

The U.S. Geological Survey Coal Quality (COALQUAL) Database Version 3.0

Data Series 975

**U.S. Department of the Interior
U.S. Geological Survey**

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By Curtis A. Palmer, Charles L. Oman, Andy J. Park, and James A. Luppens

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The U.S. Geological Survey Coal Quality (COALQUAL) Database Version 3.0

By Curtis A. Palmer¹, Charles L. Oman¹, Andy J. Park¹, and James A. Luppens²

Abstract

Coal has often been described as one of the most difficult materials to sample because of its inherent heterogeneity. Therefore, fundamental to any coal assessment is an understanding of the impacts of the geological heterogeneity on coal quality variability for a given area.

Since the mid-1970s, the U.S. Geological Survey (USGS) has maintained a coal quality database of national scope named USCHEM, which currently contains data for over 13,000 samples. A subset of the USCHEM database called COALQUAL Version 1.3 was initially published in 1994. Version 3.0 of the COALQUAL database represents a major editing effort to resolve some of the DOS software limitations used by earlier versions of the database.

Because of database size limits during the development of COALQUAL Version 1.3, many analyses of individual bench samples were merged into whole coal bed averages. The methodology for making these composite intervals was not consistent. Size limits also restricted the amount of georeferencing information and forced removal of qualifier notations such as “less than detection limit” (<) information, which can cause problems in using the data. A review of the original data sheets revealed that COALQUAL Version 2.0 was missing information, which was needed for a complete understanding of a coal section. Another important database issue to resolve was the USGS “remnant moisture” problem. Prior to 1998, tests for remnant moisture (as-determined moisture in the sample at the time of analysis) were not performed on any USGS major, minor, or trace-element coal analyses. Without the remnant moisture, it is impossible to convert the analyses to a usable basis (as-received, dry, etc.). Based on remnant moisture analyses of hundreds of samples of different ranks and known residual moisture reported (moisture reported at the time of the ultimate and proximate analysis) after 1998, it was possible to develop a method to provide reasonable estimates of remnant moisture for older data to make it more useful in COALQUAL Version 3.0. In addition, the COALQUAL Version 3.0 database is improved by (1) adding qualifiers, including statistical programming to deal with the qualifiers; (2) clarifying the sample compositing problems; and (3) adding associated samples (discussed in more detail in report). Version 3.0 of COALQUAL also represents the first attempt to incorporate data verification by mathematically crosschecking certain analytical parameters. Finally, a new database system was designed and implemented to replace the outdated DOS program used in earlier versions of the database. The COALQUAL Version 3.0 database is located at <http://ncrdspublic.er.usgs.gov/coalqual/>.

Introduction

Coal has often been described as one of the most difficult materials to sample because of its inherent heterogeneity (Luppens and others, 1992). Fundamental to any coal assessment is an understanding of the impacts of the geological heterogeneity on coal quality variability for a given area. Consequently, a coal bed may often be subsampled in several intervals (benches) rather than a single sample of the entire bed to document vertical quality variations at a sampling location.

Since the mid-1970s, the U.S. Geological Survey (USGS) has maintained a coal quality database of national scope named USCHEM, which currently contains data for over 13,000 samples. A subset of the USGS coal quality database USCHEM called COALQUAL Version 1.3 was first released in 1994 (Bragg and others, 1994). COALQUAL Version 2.0 (Bragg and others, 1997) was released in 1997 without changes to the data, to accommodate the Microsoft XP operating system. The first two releases of COALQUAL provided public data from almost 7,500 coal and coal-related samples or composites analyzed from the early 1970s until 1990.

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The USCHEM database was not published in its original format for several reasons, including the following:

- USCHEM data were stored on an as-determined basis.
- Some elements and (or) oxides were analyzed on a whole-coal basis, while others were analyzed on the coal ash and maintained in multiple basis types as originally reported. If all data were not converted to the same basis, the data could be misinterpreted or misused by those unfamiliar with coal chemical analyses. In COALQUAL Version 3.0, all elemental data for samples are converted to a dry, whole-coal basis.
- The most important analyses reported in COALQUAL Version 3.0 are from samples that represent the entire coal bed at the point of sampling. Many of the coal samples were originally collected and analyzed as a series of individual benches, particularly for the thick coal beds from the western United States. The whole- or full-bed value for each parameter was determined from the weighted mathematical composite of the bench analyses based on sample interval thicknesses. For example, for a 9-foot (ft) sample with two benches, one 3-feet thick and one 6-feet thick, with concentrations of iron (Fe) of 1.0 milligram per kilogram (mg/Kg) and 1.5 mg/Kg respectively, the concentration of Fe for the full-bed is 1.33 as follows:

$$(3\text{ft} / 9\text{ft} \times 1.0 \text{ mg / Kg}) + (6\text{ft} / 9\text{ft} \times 1.5 \text{ mg / Kg}) = 1.33 \text{ mg / Kg}$$

- In a few cases, samples were physically composited by combining properly prepared samples of each bench in the weight ratio of their thicknesses. While this method is only approximate, as differences in the densities of the benches would lead to small differences between mathematical and physical composites, we found that for samples where both types of composites were available the data were similar and we treated them as duplicates. The original USCHEM database also lacked mathematical composite data, as well as data on coal weathering and identification of duplicates. Those conditions made it difficult, and in some cases, impossible to determine chemical data for non-weathered full-bed samples, which may have originated from multiple samples and (or) samples that may have experienced various degrees of weathering. It should be emphasized that only non-weathered, full-bed (Upper Level) coal samples should be used for most coal resource studies. A total of 7,657 Upper Level samples are included in COALQUAL Version 3.0.

In addition to non-weathered, full-bed coal samples (Upper Level samples), USCHEM contained data for individual coal benches, which were combined to form Upper Level samples and data for partings, roof, floor, and miscellaneous coal and coal-related samples. These miscellaneous samples included coal byproducts, fly ash, bottom ash, chemically treated coal samples, rock samples related to the coal stratigraphy, tonsteins, or non-representative samples from partial-bed or coal mining efforts. Appendix 1 provides a complete list these miscellaneous samples.

Prior to 1998, as-determined moisture analyses (moisture in the sample at the time of analysis or remnant moisture) were not performed routinely on USGS coal samples analyzed for major, minor, or trace elements. Originally, it was felt that differences in moisture content of the dried samples were less significant than errors in trace element determinations. Therefore, all analytical values were reported on a remnant moisture basis. However, because the remnant moisture values of the samples were not measured, conversions to any other analytical basis (as-received, dry, or dry ash-free) were impossible. This is a significant limitation to the use of the data in previous versions of COALQUAL as many users often needed analytical results reported on either an as-received or a dry basis. Additionally, qualifying (censored) data such as (1) values below the detection limit, (2) upper limits caused by non-linear standards, (3) values not determined because of spectral interferences, and (4) values not determined for other reasons, were stored in the USCHEM database. If a parameter was not analyzed, a “zero” with a “B” qualifier notation was used.

When the original COALQUAL Version 1.3 database was being compiled, potential users were faced with limited computer memory, storage capacity, and media availability, as well as minimal broadband capacity. In 1994, the USCHEM database including appropriate metadata could not fit on a single CD-ROM disk. These limitations required a number of data storage compromises while compiling the COALQUAL Version 1.3 data, when database functionality relied on the DOS-based operating system. The COALQUAL Version 2.0 database revision utilized the Microsoft Windows XP operating system, but the database remained unchanged. COALQUAL Version 3.0 has been updated to include all supportive metadata, as well as revised data values as warranted during the extensive editing process.

In earlier versions of COALQUAL, analyses of individual bench samples were merged into full-bed averages for each location, even though the composited bench samples did not represent the entire bed or the mined coal in some cases. Additionally, size limitations in the Microsoft Excel spreadsheets (mainly the number of columns available in earlier COALQUAL versions) restricted the amount of georeferencing information and forced removal of qualifier notations such as “less than detection limit” (<) information. Furthermore, most partings were excluded as were bench-sample data, which prevented compilation into a full-bed sample. Although impure coal is defined as having dry ash content between 25 to 50 percent by American Society for Testing and Materials International (ASTM) Standard D121–09 (ASTM, 2014), all coal samples in USCHEM whose USGS and ASTM ash

values on an as-received basis were greater than 33 percent, were not included in COALQUAL Version 1.3 and Version 2.0 (Wood and others, 1983). These samples are incorporated into the COALQUAL Version 3.0 database.

Purpose of COALQUAL Version 3.0 Database Revision

An extensive revision of the COALQUAL database was initiated to take advantage of advances in computer technology and software design since the original versions of COALQUAL were developed. This growth in technology resolved the original compromises due to limited memory and storage capacity and also provided improved database design and an improved web-based delivery platform. The primary objectives for this revision were as follows:

1. Complete a thorough audit of the COALQUAL analytical data versus original hard copy analytical sheets (and other USGS databases) and make appropriate corrections.
2. Resolve the forced removal of data qualifier notations such as “less than detection limit” (L) by referring back to the original hardcopy analytical sheets, and resolve the problems associated with the use of “zeros” for parameters that were not analyzed.
3. Investigate and remedy the problem of missing USGS remnant moisture values.
4. Review the methodology and the consistency for compositing bench samples and add associated samples such as roof, floor, and parting analyses.
5. Revise the COALQUAL georeferencing information based on original hard copy analytical sheets and make necessary corrections and enhancements.
6. Investigate the feasibility of estimating errors associated with combining bench samples into full-bed data and estimating moisture values.
7. Investigate the viability of developing data validation tools.
8. Develop an improved web-based interface for database access.

Editing Results

The comprehensive editing effort of the COALQUAL Version 3.0 database resulted in a significant improvement, not only in the accuracy of the data, but also resulted in an improved user interface for COALQUAL Version 3.0. Additionally, several significant limitations for use of the data were also addressed.

Review of Original Data

In order to ensure that COALQUAL Version 3.0 was accurate and complete, the review started with the original data from USCHEM. The analytical data in USCHEM were extensively checked before previous versions of COALQUAL were released. For this new version, all of the stratigraphic, geologic, and geospatial data were checked with original paper copies of the analytical reports and sample description sheets. Additional columns of data were added to include all pertinent data available for each sample.

Table A2–1 of appendix 2 provides a list and brief description of all data parameters. Those parameters added to COALQUAL Version 3.0 are highlighted with asterisks and bold lettering in table A2–1. The new parameters include (1) estimated remnant moisture; (2) USGS ash on a dry basis; (3) several columns related to major coal-forming elements; (4) data verification classifications for ultimate and proximate analysis; (5) carbonate carbon, organic carbon, and total carbon; and (6) columns related to rank of coal (ASTM apparent rank, British thermal units per pound (Btu/lb), volatile matter, and fixed carbon; all on a moist, mineral-matter-free basis). Additional columns document stratigraphic relationships between samples and major ash-related elements that were originally reported only as oxides (are now also reported as elements).

Data Qualifier Restoration

Qualifier characters for censored data are defined in appendix 3. In older versions of COALQUAL, no qualifiers were reported. Data values below the detection limit were presented as 0.7 times the reported detection limit if the “L” (less than) data qualifier was used, or as “0” if the “N” (not detected) or “B” (no data) qualifier was used (appendix 3). When a “G” (greater than) qualifier was present, it was ignored and the data value was retained. The total number of qualified data values was reported as a percent of the total number of samples in the technical information metadata for COALQUAL Versions 1.3 and 2.0, but it was not possible to determine what individual values were qualified. In COALQUAL Version 3.0, qualifiers from USCHEM were retained and new qualifiers were added based on hardcopies of lab results and USGS and State Geological Survey publications.

The use of “zeros” was also problematic in older versions of COALQUAL. If a parameter was not analyzed, a “0” with a “B” qualifier was used. Unfortunately, some parameters like the free-swelling index, loss on ignition (LOI), and residual moisture have valid zero values making it impossible to distinguish between real zero values and “not analyzed” values or those with “N” qualifiers. The problems associated with the use of zeros were resolved by creating the more extensive list of data qualifiers in appendix 3.

Lack of Remnant Moisture Data Issue

The initial steps in the analysis of a coal sample is pulverizing the as-received samples to minus 8 mesh and air-drying the samples per ASTM D3302 (ASTM, 2014). The purpose of the air-drying is to allow the samples to reach equilibrium with laboratory ambient temperature and humidity. This equilibrium condition minimizes sample weight gains or losses during the subsequent handling, weighing, and analyses of the coal. The moisture content of the air-dried samples prepared for ultimate and proximate analysis is termed “residual moisture.” The moisture content in analytical samples can change when the samples are exposed to an atmosphere in which the relative humidity differs from that prevailing during sample preparation. Consequently, it is advisable to measure moisture at the same time an analytical property is determined (ASTM, 2014; see ASTM D3302). Without a moisture value, the calculation of a coal analysis from an as-determined to different bases (as-received, dry, and so forth) cannot be accurately accomplished (ASTM, 2014; see ASTM D3180).

Unfortunately, although residual moistures were determined at the time of ultimate and proximate analysis, remnant moisture was not determined for all samples in the USCHEM database at the time of the major, minor, and trace element analyses. COALQUAL Version 3.0 addresses missing values for the remnant moisture content. Ultimate and proximate analyses generally included residual moisture values. The residual moisture values were usually determined in contract laboratories generally 6 to 20 months before elemental data were generated at the USGS laboratories located near Washington, D.C. (in Reston, Va.) or near Denver, Colorado (in Lakewood). The altitude and humidity of most contract lab locations is similar to Washington, D.C., but is significantly different than that in Denver, Colorado. The altitude and the drier climate in Denver promoted the possibility of further sample drying even if sealed in polyethylene containers. Samples that were not tightly sealed may have experienced accelerated drying. Higher-rank coal samples inherently have much lower residual moisture contents, and therefore are typically less susceptible to significant moisture loss during storage. Thus, the rates of moisture loss and (or) gain is different in Denver versus Washington D.C., especially for low-rank, high-moisture coals.

After 1998, remnant moisture was determined at the time of analysis on a large number of samples with various ranks and compared to the respective residual moisture contents determined on air-dried samples at the time of proximate and ultimate coal analyses. From these comparisons, a methodology was developed to derive estimates for the remnant moisture content in the USGS laboratory samples using moisture data from samples with known residual moisture and (or) air dried-loss values and coal rank.

Major and trace element data on a dry, whole-coal basis are estimated using procedures that are described in appendix 4. Samples with estimated remnant moisture are qualified with the letter “r” (appendix 3). Procedures for estimating the remnant moisture content (for samples without air-dried loss, or residual moisture information that are based on the apparent rank only) are also described in appendix 4 and qualified with the letter “e” (appendix 3). The estimates for moisture for samples qualified with the letter “e” assume all samples of a given rank have the same moisture value, and therefore are not generally as accurate as those samples qualified with an “r” (appendix 3). Estimated moisture contents, as well as the as-determined data values, are listed in the COALQUAL Version 3.0 database. Appendix 4 describes the method developed, which was designed to minimize the errors resulting from using these estimated moisture values to calculate elemental concentrations to a dry basis.

Compositing Review

Coal data for a given location are typically most useful if the sample(s) are reported on a whole- or full-bed basis. Partial-bed samples provide some information, but are not representative of the full-bed at the point of sampling. Therefore, every attempt

to provide as much data in COALQUAL Version 3.0 on a full-bed basis (Upper Level samples) was made. Often, coal beds are sampled in two or more benches or layers to better characterize vertical variations in coal quality. The individual benches are then composited, either mathematically or physically, to provide weighted average values for coal quality parameters on a full-bed basis. COALQUAL Version 3.0 has correctly composited data to completely represent a coal bed (referred to as a “full” coal bed) like previous versions, which includes full-channel samples, core samples, and composited samples.

