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Chemical Analyses in the World Coal Quality Inventory, Version 1

Compiled by Susan J. Tewalt, Harvey E. Belkin, John R. SanFilipo, Matthew D. Merrill, Curtis A. Palmer, Peter D. Warwick, Alexander W. Karlsen, Robert B. Finkelman, and Andy J. Park

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Conversion Factors

Multiply	By	To obtain
British thermal units per pound	0.002325	Megajoules (MJ) per kilogram
meter (m)	3.281	foot (ft)
kilometer (km)	0.6214	mile (mi)
mile (mi)	1.609	kilometer (km)
Degrees Fahrenheit (°F)	(°F-32)/1.8	degrees Celsius (°C)
Percent (percent)	10,000	Parts per million (ppm)
Location		
"North American Datum of 1983 (NAD 83)"		

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Introduction

The main objective of the World Coal Quality Inventory (WoCQI) was to collect and analyze a global set of samples of mined coal during a time period from about 1995 to 2006 (Finkelman and Lovern, 2001). Coal samples were collected by foreign collaborators and submitted to country specialists in the U.S. Geological Survey (USGS) Energy Program. However, samples from certain countries, such as Afghanistan, India, and Kyrgyzstan, were collected collaboratively in the field with USGS personnel. Samples were subsequently analyzed at two laboratories: the USGS Inorganic Geochemistry Laboratory located in Denver, CO and a commercial laboratory (Geochemical Testing, Inc.) located in Somerset, PA. Thus the dataset, which is in Excel (2003) format and includes 1,580 samples from 57 countries, does not have the inter-laboratory variability that is present in many compilations. Major-, minor-, and trace-element analyses from the USGS laboratory, calculated to a consistent analytical basis (dry, whole-coal) and presented with available sample identification information, are sorted alphabetically by country name. About 70 percent of the samples also have data from the commercial laboratory, which are presented on an as-received analytical basis.

The USGS initiated a laboratory review of quality assurance in 2008, covering quality control and methodology used in inorganic chemical analyses of coal, coal power plant ash, water, and sediment samples. This quality control review found that data generated by the USGS Inorganic Geochemistry Laboratory from 1996 through 2006 were characterized by quality practices that did not meet USGS requirements commonly in use at the time. The most serious shortcomings were (1) the adjustment of raw sample data to standards when the instrument values for those standards exceeded acceptable limits or (2) the insufficient use of multiple standards to provide adequate quality assurance.

In general, adjustment of raw data to account for instrument “drift” is an acceptable practice within strictly defined limits. During the denoted period, USGS required that the maximum adjustment of instrument values, guided by calibration standards, was not allowed to exceed 10 percent. However, in some cases, the Inorganic Geochemistry Laboratory released data that were adjusted by more than 10 percent and (or) were not constrained by an adequate number of control standards. Original instrument values no longer exist for about 80 percent of the analyses during this period; therefore, the acceptability of drift corrections for most of the samples analyzed cannot be determined. For these reasons, the WoCQI data from the USGS Inorganic Geochemistry Laboratory should be used with care. For more information, individuals may contact laboratory

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management at *EnergyLabs@usgs.gov* with specific questions about particular datasets or analytical attributes.

Standard USGS sampling methods were provided and recommended to collaborators, but the analyzed samples may or may not be representative of their locale; for some samples, only limited information is available concerning sample provenance. Single samples cannot represent spatial or temporal variability within a coal area.

Geochemical datasets of U.S. coals can be found in the COALQUAL database (Bragg and others, 1997) and the National Coal Quality Inventory (Hatch and others, 2006), as only non-U.S. sample data are presented in the WoCQI. Although the WoCQI does not contain worldwide coverage of coal deposits, it is truly a unique and valuable compilation. The information in the WoCQI should prove useful for identifying possible areas for future global coal research.

