestone, (2) the Upper Freeport coal bed, (3) the Uffington Shale, and (4) the Mahoning Sandstone Member (fig. 2). In places, the Upper Freeport coal bed directly overlies the Upper Freeport limestone. The limestone ranges from a brecciated limestone which displays some laminae and collapse structures to silty brecciated claystone which, in places, resembles flint clay. Overlying the limestone horizon is claystone and underclay which form the underlying unit for most of the Upper Freeport coal bed. Where present, the coal bed commonly ranges from 48 to 83 inches thick and is overlain by the Uffington Shale which varies from a black, well-laminated shale to a light gray shale. In places, the Mahoning Sandstone Member is in direct contact with the coal and commonly lies only a few feet above the shale or coal contact.

### **COAL-BED FACIES**

The Upper Freeport coal bed is composed of subunits called coal-bed facies that have distinctive lithologic characteristics and can be traced laterally. Four to ten coal-bed facies were observed in the Upper Freeport coal bed, depending on the sampling location. The lateral extent of the facies was determined by examining and describing the bed either at mine faces or in core. Thicknesses of bright and dull layers or bands, partings, frequency of banding, type and mode of occurrence of megascopic minerals, type of fractures, occurrence of fusain, and cleat spacing were the major criteria used for differentiating the facies. These criteria are similar to those used by Schopf (1960) for describing major coal types. The number of specific coal-bed facies and their properties vary areally in the bed. In addition to mine descriptions and samples, 41 cores were obtained from unmined areas and X-ray radiographed



**FIGURE 1. INDEX MAP OF THE HOMER CITY, PA. STUDY AREA AND CONEMAUGH-ALLEGHENY CONTACT.**



**FIGURE 2. GENERALIZED STRATIGRAPHIC COLUMN OF ROCKS IN THE STUDY AREA.**

(Stanton and others, 1983). A fence diagram (fig. 3) was prepared on the basis of description of the bed at various mine locations and descriptions of core. The lower split of the coal bed (Facies C, D, lower parting, and E) persists throughout the study area. The upper split of the coal bed (Facies B, and in some places A and A') is present only in the northeastern quadrant of the area.

The importance of obtaining coal-bed facies samples instead of whole-bed samples for analyses can be understood by comparing the ash and sulfur isopleth maps and isopach maps of the lower four facies to those of the whole bed (fig. 4). The different facies show different patterns of ash and sulfur distributions. Data from over 400 drill hole locations from company files were used to prepare the patterns in figure 4. In many cases, differentiation between Facies C and D was not made in the logs. Therefore, to compare all of the data with a comparable level of confidence, data for Facies C and D were combined. Other data plotted in figure 5 show the difference in quality among the facies. Although low in ash yield, Facies C varies most in sulfur among the lower facies (fig. 5). The lower parting facies is relatively constant in sulfur content even though its ash yield changes.

During compaction and coalification, fissility and banding develop and vitrain and mineral-rich layers appear as discrete although discontinuous bands. The thickest areas of each facies (fig. 4) also correspond to the lowest ash yields in those facies suggesting that prior to compaction. It is also postulated that these areas were probably much thicker and located nearer the center of the paleopeat-forming environment than other areas on the margins. A slightly raised, acid peat body would inhibit the influx of mud-laden flood waters both physically and chemically (McCabe, 1984) thereby producing minimal variation in ash yields as evident in figure 4. From this relationship, Facies C may have resulted from a slightly raised peat accumulation in contrast to the low-lying, planar peat formation of Facies E. So long as inorganic matter is not depleted during the transformation of plant material to peat and then to coal, all the processes that operate such as dewatering and devolatilization will result in a loss of organic matter. The loss of organic matter will have the effect of concentrating the mineral matter assuming that no appreciable mineral matter is lost. If the transformation of a well preserved peat into a bituminous coal, involves a compaction ratio of about 11:1 (Ryer and Langer, 1980) and a 50 percent weight loss of the original peat organic matter (Cecil and others, 1981), these factors mean that 11 meters of peat having about 10 weight percent ash yield (dry basis) will become about one meter of bituminous coal having a minimum ash yield of about 18 percent, assuming that mineral matter is not lost during coalification. Similarly, a peat that yields about 25 percent ash would be transformed into an impure bituminous coal that yields about 45 percent ash; compaction of this material may not be as great as a low-ash peat. Changes of these magnitudes have profound implications on the interpretations of the sedimentary history and depositional conditions of coal beds.

#### ORIGIN OF COAL COMPONENTS

To predict coal quality parameters, the means by which each component in the coal is concentrated and distributed must be understood and delimited. Commonly, certain components in coal originate from more than a single source. Sulfur, for example, is subdivided into organic, pyritic, and sulfate forms in standard coal analysis. Pyrite in different coal-bed facies may have been concentrated in coal by different processes at different times. Processes that affect the concentration of pyrite may include (1) metabolic activities of