Most of the data for full coal beds are identical to the data in COALQUAL Version 1.3 and Version 2.0, but calculated to a dry basis for elemental data. All elements reported on a remnant moisture, whole-coal basis in the previous versions of COALQUAL are reported on a dry, whole-coal basis in COALQUAL Version 3.0. The ultimate and proximate data are on an as-received basis in all versions of COALQUAL. However, in COALQUAL Version 1.3 and Version 2.0, hydrogen (H) and oxygen (O) values included H and O concentrations in residual moisture, which is not consistent with coal industry practices. In some cases, full-beds were constructed the same way for all versions of COALQUAL. Each version provides information on how the full-beds were constructed. A set of rules for Version 3.0 is included in appendix 1, Acceptance Rules for Upper Level Data. A few samples in the original COALQUAL Version 1.3 were not included in this version because they did not meet the standards required, and a few new samples were added. COALQUAL Version 3.0 provides criteria for rejecting samples not included in the set of full-bed samples.

The 15,121 individual samples in this database are divided into several groups based on categories of full-bed samples and sample type. The acceptance rules for compositing bench samples into full-bed samples are provided in appendix 1. Samples in the database are organized on several classifications or levels as follows:

1. Upper Level—Samples represent unweathered, full coal bed intervals at a given location. These full-bed samples are the basis of COALQUAL Version 3.0, which is consistent with previous versions of COALQUAL. The new version of COALQUAL Version 3.0 has 7,657 full-bed samples. These samples are either single full-bed samples, or may be represented by the mathematical average of a full-bed interval sampled in multiple benches. Second Level data for multiple benches (duplicate and (or) composited samples), are composited to represent a single Upper Level sample using guidelines found in appendix 5.
2. Second Level—Individual coal samples that are composited to represent a single Upper Level sample including:
 - a. Bench samples (either drill core or face-channel samples).
 - b. Duplicates (provided as a measure of reliability).
 - c. Physical composites of partial-beds (or full-beds, if used in combination with a. and (or) b. above to determine an Upper Level sample).
3. Third Level—All samples collected at the location of the Upper Level sample.
 - a. Includes other full-bed samples, which may be other Upper Level samples or Second Level samples at a different stratigraphic location, or which may represent partial coal beds or benches.
 - b. Non-coal samples such as roof, floor, and partings, and other miscellaneous samples (see appendix 1).
4. Fourth Level—Samples that are similar to Third Level samples except they are within a limited geographic area of the Upper Level sample, but not at the same location. It should be noted that Upper Level, Second Level, and Third Level samples may be Fourth Level samples at nearby locations. Fourth Level samples are from:
 - a. The same mine.
 - b. Within a mile of the location of Upper Level samples.
5. Fifth Level—Miscellaneous samples not related to full-bed samples.

The first three levels contain samples from a single latitude and longitude location. These samples are (1) full-bed samples, (2) benches that make up full- or partial-bed samples, and (3) non-coal samples such as roof, floor, and partings at different vertical locations. Most samples do not have exact vertical locations (depth from surface), but nearly all samples have known relative vertical locations. For the few samples with unknown relative locations, those samples have been identified by using slightly different longitude or latitude coordinates a few feet from the original location. The relative vertical stratigraphic positions are given by the **Strat** parameter, which is defined in appendix 2 and shown as ***Strat*** in table A2–1. Appendix 6 also provides detailed information about the **Strat** parameter.

Web Interface

In addition to including new data in Version 3.0, a new web interface was created because the additional data and revised format required these changes, and technological advances enabled more efficient presentation of the data. This new interface makes it possible to present full-bed sample data (Upper Level samples) as in previous versions of COALQUAL (Version 1.3 and Version 2.0), as well as all data used to calculate the full-bed data including duplicate samples and benches. The data from USCHEM that were not available in the earlier versions of COALQUAL, such as roof, floor, and parting samples can also be accessed from the Upper Level samples in the database. Georeferencing efforts to identify other samples located within one mile of a sample's location, is computed by the database program using an equation based on the law of spherical cosines (appendix 7). This facilitates comparisons to nearby samples in the database. However, nearby samples may represent one or more different beds so the user needs to confirm stratigraphic equivalency.

The COALQUAL web interface consists of four horizontal tabs (fig. 1), the **Home** tab, the **Browse Coal Data** tab, the **Search and Download Data** tab, and the **Browse Miscellaneous Data** tab.

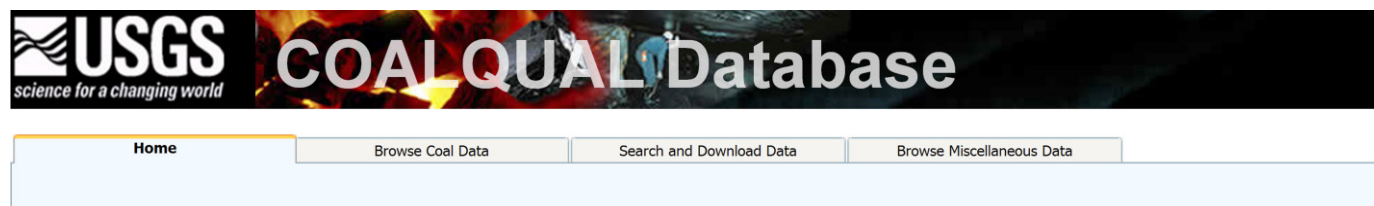


Figure 1. A screen image of the COALQUAL Version 3.0 web interface banner and tabs.

Home Tab

The **Home** tab (fig. 2) contains contact information and a link to generate a report in comma separated values (CSV) format, which shows the total number of samples that currently exist in the COALQUAL database. The index of samples is grouped by State, county, and sample type.

Browse Coal Data Tab

The **Browse Coal Data** tab provides a quick way to search data using the following search criteria related to samples: apparent rank, State, county, and coal province. When a State is selected from the **State** pull down menu, the **County** pull down menu is populated with the county names that belong to the selected State. When the **Show** button is clicked after selecting one or more of the search values, search results will be returned in table format in the left area of the tab as shown below in figure 3.

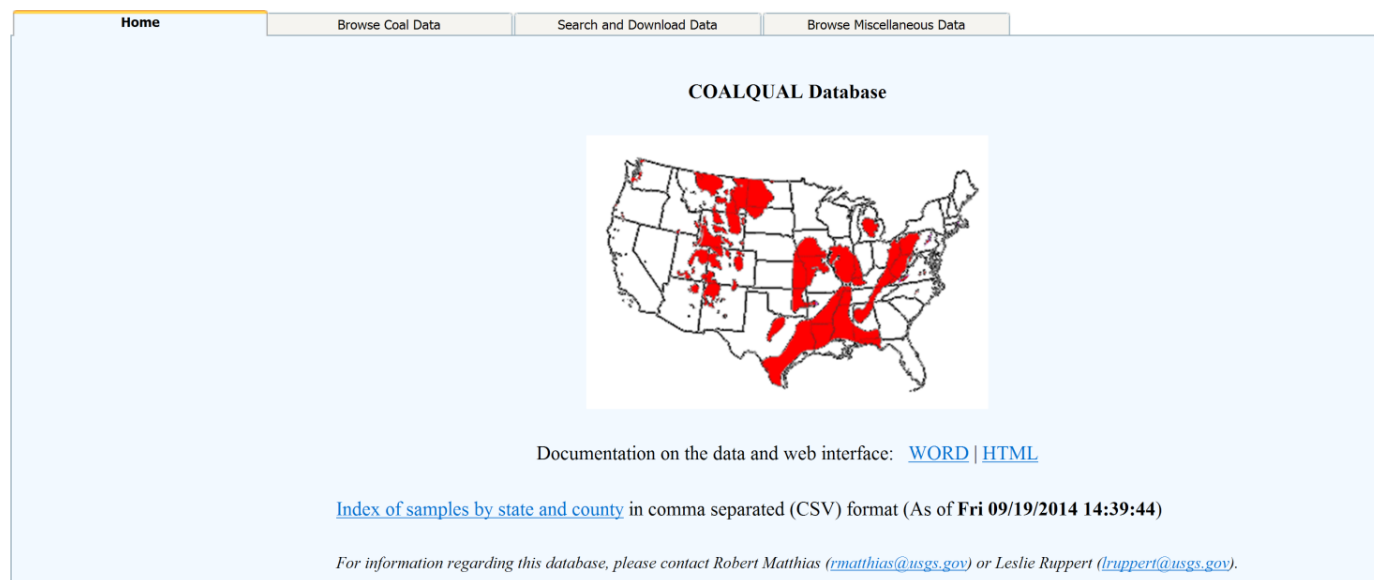


Figure 2. A screen image of the COALQUAL Version 3.0 **Home** tab.

To see additional information on each sample, the user can select a sample record by clicking on a row in the table to see other samples related to the selected sample. Other samples located at the same location (as the selected sample) will be returned in a table on the top right area of the **Browse Coal Data** tab (fig. 3). Note that samples associated directly with the selected sample are highlighted in green. Samples located within one mile radius (or that originated from the same mine or power plant) as the selected sample will be returned in a table in the bottom right area of the tab (fig. 4).

Click on the plus (+) icon in front of each sample record to see subsamples related to the selected sample (fig. 5). For example, subsamples can be bench samples composited together to make up an Upper Level sample (highlighted green in fig. 5). The plus icon appears in front of each sample row only if a sample has related subsamples. When the selected row is expanded, the plus icon is replaced by a minus (-) icon to indicate that the expanded row can be collapsed to hide the related subsamples (highlighted in light blue) as shown in figure 5.

Double click on a sample record in any table within the **Browse Coal Data** tab to see the selected sample's information in detail. A new browser window will open to show the information related to the selected sample (fig. 6).

Search and Download Data Tab

The **Search and Download Data** tab (fig. 7) is equipped with extensive search criteria to provide users the ability to select advanced filtering options giving users the power to find samples that match very specific criteria. Initially, the **Search and Download Data** tab is preset with several default options. The pull down menu for the type of report (fig. 8) is set to **Sample Descriptions** which shows mainly the geologic location of samples. Note that the **Oxides** report shows the analysis values related to major elements.

The **Report Format** pull down menu (fig. 9) is set to the **Display report in browser** option to display search results in table format within a new browser window. The other two options can be used to download results in CSV format. The last download option in the menu produces two CSV files (fig. 10) compressed into a single ZIP folder:

- The first CSV file contains only Upper Level samples.
- The other file shows subsamples that make up the Upper Level samples shown in the first file mentioned in the previous step a. The first column called “**Related To**” contains the sample numbers of the Upper Level samples to show the relationship between subsamples and Upper Level samples. Note that combining both the Upper Level sample data and the subsample data requires extreme care to obtain accurate statistical results. Subsample data may represent multiple duplicate samples and partial-bed samples.

Home Browse Coal Data Search and Download Data Browse Miscellaneous Data

Narrow down starting with * Province or State Run!

Province: ALASKA State: Alaska County: BRISTOL BAY BOROUGH Apparent Rank:

* Double-click on individual sample record to see more data

Sample ID	State	County	Province	Apparent Rank	Data Type
D172333	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
D172334	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
D177644	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
D177651	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
DA2172331	Alaska	BRISTOL BAY BOROUGH	ALASKA		Averaged
DA2177645	Alaska	BRISTOL BAY BOROUGH	ALASKA		Averaged

Sample ID Depth (in) Thickness (in) Bed Data Type

DC2177645	0	52.8	UNNAMED	ASTM Composite
D177645	0	20.4	UNNAMED	Bench with composi
D177646	20.4	32.4	UNNAMED	Bench with composi

DA2177647 Alaska BRISTOL BAY BOROUGH ALASKA Averaged

Sample ID Depth (in) Thickness (in) Bed Data Type

DC2177647	0	74.4	UNNAMED	ASTM Composite
D177647	0	55.2	UNNAMED	Bench with composi
D177649	64.8	19.2	UNNAMED	Bench with composi

Records from 1 to 7 of 7

Related Data for DA2177645

Samples At The Same Location (Highlighted samples related to the selected sample)

Sample ID	Depth (in)	Thickness (in)	Bed	Sample Type
D177644	0	56.4	UNNAMED	Channel 1
DA2177645	0	52.8	UNNAMED	Channel 2
DC2177645	0	52.8	UNNAMED	Channel 2
D177645	0	20.4	UNNAMED	Channel 2
D177646	20.4	32.4	UNNAMED	Channel 2

Records from 1 to 5 of 5

Samples Within One Mile (Same Mine or Power Plant)

Sample ID	State	County	Latitude	Longitude
D177644	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
D177645	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
D177646	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
DA2177645	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
DC2177645	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008

Records from 1 to 5 of 5

Figure 3. An example of the COALQUAL Version 3.0 **Browse Coal Data** tab and search screen.

Samples At The Same Location *(Hilighted samples related to the selected sample)*

Sample ID	Depth (in)	Thickness (in)	Bed	Sample Type
D177644	0	56.4	UNNAMED	Channel 1
DA2177645	0	52.8	UNNAMED	Channel 2
DC2177645	0	52.8	UNNAMED	Channel 2
D177645	0	20.4	UNNAMED	Channel 2
D177646	20.4	32.4	UNNAMED	Channel 2

1

Records from 1 to 5 of 5

Samples Within One Mile (Same Mine or Power Plant)

Sample ID	State	County	Latitude	Longitude
D177644	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
D177645	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
D177646	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
DA2177645	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008
DC2177645	Alaska	BRISTOL BAY BOROUGH	56.2658	-158.7008

1


Records from 1 to 5 of 5

Figure 4. An example of coal samples that are from either the same location, or located at the same mine or power plant (within one mile distance).

* Double-click on individual sample record to see more data

	Sample ID	State	County	Province	Apparent Rank	Data Type
	D172333	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
	D172334	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
	D177644	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
	D177651	Alaska	BRISTOL BAY BOROUGH	ALASKA		Single
+	DA2172331	Alaska	BRISTOL BAY BOROUGH	ALASKA		Averaged
-	DA2177645	Alaska	BRISTOL BAY BOROUGH	ALASKA		Averaged
	Sample ID	Depth (in)	Thickness (in)	Bed	Data Type	
	DC2177645	0	52.8	UNNAMED	ASTM Composite	
	D177645	0	20.4	UNNAMED	Bench with composi	
	D177646	20.4	32.4	UNNAMED	Bench with composi	
-	DA2177647	Alaska	BRISTOL BAY BOROUGH	ALASKA		Averaged
	Sample ID	Depth (in)	Thickness (in)	Bed	Data Type	
	DC2177647	0	74.4	UNNAMED	ASTM Composite	
	D177647	0	55.2	UNNAMED	Bench with composi	
	D177649	64.8	19.2	UNNAMED	Bench with composi	

Figure 5. An example of the relationship of coal subsamples to an Upper Level sample.



