

HANDBOOK OF COAL ANALYSIS

James G. Speight



A JOHN WILEY & SONS, INC., PUBLICATION

HANDBOOK OF COAL ANALYSIS

CHEMICAL ANALYSIS

A SERIES OF MONOGRAPHS ON ANALYTICAL CHEMISTRY
AND ITS APPLICATIONS

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PREFACE

Coal is an extremely complex material and exhibits a wide range of physical properties. The rapidly expanding use of coal in the twentieth century made it necessary to devise acceptable methods for coal analysis with the goal of correlating composition and properties with behavior. It is only by assiduously using careful analyses of coal that the various aspects of coal usage can be achieved in an environmentally acceptable manner. As a part of the multifaceted program of coal evaluation, new methods are continually being developed and the already accepted methods may need regular modification to increase the accuracy of the technique as well as the precision of the results. Furthermore, proper interpretation of the data resulting from the analysis of coal requires an understanding of the significance of the analytical data.

This book deals with the various aspects of coal analysis and provides a detailed explanation of the necessary standard tests and procedures that are applicable to coal in order to help define coal behavior relative to usage and environmental issues. The first items that the book covers (after nomenclature and terminology) are related to sampling, accuracy of analysis, and precision of analysis. These important aspects are necessary to provide reproducibility and repeatability of the analytical data derived from the various test methods. The book then goes on to provide coverage of the analysis of coal by various test methods, as well as the application and interpretation of the data to provide the reader with an understanding the quality and performance of coal. A glossary of terms that will be useful to the reader is also included. Each term is defined in a language that will convey the meaning to the reader in a clear and understandable way.

Sources of information that have been used include (1) the *Annual Book of ASTM Standards*, (2) the British Standards Institution, (3) the International Organization for Standardization, (4) older books, (5) collections of individual articles from symposia, and (6) chapters in general coverage books. This will be the first book that provides not only a detailed description of the tests but also the outcome of the tests and the meaning of the data. However, the actual mechanics of performing a test method are not included; such information is available from the various standards organization.

Although the focus of the book is on the relevant ASTM (American Society for Testing and Materials) test methods with the numbers given, where possible the corresponding ISO (International Organization for Standardization) and BS (British Standards Institution) test method numbers are also presented. As an aside, the ASTM may have withdrawn some of the test methods noted herein,

but the test method is still referenced because of its continued use, for whatever reason, in many analytical laboratories.

If this book helps toward a better understanding of the criteria for determining the properties of coal, leading to an understanding of coal behavior, it will have served its purpose.

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August 2004*

1 Coal Analysis

Coal is an organic sedimentary rock that contains varying amounts of carbon, hydrogen, nitrogen, oxygen, and sulfur as well as trace amounts of other elements, including mineral matter (van Krevelen, 1961; Gluskoter, 1975; Speight, 1994; ASTM D-121).

The name *coal* is thought to be derived from the Old English *col*, which was a type of charcoal used at the time. Coal is also referred to in some areas, as *sea coal* because it is occasionally found washed up on beaches, especially in northeastern England. Generally, coal was not mined to any large extent during the early Middle Ages (prior to A.D. 1000) but there are written records of coal being mined after that date. However, the use of coal expanded rapidly, throughout the nineteenth and early twentieth centuries. This increased popularity has made it necessary to devise acceptable methods for coal analysis, with the goal of correlating fuel composition and properties with behavior (Montgomery, 1978; Vorres, 1993; Speight, 1994).

Coal is a solid, brittle, combustible, carbonaceous rock formed by the decomposition and alteration of vegetation by compaction, temperature, and pressure. It varies in color from brown to black and is usually stratified. The source of the vegetation is often moss and other low plant forms, but some coals contain significant amounts of materials that originated from woody precursors.