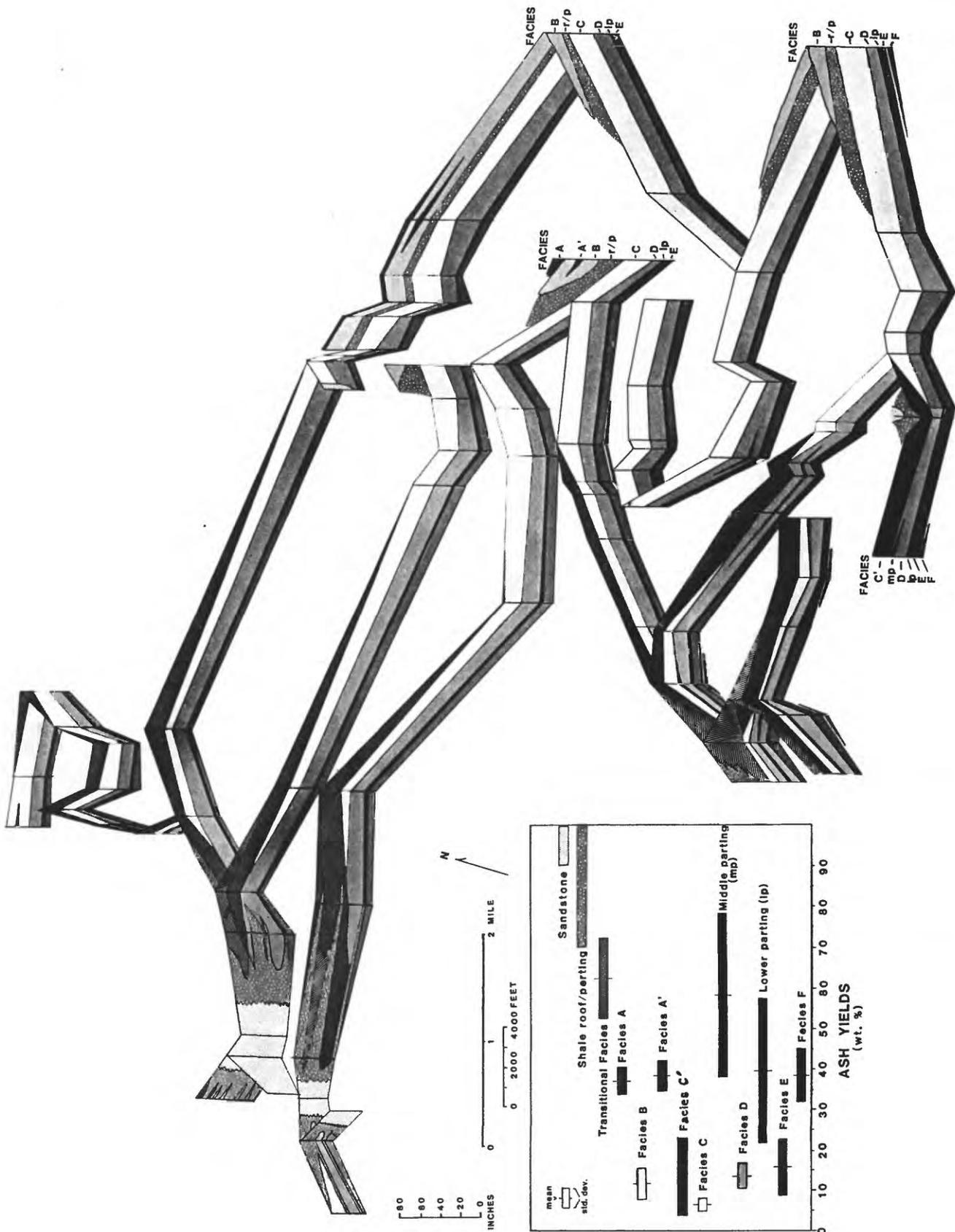
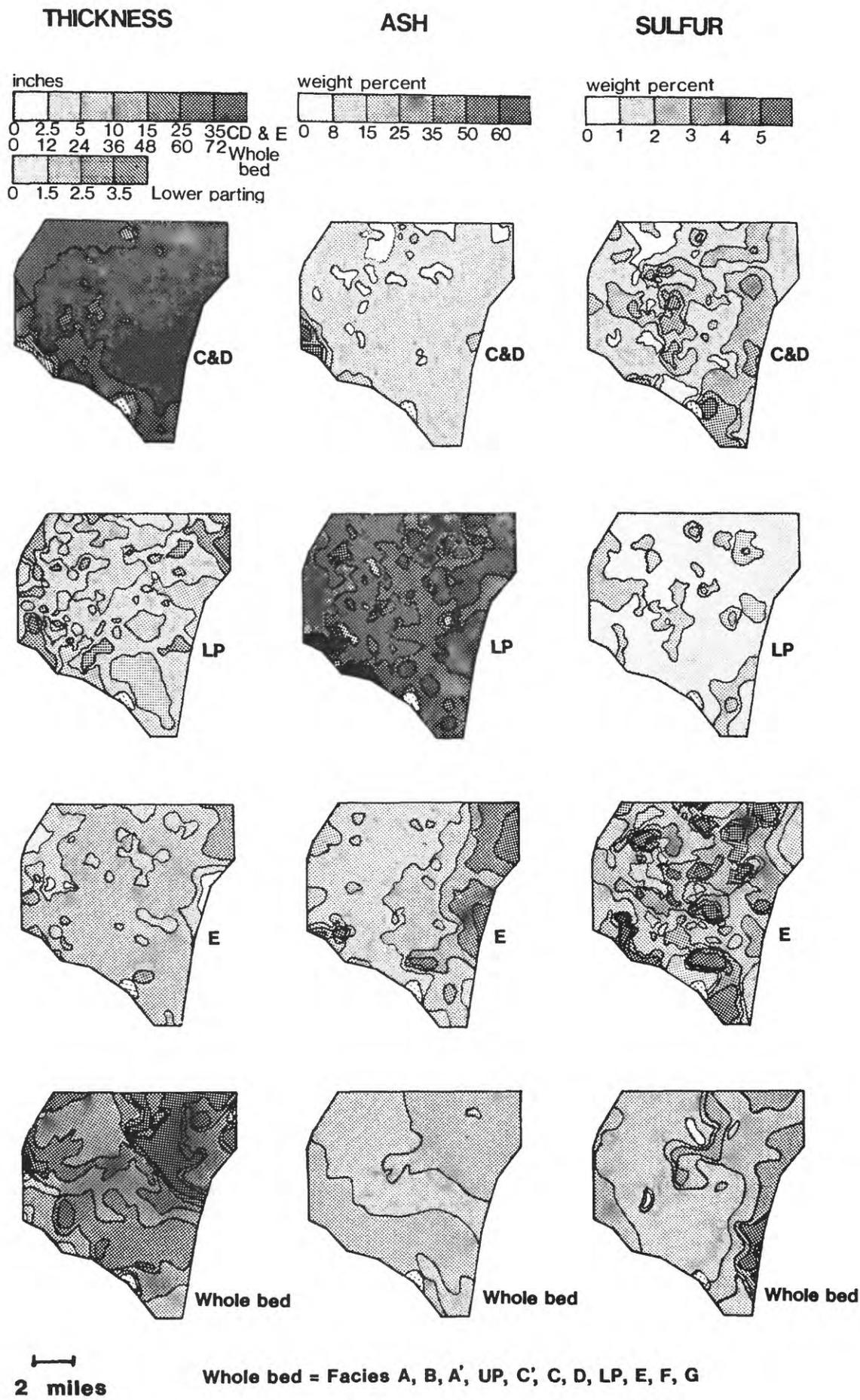
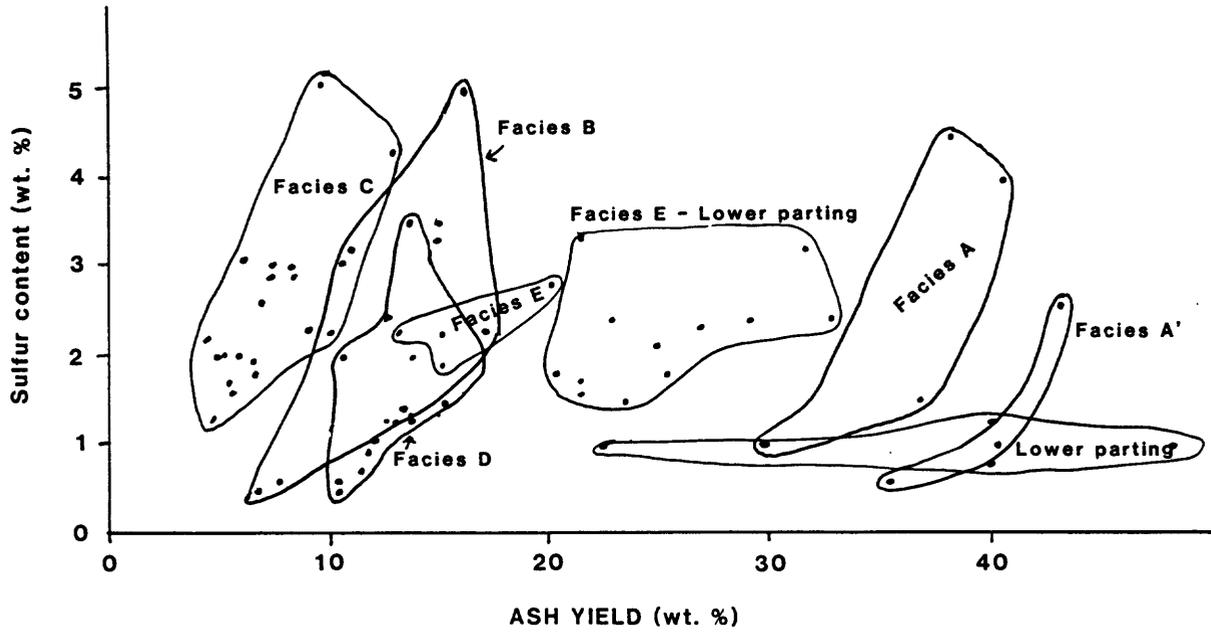