COAL QUAL Database

Sample Detail for W212981

View Definitions of Qualifiers and Parameters

Sample Description		Proximate & Ultimate		Oxide		Trace Element	
Sample ID	W212981	Sample ID	W212981	Sample ID	W212981	Sample ID	W212981
State	Alabama	Moisture		Remnant Moisture	4	GS Ash Dry	25.4
County	TUSCALOOSA	Moisture Q	B	Remnant Moisture Q	e	GS Ash Dry Q	
Latitude	33.5272	Volatile Matter		GSAsh	24.4	Si	44500
Longitude	-87.5100	Volatile Matter Q	B	GSAsh Q		Si Q	
Province	EASTERN	Fixed Carbon		SiO ₂	37.5	Al	33300
Region	SOUTHERN APPALACHIAN	Fixed Carbon Q		SiO ₂ Q	o	Al Q	
Field	WARRIOR	Standard Ash		Al ₂ O ₃	24.8	Ca	11400
District		Standard Ash Q	B	Al ₂ O ₃ Q	o	Ca Q	
Formation	POTTSVILLE	Proximate Validation	Incomplete Data	CaO	6.27	Mg	1190
Group	PRATT	Hydrogen		CaO Q	o	Mg Q	
Bed	AMERICAN	Hydrogen Q	B	MgO	0.78	Na	763
Member		Carbon		MgO Q	o	Na Q	
Coal Zone		Carbon Q	B	MnO	0.023	K	2490
Depth (in)	10621.2	Nitrogen		MnO Q		K Q	
Thickness (in)	10	Nitrogen Q	B	Na ₂ O	0.405	Fe	32800
System	Pennsylvanian	Oxygen		Na ₂ O Q	o	Fe Q	
Series/Epoch	Lower	Oxygen Q	B	K ₂ O	1.18	Ti	1550
Literature		Sulfur		K ₂ O Q	o	Ti Q	
Comments		Sulfur Q	B	Fe ₂ O ₃	18.4	S	1.53
Map	BERRY SE (7.5')	Ultimate Validation	Incomplete Data	Fe ₂ O ₃ Q	o	S Q	s,d
Collector	ALGS-WARD R	Btu		TiO ₂	1.02	Ag	0.104
Mine/Power Plant	NO DATA ENTERED	Btu Q	B	TiO ₂ Q	o	Ag Q	
Drill Core No	266166-KII-40.H	Sulfate Sulfur		P ₂ O ₅		As	111
Point Id	266166-KII-40.H	Sulfate Sulfur Q	B	P ₂ O ₅ Q		As Q	
Submit Date	03/30/1981	Pyritic Sulfur		SO ₃	3.68	Au	2.6
Sample Description	BITUMINOUS COAL	Pyritic Sulfur Q	B	SO ₃ Q	s	Au Q	L
Estimated Rank	BITUMINOUS	Organic Sulfur		LOI		B	55.9
Apparent Rank		Organic Sulfur Q	B			B Q	
Analytical Labs	USBM and USGS	Ash Deformation				Ba	661
Sample Type	Drill Core	Ash Deformation Q	B			Ba Q	
Analysis Type	As Received	Ash Softening				Be	3.05
Values Represent	Single sample	Ash Softening Q	B			Be Q	
Township		Ash Fluid				Bi	2.6
Range		Ash Fluid Q	B			Bi Q	L
Section		Free Swelling				Br	5.42
Quarters		Free Swelling Q	B			Br Q	
Tract		HGI				Cd	0.153
Location Detail		HGI Q				Cd Q	

Figure 6. An example of the COALQUAL Version 3.0 coal Sample Detail page.

Home	Browse Coal Data	Search and Download Data	Browse Miscellaneous Data
------	------------------	---------------------------------	---------------------------

Report: Sample Descriptions ▼
Report Format: Display report in browser ▼
Generate

Search Coal Samples
Search Miscellaneous Samples
Reset Criteria

Qualifier L (less than) and G (greater than) : Exclude values with L and G qualifiers ▼
☐ Search Criteria Defined
 Show Criteria

Figure 7. A screen image of the COALQUAL Version 3.0 Search and Download Data tab.

Sample Descriptions ▼

Sample Descriptions
 Oxides
 Proximate & Ultimate Analysis
 Trace Elements

Figure 8. The pull down menu for report types on the Search and Download Data tab.

Display report in browser ▼

Display report in browser
 Download report in comma separated (CSV) format
 Download report in comma separated (CSV) format with related data

Figure 9. The Report Format pull down menu on the Search and Download Data tab.

	A	B	C	D	E	F
1	Sample ID	State	County	Latitude	Longitude	Province
2	W233974	Alabama	TUSCALOOSA	37.3278	-87.2092	EASTERN
3	W233978	Alabama	TUSCALOOSA	33.2703	-87.3739	EASTERN
4	WA2204687	Alabama	TUSCALOOSA	33.4856	-87.5414	EASTERN
5	WA2211667	Alabama	TUSCALOOSA	33.5717	-87.47	EASTERN
6	WA2213006	Alabama	TUSCALOOSA	33.59	-87.4911	EASTERN
7						

	A	B	C	D	E	F
1	Related To	Sample ID	State	County	Latitude	Longitude
2	WA2204687	W204686	Alabama	TUSCALOOSA	33.4856	-87.541
3	WA2204687	W204687	Alabama	TUSCALOOSA	33.4856	-87.541
4	WA2211667	W211667	Alabama	TUSCALOOSA	33.5717	-87.4
5	WA2211667	W211669	Alabama	TUSCALOOSA	33.5717	-87.4
6	WA2213006	W213006	Alabama	TUSCALOOSA	33.59	-87.491
7	WA2213006	W213007	Alabama	TUSCALOOSA	33.59	-87.491
8						

Figure 10. Examples of two CSV files showing Upper Level samples and related subsamples.

Also note that the **Report Format** menu works in conjunction with the **Report** menu. For example, if the **Proximate & Ultimate Analysis** report is selected, search results will only show attributes associated with the proximate and ultimate analysis.

The search results window displays the search criteria defined by the user (and a table) as shown in figure 11. Radio buttons allow the user to search either coal samples or miscellaneous samples, but not both (fig. 12). By default, the *Search Coal Samples* option is selected to limit the search to coal samples.

The pull down menu (fig. 13) for data qualifiers (L for less than and G for greater than) is set to the **Exclude values with L and G qualifiers** option to filter out samples that have analysis values with L or G qualifiers. This pull down menu is only applicable when the user selects one or more attributes related to analysis values. The other options can be used to limit the search on samples that have analysis that include (1) values with L qualifier, (2) values with G qualifier, or (3) values with L and G qualifiers.

The *Search Criteria Defined* checkbox (fig. 14) will show a check mark when one or more search options are defined by the user. At any time, the current active search criteria can be displayed by clicking **Show Criteria**. When the **Show Criteria** button is clicked after defining a search criteria, a new window will open showing selected criteria for an additional search (fig. 15). Search criteria are divided into four categories (fig. 16), which are closely associated with the four types of reports and represented by the following four tabs: **Sample Description**, **Proximate/Ulimate**, **Oxides**, and **Trace element**.

Sample Description Tab

The **Sample Description** tab (fig. 17) consists of search criteria mainly associated with the geologic location of samples.

Proximate/Ulimate Tab

The **Proximate/Ulimate** tab (fig. 18) allows the user to search samples by defining ranges of values associated with proximate and (or) ultimate analysis.



COAL QUAL Database

Proximate and ultimate analysis, heat of combustion, forms of sulfur, free-swelling index, and ash-fusion temperature determination for selected coal samples.

[All analyses in percent except free-swelling index, ash fusion temperatures, Btu/lb, and Btu related analyses. For each sample number, the analyses are reported as determined. Analyses are by a commercial testing laboratory following ASTM standards.]

Your search criteria were: (Btu between 12000 and 15000)) and (Exclude Btu with L or G qualifiers) and (STDASH between 10 and 15)) and (Exclude STDASH with L or G qualifiers)

View [Definitions of Qualifiers and Parameters](#)

* Double-click on individual Sample record to see more data

Proximate Analysis										Ultimate Analysis						
Sample ID	Moisture	Moisture Q	Volatile Matter	Volatile Matter Q	Fixed Carbon	Fixed Carbon Q	Standard Ash	Standard Ash Q	Proximate Validation	Hydrogen	Hydrogen Q	Carbon	Carbon Q	Nitrogen	Nitrogen Q	Oxygen
WA2190637	2.94 a		29.62 a		56.97		10.47 a		Acceptable	4.61 a		74.4 a		1.5 a		3.13 a
Sample ID	Depth (in)	Thickness (in)	Bed	Data Type												
W190637	0	26.75	EAGLE	Bench												
W190638	26.8	15.5	EAGLE	Bench												
WA2191112	2.78 a		26.99 a		57.42		12.81 a		Acceptable	4.56 a		73.31 a		1.25 a		3.6 a
WA2191122	2.79 a		30.66 a		55.54		11.02 a		Acceptable	4.74 a		73.76 a		1.05 a		4.15 a
WA2191324	2.08 a		32.75 a		52.48		12.7 a		Acceptable	4.59 a		72.58 a		1.27 a		3.83 a
WA2191327	2.52 a		36.14 a		49.57		11.77 a		Acceptable	4.75 a		71.98 a		1.42 a		5.57 a

Figure 11. An example of search results filtered by search criteria.

- *Search Coal Samples*
- *Search Miscellaneous Samples*

Figure 12. A screen image of the radio buttons for options to search coal or miscellaneous samples.

Exclude values with L and G qualifiers

Exclude values with L and G qualifiers
 Values with L qualifier
 Values with G qualifier
 Include values with L and G qualifiers

Figure 13. A screen image of the pull down menu for the L and G data qualifiers.

☒ *Search Criteria Defined*

Show Criteria

Figure 14. A screen image of the check box and button for search criteria.

Proximate/Ulimate

(Btu between 12000 and 15000)
 Exclude Btu with L or G qualifiers
 (STDASH between 10 and 15)
 Exclude STDASH with L or G qualifiers

Figure 15. An example of additional search criteria.

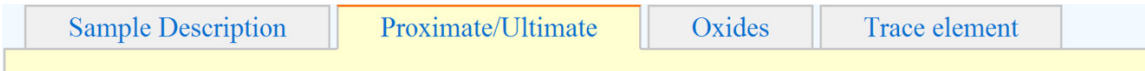


Figure 16. A screen image of the four search categories.

Sample Description

Proximate/Ultimate

Oxides

Trace element

Narrow down starting with:

Province - Region

State

Formation

Bed

Map

Province - Region(s)*:

ALASKA - ALASKA PENINSULA
ALASKA - CENTRAL ALASKA
ALASKA - COOK INLET-SUSITNA
ALASKA - NORTHERN ALASKA

State(s)*:

County(s)*:

Formation(s)*:

Bed(s)*:

Map(s)*:

* How to select multiple options in a list box

Apparent Rank:

Field:

Sample Type:

Collector:

Latitude: from to decimal degrees

Longitude: from to decimal degrees

Figure 17. The search criteria in the **Sample Description** tab.

Sample Description

Proximate/Ultimate

Oxides

Trace element

Category	from	to
Btu (Btu/lb)	12000	15000
Standard Ash (percent)	10	15
-- None selected --		
-- None selected --		
-- None selected --		
-- None selected --		
-- None selected --		
-- None selected --		
-- None selected --		
-- None selected --		

Figure 18. The search criteria in the **Proximate/Ultimate** tab.

Oxides Tab

The **Oxides** tab (fig. 19) allows the user to select samples by adding ranges of values associated with the analysis of oxides.

Trace Elements Tab

The **Trace element** tab (fig. 20) lets the user query the database with ranges of values related to the analysis of major, minor, and trace elements.

Browse Miscellaneous Data Tab

The **Browse Miscellaneous Data** tab is implemented to show non-coal, miscellaneous samples based on four search criteria related to samples, as follows: **State** and **County** (location), **Sample Type**, and **Rejected** (reason for rejection as an unacceptable coal sample). Just like the **State** and **County** pull down menus in the **Browse Coal Data** tab, when a State is selected from the **State** pull down menu, the **County** pull down menu gets populated with the county names that belong to the selected State. After selecting values from the search criteria, clicking on the **Show** button will return miscellaneous samples in a table as displayed in figure 21.

To see additional information on each sample, double click on a sample record. A new internet browser window will open with sample data related to the selected sample (fig. 22).

Sample Description			Proximate/Ulimate			Oxides			Trace element		
Category	from	to		Category	from	to					
-- None selected --			percent	-- None selected --			percent				
-- None selected --			percent	-- None selected --			percent				
-- None selected --			percent	-- None selected --			percent				
-- None selected --			percent	-- None selected --			percent				
-- None selected --			percent	-- None selected --			percent				
Oxide ratio:				Category	Category	from	to				
				-- None selected --	-- None selected --	=					

Figure 19. The search criteria in the **Oxides** tab.

Sample Description			Proximate/Ulimate			Oxides			Trace element		
Category	from	to		Category	from	to					
-- None selected --			PPM	-- None selected --			PPM				
-- None selected --			PPM	-- None selected --			PPM				
-- None selected --			PPM	-- None selected --			PPM				
-- None selected --			PPM	-- None selected --			PPM				
-- None selected --			PPM	-- None selected --			PPM				

Figure 20. The search criteria in the **Trace element** tab. [PPM, parts per million]

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Home		Browse Coal Data		Search and Download Data		Browse Miscellaneous Data	
State:	Wyoming	County:	CAMPBELL	Sample Type:		Rejected:	
* Double-click on individual Sample record to see more data							
Sample ID	State	County	Province	Apparent Rank	Rejected	Sample Type	Values Represent
D160981	Wyoming	CAMPBELL	NORTHERN GREAT		ROCK	Channel	Single sample
D160986	Wyoming	CAMPBELL	NORTHERN GREAT		RUN OF MINE	Run of Mine	Physical or mathematical composite (by thickness)
D160987	Wyoming	CAMPBELL	NORTHERN GREAT		TIPPLE	Tipple	Physical or mathematical composite (by thickness)
D160988	Wyoming	CAMPBELL	NORTHERN GREAT		TIPPLE	Tipple	Physical or mathematical composite (by thickness)
D161800	Wyoming	CAMPBELL	NORTHERN GREAT		ROAD CUT BURNED	Naturally Burned Roa	High ash yield samples
D161801	Wyoming	CAMPBELL	NORTHERN GREAT		ROAD CUT BURNED	Naturally Burned Roa	High ash yield samples
D163196	Wyoming	CAMPBELL	NORTHERN GREAT		NATURALLY BURNED	Naturally Burned	High ash yield samples
D163516	Wyoming	CAMPBELL	NORTHERN GREAT		WEATHERED	Channel	Bench
D163517	Wyoming	CAMPBELL	NORTHERN GREAT		WEATHERED	Channel	Bench
D163518	Wyoming	CAMPBELL	NORTHERN GREAT		WEATHERED	Channel	Bench
D163519	Wyoming	CAMPBELL	NORTHERN GREAT		WEATHERED	Channel	Bench
D163520	Wyoming	CAMPBELL	NORTHERN GREAT		WEATHERED	Channel	Bench
D163521	Wyoming	CAMPBELL	NORTHERN GREAT		WEATHERED	Channel	Bench
D163522	Wyoming	CAMPBELL	NORTHERN GREAT		TIPPLE	Tipple	Physical or mathematical composite (by thickness)
D164323	Wyoming	CAMPBELL	NORTHERN GREAT		DRILL ADDITIVE	Drill Fluid additive	Single sample
D164324	Wyoming	CAMPBELL	NORTHERN GREAT		DRILL ADDITIVE	Drill Fluid additive	Single sample
D164325	Wyoming	CAMPBELL	NORTHERN GREAT		DRILL ADDITIVE	Drill Fluid additive	Single sample
D164326	Wyoming	CAMPBELL	NORTHERN GREAT		DRILL ADDITIVE	Drill Fluid additive	Single sample
D164327	Wyoming	CAMPBELL	NORTHERN GREAT		DRILL ADDITIVE	Drill Fluid additive	Single sample
D164604	Wyoming	CAMPBELL	NORTHERN GREAT		LOW RECOVERY	Drill Core	Core with low recovery (< 70%)
Records from 1 to 20 of 182							

Figure 21. A screen image of the Browse Miscellaneous Data tab.