The plant precursors that eventually formed coal were compacted, hardened, chemically altered, and metamorphosed by heat and pressure over geologic time. It is suspected that coal was formed from prehistoric plants that grew in swamp ecosystems. When such plants died, their biomass was deposited in anaerobic, aquatic environments where low oxygen levels prevented their reduction (rotting and release of carbon dioxide). Successive generations of this type of plant growth and death formed deep deposits of unoxidized organic matter that were subsequently covered by sediments and compacted into carboniferous deposits such as peat or bituminous or anthracite coal. Evidence of the types of plants that contributed to carboniferous deposits can occasionally be found in the shale and sandstone sediments that overlie coal deposits.

Coal deposits, usually called *beds* or *seams*, can range from fractions of an inch to hundreds of feet in thickness. Coals are found in all geologic periods from Silurian through Quaternary, but the earliest commercially important coals are found in rocks of Mississippian age (Carboniferous in Europe). Coals generally

formed either in basins in fluvial environments or in basins open to marine incursions. Coal is found on every continent, and world coal reserves exceed 1 trillion tons. However, the largest reserves are found in the United States, the former Soviet Union, and China. The United States and former Soviet Union each have about 23% of the world's reserves, and China has about 11%.

Coal consists of more than 50% by weight and more than 70% by volume of carbonaceous material (including inherent moisture). It is used primarily as a solid fuel to produce heat by burning, which produces carbon dioxide, a greenhouse gas, along with sulfur dioxide. This produces sulfuric acid, which is responsible for the formation of sulfate aerosol and acid rain. Coal contains many trace elements, including arsenic and mercury, which are dangerous if released into the environment. Coal also contains low levels of uranium, thorium, and other naturally occurring radioactive isotopes, whose release into the environment may lead to radioactive contamination. Although these substances are trace impurities, a great deal of coal is burned, releasing significant amounts of these substances.

When coal is used in electricity generation, the heat is used to create steam, which is then used to power turbine generators. Approximately 40% of Earth's current electricity production is powered by coal, and the total known deposits recoverable by current technologies are sufficient for at least 300 years of use. Modern coal power plants utilize a variety of techniques to limit the harmfulness of their waste products and to improve the efficiency of burning, although these techniques are not widely implemented in some countries, as they add to the capital cost of the power plant.

Coal exists, or is classified, as various types, and each type has distinctly different properties from the other types. *Anthracite*, the highest rank of coal, is used primarily for residential and commercial space heating. It is hard, brittle, and black lustrous coal, often referred to as *hard coal*, containing a high percentage of fixed carbon and a low percentage of volatile matter. The moisture content of fresh-mined anthracite generally is less than 15%. The heat content of anthracite ranges from 22 to 28 million Btu/ton on a moist, mineral-matter-free basis.

Bituminous coal is a dense coal, usually black, sometimes dark brown, often with well-defined bands of bright and dull material, used primarily as fuel in steam-electric power generation, with substantial quantities also used for heat and power applications in manufacturing and to make coke. The moisture content of bituminous coal is usually less than 20% by weight. The heat content of bituminous coal ranges from 21 to 30 million Btu/ton on a moist, mineral-matter-free basis.

Subbituminous coal is coal whose properties range from those of lignite to those of bituminous coal, used primarily as fuel for steam-electric power generation. It may be dull, dark brown to black, and soft and crumbly at the lower end of the range, to bright, black, hard, and relatively strong at the upper end. Subbituminous coal contains 20 to 30% inherent moisture by weight. The heat content of subbituminous coal ranges from 17 to 24 million Btu per ton on a moist, mineral-matter-free basis.

Lignite is the lowest rank of coal, often referred to as *brown coal*, used almost exclusively as fuel for steam-electric power generation. It is brownish black and has a high inherent moisture content, sometimes as high as 45%. The heat content of lignite ranges from 9 to 17 million Btu/ton on a moist, mineral-matter-free basis.

