



Ash chemistry database for British Columbia Rocky Mountain bituminous coals

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Front cover: Bituminous coal sample from the Mist Mountain Formation, Elk River coalfield.
Photo by Janet Riddell.

Back cover: Core from the Gething Formation, Trend mine, Peace River coalfields.
Photo by Paul Jago.



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Abstract

Ash is the inorganic residue remaining after coal combusts. It is composed of oxides of the mineral content in the coal. Coal ash chemistry can have a significant influence on coke strength after reaction (CSR), an important measure of coking coal quality. Coals that were overlain by non-marine deposits (which includes most Canadian Rocky Mountain coals) generally have mineral assemblages that form ashes with low ratios of reactive oxides (i.e. Fe_2O_3 , CaO , MgO , Na_2O and K_2O) to refractory oxides (i.e. SiO_2 , Al_2O_3 and TiO_2), which favours good coke strength under blast furnace conditions. Coal ash chemistry is also used to predict slagging and fouling potential in the furnaces or kilns of all types of coals. This database compiles ash chemistry analyses of British Columbia Rocky Mountain bituminous coals from public sources into a standardized relational format to facilitate its distribution and use.

Keywords: Coal ash geochemistry database, logical data model, bituminous coal, coke strength after reaction with CO_2 (CSR), Gates Formation, Gething Formation, Mist Mountain Formation, coking coal quality, data management and maintenance

1. Introduction

A demand to store and manage geochemical data collectively, in a relational database, has emerged because of increases in the volume of data, and due to complexities introduced by increased spatial extent and resolution of sample collection, application of new analytical methods, and collaboration between multiple publically funded agencies and mineral exploration organizations. Managing data in an organization-wide database is more effective than the file-based approach. First, it enables long-term data preservation and mitigates data loss. Second, it provides an effective means to systematically and consistently integrate data collected for different projects and from different areas, making data collected for individual projects more useful. Third, it links directly into existing organizational web GIS systems, such as MapPlace, the BCGS platform for data discovery, visualization, extraction, and distribution.

Ash is the inorganic residue remaining after coal combusts. It is composed of oxides of the mineral content in the coal. Coal ash chemistry can have a significant influence on coke strength after reaction (CSR), an important measure of coking coal quality. In this GeoFile we provide a database of ash chemistry from bituminous coals in the Peace River, Elk River and Crowsnest coalfields in the Rocky Mountains of British Columbia (Fig.1). The primary source for this database is non-confidential records in BC COALFILE, the collection of

company exploration reports supplied to the British Columbia Ministry of Energy and Mines as part of the statutory reporting requirements for maintaining coal tenure. Data were also taken from CANMET (Canadian Centre for Mineral and Energy Technology) publications (Faurstou et al., 1982; Bonnell and



Fig. 1. Locations of coalfields in the Rocky Mountains of British Columbia.

Janke, 1986; Price and Gransden, 1987). COALFILE reports are available for viewing and download in PDF format, and spatial data (location co-ordinates for boreholes, bulk samples and trenches) are available for viewing and download in Access from <<http://www.empr.gov.bc.ca/Mining/Geoscience/Coal/CoalBC/Pages/CoalDataReports.aspx>>

2. Data modeling and database development

Database development commonly follows iterative stages including requirement analysis, logical design, implementation, and database population (Connolly and Begg, 1999). We followed these stages closely to develop the BCGS coal ash geochemistry database. Our relational data model (Fig. 2) consists of three data entities (DATA_PUBLISH, DATA_SAMPLE, and DATA_ANALYTE) and three meta-data entities (CODE_METHOD, CODE_LAB, and CODE_UNIT). The 3 data entities are used to model and store the related data as suggested by their names. For example DATA_SAMPLE here is for coal sample data modeling and storage. The three meta-data entities are used to model and store information such as the analytical method and laboratory for each analyte determination value and coal sample.

With minimum redundancy, our model can effectively address relationships between sample, publication, analyte, analytical method, and laboratory in cases where: 1) samples were analyzed by different methods at different laboratories;

2) samples were re-analyzed; 3) samples were re-analyzed with different minimum detection limits; and 4) samples were published in multiple publications. This model aligns with the Open Geoscience data model (Granitto et al., 2012; Watson and Evans, 2012). We constructed the coal ash geochemistry database using Microsoft Access. Peripheral applications were developed as three Python scripts to assist routine data management, including data quality control, data loading, and product generating.