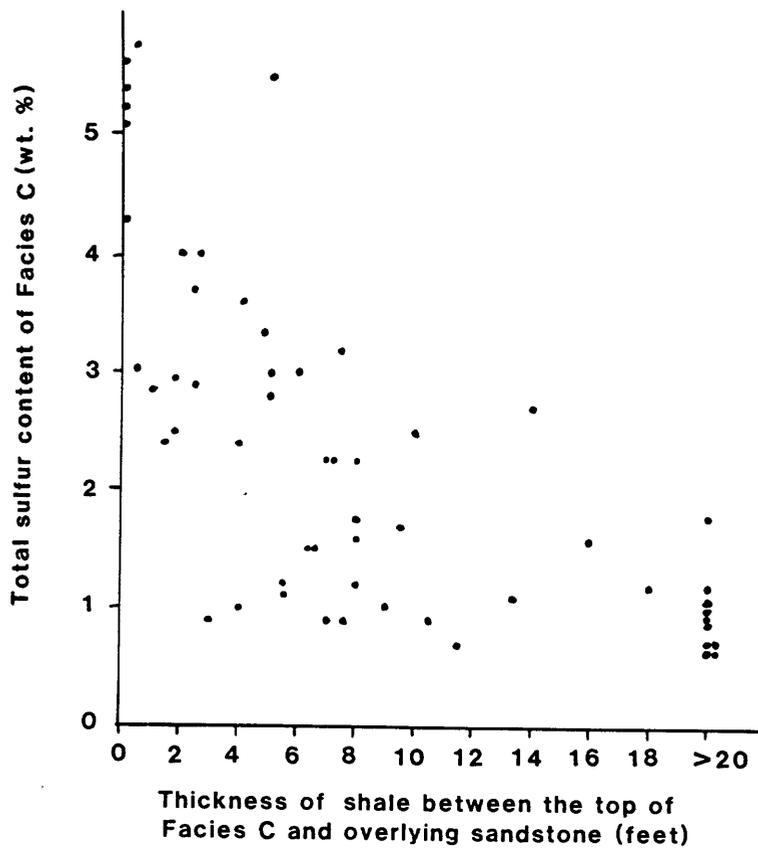
FIGURE 3. FENCE DIAGRAM OF FACIES OF THE UPPER FREEPORT COAL BED.



**FIGURE 4. ASH AND SULFUR ISOPLETHS AND THICKNESS ISOPACHS OF LOWER FOUR FACIES AND TOTAL BED.**



**FIGURE 5. COMPARATIVE QUALITY OF FACIES SAMPLES.**



**FIGURE 6. EFFECT OF SANDSTONE PROXIMITY TO SULFUR CONTENT OF FACIES C.**

plants and microorganisms during very early peat formation, (2) detrital surges from fluvial sources, or (3) biogenic and chemical reactions during coalification after burial.

The classes of coal components commonly used to describe coal composition are vitrinite, liptinite, inertinite, quartz, kaolinite, illite, calcite, and pyrite. The amounts of these components can be estimated by the combined use of petrography, chemistry, and X-ray diffraction. The concentration of any component based on bulk analysis of complete channel samples, however, is not necessarily indicative of any particular process that controlled its concentration.

### **Statistical groupings of data**

Spearman Rank correlation coefficients indicated two major groups of variables from analysis of data obtained in the initial collection of 75 facies samples (Cecil and others, 1981; table 1). These two distinct groups of elements, minerals, and macerals were interpreted to be related to processes by which the components were incorporated into the peat. Furthermore, those elements that correlate positively in Group I are interpreted to be derived from a dominant source or process. Incorporation from mixed processes or sources (such as detrital, plant and chemical) should not lead to statistically significant correlations. Because of the positive correlations of these elements with vitrinite (collinite and telinite), the concentration of the elements of Group I are interpreted to be related to material originally in the plants. The chemical elements of Group I may have been further concentrated by chemical and biochemical degradation of plant tissues during the peat stage and by the loss of organic matter during coalification. Other than for calcite and pyrite, the dominant source of major minerals in low-ash coal is interpreted to be inherent or derived from the vegetal matter (Cecil and others, 1981; 1982; 1985).

Assuming plant ash is the dominant source of the Group I chemical elements, the variations in the concentrations of the Group I elements are interpreted to have been caused primarily by variations within the peat-forming environment such as (1) differing plant communities, (2) variable water depth, and (3) variable water and peat chemistry. In general, given the effect of concentrating mineral matter during coalification, the ash yields of the coal in the study area, with the possible exception of A and A' facies, are too low and are interpreted to have resulted other than from a dominant detrital source.

Those chemical elements that correlate with sulfur (Group II) are interpreted as primarily of chemical and biochemical origin. The pH of the peat-forming environment affected and/or controlled bacterial degradation of the peat, the sulfate reduction, and the resultant sulfur fixation. This conclusion is based on the positive correlations among Ca, S, Fe, micrinite, and sporinite (Cecil and others, 1981). Micrinite is interpreted to be related to decomposition of cell contents (Cohen and Spackman, 1980). Sporinite is resistant to decay and because of its resistance will be relatively enriched in peats that are subject to degradation (Thiessen, 1925). Calcium fixation by organic acids during the peat stage of coal formation can partially neutralize peat acidity (pH>5), thereby allowing the functioning of sulfate reducing bacteria, which need a pH > 5 (Baas-Becking and others, 1960). Vertical and lateral variations in sulfur content may have been controlled primarily by variations in water and peat chemistry during the peat stage. High sulfur coal

Table 1 - Groupings of elements, minerals, and macerals based on nonparametric associations (modified from Cecil and others, 1981)

	GROUP I				GROUP II	
MACERALS	Collinite/Telinite				Sporinite	
	Fusinite				Micrinite	
	Semifusinite					
ELEMENTS AND SULFUR FORMS	B	Ga	Rb	Yb	Ca	
	Ba	Gc	Sb	Zn	Pyritic Sulfur	
	Be	Hf	Sc	Zr	Organic Sulfur	
	Cd	La	Se	Si	Fe oxide	
	Ce	Li	Sm	Al	As	
	Cr	Lu	Sn	Mg	Ge	
	Cs	Nb	Tb	Na	Hg	
	Cu	Nd	U	K		
	Eu	Ni	V	Ti		
	F	Pb	Y			
MINERALS	Quartz				Calcite	
	Illite				Pyrite	
	Kaolinite					