USGS COALQUAL Database							
Sample Detail for D176537							
View Definitions of Qualifiers and Parameters							
Sample Description		Proximate & Ultimate		Oxide		Trace Element	
Sample ID	D176537	Sample ID	D176537	Sample ID	D176537	Sample ID	D176537
State	Wyoming			Remnant Moisture	0	GS Ash Dry	78.6
County	CAMPBELL	Moisture Q		Remnant Moisture Q	g	GS Ash Dry Q	
Latitude	44.8117	Volatile Matter		GS Ash	78.6	Si	110000
Longitude	-105.5908	Volatile Matter Q		GS Ash Q		Si Q	d
Province	NORTHERN GREAT PLAINS	Fixed Carbon		SiO ₂	30	Al	37000
Region	POWDER RIVER	Fixed Carbon Q		SiO ₂ Q		Al Q	d
Field	LITTLE POWDER RIVER	Standard Ash		Al ₂ O ₃	8.9	Ca	26900
District		Standard Ash Q		Al ₂ O ₃ Q		Ca Q	d
Formation	FORT UNION	Proximate Validation		CaO	4.8	Mg	17000
Group		Hydrogen		CaO Q		Mg Q	d
Bed		Hydrogen Q		MgO	3.58	Na	990
Member	TONGUE RIVER	Carbon		MgO Q		Na Q	d
Coal Zone	TONGUE RIVER	Carbon Q		MnO	0.206	K	7190
Depth (in)	1612.8	Nitrogen		MnO Q		K Q	d
Thickness (in)	8.4	Nitrogen Q		Na ₂ O	0.17	Fe	264000
System	Tertiary	Oxygen		Na ₂ O Q		Fe Q	d
Series/Epoch	Paleocene	Oxygen Q		K ₂ O	1.1	Ti	1740
Literature		Sulfur		K ₂ O Q		Ti Q	d
Comments		Sulfur Q		Fe ₂ O ₃	48	S	0.1
Map	WHITE TAIL BUTTE (7.5')	Ultimate Validation		Fe ₂ O ₃ Q		S Q	L
Collector	USGS-HOBBS R G	Btu		TiO ₂	0.37	Ag	
Mine/Power Plant	NO DATA ENTERED	Btu Q		TiO ₂ Q		Ag Q	
Drill Core No	HOLE NO RM-3	Sulfate Sulfur		P ₂ O ₅		As	8
Point Id	RM-3-RS-6	Sulfate Sulfur Q		P ₂ O ₅ Q		As Q	
Submit Date	07/21/1975	Pyritic Sulfur		SO ₃	0.1	Au	
Sample Description	ROCK	Pyritic Sulfur Q		SO ₃ Q	s.L	Au Q	
Apparent Rank		Organic Sulfur		LOI		B	40
Analytical Labs	U.S. Geological Survey (USGS)	Organic Sulfur Q				B Q	L
Sample Type	Rock Core sample	Ash Deformation				Ba	550

Figure 22. A detailed example of miscellaneous data.

Error Estimation

Several errors associated with using these data were also estimated. Rules associated with error estimation, when combining bench samples to create a Upper Level sample, are given in appendix 5. Errors associated with remnant moisture effect on all elemental data, as well as the determination of whether a sample is a rock or coal, are discussed in appendix 4.

In some cases, only the type of error is identified. For example, qualifiers are used when data are incomplete or approximated using various procedures (appendix 3). This resulted in two levels of qualifiers. Those with a capital letter provided some additional information, but often not enough to allow the parameter to be used for statistical purposes. Small letter qualifiers were used for alternate procedures, which generally had smaller errors associated with them, and did not require censor from statistical procedures. In some instances, these qualifiers identified cases where data were not analyzed in complete compliance with ASTM standards, but errors were determined to be insignificant in determining the final value.

Data Validation

The degree of consistency and reliability of analytical results for any database is always a concern. Version 3.0 of COALQUAL represents the first attempt to develop verified data by crosschecking certain analytical parameters. The verification process is based on the fact that data interrelationships are often axiomatic in coal analyses. As the analytical result for one parameter changes, the results for related parameters also change. The pair of test results may vary inversely or be in direct proportion to each other. Correlations based on these data interrelationships can be used to estimate missing data (Hoeft and others, 1983). Data verification was performed on two suites of analyses, the ultimate and proximate data.

Data Validation Methodology

One of P.L. Dulong's contributions to coal chemistry is the idea that the heat of combustion of coal can be estimated by summing the weighted heats of combustion of their constituent elements (Francis and Lloyd, 1983). While it is widely circulated, P.L. Dulong never formally published his equation. By applying this principle to coal, predictive formulas have been developed to estimate higher heating values (HHV). A good predictive correlation is useful as an additional quality control tool, and it provides an independent measure of consistency.

The data validation in COALQUAL Version 3.0 is based on a proprietary algorithm developed by Quality Associates International Ltd., which is a refinement of the Dulong approach. This algorithm uses carbon, hydrogen, sulfur, and nitrogen values from the ultimate analyses to derive a predicted HHV. For each sample, the predicted HHV value is then compared to the measured HHV. The following relative rating scale was developed to rate the degree of agreement between the predicted and measured HHV results:

- EXCELLENT: HHV results are within 1 percent relative.
- GOOD: HHV results are within 2 percent relative.
- ACCEPTABLE: HHV results are within 3 percent relative.
- INVESTIGATE: HHV results exceed 3 percent relative.

Those samples that exceed 3 percent should be further investigated to determine a potential cause. For the Upper Level coal analyses in COALQUAL Version 3.0, 961 samples had either insufficient data or no HHV data.

The verification of the proximate analyses is based on the data interrelationships between parameters from the proximate and ultimate analyses. The proximate analysis values of residual moisture (moisture in the analytical sample), ash yield, and volatile matter are used to calculate fixed carbon by difference. Subtracting the fixed carbon from carbon from the ultimate analysis yields volatile carbon (dividing this result by 12 yields the number of moles of volatile carbon). Dividing the moles of volatile carbon by the number of moles of hydrogen from the ultimate analysis yields the number of moles of volatile coal, which should be between 0.0 and 0.5 moles. This validation serves to confirm the reliability of the proximate results, as well as the reliability of the carbon and hydrogen from the ultimate analyses. Results that fall in the 0.0 to 0.5 range are designated as ACCEPTABLE. Results that do not fall in the 0.0 to 0.5 range are designated as INVESTIGATE. An "incomplete" data designation indicates that a sample is missing critical test results required to carry out the validation process.

Validation Results

COALQUAL Version 2.0 (Bragg and others, 1997) was submitted to Quality Associates International Ltd. for validation. A validation algorithm was applied to the ultimate analysis values and HHV. Although about 98 percent of all ultimate and HHV results passed at least the ACCEPTABLE quality level (as specified by the validation algorithm) the validation revealed the following problems:

1. The hydrogen and oxygen data recorded in the 1997 version included the hydrogen and oxygen associated with the moisture in the coal. Conventional coal industry practice does not include the hydrogen and oxygen in water when reporting these parameters in coal. The USGS corrected the hydrogen and oxygen numbers to exclude the hydrogen and oxygen from water in COALQUAL Version 3.0.
2. Approximately 3 percent of the samples failed to meet the ACCEPTABLE quality level set by the validation algorithm. The USGS attempted to verify whether any of these failures were a result of data entry errors, and determined that about 600 samples lacked all of the data required to carry out an ultimate and HHV validation. The USGS attempted to determine reasons for missing data.

During the investigation of these two validation problems it became evident that some composites consisted of combinations of bench samples from different lateral locations in the same bed, especially in the western United States, where unusually thick coal beds are encountered. If the results from both bench samples are ACCEPTABLE, then any properly calculated mathematical combination would also be ACCEPTABLE. However, such a combination would not be representative of the bed at a specific vertical sampling location. This revelation required a complete re-evaluation of all samples in the 1997 database to ensure bench samples had been properly composited. This resulted in the removal of a number of composite samples from the database, as well as recombination of properly selected benches to yield new composites. This process resulted in the Version 3.0 database, which contains 7,658 samples.

The edited COALQUAL Version 3.0 database was sent to Quality Associates International Ltd. for validation using the same algorithm (for ultimate and HHV) as used for the 1997 version, as well as the additional algorithm for validation of proximate data. The validation proceeded as a series of verification steps. It was confirmed for all 5,517 samples (that were also in the 1997 database) that the hydrogen and oxygen results did not originate from the water in coal in Version 3.0. Furthermore, the validation confirmed the ultimate and HHV ratings had not changed for these 5,517 coal samples. These two steps suggest there were no errors introduced in the correction of the hydrogen and oxygen data or in the transfer of entire datasets from the 1997 Version 2.0 database. We conclude the same level of scrutiny was employed when entering the 2,141 additional samples into the Version 3.0 database. This is confirmed in part by the validation of ultimate and HHV results of the COALQUAL Version 3.0 database, which resulted in 6,545 of the 6,683 complete datasets of ultimate and HHV results passing an ACCEPTABLE or better rating (97.94 percent of the complete sets passed), an improvement over the 1997 database Version 2.0 where 97.5 percent of the complete datasets passed. The summary of results for algorithm verification of the ultimate and HHV is shown in table 1.

Table 1. Validation summary for the degree of agreement between the predicted higher heating value (HHV) and the ultimate and measured HHV analyses. [Validated samples (6,683) equals the total number of samples (7,644) minus the number of incomplete samples (961), and refers to the number of complete datasets. Percent (%) is of 6,683.]

Ultimate and HHV Validation		
Number of samples	Total	7,644
	Incomplete	961
	Validated	6,683
Rating scale	EXCELLENT	71.55%
	GOOD	21.44%
	ACCEPTABLE	4.95%
	INVESTIGATE	2.05%

There is a difference in the quality rating scales applied to ultimate and HHV validation versus that for proximate value verification. The ultimate and HHV algorithm is based on thermo-chemical calculations derived from heats of combustions of pure substances. As such, it is possible to calculate uncertainties that are not based on an empirical correlation derived from ultimate and HHV results extracted from the data in the USGS coal quality database.

Conversely, the proximate validation algorithm is based on an empirical correlation, albeit developed from the results of several independent coal quality databases (Swartzman, 1953; Swartzman and Tibbetts, 1955; Tibbetts and Montgomery, 1960; Tibbetts and others, 1978; Faurschou and others, 1982; Bonnell and others, 1983; Joint Coal Board and Queensland Coal Board, 1979; and CANSPEX, a proprietary database by Quality Associates International Ltd.). For this reason, the validation rating categories for proximate are set only as either ACCEPTABLE or SUSPECT. The summary for the proximate validation algorithm is shown in table 2. The proximate validation resulted in 6,659 of the 6,692 complete proximate datasets (99.51%) passing with a rating of ACCEPTABLE. In a case where the proximate rating is SUSPECT and the ultimate and HHV rating is not INVESTIGATE, the most likely cause is a questionable volatile matter result. This is because moisture, ash yield, and volatile matter are used in the proximate validation. Moisture and ash yield are also used in the ultimate and HHV validation, but volatile matter is not used.

Two parameter columns labeled as Ultimate Validation and Proximate Validation (*Ultimate Validation* and *Proximate Validation* in table A2–1) were added to COALQUAL Version 3.0 (see appendix 2) to present the results of the validation process for all samples with sufficient data required by the validation algorithms. The validation results provide the user of the data an additional tool that can be used to help decide which data would be most appropriate for a particular use. For example, a sample with an INVESTIGATE rating for the HHV and ultimate validation may not be chosen for inclusion in the determination of apparent rank for a particular area, but the use of the trace element analyses for that same sample may be acceptable.

Table 2. Validation summary for the degree of agreement between the proximate analyses and the carbon and hydrogen values from the ultimate analyses. [Validated samples (6,692) equals the total number of samples (7,644) minus the number of incomplete samples (952), and refers to number of complete datasets. Percent (%) is of 6,692.]

Proximate Validation		
Number of samples	Total	7,644
	Incomplete	952
	Validated	6,692
Rating scale	ACCEPTABLE	99.51%
	SUSPECT	0.49%

Conclusion

COALQUAL Version 3.0 represents the latest revision of the U.S. Geological Survey COALQUAL database. Unlike previous versions more than 95 percent of the data in the USCHEM database are included, while still maintaining the emphasis of full-bed data. All bench data used to calculate the full-bed data are included, as well as complete stratigraphic sections that include roof, floor, and parting samples. Improved georeferencing data makes it possible to easily determine which samples are related to a full-bed sample. The data qualifiers from USCHEM are included, as well as additional qualifiers, to more clearly explain how the data were collected and analyzed. Limitations on data usage are also more fully documented.

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Appendixes 1–7

Appendix 1. Acceptance Rules for Upper Level Data

Appendix 2. Data Parameters

Appendix 3. Data Qualifiers

Appendix 4. Remnant Moisture Estimate Method

Appendix 5. Averaging Components Used to Calculate Upper Level Samples

Appendix 6. Strat Parameter

Appendix 7. Identification of Nearby Samples

Appendix 1. Acceptance Rules for Upper Level Data

1. An Upper Level analysis in COALQUAL Version 3.0 is a sample or multiple samples that represents a full coal bed (full-bed samples) (from bottom to top), or meets the following criteria:
 - a. Channel samples must be composed of 100 percent of the coal bed thickness less any partings of material greater than 50 percent ash on a dry basis.
 - b. Core samples which are incomplete due to poor recovery are assumed to be representative if the percent core loss is less than 30 percent.
 - c. If any single parting is 12 inches or more, the coal bed is separated into two beds. If there are multiple partings 12 inches or more, 3 or more separate coal beds will be defined. Note that full-bed samples are only one criteria that defines Upper Level samples, but all Upper Level samples are full-bed samples.
 - d. Coal must be representative of a full coal bed, and not be oxidized or processed.
2. Samples may be rejected as representative of Upper Level samples for a variety of reasons. Rejected samples are included in miscellaneous data and can be searched by reason for rejection. The reasons for rejected samples include the following:
 - a. Grab samples: These are not considered representative of a full-bed or the mine from which they originated because of the typical high vertical inhomogeneity within a coal bed.
 - b. Tipple samples: These mined samples are collected at the coal processing site and are not representative of a single bed at a single location.
 - c. Run of mine samples: These mine samples are collected at the coal processing site and are not representative of a single bed at a single location (see tipple samples).
 - d. Pit samples: See grab samples.
 - e. Blend pile: These samples are taken from a pile of coal often from a specific bed, part of bed, or group of beds, but not collected in a manner to ensure a representative full-bed sample.
 - f. Stockpile: These samples are generally in a storage pile either at the mine, load-out facility, or power plant. In many cases, the exact origin of the coal is not known and they are not representative of a single bed.
 - g. Feed coal: Coal being fed into a power plant, sometimes blended from several sources or taken from a stockpile.
 - h. Limestone sludge: Reacted limestone after it is used in the desulfurization process at a power plant.
 - i. Shot pile: Samples taken from coal that result from blasting at the coal face, which is commonly needed to break-up thick coal beds of the western United States before loading, and may not be representative of a single bed at a single location.
 - j. Dump: A pile of poor quality coal and (or) rock, often weathered, and not representative of mined coal or representative of a single bed at a single location.
 - k. Partial bed: An incomplete bed sample that is not representative of the full-bed primarily because of typical vertical inhomogeneity differences.
 - l. Partings greater than one foot: In some cases, a single sample is a physically composited sample of two coal intervals separated by a parting that is 1 foot or more thick. These samples are rejected because we define the 1-foot parting as two beds, and therefore the sample is not properly composited.
 - m. Rock: Samples with a dry ash content of greater than 50 percent are not coal samples (ASTM, 2014; see ASTM D121–09). They may represent partings, if less than 1 foot thick, or other related rock samples such as roof, floor, concretions, lenses, or other high-ash samples (also see tonsteins).
 - n. Drill cuttings, chip samples from a coal bed, an auger, or a churn drill: These coal samples from drilling operations are contaminated by non-coal rock fragments and are not considered representative of a full coal bed.
 - o. Less than 70 percent recovery: Drill core recovery less than 70 percent is not considered representative of a full coal bed.
 - p. Naturally burned or road cut burned: Burned samples that do not represent the original coal.
 - q. Materials that are not coal: These include materials such as drill additives, drill mud, drill fluid mix, fly ash, bottom ash, and slag.
 - r. Tonsteins: Thin layers of altered volcanic ash that can be used to determine the age of coal beds and sometimes used to help determine coal bed names.

- s. Weathered: We define a weathered sample as a sample that has a calorific value on a moisture- and ash-free basis of 11,500 Btu/lb or less. Single full-bed samples that are weathered are rejected as non-representative samples. Weathered bench samples are considered as representative only if they are composited with other bench samples in the full-bed. The composited samples are not considered weathered.
- t. Washed: Coal that has been cleaned typically by a gravity separation process where the denser material (rocks, high-ash coal particles, and minerals such as pyrite) are separated and removed from the coal.
- u. Alkaline extracts: Low-rank coal samples that have been leached in a weak alkaline solution, which is believed to represent coal before contact with ground water. Because these samples are treated they are not equivalent to unleached samples throughout the database.
- v. Density: A sample divided into a specific gravity separate, which is not representative of in-situ coal.
- w. No location: If there is no location known, then it is automatically rejected as an Upper Level sample.