1.1 ANALYSIS CONSIDERATIONS

The data obtained from coal analyses (Table 1.1) establish the price of the coal by allocation of production costs as well as to control mining and cleaning operations and to determine plant efficiency. However, the limitations of the analytical methods must be recognized (Rees, 1966). In commercial operations, the price of coal not only reflects the quantity of coal but also invariably reflects the relationship of a desirable property or even a combination of properties to performance of coal under service conditions (Vorres, 1993).

Measurements of the desired property or properties (usually grouped together under the general title *specifications*) are expressed as numerical values; therefore, the accuracy of these measurements is of the utmost importance. The measurements need to be sufficiently accurate so as to preclude negative scientific or economic consequences. In other words, the data resulting from the test methods used must fall within the recognized limits of error of the experimental procedure so that the numerical data can be taken as fixed absolute values and

TABLE 1.1 Sampling and Analytical Methods Used for Coal Evaluation

Test/Property	Results/Comments
Sample information	
Sample history	Sampling date, sample type, sample origin (mine, location)
Sampling protocols	Assurance that sample represents gross consignment
Chemical properties	
Proximate analysis	Determination of the "approximate" overall composition (i.e., moisture, volatile matter, ash, and fixed carbon content)
Ultimate analysis	Absolute measurement of the elemental composition (i.e., carbon, hydrogen, sulfur, nitrogen, and oxygen content)
Sulfur forms	Chemically bonded sulfur: organic, sulfide, or sulfate
Ash properties	
Elemental analysis	Major elements
Mineralogical analysis	Analysis of the mineral content
Trace element analysis	Analysis of trace elements; some enrichment in ash
Ash fusibility	Qualitative observation of temperature at which ash passes through defined stages of fusing and flow

Source: Smith and Smoot (1990).

not as approximations. Indeed, the application of statistical analysis to such test methods must be treated with extreme caution. Such analysis must be based on valid assumptions and not be subject to a claim of mathematical manipulation to achieve the *required result*. In other words, there is a requirement that reliable *standard* test methods be applied to coal analysis.

There are many problems associated with the analysis of coal (Lowry, 1963; Karr, 1978) not the least of which is its heterogeneous nature. Other problems include the tendency of coal to gain or lose moisture and to undergo oxidation when exposed to the atmosphere. In addition, the large number of tests and analyses required to characterize coal adequately also raise issues.

Many of the test methods applied to coal analysis are empirical in nature, and strict adherence to the procedural guidelines is necessary to obtain repeatable and reproducible results. The type of analysis normally requested by the coal industry may be a proximate analysis (moisture, ash, volatile matter, and fixed carbon) or an ultimate analysis (carbon, hydrogen, sulfur, nitrogen, oxygen, and ash).

By definition, a *standard* is defined as a document, established by consensus and approved by a recognized body, that provides, for common and repeated use, rules, guidelines, or characteristics for activities or their results. Many industry bodies and trade associations require a product (e.g., coal) to conform to a standard or directive before it can be offered for sale. In fact, the use of standards is becoming more and more of a prerequisite to worldwide trade. Above all, any business, large or small, can benefit from the conformity and integrity that standards assure.

As a result, the formation of various national standards associations has led to the development of methods for coal evaluation. For example, the American Society for Testing and Materials (ASTM) has carried out uninterrupted work in this field for many decades, and investigations on the development of the standardization of methods for coal evaluation has occurred in all the major coal-producing countries (Montgomery, 1978; Patrick and Wilkinson, 1978). There are in addition to the ASTM, organizations for methods development and standardization that operate on a national level; examples are the International Organization for Standardization (ISO) and the British Standards Institution (BS), which covers the analysis of coal under one standard number (BS 1016) (Table 1.2).

Furthermore, the increased trade between various coal-producing countries that followed World War II meant that cross-referencing of already accepted standards was a necessity, and the mandate for such work fell to the ISO, located in Geneva, Switzerland; membership in this organization is allocated to participating (and observer) countries. Moreover, as a part of the multifaceted program of coal evaluation, new methods are continually being developed and the methods already accepted may need regular modification to increase the accuracy of the technique as well as the precision of the results.