Data: Use and Caveats

The WoCQI dataset, WoCQI_v1.xls, was compiled from an Access database maintained by the USGS Geochemistry Laboratory, as well as from hardcopy reports and digital files from the commercial laboratory, into an Excel (2003) dataset. WoCQI includes available sample information and major-, minor-, and trace-element analyses presented on a dry, whole-coal analytical basis. A metadata file, WoCQI_v1_meta.txt, lists information on the chemical attributes in text format. Explanations for some data conversion formulas, as well as citations of analytical methods, can be found in this document.

Some sample (remnant) moistures were not available from the USGS lab, and concentrations are estimated to a dry basis from other available parameters, such as the residual moisture values generated by the commercial laboratory. USGS analytical methods are described in Bullock and others (2002), but changes in instrumentation and sample preparation methods occurred for mercury and chlorine in July 2004 and March 2005, respectively (see lab1_date attribute in WoCQI_v1.xls). Current instrumentation is listed in the dataset and descriptions of USGS analytical procedures may be found on-line at *http://energy.cr.usgs.gov/gg/geochemlab/methodology.html.* Owing to the analytical quality control issue for some analyses, the estimation of moisture content for some samples, and the uncertainty associated with sample representativeness, the WoCQI data should be considered semi-quantitative. As a practical matter, if the results reported have been confirmed by other, independent samples and analyses, the data may be treated quantitatively. Alternatively, if the data cannot be independently confirmed but the conclusions drawn from them are qualitative, results should be adequate to support those conclusions. WoCQI data, however, should not be used to draw conclusions or to base decisions that are critically dependent upon quantitative results.

About 70 percent of WoCQI samples had proximate and ultimate analyses, calorific value, and forms of sulfur analyzed by Geochemical Testing, and these are presented on an as-received basis in WoCQI_v1.xls. In addition, ash-fusion temperatures (degrees Fahrenheit, reducing atmosphere), Hardgrove grindability index (HGI), and free swelling index (FSI) were routinely performed by the commercial laboratory, as well as apparent specific gravity and fluorine analyses (on a dry, whole-coal basis) for a subset of samples.

When selecting samples, the user is cautioned to check sample lithology, sample type, and sample processing method (processing done prior to analysis, for example, raw versus washed) in the spreadsheet. The dataset includes not only run-of-mine and standard channel samples but also grab, benched, washed, sized, coal bed partings, and briquetted samples, so it is extremely

important to read the associated metadata for an explanation of attributes and data processing to prevent misinterpretation of the data.

To use the data in WoCQI_v1.xls, the user must assume that included data are representative of their respective coal-bearing areas. Because sample locations vary widely in confidence and most locations have some degree of uncertainty, an attribute estimating the accuracy of the presented geographic coordinates of the sample to the true location of the sample has been assigned. This attribute should be considered in conjunction with the presented precision (number of decimal places) in the latitude and longitude coordinates.

A secondary EXCEL file (WoCQI_ADD_v1.xls) contains the following: proximate and ultimate analytical data from laboratories other than Geochemical Testing for samples that have analyses in the WoCQI_v1.xls dataset, a few samples of insufficient bulk size for the inorganic analysis, and foreign coal samples from other USGS projects preceding or nearly contemporaneous with WoCQI sample collection. Other laboratories may have used foreign standard methods with different ashing temperatures or preparation methods than Geochemical Testing, which uses ASTM standards (ASTM, 2007). These external data are also not likely to be as comprehensive as the data in WoCQI_v1.xls.

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Samples from some countries, such as North Korea, were obtained from collaborators who were not residents of those countries. Iranian samples were obtained through License No. IA-5012 issued by the U.S. Department of Treasury, Office of Foreign Assets Control to John R. SanFilipo, for the purpose of obtaining, analyzing, and including the data in the WoCQI. Funding for commercial analyses of Afghanistan samples was provided by the U.S. Agency for International Development.

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Appendixes

EXCEL FILES LINK