Appendix 2. Data Parameters

Appendix 2 provides a description of all data parameters (table A2–1) used in COALQUAL Version 3.0. Parameter names surrounded by asterisks and in bold such as ***Sample ID***, are new parameters to COALQUAL Version 3.0. Other parameters were also in COALQUAL Version 1.3 and Version 2.0, but may have been referred to differently than in Version 3.0, which is explained in the individual descriptions provided in table A2–1.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Sample ID	Unique sample identification number generated by combining the Lab ID (W for samples analyzed in Washington D.C. or Reston, Virginia, or D for samples analyzed in Denver, Colorado) and the sample number from COALQUAL Version 1.3 and Version 2.0. For full-bed samples that are determined by mathematically compositing coal bench samples (according to rules in appendix 5) with duplicates and composites (if applicable), an A (for averaged) or a C (for composites) is used. The number of samples used for the composited value is placed after the Lab ID and before the sample number of the upper most bench coal sample. For example, DA2161315 is a mathematically averaged sample of D161315 and D161316. For composited samples using U.S. Geological Survey data only, the Sample ID may contain a decimal point and a number as part of the sample number, for example W217379.1 (appendix 6; table A6–8).
Related To	Related to Sample ID of an Upper Level sample. Only used for lower level samples such a bench samples, partings, or miscellaneous samples. Only Upper Level samples were shown in COALQUAL Version 1.3 and Version 2.0.
State	Name of State where sample was collected. This parameter was STATE in COALQUAL Version 1.3 and Version 2.0.
County	Name of county in State (or borough name in Alaska) where sample was collected. This parameter was COUNTY in COALQUAL Version 1.3 and Version 2.0.
Latitude	Latitude coordinate for point source location of coal sample (decimal degrees). This parameter was LATITUDE in COALQUAL Version 1.3 and Version 2.0. The N/S (north/south) parameter was eliminated because a positive number for latitude is understood to be north of the equator, and therefore all values in this database are positive.
Longitude	Longitude coordinate for point source location of coal sample (decimal degrees). This parameter was LONGITUD in COALQUAL Version 1.3 and Version 2.0. The E/W (east/west) parameter was eliminated by converting all longitude data to a negative number because a negative number for longitude is understood to be west of the Greenwich meridian. All values in this database are negative, therefore all locations in the database are in the Western Hemisphere. The values in COALQUAL Version 1.3 and Version 2.0 were positive with a parameter “W” telling the user of the database that the numbers are in the Western Hemisphere.
Province	Coal province name from Wood and others (1983). This parameter was CPROVINC in COALQUAL Version 1.3 and Version 2.0.
Region	Coal region name from Wood and others (1983). This parameter was called CREGION in COALQUAL Version 1.3 and Version 2.0.
Field	Coal field name from Barnes (1961). Also see Trumbull (1960). This parameter was called CFIELD in COALQUAL Version 1.3 and Version 2.0.
District	District name. Depending on the state, this field may be mining districts, political divisions (such as townships or boroughs), or other subdivisions of the state. This parameter was called DISTRICT in COALQUAL Version 1.3 and Version 2.0.
Formation	Formation name. Stratigraphic formation name specified by the collector of the sample, usually a state geologist; or if collected by U.S. Geological Survey personnel see GEOLEX database (U.S. Geological Survey, 2011). This parameter was called CFORMATN in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Group	Group name. Stratigraphic group name specified by the collector of the sample, usually a state geologist; or if collected by U.S. Geological Survey see GEOLEX database (U.S. Geological Survey, 2011). This parameter was called CGROUP in COALQUAL Version 1.3 and Version 2.0.
Bed	Bed name. Stratigraphic bed name specified by the collector of the sample, usually a state geologist; or if collected by U.S. Geological Survey see GEOLEX database (U.S. Geological Survey, 2011). This parameter was called CBED in COALQUAL Version 1.3 and Version 2.0.
Member	Member name. Stratigraphic member name specified by the collector of the sample, usually a state geologist; or if collected by U.S. Geological Survey see GEOLEX database (U.S. Geological Survey, 2011). This parameter was CMEMBER in COALQUAL Version 1.3 and Version 2.0.
Coal Zone	Relationship between non-coal material and the coal bed (parting, roof, or floor). This parameter was CZONE in COALQUAL Version 1.3 and Version 2.0.
Depth (in)	Depth from the surface of the earth to the top of the sample, if the sample is part of a drill core. If samples are not from a drill core, but the sample is a bench sample, then the depth is a measure from the top of the uppermost bench to the top of the next sample in the benched series (depth is measured in inches). This parameter was DEPTH in COALQUAL Version 1.3 and Version 2.0.
Thickness (in)	Thickness of the sample, measured in inches. This parameter was SAMPTHK in COALQUAL Version 1.3 and Version 2.0.
System	Designates a fundamental chronostratigraphic unit of the samples geologic age (U.S. Geological Survey, 2011). This parameter was SYSTEM in COALQUAL Version 1.3 and Version 2.0.
Series/Epoch	Designates a fundamental chronostratigraphic/geochronologic unit of the samples geologic age; the database provides either series or epoch (U.S. Geological Survey, 2011). This parameter was SER_EPOC in COALQUAL Version 1.3 and Version 2.0.
Literature	References to published data about a sample.
Comments	Miscellaneous comments. This parameter was COMMENTS in COALQUAL Version 1.3 and Version 2.0.
Map	Usually the topographic quadrangle map name and series. Occasionally another type of map name may be used along with the scale of the map. This parameter was MAP in COALQUAL Version 1.3 and Version 2.0.
Collector	Agency and name of collector. This parameter was COLLECTR in COALQUAL Version 1.3 and COLLECR in COALQUAL Version 2.0.
Mine/Power Plant	Coal mine or power plant.
Drill Core No	Drill core number.
Point Id	Field number assigned by the collector or submitter of the sample. This parameter was POINTID in COALQUAL Version 1.3 and Version 2.0.
Submit Date	The date the sample was confirmed by the analytical labs as having been submitted for analysis (MM/DD/YYYY). This parameter was SUBDATE in COALQUAL Version 1.3 and Version 2.0.
Sample Description	Complete sample description.
Estimated Rank	Rank identified by the collector in the field. Because the ash content was not known in the field some rocks were identified as coals and some coals identified as rocks (see Sample Description for complete description of sample). This parameter was ESTRANK in COALQUAL Version 1.3 and Version 2.0.
Apparent Rank	Standard classification of coal by rank; ASTM D388 method determined based on ASTM (2014). Calculations used ASTM data of samples to produce: (1) moist, mineral-matter-free Btu/lb, (2) dry, mineral-matter-free fixed carbon, and (3) volatile matter values.
Analytical Labs	Laboratory where sample was analyzed. This parameter was LABCODE in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Sample Type	Description of sampling and condition of sample. This parameter was SAMPTYPE in COALQUAL Version 1.3 and Version 2.0.
Analysis Type	Analysis type. This parameter was ANALTYPE in COALQUAL Version 1.3 and Version 2.0.
Values Represent	Description of sampling and condition of sample. This parameter was VALREP in COALQUAL Version 1.3 and Version 2.0.
Township	Geographic township.
Range	Geographic range.
Section	Section number in township and range.
Quarters	Quarters in section.
Tract	Subdivision of location information.
Location Detail	Details of location information.
Strat	This parameter is used to identify the stratigraphic (vertical) position of the sample for a single latitude and longitude location. A full description of this parameter is provided in appendix 6.
Rejected	Reason for rejected as an unacceptable coal sample. These samples are classified as miscellaneous samples.
Moisture	Moisture content (as-received basis) in percent by weight as determined by ASTM method D3173 of ASTM (2014). This parameter is MOISTR in COALQUAL Version 1.3 and Version 2.0.
Moisture Q	Qualifier (Q) for Moisture.
Volatile Matter	Volatile matter content in percent as determined by ASTM method D3175 of ASTM (2014). This parameter was VOLMAT in COALQUAL Version 1.3 and Version 2.0.
Volatile Matter Q	Qualifier for Volatile Matter.
Fixed Carbon	Fixed carbon content in percent as determined by ASTM method D3172 of ASTM (2014). This parameter was FIXEDC in COALQUAL Version 1.3 and Version 2.0.
Fixed Carbon Q	Qualifier for Fixed Carbon.
Standard Ash	Ash yield in percent as determined by ASTM method D3174 (ash obtained at 750 degrees Celsius) of ASTM (2014). This parameter was STDASH in COALQUAL Version 1.3 and Version 2.0.
Standard Ash Q	Qualifier for Standard Ash.
Proximate Validation	<p>Validation rating for the proximate analysis. The proximate values of residual moisture, ash, and volatile matter are used to calculate fixed carbon by the difference. Subtracting the fixed carbon from the total carbon yields volatile carbon. Dividing this by 12 (atomic weight of carbon) gives moles of volatile carbon. Dividing the volatile carbon by the moles of hydrogen gives moles of volatile coal. This result should be between 0.0 and 0.5. This validation serves to confirm the reliability of the proximate results as well as the ultimate carbon and hydrogen.</p> <ol style="list-style-type: none"> 1. ACCEPTABLE: designation of results that fall in the range of 0.0–0.5. 2. SUSPECT: designation of results that do not fall in the range of 0.0–0.5. <p>Incomplete data indicates that a sample is missing critical test results required to carry out a proper validation.</p>
Hydrogen	Hydrogen content in percent as determined by ASTM method D3178 of ASTM (2014). This parameter was HYDRGN in COALQUAL Version 1.3 and Version 2.0; hydrogen in Version 3.0 does not include hydrogen from moisture.
Hydrogen Q	Qualifier for Hydrogen.
Carbon	Carbon content in percent as determined by ASTM method D3178 of ASTM (2014) in U.S. Geological Survey labs or other labs. This parameter was CARBON in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Carbon Q	Qualifier for Carbon.
Nitrogen	Nitrogen content in percent as determined by ASTM method D3179 of ASTM (2014). This parameter was NITRGN in COALQUAL Version 1.3 and Version 2.0.
Nitrogen Q	Qualifier for Nitrogen.
Oxygen	Oxygen content in percent as determined by ASTM method D3176 of ASTM (2014). This parameter was OXYGEN in COALQUAL Version 1.3 and Version 2.0; oxygen in Version 3.0 does not include oxygen from moisture.
Oxygen Q	Qualifier for Oxygen.
Sulfur	Sulfur content in percent as determined by ASTM method D3177 of ASTM (2014) in U.S. Geological Survey labs or other labs. This parameter was SULFUR in COALQUAL Version 1.3 and Version 2.0.
Sulfur Q	Qualifier for Sulfur.
Ultimate Validation	<p>The validation of ultimate data is based on a proprietary equation developed by Quality Associates International Ltd., which refines the Dulong approach. This algorithm employs carbon, hydrogen, sulfur, and nitrogen values from the ultimate analyses to derive a predicted higher heating value (HHV). For each sample, the predicted HHV value is then compared to the measured HHV value. The following relative scale was developed to rate the degree of agreement between the predicted and measured HHV results:</p> <ol style="list-style-type: none"> 1. EXCELLENT: HHV results are within 1 percent relative 2. GOOD: HHV results are within 2 percent relative 3. ACCEPTABLE: HHV results are within 3 percent relative 4. INVESTIGATE: HHV results exceed 3 percent relative <p>Those samples that exceed 3 percent relative should be investigated to determine a potential cause. For the Upper Level coal analyses in COALQUAL, 961 samples had either insufficient data or no HHV data.</p> <p>Incomplete data indicates that a sample is missing critical test results required to carry out the validation process.</p>
Btu	Gross calorific value of a coal sample as determined by ASTM method D2015 of ASTM (2014).
Btu Q	Qualifier for Btu.
Sulfate Sulfur	Sulfate sulfur content in percent by weight as determined by ASTM method D2492 of ASTM (2014) in other labs, or similar method in U.S. Geological Survey labs. This parameter was SULFATE in COALQUAL Version 1.3 and Version 2.0.
Sulfate Sulfur Q	Qualifier for Sulfate Sulfur.
Pyritic Sulfur	Pyritic sulfur content in percent as determined by ASTM method D2492 of ASTM (2014) in other labs, or similar method in U.S. Geological Survey labs. This parameter was SLFPYR in COALQUAL Version 1.3 and Version 2.0.
Pyritic Sulfur Q	Qualifier for Pyritic Sulfur.
Organic Sulfur	Organic sulfur content in percent as determined by ASTM method D2492 of ASTM (2014) in U.S. Geological Survey labs or other labs. This parameter was SLFORG in COALQUAL Version 1.3 and Version 2.0.
Organic Sulfur Q	Qualifier for Organic Sulfur.
Ash Deformation	Ash deformation temperature in degrees Fahrenheit as determined by ASTM method D1857 in reducing atmosphere (ASTM, 2014). This parameter was ASHDEF in COALQUAL Version 1.3 and Version 2.0.
Ash Deformation Q	Qualifier for Ash Deformation.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Ash Softening	Ash softening temperature in degrees Fahrenheit as determined by ASTM method D1857 in reducing atmosphere (ASTM, 2014). This parameter was ASHSOF in COALQUAL Version 1.3 and Version 2.0.
Ash Softening Q	Qualifier for Ash Softening.
Ash Fluid	Ash fluid temperature in degrees Fahrenheit as determined by ASTM method D1857 in reducing atmosphere (ASTM, 2014). This parameter was ASHFLD in COALQUAL Version 1.3 and Version 2.0.
Ash Fluid Q	Qualifier for Ash Fluid.
Free Swelling	Free swelling index as determined by ASTM method D720 of ASTM (2014). This parameter was FRESWL in COALQUAL Version 1.3 and Version 2.0.
*Free Swelling Q *	Qualifier for Free Swelling.
HGI	Hardgrove Grindability Index (HGI) as determined by ASTM method D409 of ASTM (2014).
HGI Q	Qualifier for HGI.
EQ Moisture	Equilibrium (EQ) moisture content in percent as determined by ASTM method D1412 of ASTM (2014). This parameter was EQMOIS in COALQUAL Version 1.3 and Version 2.0.
EQ Moisture Q	Qualifier for EQ moisture.
Btu Moist MMF	Calorific value (Btu/lb) on a moist, mineral-matter-free basis (MMF) calculated using Standard Practice D3180 determined based on ASTM (2014). Note that some sulfur and SO ₃ concentration values used in this calculation were approximated from other sulfur concentration values (for example: SO ₃ determined in ash produced by heating the sample to 525 degrees Celsius by U.S. Geological Survey). See appendix 3.
Btu Moist MMF Q	Qualifier for Btu Moist MMF.
VM Dry MMF	Volatile matter (VM) on a dry mineral-matter-free basis (MMF) calculated using Standard Practice D3180 determined based on ASTM (2014). Note that some sulfur and SO ₃ concentration values used in this calculation were approximated from other sulfur concentration values (for example: SO ₃ determined in ash produced by heating the sample to 525 degrees Celsius by U.S. Geological Survey). See appendix 3.
VM Dry MMF Q	Qualifier for VM Dry MMF.
Fixed C Dry MMF	Fixed carbon (C) on a dry mineral-matter-free basis (MMF) calculated using Standard Practice D3180 determined based on ASTM (2014). Note that some sulfur and SO ₃ concentration values used in this calculation were approximated from other sulfur concentration values (for example: SO ₃ determined in ash produced by heating the sample to 525 degrees Celsius by U.S. Geological Survey). See appendix 3.
Fixed C Dry MMF Q	Qualifier for Fixed C Dry MMF.
Moisture, Ash Free Btu	Moisture, ash-free calorific value (Btu/lb). If the value is greater than 0 and less than 11,500 Btu/lb the sample is assumed to be weathered (also see appendix 1, number 2s).
MAFBtu Q	Qualifier for Moisture, Ash Free Btu.
Total C	Total carbon.
Total C Q	Qualifier for Total C.
Carbonate C	Carbonate carbon.
Carbonate C Q	Qualifier for Carbonate C.
Organic C	Organic carbon.
Organic C Q	Qualifier for Organic C.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Air Dry Loss	Air dry loss in percent by weight as determined by ASTM method D2013 of ASTM (2014). This parameter was ADLOSS in COALQUAL Version 1.3 and Version 2.0.
Air Dry Loss Q	Qualifier for Air Dry Loss.
Residual Moisture	Residual moisture is the moisture remaining in the sample after air drying required prior to many ASTM test methods.
Residual moisture Q	Qualifier for Residual Moisture.
Remnant Moisture	Moisture of sample at the time of U.S. Geological Survey analysis. See appendix 4, and data qualifiers in appendix 3 for more details.
Remnant Moisture Q	Qualifier for Remnant Moisture.
GSash	Ash yield in percent as determined by U.S. Geological Survey (GS) laboratories (ash obtained at 525 degrees Celsius). This parameter was GSASH in COALQUAL Version 1.3 and Version 2.0.
GSash Q	Qualifier for GSash.
SiO ₂	Silicon dioxide (SiO ₂) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from Si concentration in parts-per-million. This parameter was SIO2 in COALQUAL Version 1.3 and Version 2.0.
SiO₂ Q	Qualifier for SiO ₂ .
LOI	Loss on ignition.
Al ₂ O ₃	Aluminum oxide (Al ₂ O ₃) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from Al concentration in parts-per-million. This parameter was AL2O3 in COALQUAL Version 1.3 and Version 2.0.
Al₂O₃ Q	Qualifier for Al ₂ O ₃ .
CaO	Calcium oxide (CaO) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from Ca concentration in parts-per-million. Note that this calculation assumes all Ca is converted to CaO. Samples containing large amounts of CaCO ₃ may only be partially converted to CaO at this temperature. This parameter was CAO in COALQUAL Version 1.3 and Version 2.0.
CaO Q	Qualifier for CaO.
MgO	Magnesium oxide (MgO) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius, and converted from Mg concentration in parts-per-million or percent. This parameter was MGO in COALQUAL Version 1.3 and Version 2.0.
MgO Q	Qualifier for MgO.
MnO	Manganese oxide (MnO) concentration in percent. Converted from Mn as-determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius), and (3) later using atomic absorption spectroscopy on the ash to analyze for Mn. This parameter was MNO in COALQUAL Version 1.3 and Version 2.0.
MnO Q	Qualifier for MnO.
Na ₂ O	Sodium oxide (Na ₂ O) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. It was converted from Na concentration in parts-per-million or percent. This parameter was NA2O in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Na2O Q	Qualifier for Na2O.
K2O	Potassium oxide (K ₂ O) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from K concentration in parts-per-million.
K2O Q	Qualifier for K2O.
Fe2O3	Ferric oxide (Fe ₂ O ₃) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from Fe concentration in parts-per-million.
Fe2O3 Q	Qualifier for Fe2O3.
TiO2	Titanium dioxide (TiO ₂) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from Ti concentration in parts-per-million. This parameter was TIO2 in COALQUAL Version 1.3 and Version 2.0.
TiO2 Q	Qualifier for TiO2.
P2O5	Phosphorous pentoxide (P ₂ O ₅) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from P concentration in parts-per-million.
P2O5 Q	Qualifier for P2O5.
SO3	Sulfur trioxide (SO ₃) concentration in percent as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from S concentration in parts-per-million.
SO3 Q	Qualifier for SO3.
GSAsh Dry	Moisture-free ash yield in percent determined from GSASH corrected for remnant moisture from U.S. Geological Survey (GS) laboratories on ash obtained at 525 degrees Celsius. Used to differentiate between coal and non-coal lithologies. A GSASH Dry value greater than 50 percent is defined as a rock, not a coal. Also for bench samples GSASH Dry is used to determine if a bench is part of the bed or a parting.
GSASH Dry Q	Qualifier for GSASH Dry.
Si	Silicon (Si) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from SiO ₂ concentration in percent. This parameter was SI_E in COALQUAL Version 1.3 and Version 2.0.
Si Q	Qualifier for Si.
Al	Aluminum (Al) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from Al ₂ O ₃ concentration in percent. This parameter was AL_E in COALQUAL Version 1.3 and Version 2.0.
Al Q	Qualifier for Al.
Ca	Calcium (Ca) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from CaO concentration in percent. This parameter was CA_E in COALQUAL Version 1.3 and Version 2.0.
Ca Q	Qualifier for Ca.
Mg	Magnesium (Mg) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. It was converted from MgO concentration in percent. This parameter was MG_E in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
*Mg Q *	Qualifier for Mg.
Na	Sodium (Na) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. It was converted from Na ₂ O concentration in percent. This parameter was NA_E in COALQUAL Version 1.3 and Version 2.0.
*Na Q *	Qualifier for Na.
K	Potassium (K) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from K ₂ O concentration in percent. This parameter was K_E in COALQUAL Version 1.3 and Version 2.0.
*K Q *	Qualifier for K.
Fe	Iron (Fe) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from Fe ₂ O ₃ concentration in percent. This parameter was FE_E in COALQUAL Version 1.3 and Version 2.0.
*Fe Q *	Qualifier for Fe.
Ti	Titanium (Ti) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from TiO ₂ concentration in percent. This parameter was TI_E in COALQUAL Version 1.3 and Version 2.0.
*Ti Q *	Qualifier for Ti.
TS	Total sulfur (TS) concentration in parts-per-million on a whole-coal basis, converted from concentration as determined on coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from SO ₃ concentration in percent. Note that this is not the standard ASTM sulfur method.
*TS Q *	Qualifier for TS.
Ag	Silver (Ag) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was AG_E in COALQUAL Version 1.3 and Version 2.0.
*Ag Q *	Qualifier for Ag.
As	Arsenic (As) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories using either (1) wet chemistry analysis for samples analyzed in Denver, Colorado (where the first letter of Sample ID is D) before 1976, or (2) Instrumental Neutron Activation Analysis (INAA) for samples analyzed in Reston, Virginia (where the first letter of Sample ID is W) and for samples analyzed after 1976 in Denver. This parameter was AS_E in COALQUAL Version 1.3 and Version 2.0.
*As Q *	Qualifier for As.
Au	Gold (Au) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was AU_E in COALQUAL Version 1.3 and Version 2.0.
*Au Q *	Qualifier for Au.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
B	Boron (B) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was B_E in COALQUAL Version 1.3 and Version 2.0.
B Q	Qualifier for B.
Ba	Barium (Ba) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was BA_E in COALQUAL Version 1.3 and Version 2.0.
Ba Q	Qualifier for Ba.
Be	Beryllium (Be) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was BE_E in COALQUAL Version 1.3 and Version 2.0.
Be Q	Qualifier for Be.
Bi	Bismuth (Bi) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was BI_E in COALQUAL Version 1.3 and Version 2.0.
Bi Q	Qualifier for Bi.
Br	Bromine (Br) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories using INAA. This parameter was BR_E in COALQUAL Version 1.3 and Version 2.0.
Br Q	Qualifier for Br.
Cd	Cadmium (Cd) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. This parameter was CD_E in COALQUAL Version 1.3 and Version 2.0.
Cd Q	Qualifier for Cd.
Ce	Cerium (Ce) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) semi-quantitative 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of the Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was CE_E in COALQUAL Version 1.3 and Version 2.0.
Ce Q	Qualifier for Ce.
Cl	Chlorine (Cl) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories using X-ray fluorescence analysis. This parameter was CL_E in COALQUAL Version 1.3 and Version 2.0.
Cl Q	Qualifier for Cl.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Co	Cobalt (Co) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) semi-quantitative 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D with Submit Date on or before 08/19/1976, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975, or the first letter of Sample ID = D and Submit Date after 08/19/1976 were analyzed on a whole-coal basis using INAA. This parameter was CO_E in COALQUAL Version 1.3 and Version 2.0
Co Q	Qualifier for Co.
Cr	Chromium (Cr) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) semi-quantitative 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D with Submit Date 08/19/1976, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975, or the first letter of Sample ID = D and Submit Date after 08/19/1976 were analyzed on a whole-coal basis using INAA. This parameter was CR_E in COALQUAL Version 1.3 and Version 2.0.
Cr Q	Qualifier for Cr.
Cs	Cesium (Cs) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) semi-quantitative 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was CS_E in COALQUAL Version 1.3 and Version 2.0.
Cs Q	Qualifier for Cs.
Cu	Copper (Cu) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. This parameter was CU_E in COALQUAL Version 1.3 and Version 2.0.
Cu Q	Qualifier for Cu.
Dy	Dysprosium (Dy) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was DY_E in COALQUAL Version 1.3 and Version 2.0.
Dy Q	Qualifier for Dy.
Er	Erbium (Er) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was ER_E in COALQUAL Version 1.3 and Version 2.0.
Er Q	Qualifier for Er.