3. Data management

The development and operation of this database makes it possible for the British Columbia Geological Survey to centrally manage coal ash geochemistry data through time, which leads to improved data consistency, timely data update, routine delivery of customized data products, and data loss mitigation. The operation and dataflow of the database follows five steps (Fig.3): 1) data compilation; 2) data screening for initial QA/QC; 3) data loading; 4) product generating; and 5) Product QA/QC. If errors are found in step 5, steps 1 to 4 are repeated.

During compilation, data are located and retrieved from different sources and saved to XLS files in a standardized format. Commonly, a single source fails to provide all the data and meta-data required by the database, or multiple sources give inconsistent results. Data completion, verification, and

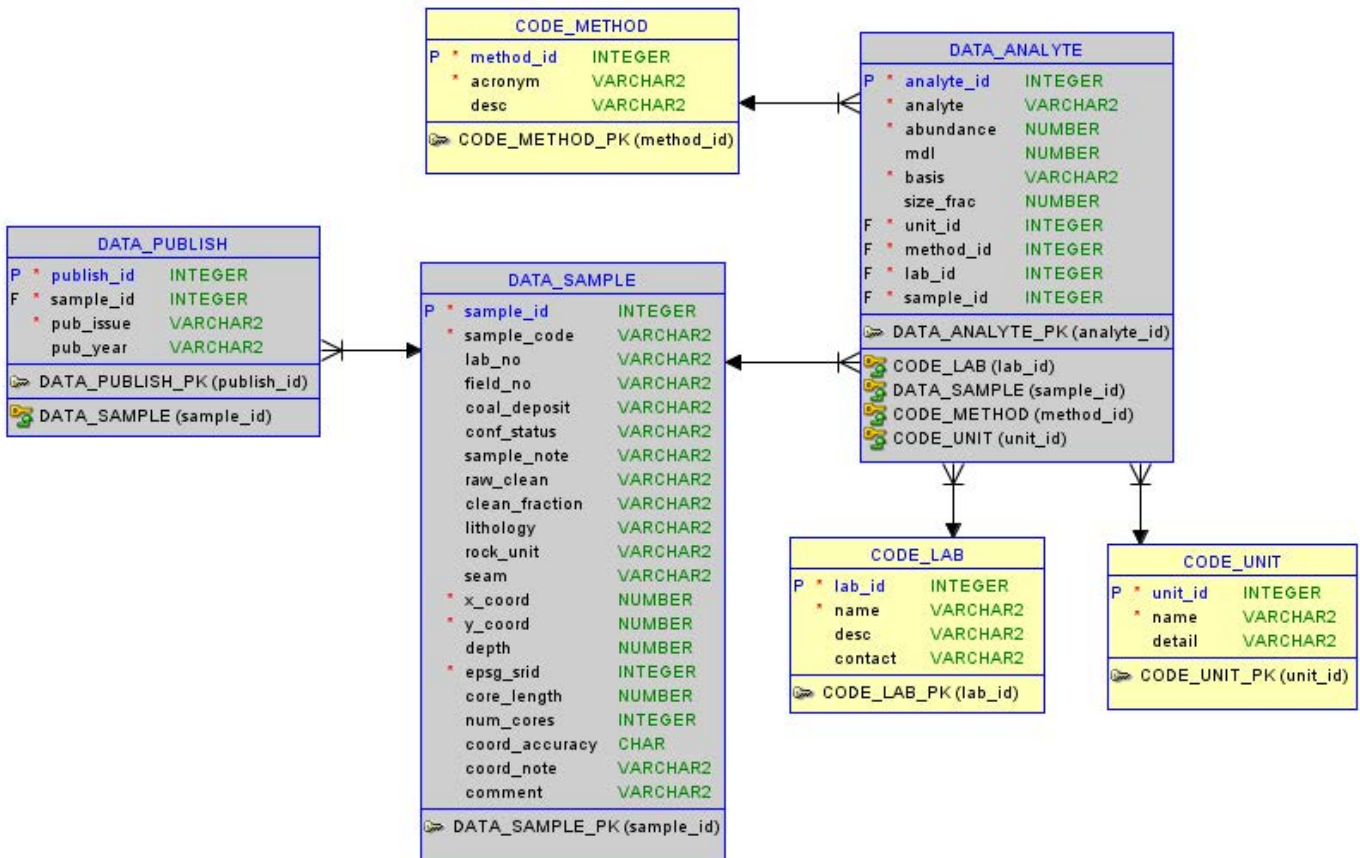


Fig. 2. Logical data model of the coal ash chemistry database.