(>3 wt. %) has been correlated with marine roof rocks (Williams and Keith, 1963) but this correlation is a special case which permits sulfur fixation in environments in which pH > 5. The occurrence of medium (1 to 3 wt. %) to high sulfur (>3 wt. %) coals associated with nonmarine sediments (such as those associated with the Upper Freeport) can be attributed to formation in environments in which iron is available (Neavel, 1966), nearly 'neutral geochemistry,' dissolved calcium carbonate, and sulfate content during the peat stage of coal formation (Cecil and others, 1985). Additional factors influencing pyrite enrichment in coal are related to roof rock lithology. Coal-bed facies in the Upper Freeport coal bed that are overlain by nonmarine sandstone roof generally have higher sulfur contents than those overlain by a shale roof (fig. 6), possibly indicating an additional control by the availability of iron. Neutralizing effects on the paleopeat may also have been introduced by water associated with the overlying sandstone thereby reactivating bacterial sulfate reduction in the upper part of the paleopeat.

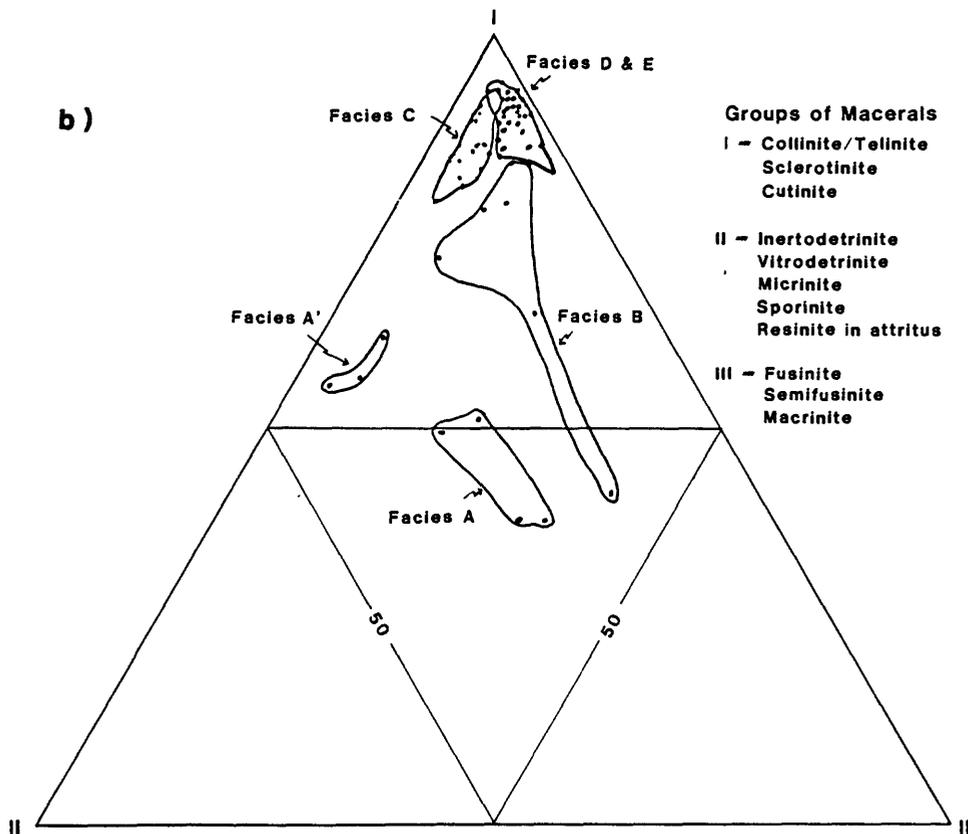
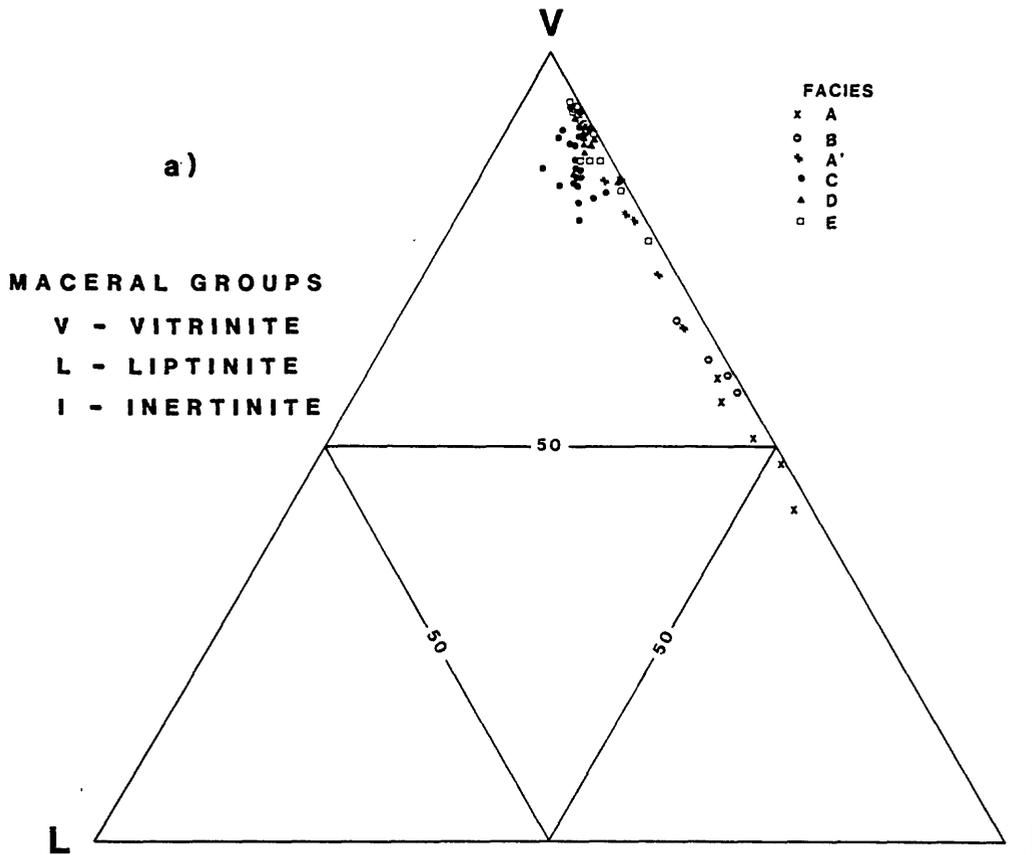
High concentrations of pyrite commonly are observed in fusain layers in Facies C. Fusain provides open sites for pyrite formation; and another factor in the pyritization of fusain may have been more favorable microchemical conditions within prefusain layers than in other peat layers. Favorable pH conditions (pH>5) could have been produced by the hydrolysis of alkali and alkaline earth ions, which were concentrated by oxidation or carbonization of plant tissues during peat formation (Cecil and others, 1982).