Table A2-1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Eu	Europium (Eu) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was EU_E in COALQUAL Version 1.3 and Version 2.0.
Eu Q	Qualifier for Eu.
F	Fluorine (F) concentration in parts-per-million as determined on a whole-coal by U.S. Geological Survey laboratories using an ion-selective electrode method. This parameter was F_E in COALQUAL Version 1.3 and Version 2.0.
F Q	Qualifier for F.
Ga	Gallium (Ga) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was GA_E in COALQUAL Version 1.3 and Version 2.0.
Ga Q	Qualifier for Ga.
Gd	Gadolinium (Gd) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was GD_E in COALQUAL Version 1.3 and Version 2.0.
*Gd Q *	Qualifier for Gd.
Ge	Germanium (Ge) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was GE_E in COALQUAL Version 1.3 and Version 2.0.
Ge Q	Qualifier for Ge.
Hf	Hafnium (Hf) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was HF_E in COALQUAL Version 1.3 and Version 2.0.
Hf Q	Qualifier for Hf.
Hg	Mercury (Hg) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories using cold vapor atomic absorption spectroscopy. This parameter was HG_E in COALQUAL Version 1.3 and Version 2.0.
Hg Q	Qualifier for Hg.
Ho	Holmium (Ho) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was HO_E in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Ho Q	Qualifier for Ho.
In	Indium (In) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was IN_E in COALQUAL Version 1.3 and Version 2.0.
In Q	Qualifier for In.
Ir	Iridium (Ir) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was IR_E in COALQUAL Version 1.3 and Version 2.0.
Ir Q	Qualifier for Ir.
La	Lanthanum (La) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was LA_E in COALQUAL Version 1.3 and Version 2.0.
La Q	Qualifier for La.
Li	Lithium (Li) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. This parameter was LI_E in COALQUAL Version 1.3 and Version 2.0.
Li Q	Qualifier for Li.
Lu	Lutetium (Lu) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was LU_E in COALQUAL Version 1.3 and Version 2.0.
Lu Q	Qualifier for Lu.
Mn	Manganese (Mn) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius), and (3) later using atomic absorption spectroscopy on the ash. This parameter was MN_E in COALQUAL Version 1.3 and Version 2.0.
Mn Q	Qualifier for Mn.
Mo	Molybdenum (Mo) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was MO_E in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Mo Q	Qualifier for Mo.
Nb	Niobium (Nb) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was NB_E in COALQUAL Version 1.3 and Version 2.0.
Nb Q	Qualifier for Nb.
Nd	Neodymium (Nd) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was ND_E in COALQUAL Version 1.3 and Version 2.0.
Nd Q	Qualifier for Nd.
Ni	Nickel (Ni) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was NI_E in COALQUAL Version 1.3 and Version 2.0.
Ni Q	Qualifier for Ni.
Os	Osmium (Os) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was OS_E in COALQUAL Version 1.3 and Version 2.0.
Os Q	Qualifier for Os.
P	Phosphorus (P) concentration in parts-per-million as determined on the coal ash by U.S. Geological Survey laboratories using X-ray fluorescence analysis on ash obtained at 525 degrees Celsius. It was converted from P ₂ O ₅ concentration in percent. This parameter was P_E in COALQUAL Version 1.3 and Version 2.0.
P Q	Qualifier for P.
Pb	Lead (Pb) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. This parameter was PB_E in COALQUAL Version 1.3 and Version 2.0.
Pb Q	Qualifier for Pb.
Pd	Palladium (Pd) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was PD_E in COALQUAL Version 1.3 and Version 2.0.
Pd Q	Qualifier for Pd.
Pr	Praseodymium (Pr) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was PR_E in COALQUAL Version 1.3 and Version 2.0.
Pr Q	Qualifier for Pr.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Pt	Platinum (Pt) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was PT_E in COALQUAL Version 1.3 and Version 2.0.
Pt Q	Qualifier for Pt.
Rb	Rubidium (Rb) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was RB_E in COALQUAL Version 1.3 and Version 2.0.
Rb Q	Qualifier for Rb.
Re	Rhenium (Re) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was RE_E in COALQUAL Version 1.3 and Version 2.0
Re Q	Qualifier for Re.
Rh	Rhodium (Rh) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was RH_E in COALQUAL Version 1.3 and Version 2.0
Rh Q	Qualifier for Rh.
Ru	Ruthenium (Ru) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was RU_E in COALQUAL Version 1.3 and Version 2.0.
Ru Q	Qualifier for Ru.
Sb	Antimony (Sb) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories (using the Rhodamine B method) with the first letter of Sample ID = D and Submit Date on or before 08/19/1976. Samples with the first letter of Sample ID = D and Submit Date after 08/19/1976, and samples with the first letter of Sample ID = W were analyzed using INAA. This parameter was SB_E in COALQUAL Version 1.3 and Version 2.0
Sb Q	Qualifier for Sb.
Sc	Scandium (Sc) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-Step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was SC_E in COALQUAL Version 1.3 and Version 2.0.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Sc Q	Qualifier for Sc.
Se	Selenium (Se) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories using X-ray fluorescence on all older samples with the first letter of Sample ID = D and Submit Date on or before 01/05/1978, and all samples with the first letter of Sample ID = W and Submit Date on or before 06/01/1975. Samples with the first letter of Sample ID = D and Submit Date after 01/05/1976, and all samples with the first letter of Sample ID = W and Submit Date after 06/01/1976 were analyzed on a whole-coal basis using INAA. This parameter was SE_E in COALQUAL Version 1.3 and Version 2.0.
Se Q	Qualifier for Se.
Sm	Samarium (Sm) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 07/01/1975. Samples with the first letter of Sample ID = W and Submit Date after 07/01/1975 were analyzed on a whole-coal basis using INAA. This parameter was SM_E in COALQUAL Version 1.3 and Version 2.0.
Sm Q	Qualifier for Sm.
Sn	Tin (Sn) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was SN_E in COALQUAL Version 1.3 and Version 2.0.
Sn Q	Qualifier for Sn.
Sr	Strontium (Sr) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was SR_E in COALQUAL Version 1.3 and Version 2.0.
Sr Q	Qualifier for Sr.
Ta	Tantalum (Ta) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D. Samples with the first letter of Sample ID = W were analyzed on a whole-coal basis using INAA. This parameter was TA_E in COALQUAL Version 1.3 and Version 2.0.
Ta Q	Qualifier for Ta.
Tb	Terbium (Tb) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was TB_E in COALQUAL Version 1.3 and Version 2.0.
Tb Q	Qualifier for Tb.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Te	Tellurium (Te) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was TE_E in COALQUAL Version 1.3 and Version 2.0.
Te Q	Qualifier for Te.
Th	Thorium (Th) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories using Delayed Neutron Analysis (DNA) (for older samples) and INAA. This parameter was TH_E in COALQUAL Version 1.3 and Version 2.0.
Th Q	Qualifier for Th.
Tl	Thallium (Tl) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was TL_E in COALQUAL Version 1.3 and Version 2.0.
Tl Q	Qualifier for Tl.
Tm	Thulium (Tm) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was TM_E in COALQUAL Version 1.3 and Version 2.0.
Tm Q	Qualifier for Tm.
U	Uranium (U) concentration in parts-per-million as determined on a whole-coal basis by U.S. Geological Survey laboratories using Delayed Neutron Analysis (DNA). This parameter was U_E in COALQUAL Version 1.3 and Version 2.0.
U Q	Qualifier for U.
V	Vanadium (V) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was V_E in COALQUAL Version 1.3 and Version 2.0.
V Q	Qualifier for V.
W	Tungsten (W) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D. Samples with the first letter of Sample ID = W were analyzed on a whole-coal basis using INAA. This parameter was W_E in COALQUAL Version 1.3 and Version 2.0.
W Q	Qualifier for W.
Y	Yttrium (Y) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was Y_E in COALQUAL Version 1.3 and Version 2.0.
Y Q	Qualifier for Y.