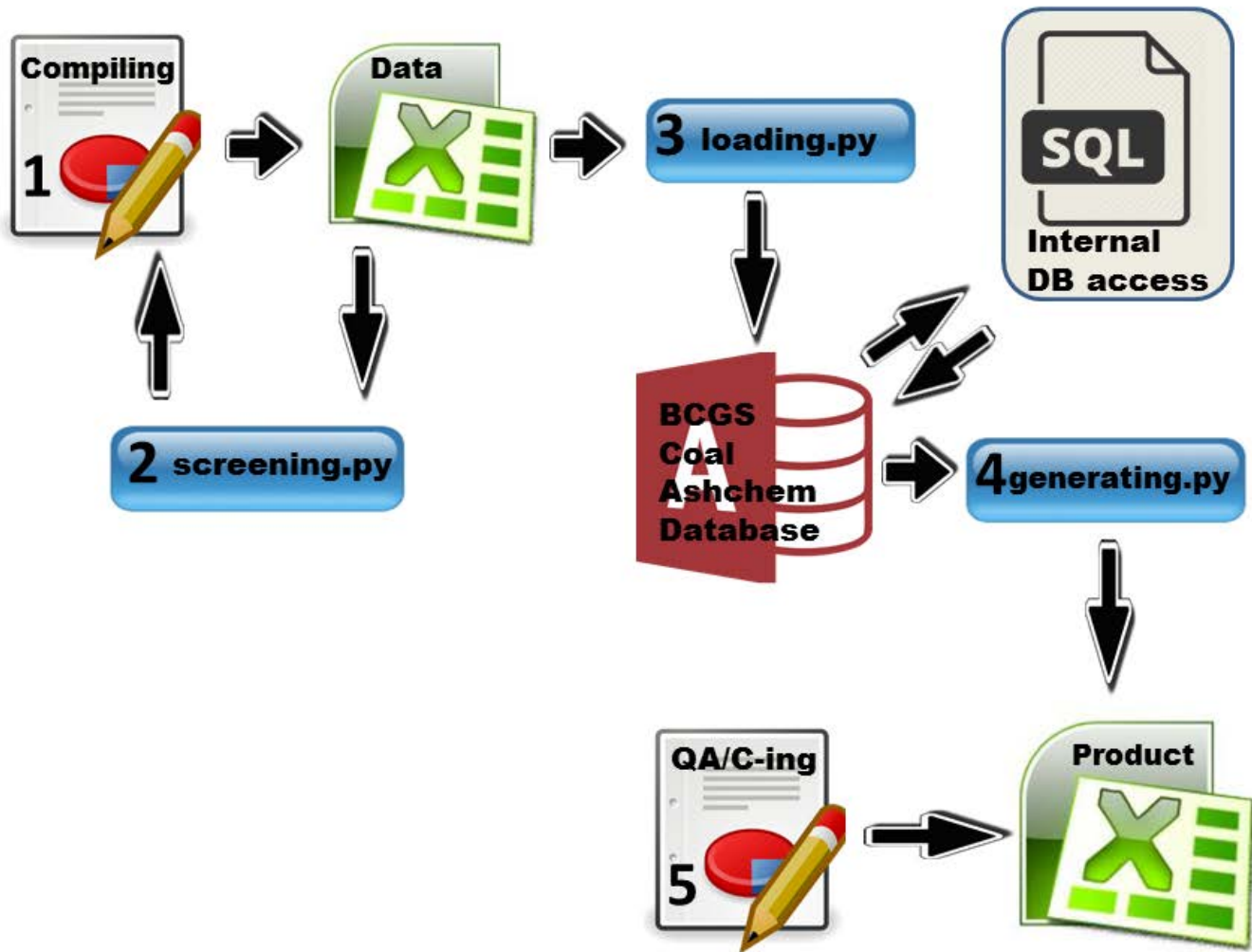


Fig. 3. British Columbia Geological Survey coal ash chemistry data management.

correction are commonly needed to deal with these situations. Data QA/QC is then conducted by the corresponding Python script (`screening.py`), which was designed to flag the most common data errors in the source or introduced in the data compilation. These include errors such as unrealistic determinations and units, improper methods, inappropriate sample locations, and redundant samples. The flagged errors are then corrected manually. Following QA/QC, data are loaded into the database. This is an automatic step done by the corresponding Python script (`loading.py`). To avoid generating duplicate entries, the script checks if a sample is already in the database. Product generating, also conducted by a Python script (`generating.py`), extracts data and outputs them in formats suited to the user (e.g., Comma-Separated-Value (CSV) files, ESRI shapefiles, or MS Access files).