From statistical relationships established among data, more than a single process or source for most coal quality parameters is indicated. Further parameter-specific investigations that require a combination of analytical techniques are necessary to delimit the dominance of one source in each facies and to further subdivide each quality parameter into process-related or source-related subclasses. These additional studies may lead to the derivation of peat-developmental succession models to explain the variability of coal quality among coal-bed facies and to predict the differences in behavior during utilization.

### **Macerals**

Although the elemental compositions of the facies differ, the maceral compositions of the facies as determined by the generally accepted maceral groupings of vitrinite, liptinite, and inertinite end members (fig. 7a) overlap. The differentiation among the maceral groupings is based on their relative reflectances, which indicate chemical differences and which do not necessarily indicate a similar genesis for macerals within a group or among groups. Characterization of coal samples based solely on these commonly used macerals groupings may be of little value in considering the origins of the coal-bed facies and the genetic relationships among the macerals and minerals. For example, fusinite and micrinite are both of the inertinite group although the processes responsible for their origins are not similar--charring, oxidation, moldering, or fungal attack for fusinite (Teichmuller, 1982) and bacterial attack (Cohen and Spackman, 1980) or coalification (Teichmuller and Wolf, 1977) for micrinite.

In this study, groupings based on maceral concentrations that resulted from the relative enrichment by specific independent processes, such as degradation, preservation, and plant-type abundance, were used to compare facies data (fig. 7b). These groupings were chosen on the basis of possible genetic relationships and statistical correlations that were determined among certain macerals. However, even these groupings may not fully explain the differences



**FIGURE 7 - MACERAL GROUP COMPOSITIONS OF FACIES SAMPLES OF THE UPPER FREEPORT COAL, HOMER CITY, PA.**

among samples and all of the maceral varieties in each grouping may not be genetically similar. Further subdivision of the collinite/telinite class during initial analyses might have yielded additional genetic information. Nevertheless, these process-related groupings do permit differentiation among samples to a greater degree than was possible using the individual maceral groups (vitrinite, liptinite, and inertinite in fig. 7a). Although the differences among these process-related groupings may not be indicative of particular environments of deposition with a peat-accumulating area, the groupings do reflect differing degrees of preservation. For example, samples of Facies C which contain more degradation indicators such as micrinite and sporinite (table 2) than do those of Facies D and E (fig. 7b).

### Pyrite and Marcasite

Petrographically, pyrite and marcasite can be classed according to their forms (Neavel, 1966) and associations (fig. 8; Stanton and others, 1980). Quantitatively, forms differ among Facies C, D, and E (fig. 8) which indicates possible multiple processes for formation. Petrographic data from our study suggests different times of formation for pyrite and marcasite forms that can be interpreted as follows:

- |  |   |
|--|---|
| early peat formation prior to compaction | -- submicron crystals in corpocollinite (humic gel)<br>-- crystals (>1um) in vitrinite<br>-- framboids encapsulated in macerals<br>-- irregular forms filling cells of fusinite and vitrinite (telocollinite) |
| prior, during, and following compaction  | -- irregular forms replacing cell walls   |
| late peat formation                      | -- marcasite overgrowths on pyrite  |
| post compaction                          | -- irregular forms that fill cleat  |

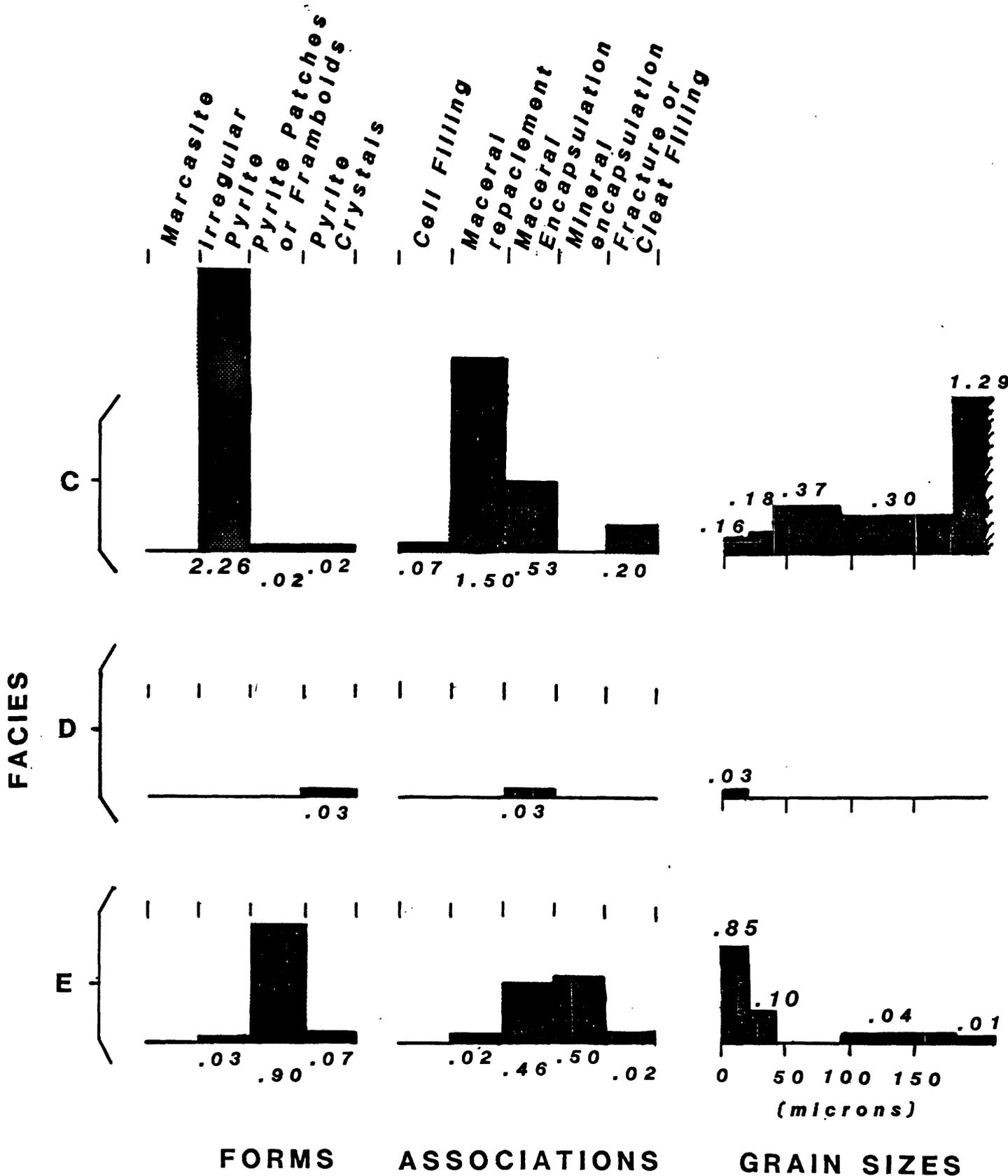
Indications of sulfur sources can be obtained from sulfur isotope data as in the study by Westgate and Anderson (1984). They concluded that the wide variability in the isotope values suggests a complex microbial origin involving sulfate reservoirs of different isotopic compositions.