It is also appropriate that in any discussion of the particular methods used to evaluate coal for coal products, reference should be made to the relevant test. Accordingly, where possible, the necessary test numbers (ASTM) have been included as well as those, where appropriate, of the BS and the ISO.

TABLE 1.2 British Standard 1016: *Methods for Analysis and Testing of Coal and Coke*

Section	Topics
BS 1016-1	Total moisture of coal
BS 1016-6	Ultimate analysis of coal
BS 1016-7	Ultimate analysis of coke
BS 1016-8	Chlorine in coal and coke
BS 1016-9	Phosphorus in coal and coke
BS 1016-10	Arsenic in coal and coke
BS 1016-14	Analysis of coal ash and coke ash
BS 1016-21	Determination of moisture-holding capacity of hard coal
BS 1016-100	General introduction and methods for reporting results
BS 1016-102	Determination of total moisture of coke
BS 1016-104.1	Proximate analysis, determination of moisture content of the general analysis test sample
BS 1016-104.2	Proximate analysis, determination of moisture content of the general analysis sample of coke
BS 1016-104.3	Proximate analysis, determination of volatile matter content
BS 1016-104.4	Proximate analysis, determination of ash content
BS 1016-105	Determination of gross calorific value
BS 1016-106.1.1	Ultimate analysis of coal and coke, determination of carbon and hydrogen content, high temperature combustion method
BS 1016-106.1.2	Liebig method
BS 1016-106.2	Ultimate analysis of coal and coke, determination of nitrogen content
BS 1016-106.4.1	Ultimate analysis of coal and coke, determination of total sulfur content, Eschka method
BS 1016-106.4.2	Ultimate analysis of coal and coke, determination of total sulfur content, high temperature combustion method

Source: BS (2003).

A complete discussion of the large number of tests that are used for the evaluation of coal (and coal products) would fill several volumes (see, e.g., Ode, 1963; Karr, 1978, 1979; Montgomery, 1978; Zimmerman, 1979; Gluskoter et al., 1981; Smith and Smoot, 1990), and such detailed treatment is not the goal of this book. The focus is on a description, with some degree of detail, of the test methods in common use, as well as a critique of various procedures that are not obvious from the official descriptions of test methods and a description of pitfalls that can occur during application of a test method for coal analysis.

Quite often, a variation of a proximate analysis or an ultimate analysis is requested, together with one or more of the miscellaneous analyses or tests discussed in this chapter. Restrictions that have been placed on the coal used in coal-fired power plants and other coal-burning facilities have created a need for more coal analyses as well as a need for more accurate and faster methods of analysis. This trend will continue, and more testing will be required with increased use of coal in liquefaction and gasification plants.

1.2 ACCURACY AND PRECISION

In any form of analysis, accuracy and precision are required; otherwise, the analytical data are suspect and cannot be used with any degree of certainty. This is especially true of analytical data used for commercial operations where the material is sold on the basis of *purity*. Being a complex material, one may wonder about the purity of coal, but in this sense the term *purity* refers to the occurrence (or lack thereof) of foreign constituents within the organic coal matrix. Such foreign constituents (impurities) are water, pyrite, and mineral matter. Therefore, at this point, it is advisable to note the differences inherent in the terms *accuracy* and *precision*.

The word *accuracy* is used to indicate the reliability of a measurement or an observation, but it is, more specifically, a measure of the closeness of agreement between an experimental result and the true value. Thus, the accuracy of a test method is the degree of agreement of individual test results with an accepted reference value.

On the other hand, *precision* is a measure of the degree to which replicate data and/or measurements conform to each other, the degree of agreement among individual test results obtained under prescribed similar conditions. Hence, it is possible that data can be very precise without necessarily being correct or accurate. These terms will be found throughout any book devoted to a description of standard methods of analysis and/or testing, and have sometimes been used (incorrectly) interchangeably. Precision is commonly expressed inversely by the imprecision of results in terms of their standard deviation or their variance. Precision, by definition, does not include systematic error or bias.