Table A2–1. Descriptions of data parameters used in COALQUAL Version 3.0.—Continued

[Abbreviations: ASTM, American Society for Testing and Materials; Btu, British thermal units; ID, identification number; INAA, Instrumental Neutron Activation Analysis. ASTM (2014) is the current reference for ASTM Annual Book of Standards. Database samples were analyzed over a period of years beginning in 1973, and the ASTM methods used were from the current ASTM Book of Standards at the time of sample analysis.]

Parameter name	Description
Yb	Ytterbium (Yb) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples; or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius) for all samples with the first letter of Sample ID = D, or all samples with the first letter of Sample ID = W and Submit Date on or before 05/27/1975. Samples with the first letter of Sample ID = W and Submit Date after 05/27/1975 were analyzed on a whole-coal basis using INAA. This parameter was YB_E in COALQUAL Version 1.3 and Version 2.0.
Yb Q	Qualifier for Yb.
Zn	Zinc (Zn) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using atomic absorption spectroscopy on ash obtained at 525 degrees Celsius. This parameter was ZN_E in COALQUAL Version 1.3 and Version 2.0.
Zn Q	Qualifier for Zn.
Zr	Zirconium (Zr) concentration in parts-per-million on a whole-coal basis, converted from concentration determined on coal ash by U.S. Geological Survey laboratories using either (1) 6-step emission spectrographic analysis for older samples, or (2) automatic plate reading computer-assisted emission spectrographic analysis (ash obtained at 525 degrees Celsius). This parameter was ZR_E in COALQUAL Version 1.3 and Version 2.0
Zr Q	Qualifier for Zr.

Appendix 3. Data Qualifiers

Appendix 3 provides a description of all data qualifiers used in COALQUAL Version 3.0 (table A3–1).

Table A3–1. Descriptions of data qualifiers used in COALQUAL Version. 3.0.

[Codes in uppercase indicate a value cannot be used as reported. Codes in lowercase mean a value has an error small enough not to affect the overall result, and therefore can be used as reported. Abbreviations: ASTM, American Society of Testing and Materials.]

Qualifier Code	Description
L	Less than.
G	Greater than.
B	Blank (no data)
N	Not detected.
X	Cannot be composited or averaged.
C	Composite
a	See note in comment field in database.
m	Miscellaneous
a	Average
e	Estimated moisture (derived directly from estimated rank).
r	Estimated for remnant moisture, based on residual moisture for trace elements. See appendix 4 for procedures.
c	Estimated using composited data (trace element data).
o	Computed oxides using elemental data.
d	Computed chemical concentration using oxide data.
i	Small or insignificant error for composited data.
u	Analyzed by the U.S. Geological Survey.
s	Originally reported as sulfur in the ash.
m	More data available.
t	Total sulfur determined by the U.S. Geological Survey using methods similar to ASTM standard for sulfur D3177 (ASTM, 2014).
l	SO ₃ was estimated using loss of ignition (LOI).
f	SO ₃ was estimated using the equation $(TS/0.4) \times (100/(100-M))$, where TS is total sulfur, and M is percent moisture; or SO ₃ was estimated using the equation (dry sulfur)/0.4).

Appendix 4. Remnant Moisture Estimate Method

All Samples

The discussion here in appendix 4 is based on a statistical evaluation of an independent data set with a large number of samples (with variable ranks) when both remnant and residual moisture values were both available. For high-rank coal, the statistical evaluation may tend to slightly overestimate the residual moisture. It may, in many cases, be an overestimation for low-rank coal, but reduces the likelihood of being incorrect on extremely high residual moisture values, and provides the lowest overall error for the database. Note that the samples used in the statistical evaluation are not part of the database.

If remnant moisture (as-determined moisture of sample at the time of USGS analysis) is known (or can be calculated), use it subject to the following conditions (also shown in table A4–1):

- If only residual moisture is known and is less than or equal to 4 percent, then residual moisture equals remnant moisture.
- If residual moisture is greater than 4 percent and less than or equal to 6 percent, subtract 4 percent from the residual moisture and divide by 2, then add 4 percent to the result to determine the estimated remnant moisture.
- If residual moisture is greater than 6 percent and less than or equal to 7 percent, subtract 1 percent from the residual moisture to determine estimated remnant moisture.
- If residual moisture is greater than 7 percent and less than or equal to 9 percent, subtract 7 percent from the residual moisture and divide by 2, then add 6 percent to the result to determine the estimated remnant moisture.
- If residual moisture is greater than 9 percent and less than or equal to 11 percent, subtract 2 percent from the residual moisture to determine the estimated remnant moisture.
- If residual moisture is greater than 11 percent and less than or equal to 13 percent, subtract 11 percent from the residual moisture and divide by 2, then add 9 percent to the result to determine estimated remnant moisture.
- If residual moisture is greater than 13 percent and less than or equal to 19 percent, subtract 3 percent from the residual moisture to determine the estimated remnant moisture.
- If residual moisture is greater than 19 percent and less than or equal to 21 percent, subtract 19 percent from the residual moisture and divide by 2, then add 16 percent to the result to determine estimated remnant moisture.
- If residual moisture is greater than 21 percent and less than or equal to 29 percent, subtract 4 percent from the residual moisture to determine the estimated remnant moisture.
- If residual moisture is greater than 29 percent and less than or equal to 31 percent, subtract 29 percent from the residual moisture and divide by 2, then add 25 percent to the result to determine estimated remnant moisture.
- If residual moisture is greater than 31 percent, subtract 5 percent from the residual moisture value to determine the estimated remnant moisture.

Table A4–1. Input and criteria for estimating remnant moisture.

Residual moisture (RM percent)	Formula used	Estimated remnant moisture (percent)
≤4	RM	≤4
>4 and ≤6	$((RM-4)/2)+4$	>4 and ≤5
>6 and ≤7	RM-1	>5 and ≤6
>7 and ≤9	$((RM-7)/2)+6$	>6 and ≤7
>9 and ≤11	RM-2	>7 and ≤9
>11 and ≤13	$((RM-11)/2)+9$	>9 and ≤10
>13 and ≤19	RM-3	>10 and ≤16
>19 and ≤21	$((RM-19)/2)+16$	>16 and ≤17
>21 and ≤29	RM-4	>17 and ≤25

Table A4-1. Input and criteria for estimating remnant moisture.—Continued

Residual moisture (RM percent)	Formula used	Estimated remnant moisture (percent)
>29 and ≤31	$((RM-29/2)+25)$	>25 and ≤26
>31	RM-5	>26

Remnant moisture should be less than 30 percent (if higher than 30 percent it is rejected from the database). The residual moisture value should not be used if it exceeds the as-received moisture value. If the ash content is greater than 50 percent on a dry basis, it is defined as a non-coal sample.

Semi-Anthracite and Anthracite Rank Samples

If remnant moisture is known, use it as long as it is less than 10 percent. If residual moisture is not known, use 3 percent for residual moisture. A 1-sigma error (standard deviation) is less than 2 percent, although individual errors could be as high as 4 percent.

Bituminous Rank Samples

If remnant moisture is known, use it as long as it is less than 10 percent. If the residual moisture is high, it is likely that the rank is misidentified. If residual moisture is not known, use 4 percent for residual moisture. A 1-sigma error is less than 2 percent, although individual errors could be as high as 4 percent.

The tiered reduction of the residual moisture is based primarily on data for low-rank coals originally air dried in Somerset, Pennsylvania and analyzed in Denver, Colorado. The altitude and the drier climate in Denver can promote further drying of samples, even if sealed in polyethylene containers. Some samples that are not tightly sealed may experience even further drying, while samples with low as-received moisture content may already have experienced some drying, and may not experience additional moisture loss. Samples analyzed in Reston, Virginia, will often experience less drying than in Somerset or Denver due to higher humidity and lower elevation in Reston.

Subbituminous Rank Samples

If remnant moisture is known, use it as long as it is less than 20 percent. If residual moisture is not known, use 6 percent for residual moisture. A 1-sigma error is less than 5 percent error, although individual errors could be as high as 15 percent. Less than 0.6 percent of the samples with known residual moistures would have an error of 10 percent or more, if 6 percent residual moisture was used.

Lignite Rank Samples

If remnant moisture is known, use it as long as it is less than 30 percent. If residual moisture is not known, use 11 percent for residual moisture. A 1-sigma error is less than 5 percent error for the full dataset, although individual errors could be as high as 20 percent. Less than 0.5 percent of the samples with known residual moistures would have an error of 10 percent or more, if 11 percent residual moisture was used.

Non-Coal and Unidentified Samples

For samples with more than 50 percent ash or identified as non-coal samples, the moisture values are generally low. If there is no moisture information, assume 0 percent moisture. For samples that have no estimated rank and no ash content, or ash content less than 50 percent, use 10 percent estimated moisture to minimize overall errors.

Appendix 5. Averaging Components Used to Calculate Upper Level Samples

When Upper Level samples represent multiple benches, duplicates, or triplicates (etc.), a weighted average (AVE_{wp}) based on sample thickness and concentration (of any analyzed coal parameter) is used to determine the value of the weighted average using equation A5F1.

$$AVE_{wp} = \sum V_{ps} T_s / \sum T_s \quad A5F1$$

Where AVE_{wp} is the weighted (w) average (AVE) of a specific parameter/element (p). V_{ps} is the value V for a specific parameter (p) in a given sample or subsample (s), and T_s is the thickness (T) of the sample or subsample (s). In cases where only relative sample thickness was known, the ratios were used instead of the actual sample thickness. See appendix 2 for the format of sample identification (**Sample ID**) for these types of samples.

When subsamples are composited and some analytical results are qualified with “less than” (L) or “greater than” (G), the following adjustments are made to the average of analysis values.

1. When the average is calculated with values qualified with “e” (greater than), a qualifier code “G” is assigned to the average.
2. When the average is calculated with values qualified with “L” (less than), the following calculations are performed.
 - 2.1. Compute the upper limit of the average values (A_u) of all values by ignoring the “L” qualifier using equation A5F1.
 - 2.2. Compute the average lower limit of the average values (A_l) by substituting “0” for the value with the “L” qualifier.
 - 2.3. Compute the average (A_a) of the two averages (A_u and A_l), obtained from the previous steps, 2.1 and 2.2, respectively.
 - 2.4. The maximum absolute error (E_{am}) is computed by calculating the difference between the two averages using equation A5F2.

$$E_{am} = A_u - A_l \quad A5F2$$

- 2.5. The maximum percent error (E_{pm}) is computed as shown in equation A5F3.

$$E_{pm} = E_{am} / A_a \times 100 \quad A5F3$$

- 2.6. Finally, if the maximum percent error (E_{pm}) is less than or equal to 5 percent, the error is considered to be insignificant with respect to the errors of analysis, and A_a (average of A_u and A_l) is taken as the final value. Otherwise, the largest value of A_u is chosen to be the final value and is qualified with “L” (less than).

Note that an average cannot be computed if the subsample’s analytical results contain both “less than” and “greater than” qualifiers.

3. There are three ways of determining the average value of a parameter when samples are physically composited as identified by the **Strat** data (given as ***Strat*** in table A2–1).
 - 3.1. If there is only one value for a given parameter (or more generally a group of parameters such as all ASTM data or all USGS data) for all benches representing the entire bed sample, and all coal benches have been physically composited, those values become the average for that sample for that parameter.
 - 3.2. If individual benches have data, and the data for all benches are physically composited, then the individual benches are combined using the weighted average (equation A5F1) and that result is further averaged with the composited data.

If only part of the full-bed is physically composited for some values as in 3.1, or all values as in 3.2, then the partial is treated as in 3.1 or 3.2 and further averaged with the remaining benches using equation A5F1.

Appendix 6. Strat Parameter

The **Strat** parameter (***Strat*** in table A2–1) is used to identify the stratigraphic (vertical) relationships of samples in the stratigraphic column for a single latitude and longitude location. This appendix explains the **Strat** parameter complexity, which is caused in part by the diversity of coal types and coal sequences throughout the United States, necessitating differing sample collection methods and sample types such as drill cores, bench sampling, roof, floor, parting, whole bed, and face-channel sampling.

Additionally, the diversity of objectives, differing laboratories, and frequent funding constraints added complexity to the sampling criteria. Samples were collected by many scientists from the USGS and State Geological Surveys for a variety of purposes. Furthermore, samples were prepared for analysis for major and trace elements in two different laboratories, and other coal parameters were analyzed by multiple contract laboratories. Uneven budget yearly funding occasionally forced reductions in the frequency of duplicate analyses, as well as the total number of samples analyzed. This required either the physical compositing of bench samples, or eliminating certain analytical procedures, or both. The following paragraphs describe the **Strat** parameter and provide examples for the different situations, beginning with less complex situations.

Single, Upper Level, full-bed samples at a given location are designated by their **Sample ID** followed by “-00.” For example, the **Strat** parameter for the single, full-bed sample W196338 would be designated W196338-00. For individual samples that do not qualify as Upper Level samples at a given location, such as miscellaneous samples, there is no designation and the field is left blank, for example D163527.

When a full-bed Upper Level sample consists of multiple coal benches, sample values are mathematically composited according to the rules in appendix 5. The **Sample ID** for these contains an “A” for average and the number of benches averaged (see ***Sample ID*** in table A2–1), for example DA2161315. The **Strat** parameter notation for the composited average for the benches is D161315-00A:01,02. The sample number for the uppermost bench is assigned “-00A” for an Upper Level mathematically composited sample with the notation 01, 02 denoting the individual benches (numbered from top to bottom) used for the composited analyses (table A6–1). The thickness of the Upper Level sample is the total thickness of the composited coal benches. Samples mathematically composited to produce the Upper Level and other non-coal samples such as partings, roof, and floor rocks etc., are organized in order from top to bottom. In most cases, the actual mean sea level elevations of the sample intervals are not known, but the thickness within a bed and relative stratigraphic positions are known. The samples of a sequence is identified by the **Sample ID** of the uppermost coal sample analyzed (full-bed or bench) followed by the sequence number. Table A6–1 presents a simple example of a stratigraphic sequence with two coal benches, and an Upper Level (full-bed) sample mathematically composited from the two bench samples.

Table A6–1. A simple example of a stratigraphic sequence with two coal benches, and an Upper Level sample mathematically composited from the two coal bench samples.

Sample ID	Strat	Thickness (feet)	Explanation
DA2161315	D161315-00A:01,02	9.5	Upper Level (-00) sample mathematically obtained by combining two coal benches (01 and 02) per appendix 5.
D161315	D161315-01	4.5	1st coal bench (01).
D161316	D161316-02	5	2nd coal bench (02).

For more complex cases, additional letter designations are added for non-coal material associated with coal bed and coal materials (shown in table A6–2). These identifiers are defined by 5 different categories as follows:

1. Non-coal identifiers.
2. Stratigraphic identifiers.
3. Coal identifiers that identify samples used to create Upper Level samples. In many cases, these samples have no qualifier and are simply numbered as shown in table A6–1.
4. Coal identifiers that identify samples not used in Upper Level samples.
5. Identifiers containing both coal and non-coal material, which are not used in Upper Level samples.