In a preliminary study, sulfur isotope values were determined on petrographically characterized pyrite separates from coal-bed facies samples of the Upper Freeport coal bed (Whelan and others, 1985; fig. 9). Isotope values ranged from 0 to +10.35 ‰ and the two major forms--(1) crystals/framboids and (2) irregular--differ (with one exception). These data indicate either different sulfate sources for the formation of the two major forms or fractionation by means of reduction of greater proportions of the sulfate available during the formation of the irregular forms of pyrite. In either case, these data and the relationship shown in figure 8 support an interpretation that the different pyrite forms may differ genetically.

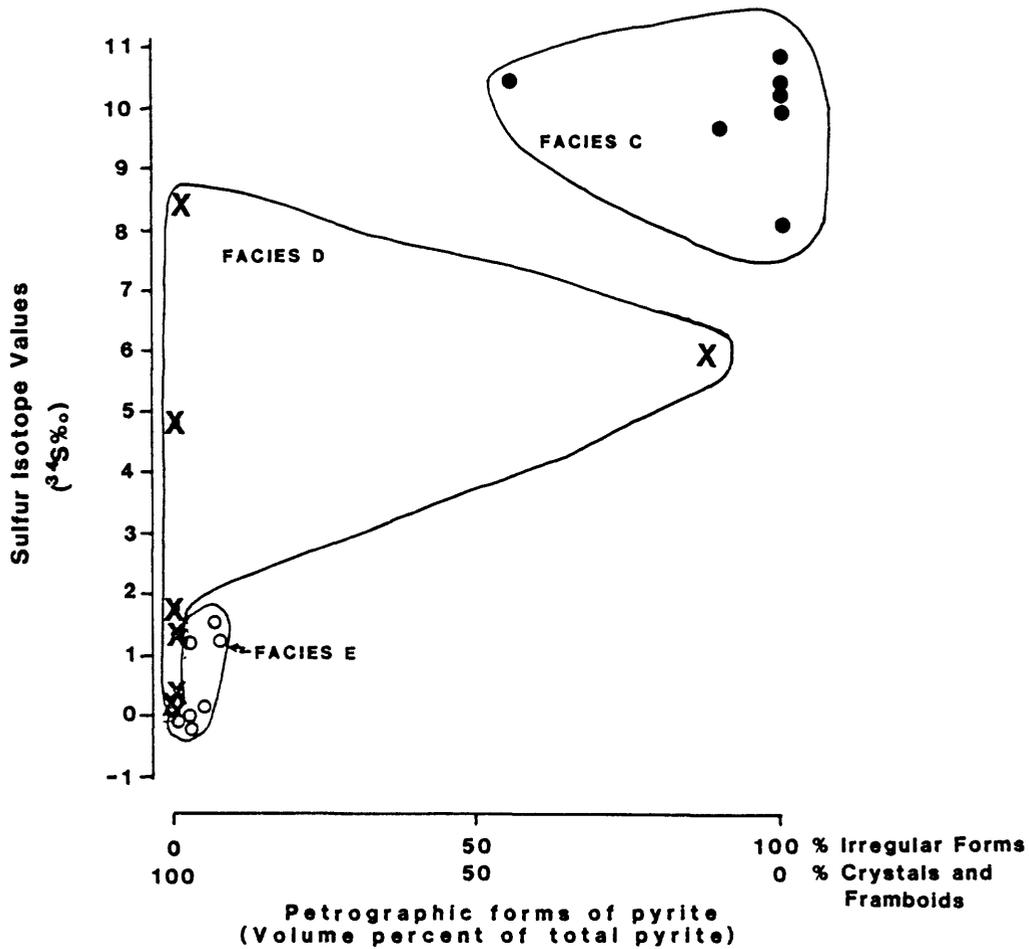
Framboidal pyrite is particularly common in the lowermost facies (E) and is less common to absent in other facies (fig. 9). The occurrence of pyrite framboids in coal has been attributed to a marine environment (Reyes-Navarro and Davis, 1976) or lower delta plain environment (Caruccio and others, 1977). Other authors have pointed out that framboids form in freshwater sediments

Table 2 : Maceral composition of Upper Freeport coal samples by facies.  
 (Mineral-free, volume percent basis; C&T=collinite and telinite; VD=vitro-detrinite; SP=sporinite; CU=cutinite; R=resinite; FU=fusinite; SF=semifusinite; MI=micrinite; MA=macrinite; SC=sclerotinite; ID=inertodetrinite; V=vittrinite; L=Liptinite; I=Inertinite; t=trace or less than 1 %; (-)=less than 1 count in 1000.)

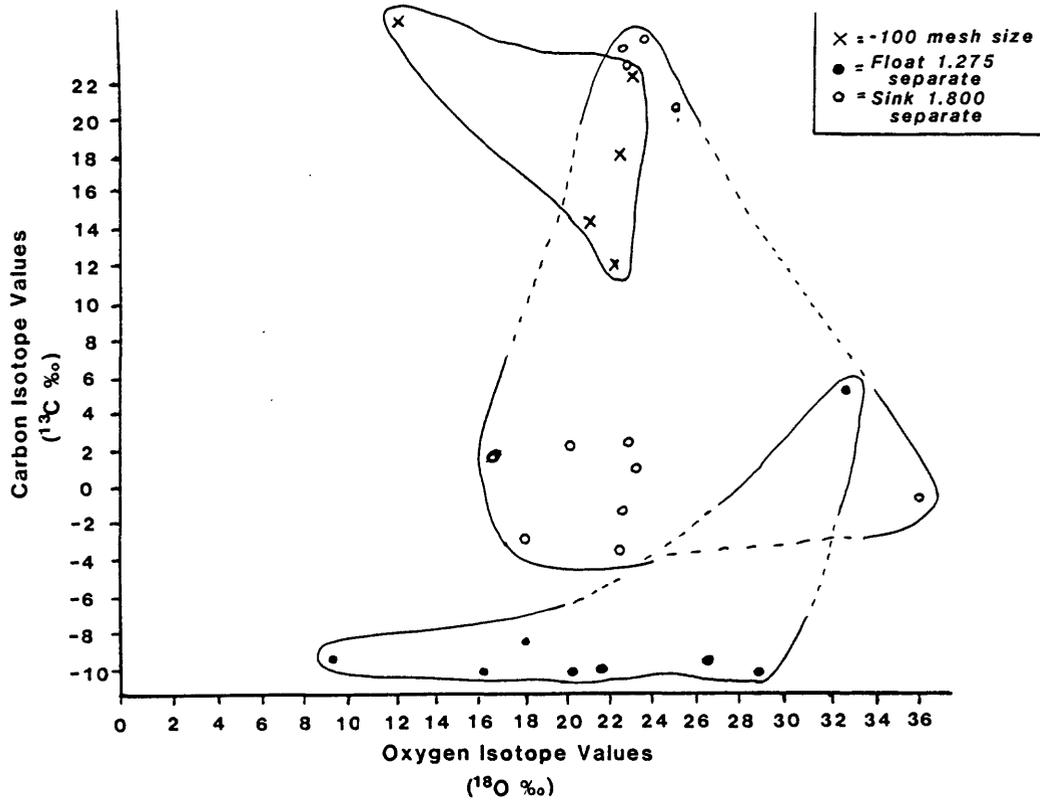
FACIES	C&T	VD	SP	CU	R	FU	SF	MI	MA	SC	ID	V	L	IN
A	45	6	T	T	-	2	13	3	12	-	17	51	2	47
B	72	-	2	T	-	4	7	7	6	-	2	72	2	26
A'	58	2	1	T	-	1	2	28	2	-	4	61	2	38
Parting	82	T	T	T	-	3	11	-	1	-	1	82	T	17
C	86	-	4	T	-	2	3	5	-	-	-	86	4	10
D	89	-	T	T	-	4	4	T	-	-	-	89	2	9
E +lower parting	89	-	T	T	-	3	5	1	-	-	1	89	1	10
D+E+lower parting	90	-	T	T	-	3	4	1	-	-	-	94	T	5