Accuracy is often expressed inversely in terms of the standard deviation or variance and includes any systematic error or bias. Accuracy includes both the random error of precision and any systematic error. The effect of systematic error on the standard deviation is to inflate it. In the measurement of coal quality for commercial purposes, accuracy expressed in this manner is generally of less interest than is systematic error itself. When systematic error is reduced to a magnitude that is not of practical importance, accuracy and precision can become meaningful parameters for defining truly representative sampling and for interpretation of the results of various test methods.

Estimation of the limits of accuracy (deviation from a true or theoretical value) is not ordinarily attempted in coal analysis. Precision, on the other hand, is determined by means of cooperative test programs. Both *repeatability*, the precision with which a test can be repeated in the same laboratory, usually but not always by the same analyst using the same equipment and following the prescribed method(s), and *reproducibility*, the precision expected of results from different laboratories, are determined. Values quoted in test methods are the differences between two results that should be exceeded in only 5 out of 100 pairs of results, equal to $2\sqrt{2}$ times the standard deviation of a large population of results.

The specification of repeatability and reproducibility intervals, without specification of a statistical confidence level, weakens the precision and accuracy

specifications to the extent that this leaves open to question the magnitude of the underlying variance. If, for example, the repeatability interval is never to be exceeded, the variance would have to be zero. From a practical standpoint, this is difficult, if not impossible. Furthermore, the variances (standard deviations) are of direct importance with regard to the details of performing sampling and testing operations because the overall variances can be partitioned into components associated with identifiable sources of variation. This permits assessment of the relative importance of specific details with regard to precision and accuracy. With regard to reproducibility, for example, there is a component of random variance that affects the degree of agreement between laboratories but does not affect the degree of agreement within laboratories (repeatability). Virtually nothing is known about this component of variance except that it exists, and the standard methods do not address this factor directly. However, recognition of it is evidenced in the standard methods by specification of reproducibility intervals that are universally larger than would be accounted for by the variances associated exclusively with the repeatability intervals specified.

In the overall accuracy of results, the sampling variance is but one component, but it is the largest single component. This is a matter of major importance that is frequently missed by the uninitiated. There are test methods (ASTM D-2234; ISO 1988) that describe not only the procedure for the collection of a gross sample of coal but also the method for estimating the overall variance for increments of one fixed weight of a given coal. The precision is such that if gross samples are taken repeatedly from a lot or consignment and one ash determination is made on the analysis sample from each gross sample, 95 out of 100 of these determinations will fall within $\pm 10\%$ of the average of all the determinations. However, under some conditions, this precision may not be obtained, and in terms of performance, the statement should be held in the correct perspective.

At present, when multiseam blended coal samples ranging from 10% by weight mineral matter to as much as 30% by weight mineral matter occur, such precision could result in a corresponding difference as large as 4 to 5% with corresponding differences in the amount of ash that remains after combustion. The response to such concerns is the design of a sampling program that will take into consideration the potential for differences in the analytical data. Such a program should involve acquiring samples from several planned and designated points within (in this case) the coal pile so that allowance is made for changes in the character of the coal as well as for the segregation of the mineral matter during and up to that point in coal's history. That is, the sampling characteristics of the coal play an extremely important role in the application of test methods to produce data for sales.

For coal that is sampled in accordance with standard methods (ASTM D-2234; ASTM D-4596; ASTM D-4916; ASTM D-6315; ASTM D-6518; ISO 13909) and with the standard preparation of the samples for analysis (ASTM D-346; ASTM D-2013), the overall variance of the final analytical data is minimized and falls within the limits of anticipated experimental difference.