The database and the data products derived from the database differ. First, the format of a data product is determined by the user, whereas the format of the database is defined by the data model and is fixed once database development is finished. Second, data products are commonly derived as the views of a database. As such, they represent only part of the information

contained in the database. Separating the database from the data product is important, because it helps the user generate multiple tailored data products from a single database.

4. The coal ash data set

The database presented herein is provided in a single MS Excel file, in which each row corresponds to a sample described by multiple attributes (Table 1). This format was chosen because it is simple and easily transferred to other software.

Table 1. Structure and content of “coalashchem_data.xls”

Column	Description	Format	Example
Sample_ID	Sequential number used as the row counter (generated by the database)	Integer	5
Lab_No	Lab number	Character string	2047-85
Field_No	Field station number	Character string	7882-CM Adit 21
Coal_Deposit	Coal mine or project	Text	Bullmoose
Conf_Status	Confidentiality status	Text	O or C
Sample_Note	Other sample information	Text	Bulk sample
Raw_Clean	Raw or clean (if specified)	Text	R or C
Clean_Fraction	Clean fraction, specific gravity	Decimal	1.6 float
Lithology	Rock type	Text	Coal
Rock_Unit	Formation or Group	Text	Gates
Seam	Seam identifiers; project specific	Character string	B upper
Core_Length(m)	Length of core sampled in metres	Decimal	1.5
Num_Cores	The number of cores used for the sample	Text	5 or multiple
NAD83_Long	Sample longitude in NAD83	Decimal	-115.227
NAD83_Lat	Sample latitude in NAD83	Decimal	52.336
Depth(m)	Sample depth in meters	Decimal	30.5
NTS_Map	1:50,000 NTS map sample location	Character string	082G15
UTM_Easting	Sample coordinate	Datum NAD83	655490
UTM_Northing	Sample coordinate	Datum NAD83	5513287
UTM_Zone	UTM zone	Northern hemisphere	10
Coord_Accuracy	Accuracy of location; high, medium, or low, as defined in text	Text	H, M or L
Coord_Note	Co-ordinate information not captured in other columns	Text	Adit 1
Comment	Information not captured in other columns	Text	No proximate analysis
Pub_Issue	Issue of publication of data source	Character string	Coal Assessment Report (CAR) 415
Pub_Year	Year of the publication of data source	Integer	1995
Al ₂ O ₃ _%	Al ₂ O ₃ in percent of the ash in the sample	Decimal	25.38
BaO_%	BaO in percent of the ash in the sample	Decimal	0.40
CaO_%	CaO in percent of the ash in the sample	Decimal	2.26

Table 1 continued. Structure and content of "coalashchem_data.xls"

Column	Description	Format	Example
Cao+MnO_%	CaO and MnO in percent of the ash in the sample	Decimal	3.80
Fe ₂ O ₃ _%	Fe ₂ O ₃ in percent of the ash in the sample	Decimal	3.72
K ₂ O_%	K ₂ O in percent of the ash in the sample	Decimal	0.74
MgO_%	MgO in percent of the ash in the sample	Decimal	0.80
Mn ₂ O ₃ _%	Mn ₂ O ₃ in percent of the ash in the sample	Decimal	0.01
Na ₂ O_%	Na ₂ O in percent of the ash in the sample	Decimal	0.05
P ₂ O ₅ _%	P ₂ O ₅ in percent of the ash in the sample	Decimal	1.09
SiO ₂ _%	SiO ₂ in percent of the ash in the sample	Decimal	56.80
SO ₃ _%	SO ₃ in percent of the ash in the sample	Decimal	1.05
SrO_%	SrO in percent of the ash in the sample	Decimal	0.08
TiO ₂ _%	TiO ₂ in percent of the ash in the sample	Decimal	1.15
Undet_%	Undetermined in percent of the ash in the sample	Decimal	0.44
Oxide_lab	Laboratory where ash oxide analyses were done	Text	Birtley
ADM_%_ar	Adsorbed moisture, as received basis	Decimal	8.2
Moisture_%_adb	Inherent moisture, air-dried basis	Decimal	1.2
Moisture_%_ar	Inherent moisture, as received basis	Decimal	2.4
CalorificValue_MJ/kg_ar	Calorific value, in Megajoules per kilogram, air-dried basis	Decimal	32.54
CalorificValue_MJ/kg_db	Calorific value, in Megajoules per kilogram, dry basis	Decimal	32.54
CalorificValue_MJ/kg_adb	Calorific value, in Megajoules per kilogram, air-dried basis	Decimal	32.54
CalorificValue MJ/kg	Calorific value, in Megajoules per kilogram, basis was not specified in source	Decimal	32.54
VolatileMatter_%_db	Volatile matter, dry basis	Decimal	26.5
VolatileMatter_%_adb	Volatile matter, air-dried basis	Decimal	24.5
VolatileMatter_%	Volatile matter, basis not specified in source	Decimal	25.3
FixedCarbon_%_db	Fixed carbon, dry basis	Decimal	66.5
FixedCarbon_%_adb	Fixed carbon, air-dried basis	Decimal	66.5
FixedCarbon_%	Fixed carbon, basis not specified in sources	Decimal	66.5
Ash_%_db	Amount of ash, dry basis	Decimal	11.2
Ash_%_adb	Amount of ash, air-dried basis	Decimal	11.2
Ash_%	Amount of ash, basis not specified in source	Decimal	11.2