**FIGURE 8 - IRON SULFIDE FORMS, ASSOCIATIONS, AND GRAIN SIZES IN FACIES SAMPLES FROM H2-42P, UPPER FREEPORT COAL, HOMER CITY, PA. (values represent weight percent of pyritic sulfur)**



**FIGURE 9. PYRITE FORMS AND SULFUR ISOTOPE VALUES FOR FACIES SAMPLES OF THE UPPER FREEPORT COAL BED.**



**FIGURE 10. CARBON AND OXYGEN ISOTOPE VALUES OF CALCITE OBTAINED FROM SIZE/GRAVITY SEPARATES.**

(Valleyntyne, 1963) and coal (King, 1978). Marine sediments are not associated with the Upper Freeport coal bed; however, the coal commonly overlies a once subaerially exposed freshwater limestone or limy mudstone. Apparently, a pH environment of 5 or greater was the primary controlling factor of pyrite formation and, in particular, of framboid formation in this coal bed (Cecil and others, 1981).

Some facies in the coal have little or no pyrite or marcasite. Elemental concentrations in the swamp environment and Eh-pH conditions determined the mineral phases formed; thus, siderite, an iron carbonate, formed where iron concentrations were high but sulfur concentrations were low (Kemezys and Taylor, 1964). During fermentation or coalification, methane and carbon dioxide are generated and if hydrogen disulfide is present, pyrite formation may occur; if hydrogen disulfide is not available, Eh conditions may be more favorable for the formation of siderite or calcite (Krumbein and Garrels, 1952).

### **Calcite**

In an analysis of the occurrence of calcite in coals in Illinois, Rao and Gluskoter (1973) stated that calcite is the dominant carbonate mineral in coals of Illinois and possibly resulted from infiltration of solutions that were similar to the composition of solutions that deposited the calcite in associated lithologies or resulted from the coal bed being sealed from solutions of different compositions. Another study of carbonate in Illinois coal beds (Anderson and others, 1980) concluded that carbonate coal balls result from spatial and temporal variations in proportions of biogenic and inorganic carbon and that cleat calcite probably resulted from the permeation of ground water.

The strong correlation of calcite, pyrite, and certain macerals (micrinite and sporinite) in the Upper Freeport coal suggest an association with degradation processes. Biogenic calcite formation could result from the release of carbon dioxide during sulfate reduction and fermentation in the early stages of peat formation. Carbon isotope values obtained on cleat calcite range from about +7 to +25 per mil (Dulong and others, 1985) in contrast to -4 to -8 per mil values obtained on cleat calcite from the Herrin (No. 6) coal bed in Illinois (Anderson and others, 1980). Carbon and oxygen isotope data for gravity separates of Upper Freeport coal-bed facies samples suggest that at least two, possibly three stages of calcite formation (fig. 10). These differences suggest that cleat calcite (enriched in sink 1.80 gravity and -100 mesh separates) originated as a result of fermentation reactions and calcite cell filling (enriched in float 1.275 gravity separates) originated as a result of either abiotic reactions or sulfate reduction (fig. 10; Dulong and others, 1985).

### **Quartz**

Quartz in the Upper Freeport coal, in addition to illite and kaolinite, was interpreted to have been dominantly derived from plants on the basis of the statistical groupings (Cecil and others, 1981; 1982). Cathodoluminescence spectra of quartz indicate that quartz is dominantly authigenic in coal with ash yields of <25 wt. %, and that the dominant source of quartz may have been from plants (Ruppert and others, 1985). Quartz grains analyzed in samples from of coal and shale from the Upper Freeport coal bed ranged from 3 to 15 microns in size and were generally subround. In low ash (<8 wt. %) coal samples, most quartz (over 80 percent) did not luminesce, indicating an authigenic (derived

from solutions under low temperature conditions) origin. In contrast, samples analyzed from the roof shale contained dominantly luminescent (detrital) type quartz and samples from the lower parting contained quartz grains derived from both sources (Ruppert and others, 1985).

One possible source for nonluminescing grains in coal may be spalled quartz overgrowths that were produced from the reworking of quartz-rich sediments. However, this is not probable because if this were the case, then the paleopeat environment would have selectively separated overgrowths from their detrital cores; the ratios of luminescent/nonluminescent quartz are very different in the shales from those in low-ash coal samples. Other more probable sources of the nonluminescing grains may be from paleoplant silica phytoliths or products of weathering of clay minerals.

Because sizes, shapes, and cathodoluminescence properties of quartz grains in the coal samples differed from those in shale samples, at least two sources for quartz in the Upper Freeport coal bed are postulated: (1) plant phytoliths or weathering products from clay minerals and (2) transported muds from nearby streams (in high-ash, coal-bed facies)(Ruppert and others, 1985).

### POSTULATED DEPOSITIONAL HISTORY

The lithologies underlying the coal are the result of a variety of processes which began with the deposition of the Upper Freeport limestone in a freshwater environment (Williams and others, 1968). From core and outcrop data, this limestone is interpreted to have undergone extensive subaerial exposure resulting in the formation of calcite-poor, brecciated units after deposition and prior to peat accumulation. This interpretation is supported by the presence of (1) extensive brecciation, (2) crusts of cemented grains interpreted to have formed by subaerial exposure, and (3) a highly irregular microkarst surface which was partially covered with clays and silt prior to the development of the ancestral peat-forming environment.