1.3 BIAS

The purpose of introducing the term *bias* into coal analysis is to ensure the correctness of the analytical data. Understanding the terms *precision* and *bias* as used in quantitative test methods (ASTM D-3670; ASTM D-6300; ASTM D-6708; ASTM E-177) is a necessary part of ensuring the accuracy of the data produced by analytical test methods.

The issue of testing for bias in a coal sampling system (ASTM D-6518; ISO 13 909) is an essential part of coal analysis and is of significant importance (Gould and Visman, 1981). Accordingly, the term *bias* represents the occurrence of a systematic error (or errors) that is (are) of practical importance.

The measurement of systematic error is carried out by taking the differences of replicate results. From a statistical standpoint, to detect a systematic error, it is necessary to reduce the precision limits of the mean to a value less than some multiple of the standard deviation of the differences. To be classified as bias, systematic error must be of a magnitude that is of practical importance. Without proper experimental design, the systematic error may be of a magnitude that is of practical importance because of the various errors. These errors (errors of omission) render the data confusing or misleading and indicate the unreliability of the test method(s).

However, rather than attempt to remove all bias, the aim is to reduce the bias to acceptable levels that do not, in each case, exceed a designated magnitude. Then the test for bias can be designed to confirm the presence of bias when the probability of a bias of that magnitude exists. Indeed, the nature of the problem is such that the absence of bias cannot be proven.

The issues of *relative bias* or *absolute bias* also need consideration. Relative bias is likely to involve comparisons of gross sample results, whereas absolute bias is based on comparison with bias-free reference values and usually involves increment-by-increment comparisons.

The test for bias includes the following essential steps:

1. Pretest inspection
2. Choice of test method specifications
3. Establishment of detailed procedures for conduct of the test method
4. Preliminary test method increment (sample) collection, processing, and analysis
5. Determination of the number of observations required
6. Final increment (sample) collection, processing, and analysis
7. Statistical analysis and interpretation of data

Each variable coal constituent or property to be examined requires assignment of a test method for that variable. As a practical matter, each constituent or property is determined by a test method that can often be viewed on a stand-alone

basis. Furthermore, exclusive of moisture, all constituents should be evaluated on a dry basis using a standard size of the coal. Most constituents of coal are affected by errors in size distribution that are associated with size selectivity. Screen tests to obtain size distribution information, particularly in the tails of the size distribution (ISO, 1953), can sometimes prove helpful, but size is not always suitable as a test variable.

Once the data are available, certification of sampling systems as unbiased, without qualification, is insufficient, and certification should also be accompanied by a statement of (1) the mean levels of each variable constituent that prevailed during conduct of the test, (2) the nominal sizing of the coal, and (3) some indication of the preparation (washing) to which the coal has been subjected, since these influence the sampling constants and may affect the magnitude of bias observed.

1.4 REPORTING COAL ANALYSIS

Analyses may be reported on different bases (ASTM D-3180; ISO 1170) with regard to moisture and ash content. Indeed, results that are *as-determined* refer to the moisture condition of the sample during analyses in the laboratory. A frequent practice is to air-dry the sample, thereby bringing the moisture content to approximate equilibrium with the laboratory atmosphere in order to minimize gain or loss during sampling operations (ASTM D-2013; ISO 1988). Loss of weight during air drying is determined to enable calculation on an *as-received basis* (the moisture condition when the sample arrived in the laboratory). This is, of course, equivalent to the *as-sampled basis* if no gain or loss of moisture occurs during transportation to the laboratory from the sampling site. Attempts to retain the moisture at the as-sampled level include shipping in sealed containers with sealed plastic liners or in sealed plastic bags.

Analyses reported on a *dry basis* are calculated on the basis that there is no moisture associated with the sample. The moisture value (ASTM D-3173; ISO 331; ISO 589; ISO 1015; ISO 1018; ISO 11722) is used for converting as determined data to the dry basis. Analytical data that are reported on a *dry, ash-free basis* are calculated on the assumption that there is no moisture or mineral matter associated with the sample. The values obtained for moisture determination (ASTM D-3173; ISO 589) and ash determination (ASTM D-3174) are used for the conversion. Finally, data calculated on an *equilibrium moisture basis* are calculated to the moisture level determined (ASTM D-1412) as the equilibrium (capacity) moisture.