Examples of each of these cases are provided below. There is no single location where all of these designations exist, however there are many locations where multiple designations are used. Note that the comments in the last column of table A6–2 (Strat Type) are for descriptive purposes only and are not included the database.

Table A6–2. A list of additional letter designations used for non-coal material associated with coal bed and coal materials.

Category	Identifier	Letter	Strat Type
1	Non-coal identifiers	R	Roof
		F	Floor
		P	Parting
		M	Miscellaneous (non-coal material)
		D	Duplicate analysis.
2	Stratigraphic identifiers	SX	Stratigraphic coal or non-coal sequence separated by at least a foot of rock material. Where X is the stratigraphic bed number, top to bottom.
		LX	This indicator is used for stratigraphic sequences that are so similar in location there is no apparent difference in the longitude and latitude, or used for stratigraphic sequences that are at the same location but their relative stratigraphic positions are unknown. X is the number of samples at the location.
3	Coal identifiers that identify samples used to create Upper Level samples	D	Duplicate analysis
		T	ASTM data determined in physically composited samples.
		U	U.S. Geological Survey data (major and trace elements) determined in physically composited samples.
		B	Both ASTM and U.S. Geological Survey data determined in physically composited samples.
4	Coal identifiers that identify samples not used in Upper Level samples	K	Samples treated with alkaline solution of ammonium acetate.
		M	Miscellaneous coal samples rejected as Upper Level samples (see appendix 1, number 2).
5	Identifier containing both coal and non-coal material	I	Informational samples composited to contain both coal and non-coal material, or whole seam samples including partings.

In the first example (table A6–3), the Upper Level sample DA4169011 indicates the three benches starting with 169011 were analyzed in Denver (D) and were averaged (A) using rules in appendix 5. The **Strat** parameter D169011-00A:02,04,06 indicates that the Upper Level sample (-00) mathematically averages (A) coal benches 02, 04, and 06. Benches 01R (roof), 03P and 05P (partings), and 07F (floor) are not coal samples, and are therefore not part of the Upper Level sample. None of the partings have thickness of 1 foot or more, so all coal benches are part of the same Upper Level sample.

Table A6–3. An example of a location with a coal sequence with roof, parting, and floor samples.

Sample ID	Strat	Thickness (feet)	Explanation
DA4169011	D169011-00A:02,04,06	8.25	Upper Level sample (-00) mathematically obtained by combining three coal benches (02, 04, and 06) per appendix 5.
D169026	D169011-01R	0.5	Roof (R)
D169011	D169011-02	0.583	1st coal bench (02).
D169025	D169011-03P	0.25	Parting (P)
D169010	D169011-04	6.5	2nd coal bench (04).
D169024	D169011-05P	0.417	Parting (P)
D169009	D169011-06	1.17	3rd coal bench (06).
D169023	D169011-07F	0.25	Floor (F)

The next example (table A6–4) has two different stratigraphic sequences at the same location. In this case, the upper most sequence (stratigraphic bed S1) has only one (01) miscellaneous (M) rock sample D165057, therefore the **Strat** parameter is D165057-01M-S1. This sequence has no Upper Level sample. The second stratigraphic sequence (S2) is below the first stratigraphic sequence, and contains a mathematically composited Upper Level sample DA2165058 from the combination of two coal bench samples D165058 and D165059 that are identified by the **Strat** parameters D165058-01-S2 and D165058-02-S2 in table A6–4.

Table A6–4. An example of a location with a miscellaneous rock sample and a coal sequence in two different stratigraphic sequences (S1 and S2).

Sample ID	Strat	Thickness (feet)	Explanation
D165057	D165057-01M-S1	3.6	Miscellaneous (M) rock sample at least one foot above D165058.
DA2165058	D165058-00A:01,02-S2	9	Upper Level sample (-00) for stratigraphic bed 2 (S2) mathematically obtained by compositing two coal benches (01 and 02) per appendix 5.
D165058	D165058-01-S2	4.5	1st coal bench (01).
D165059	D165058-02-S2	4.5	2nd coal bench (02).

Table A6–5 illustrates stratigraphic sequences, which are at the same location but their relative stratigraphic positions are unknown, or samples that are known to be at a slightly different location, but the difference cannot be detected within the precision of the latitude and longitude in the database (usually within a few feet). The third example, shown in table A6–5, illustrates three different stratigraphic sequences with all samples so similar in location there is no apparent difference in latitude and longitude (locations L1, L2, and L3). The relative stratigraphic locations of the mathematically averaged (A) Upper Level samples for two of these locations are not known, location L1 (WA5232482) consists of four benches, and location L3 (WA2232573) consists of two benches. The Upper level single sample at location L2 (W232486) is below the bottom of location L1 by 6.4 feet. It should be noted that the “L” qualifier here is always followed by a number, and is different from the “L” qualifier in the elemental data, which always follows the number.

Table A6-5. An example of three stratigraphic sequences that are at the same location, or so similar in location there is no apparent difference in latitude and longitude.

Sample ID	Strat	Thickness (feet)	Explanation
WA5232482	W232482-00A:01,02,03,04-L1	4.9	Upper Level sample (-00) for location 1 (L1).
W232482	W232482-01-L1	0.9	1st coal bench (01) location 1.
W232487	W232482-02D-L1	0.9	2nd coal bench (02) location 1.
W232483	W232482-02D-L1	0.9	Duplicate (D) of 2nd coal bench
W232484	W232482-03-L1	1.5	3rd coal bench (03) location 1.
W232485	W232482-04-L1	1.6	4th coal bench (04) location 1.
W232486	W232486-00-L2	1	Upper Level (-00) single sample at location 2 (L2); this bed is below the bed at location 1.
WA2232573	W232573-00A:01,02-L3	1.2	Upper Level (-00) sample for location 3 (L3).
W232573	W232573-01-L3	0.6	1st coal bench (01) location 3.
W232572	W232573-02-L3	0.6	2nd coal bench (02) location 3.

Table A6-6 shows an example of a stratigraphic sequence that contains a duplicate (D) of the stratigraphic bed S1 and a floor (F) non-coal sample. Since the duplicates represent the same sample interval they both have the identifier “01D,” after their **Sample ID** (of the **Strat** parameter designation). Note that if the sample was analyzed in Denver it has a letter “D” at the beginning of the sample ID, in contrast the “D” for duplicate sample is after the **Strat** parameter, for example D202213-1D. In this case, the sample number of the Upper Level sample is arbitrary since both samples represent the upper-most coal sample. These two samples are averaged (A) to obtain the mathematically composited Upper Level sample. If additional coal benches were in this sequence, the duplicates would have been averaged first, before being composited with the other coal bench samples according to the guidelines in appendix 5.

Table A6-6. An example of a location with a stratigraphic sequence (S1) that contains both a duplicate and a floor sample.

Sample ID	Strat	Thickness (feet)	Explanation
WA2211942	W211942-00A:01-S1	1.4	Upper Level sample (-00) obtained mathematically by combining full-bed duplicates.
W211942	W211942-01D-S1	1.4	Full-bed duplicate (D) of W211859.
W211859	W211942-01D-S1	1.4	Full-bed duplicate (D) of W211942.
W211939	W211942-02F-S1	0.17	Floor (F) sample for the full-bed samples above.

The next three examples show how composited data are handled in the database. There are three types of composited data. The first example relates to the two different types of analytical parameters determined in the database. Coal parameters analyzed in accordance with ASTM procedures are indicated by a “T” qualifier. In the second example, major and trace element data analyzed in USGS laboratories are indicated with a “U” qualifier. In the first two examples, depending on the original purpose for acquiring the data (and in some cases financial restrictions at the time of analysis), coal benches were physically composited to reduce the number of samples analyzed. In the third example, the composited sample was analyzed by both ASTM and USGS laboratories and indicated by the qualifier “B.” In this last example, the data are treated as a single sample without a qualifier (since there are no data for individual benches). Otherwise, the physically composited benches are treated as duplicates of the whole sample, or of those benches composited. It should be noted that this qualifier is not the same as the qualifier “B” (blank) used to indicate blank data. Blank data is canceled by USGS and ASTM data fields, whereas the “B” (both) parameters is only found in **Strat** data.

The following paragraphs discuss each of these examples in more detail. The first, illustrates coal parameters (ASTM composite data) for three benches (table A6-7) at a location (L1). The “C” in the **Sample ID** number (DC3172313) represents composited data, the first “3” (after “DC”) represents the number of coal benches composited, and the “T” in the **Strat** parameter (D172313-00T:01,02,03-L1) represents ASTM composite data as discussed above. In this example, data for **Sample ID** DC3172313 contains only ASTM data. The coal bench samples contain only USGS data (major and trace element associated ash values, and so forth). The Upper Level sample (DA3172313) composites the coal bench samples according to appendix 5 for

USGS data and ASTM data. Additional locations (L2 and L3) are not included in table A6–7 because they do not contain new information.

Table A6–7. An example of a location with ASTM composite data and three bench samples without ASTM data. The table includes only one of three locations found in the database at the associated latitude and longitude.

Sample ID	Strat	Thickness (feet)	Explanation
DA3172313	D172313-00A:01,02,03-L1	64.8	Upper Level sample (-00) obtained by using the physically composited ASTM data (DC3172313) and compositing the USGS data from the three benches from location 1 (L1).
DC3172313	D172313-00T:01,02,03-L1	64.8	Physically composited sample of three bench samples (01, 02, and 03) analyzed for ASTM parameters only (T).
D172313	D172313-01-L1	21.6	1st coal bench (01) analyzed for USGS parameters only.
D172314	D172313-02-L1	21.6	2nd coal bench (02) analyzed for USGS parameters only.
D172315	D172313-03-L1	21.6	3rd coal bench (03) analyzed for USGS parameters only.

The next example (table A6–8) shows USGS data were analyzed for a sample physically composited from two coal benches. In this case, the full-bed sample W217379 was the only sample analyzed for major and trace elements. This sample was composited from two bench samples for which ASTM data were obtained. Because these samples had no USGS sample numbers, and all data in this database use USGS sample numbers, a decimal identification was attached to each bench resulting in **Sample IDs** W217379.1 and W217379.2. The **Strat parameter** for sample W217379 is W217379.1-00U:01,02-S4, because it is a USGS composite (U) of coal benches W217379.1 and W217379.2, “01” and “02,” respectively. The Upper Level sample WA3217379.1 contains the USGS data from W217379 and the mathematically averaged ASTM data from W217379.1 and W217379.2. The stratigraphic sequence (S4) is one of five stratigraphic sequences sampled at this location; the other four sequences contained no new information, and therefore are not described in table A6–8.

Table A6–8. An example of a stratigraphic sequence (S4) at a location with U.S. Geological Survey (USGS) composite data and two bench samples without USGS data. Only one of five stratigraphic sequences from the database is included in the table.

Sample ID	Strat	Thickness (feet)	Explanation
W217379	W217379.1-00U:01,02-S4	1.75	Physically composited sample of the two coal benches (01 and 02) analyzed for USGS parameters only (U).
W217379.1	W217379.1-01-S4	1.35	1st coal bench sample (01) analyzed for ASTM parameters only.
W217379.2	W217379.1-02-S4	0.4	2nd coal bench sample (02) analyzed for ASTM parameters only.
WA3217379.1	W217379.1-00A:01,02-S4	1.75	Upper Level sample (-00) mathematically composited using USGS data from the two coal bench samples (01 and 02) and the physically composited sample.

The next example in table A6–9 shows a physically composited sample representing a full coal bed. Unlike the previous two examples, where all parameters were analyzed in all samples, the ASTM data were analyzed in a separate physically composited sample, which was considered to be essentially a duplicate of the mathematically averaged sample. The Upper Level sample WA4202051 is a combination of the mathematically composited data for benches 02, 03, and 04 containing USGS data, and the physically composited sample W202050 containing the ASTM data.

Table A6–9. An example of a location with an Upper Level physically composited sample using both ASTM and U.S. Geological Survey (USGS) data, a roof, three coal benches, and a floor.

Sample ID	Strat	Thickness (feet)	Explanation
WA4202051	W202051-00A:02,03,04	3.83	Upper Level sample (-00) mathematically obtained by combining three coal benches (02, 03, and 04) and the Upper Level composite per appendix 5.
W202050	W202051-00B:02,03,04	3.83	Physical composite of the three coal benches (02, 03, and 04) analyzed for ASTM data only.
W202054	W202051-01R	0.33	Roof (R)
W202051	W202051-02	1.75	1st coal bench (02) analyzed for USGS data only.
W202052	W202051-03	1.16	2nd coal bench (03) analyzed for USGS data only.
W202053	W202051-04	0.92	3rd coal bench (04) analyzed for USGS data only.
W202055	W202051-05F	0.17	Floor (F)

Table A6–10 shows an example of two samples at two stratigraphic sequences treated with alkaline solution of ammonium acetate (identified with “K” after the sample number). The ammonium acetate solution removes elements attached to low-rank coal at ion exchangeable sites by groundwater. Since only a few samples of this kind are included in the database, they are not included in the Upper Level samples. In this example, the untreated sample splits are the Upper Level samples.

Table A6–10. An example of a location with two single Upper Level samples with splits treated with alkaline solution (K). The two Upper Level samples are separated by rock material by more than a foot forming two stratigraphic levels and an additional coal sequence at a third stratigraphic level.

Sample ID	Strat	Thickness (feet)	Explanation
D165598	D165598-00-S1	6	Single Upper Level sample (-00) above S2 and S3 samples (stratigraphic levels 2 and 3).
D166369	D165598-01K-S1	6	Alkaline solution (K) treated split of D165598.
D165599	D165599-00-S2	4.6	Single Upper Level sample (-00) above S3 and below S1 samples (stratigraphic level 1).
D166370	D165599-01K-S2	4.6	Alkaline solution (K) treated split of D165599.
DA2165600	D165600-00A:01,02-S3	15.9	Stratigraphic level 3 (S3) mathematically obtained by combining two coal benches (01 and 02) as per appendix 5.
D165600	D165600-01-S3	10	1st coal bench (01) for S3.
D165601	D165600-02-S3	5.9	2nd coal bench (02) for S3.

Table A6–11 shows an example of a location with a single sample. The **Strat** parameter includes an “I” for informational sample. The sample contains non-coal material (parting), and therefore it is not an Upper Level sample.

Table A6–11. An example of a location with an informational sample (I) that contains a parting (P).

Sample ID	Strat	Thickness (feet)	Explanation
W202073	W202073-00I:01,02P,03	36	Not an Upper Level sample because it includes a parting (P).

Table A6–12 shows an example where a parting (P) is removed from a sample and the coal material from above and below the parting is recomposited to form a new sample D169253 (coal material). The parting was analyzed separately as D169264.

Table A6-12. An example of a location with a stratigraphic sequence (S3) with a parting (P) removed and analyzed separately.

Sample ID	Strat	Thickness (feet)	Explanation
DA2169254	D169254-00A:01,02,04-S3	8.3	Upper Level sample (-00) mathematical composite obtained by combining the upper and lower sections of a single sample containing a parting.
D169254	D169254-01-S3	5.5	1st coal bench (01).
D169253	D169254-02,04-S3	2.8	2nd coal bench (combination of stratigraphic levels 02 and 04) without the parting (03P).
D169264	D169254-03P-S3	0.1	Parting (03P)

Appendix 7. Identification of Nearby Samples

Georeferencing, used to identify samples that are located within one mile of another sample's location, is computed by the database using the following equation based on the law of spherical cosines (Veness, 2010):

$$D = \text{acos} [\sin (\text{lat}_1) \times \sin (\text{lat}_2) + \cos (\text{lat}_1) \times \cos (\text{lat}_2) \times \cos (\text{long}_2 - \text{long}_1)] \times R$$

where:

- D is distance in miles between two geographical points
- R is mean radius of earth, equal to 3,959 miles
- lat₁ is latitude of sample 1
- long₁ is longitude of sample 1
- lat₂ is latitude of sample 2
- long₂ is longitude of sample 2