Formation of the first peat facies (Facies F, fig. 3) resulted in patchy peat development in topographically low areas in a shallow lacustrine environment. Peat accumulation eventually blanketed the study area, resulting in Facies E which was interrupted by deposition of the mud-laden precursor to the lower parting facies based on patterns of figure 4. This parting resulted from detrital influx from stream flooding or ponding of the active drainage system that formed the western, southern, and eastern boundaries of the swamp. On these respective margins, the parting is high in ash (fig. 5)--a shale or claystone; in contrast, the parting is a high-ash durain in the interior part of the study area. Peat accumulation subsequently resumed and resulted in the formation of Facies D which is petrographically similar to Facies E. Conditions next changed from low-lying peat formation (planar) to slightly raised, less wet, possibly acid peat formation (Facies C) that physically or chemically restricted the influx of sediment and mud-laden waters during periods of high stream flow. Evidence for this change consists of the compositional differences between Facies D and C, the low-ash yield of Facies C, the lack of clay-rich layers in Facies C, the abundance of fusain layers in Facies C, and the random pattern of ash-yield of Facies C and D as compared to the isopleths of the lower parting facies and Facies E (fig. 4).

In the western and southern part of the study area, Facies C', which consists of alternating clay-rich and vitrain layers, may have resulted from lush vegetation along the margins of a stream that supplied nutrients for growth. In contrast, Facies C may have formed from a slightly raised peat and decreased in areal extent probably as a result of increased water levels. Peataccumulation was apparently terminated by increased water levels and the

formation of a nonmarine lake in which laminated clay and silt were deposited. In the northeastern part of the study area peat deposition resumed, probably on topographically high areas of the underlying low-ash, thick areas of Facies C. The peat that formed Facies B consisted of a long, linear, peat island similar to that described by Ferm and Staub (1984). Nonbanded coal Facies A' and A resulted from variations of peat-forming conditions influenced most by the water level of the surrounding lake. Peat accumulation was finally terminated by flooding of the island; clay and silt were deposited over the entire area thus forming the Uffington Shale.

The Mahoning Sandstone Member was deposited over much of the area as part of a fluvial sequence that prograded into the lake environment. In most cases that were examined underground where the sand was in contact with the coal, the coal bed was not eroded but was less thick because of differential compaction of the sand, mud, and peat, as evidenced by slickensides in the coal bed, thickening of the coal bed marginal to the channel sandstone roof areas, and the paucity of coaly clasts in the basal part of the sandstone. Rarely was the peat itself eroded. In addition, sharp, scoured contacts between the shale and sandstone in core and exposed sections indicate that the overlying sandstone was deposited after the deposition of the Uffington muds (Cecil and others, 1981). In some places the streams transporting the sands eroded the previously deposited Uffington muds resulting in the deposition of sand directly on the buried peat.

#### **GEOCHEMICAL MODEL**

A geochemical model for coal formation and the effect of paleoclimate on peat formation is detailed in Cecil and others (1985). Low-ash coal must result from very low-ash peats (<5 percent, dry basis) or from peats that had significant quantities of mineral matter removed before or during coalification. Although we cannot determine the ash content and compaction of the plant precursors of the Upper Freeport coal, it does seem reasonable to assume that Pennsylvanian plants did contain ash-forming elements similar to modern plants. The content and variability of ash and sulfur in modern environments are affected by the chemistry and climatic conditions of the peat-forming environment (Cecil and others, 1981; 1985). High-ash, high-sulfur peats are associated with nearly neutral pH conditions, and low-ash, low-sulfur peats are associated with acid peat conditions (Cecil and others, 1985). The most probable source of the mineral-matter in low-ash peats is the inherent plant ash. The two factors most affecting the variability of the mineral matter are (1) the type of peat formation (planar or raised) and (2) the degree of differential decay of the plant tissues in the peat (Thiessen, 1925). High-ash layers are interpreted by the authors to result from detrital influxes only if the peat type was planar (criteria for planar peat accumulation includes the existence of correlative coal-bed facies across a large area (miles) and very extensive inorganic-rich facies, such as the lower parting facies). Even under planar peat formation, the highest ash yields are where the peat was marginal to active streams.

The significance of the plant ash contribution to mineral matter in the Upper Freeport coal bed initially was recognized from the statistical analysis of the data (Cecil and others, 1981). Those elements of Group I (table 1) are interpreted to be principally derived from a common source and caused primarily by variations within the peat-forming environment such as (1) differing plant communities, (2) variable water depth, and (3) variable peat and water chemistry. In general, given the effects of compaction, dewatering, and coalification, we regard the ash contents of the coal-bed facies of the study

area (Facies B, C, D, E, and F) as too low to have resulted from a dominant detrital source. Facies A and A', the parting facies, and the western and southern margins of the lower facies have high ash yields and probably resulted from mixed sources.

During the peat stage of coal formation, mineral matter in the Upper Freeport coal bed is interpreted to have been derived from multiple sources, (1) a dominant source--inherent plant chemical composition, (2) sorption of ions in solution on surfaces of peat particles, (3) precipitation from solution by chemical and/or biochemical processes, and (4) a source of limited areal influence and during planar peat formation--detrital minerals that were washed or blown into the peat-forming environment. After burial, mineral matter may have been precipitated from formation waters in pores and fractures. This later stage of mineral-matter fixation may be the result of diagenetic processes operating on mineral matter already present in the coal, or it may be the result of enrichment of elements from ground water moving through the coal. Techniques such as spectral cathodoluminescence and isotopic analysis allow discriminant interpretation of the primary sources that concentrated a particular element or formed a particular mineral.

### CONCLUSIONS

Classification of coal-bed facies successions which are related to paleopeat formation may be a key to classifying and modeling the quality of coal beds. Facies succession will differ for different physical and chemical environments which existed during peat formation. However, coupled with a geochemical model, facies analysis of a coal bed may be the best way to identify the dominant geologic processes that affect the quality of the bed. Tools useful for classification include facies description and sampling, aided by X-ray radiography of core. By delimiting the dominant processes that affect the variability of coal quality, those quality-parameters that are undesirable or desirable for a specific use can be determined more precisely.

In the Upper Freeport coal bed, successive intervals of peat formation resulted in the formation of coal-bed facies that show different patterns in quality than patterns of the whole bed data. The dominant processes that formed each facies also controlled the type, amount, and distribution of the major quality parameters such as macerals, quartz, clay minerals, pyrite, and calcite.

Coal composition is controlled by multiple parameters that are interrelated. The variations in composition of facies are determined mostly by (1) the pH and Eh of the environment, (2) dominant plant communities and their relative differential decay, (3) degree of microbial and chemical degradation of macerals and minerals, (4) the concentrations of the inherent ash, calcium, iron, and sulfur, and (5) the type of peat formation, domed or planar, and the hydrologic effects on the peat formation. Quantification of the genetic types of compositional parameters is the next step in developing effective and practical coal quality models.

Exploration for low-sulfur coal bodies should focus on stratigraphic sequences where calcareous sediments are uncommon. Coals in such sequences should normally have low sulfur contents and low ash yields with minimal variability. Ash and sulfur should be more highly variable as the calcium carbonate content of a given coal and associated rocks increases. If the peat succession types can be determined and the quality of contributing facies is established and matched with the proper model, exploration and development costs can be minimized and mine planning can be adjusted to optimize production quality of a coal resource.

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