Hydrogen and oxygen reported on the moist basis may or may not contain the hydrogen and oxygen of the associated moisture, and the analytical report should stipulate which is the case because of the variation in conversion factors (Table 1.3). These factors apply to calorific values as well as to proximate analysis (Table 1.4) and to ultimate analysis (Table 1.5).

TABLE 1.3 Conversion Factors of Components Other Than Hydrogen and Oxygen^a

Given	As-Determined (ad)	As-Received (ar)	Dry (d)	Dry Ash-Free (daf)
As-determined (ad)	—	$\frac{100 - M_{ar}}{100 - M_{ad}}$	$\frac{100}{100 - M_{ar}}$	$\frac{100}{100 - M_{ad} - A_{ad}}$
As-received (ar)	$\frac{100 - M_{ad}}{100 - M_{ar}}$	—	$\frac{100}{100 - M_{ar}}$	$\frac{100}{100 - M_{ar} - A_{ar}}$
Dry (d)	$\frac{100 - M_{ad}}{100}$	$\frac{100 - M_{ar}}{100}$	—	$\frac{100}{100 - A_d}$
Dry, ash-free (daf)	$\frac{100 - M_{ad} - A_{ad}}{100}$	$\frac{100 - M_{ar} - A_{ar}}{100}$	$\frac{100 - A_d}{100}$	—

Source: ASTM D-3180.

^aM, percent moisture by weight; A, percent ash by weight. For example, given ad, to find ar, use the formula

$$ar = ad \times \frac{100 - M_{ar}}{100 - M_{ad}}$$

TABLE 1.4 Data Derived from Proximate Analysis

	Moisture	Ash	Volatile	Fixed Carbon
Air-dried	8.23	4.46	40.05	47.26
Dry	—	4.86	43.64	51.50
As-received ^a	23.24	3.73	33.50	39.53

^aAir-dry loss in accordance with ASTM D-2013 = 16.36%.

TABLE 1.5 Data Derived from Ultimate Analysis

Basis	Component (% w/w)						Moisture	Total (%)
	Carbon	Hydrogen	Nitrogen	Sulfur	Ash	Oxygen ^a		
As-determined ^{b,c}	60.08	5.44	0.88	0.73	7.86	25.01	9.00	100.0
Dry	66.02	4.87	0.97	0.80	8.64	18.70	0.00	100.0
As-received ^d	46.86	6.70	0.69	0.57	6.13	39.05	(29.02)	100.0
As-received ^e	46.86	3.46	0.69	0.57	6.13	13.27	29.02	100.0

^aBy difference.

^bAfter air-dry loss (22.00%) in accordance with ASTM D-2013.

^cHydrogen and oxygen include hydrogen and oxygen in sample moisture, M_{ad} .

^dHydrogen and oxygen include hydrogen and oxygen in sample moisture, M_{ar} .

^eHydrogen and oxygen do not include hydrogen and oxygen in sample moisture, M_{ar} .

When hydrogen and oxygen percentages do contain hydrogen and oxygen of the moisture, values on the dry basis may be calculated according to the formulas

$$H_d = (H^1 - 0.1111M^1) \times \frac{100}{100 - M^1} \quad (1.1)$$

$$O_d = (O^1 - 0.8881M^1) \times \frac{100}{100 - M^1} \quad (1.2)$$

where H_d and O_d are the weight percent of hydrogen and oxygen on the dry basis, and H^1 and O^1 are the given or determined weight percents of hydrogen and oxygen, respectively, for the given or determined weight percent of moisture M^1 . Rearrangement of these equations to solve for H^1 and O^1 yields equations for calculating moisture containing hydrogen and oxygen contents H^1 and O^1 at any desired moisture level M^1 .

The mineral matter (Ode, 1963) in coal loses weight during thermal conversion to ash because of the loss of water from clays, the loss of carbon dioxide from carbonate minerals such as calcite, and the oxidation of pyrite (FeS_2) to ferric oxide (Fe_2O_3). In addition, any chlorine in the coal is converted to hydrogen chloride, but the change in weight may not be significant.

Analyses and calorific values are determined on a mineral-matter-free basis by the Parr formulas (ASTM D-388), with corrections for pyrite and other mineral matter. The amount of pyrite is taken to be that equivalent to the total sulfur of the coal, which despite the potential error has been found to correlate well in studies of mineral matter. The remaining mineral matter is taken to be 1.08 times the weight of the corresponding (iron-oxide-free) ash:

$$mm = 1.08A + 0.55S \quad (1.3)$$

where mm , A , and S are the weight percent of mineral matter, ash, and total sulfur, respectively.

Such data are necessary for calculation of parameters in the classification of coal by rank: dry, mineral-matter-free volatile matter (or fixed carbon) as well as moist, mineral-matter-free gross calorific value. For volatile matter and fixed-carbon data, it is also necessary to assume that 50% by weight of the sulfur is volatilized in the volatile matter test and therefore should not be included as part of the organic volatile matter (nor should the loss from clays and carbonate minerals):

$$FC_{dmmf} = \frac{100(FC - 0.15S)}{100 - (M + 1.08A + 0.55S)} \quad (1.4)$$

$$VM_{dmmf} = 100 - FC \quad (1.5)$$

where FC_{dmmf} and VM_{dmmf} are fixed carbon and volatile matter, respectively, on a dry, mineral-matter-free basis; and FC , M , A , and S are the determined fixed carbon, moisture, ash, and total sulfur, respectively.

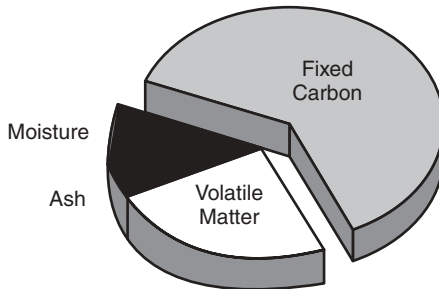
In the Parr formula for moist, mineral-matter-free calorific value, the moisture basis used is that of the inherent moisture of the coal in the seam (natural bed moisture, capacity moisture):

$$\text{moist, mineral-matter-free Btu} = \frac{100(\text{Btu} - 50\text{S})}{100 - (1.08\text{A} + 0.55\text{S})} \quad (1.6)$$

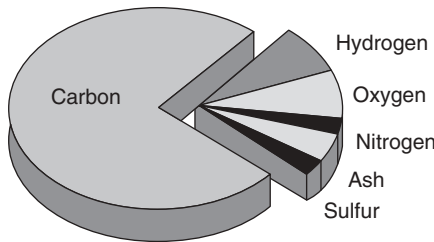
where Btu is the calorific value (Btu/lb), A is the ash (% w/w), and S is sulfur (% w/w); all are on the moist (natural bed) basis.

Coal analyses are generally reported in tabular form (Tables 1.4 and 1.5) and the data can be represented graphically as in these EIA coal data from the U.S. Department of Energy:

1. Proximate analysis (see also Table 1.6):



2. Ultimate analysis:



1.5 INTERRELATIONSHIPS OF THE DATA

Just as a relationship exists between the various properties of petroleum with parameters such as depth of burial of the reservoir (Speight, 1999), similar relationships exist for the properties of coal (e.g., Solomon, 1981; Speight, 1994). Variations in hydrogen content with carbon content or oxygen content with carbon content and with each other have also been noted. However, it should be noted that many of the published reports cite the variation of analytical data or test results not with rank in the true sense of the word but with elemental carbon content that can only be approximately equated to rank.