Table 1 continued. Structure and content of “coalashchem_data.xls”

Column	Description	Format	Example
ProximateAnalysis_lab	Proximate analysis laboratory	Text	Sunnyvale Minerals Laboratory
Sulphate_%_db	Percent of whole coal sample that is sulphur in the form of sulphate, dry basis	Decimal	0.01
Sulphate_%_adb	Percent of whole coal sample that is sulphur in the form of sulphate, air-dried basis	Decimal	0.01
Pyrite_%_db	Percent of whole coal sample that is sulphur in the form of pyrite, dry basis	Decimal	0.1
Pyrite_%_adb	Percent of whole coal sample that is sulphur in the form of pyrite, air-dried basis	Decimal	0.1
Organic_%_db	Percent of whole coal sample that is in organic form, dry basis	Decimal	0.21
Organic_%_adb	Percent of whole coal sample that is sulphur inorganic form, air-dried basis	Decimal	0.21
TotalSulphur_%_db	Percentage of whole coal sample that is Sulphur, dry basis	Decimal	0.31
TotalSulphur_%_adb	Percentage of whole coal sample that is sulphur, air-dried basis	Decimal	0.31
TotalSulphur_%	Percentage of whole coal sample that is sulphur, basis not specified in source	Decimal	0.31
SulphurForms_lab	Sulphur forms analysis laboratory	Text	CANMET
FSI	Free swelling index	Decimal	4.5
FSI_lab	FSI test laboratory	Text	Sunnyvale
CSR-SHO_%	Coke strength after reaction, sole-heated oven test	Decimal	58.0
CSR_lab	CSR analysis laboratory	Text	CANMET

4.1. Data type and quality

The dataset contains coal ash oxide and related analyses for 478 samples from the Gates, Gething, Minnes and Boulder Creek formations (Fig. 4) in the Peace River coalfields (Fig. 5) in the northeast part of the province, and from the Mist Mountain Formation (Fig. 6) in the Elk River and Crowsnest coalfields of southeastern British Columbia. These coals are mainly bituminous in rank; a few range to the sub-anthracite range. Not all samples in the dataset are coking coals.

The dataset contains the standard ash analyses, including major oxides (SiO₂, Al₂O₃, TiO₂, Fe₂O₃, CaO, Na₂O, K₂O, MgO, P₂O₅, SO₃) and minor oxides (some reports include BaO and SrO). Where available and directly attributable to the same sample or seam, the following attributes were captured.

- Ash content
- Calorific value
- Volatile matter
- Fixed carbon

- Total sulphur
- FSI
- Sulphur forms
- CSR (coke strength after reaction with CO₂)

Sample information includes

- field and lab identifying names or numbers
- data source
- deposit
- formation
- seam
- sample type,
- sample UTM coordinates,
- location coordinate accuracy,
- sample depth,
- analysis method where specified
- if clean, clean fraction sampled

Era	Period & Epoch	BC Rocky Mountains			
		Peace River Coalfields	Elk River & Crowsnest Coalfields		
Mesozoic	Cenozoic	Quaternary			
		Tertiary			
	Cretaceous	Upper			
		Lower	Fort St. John Group	Dunvegan	Alberta Group
				Boulder Creek	
			Gates	Blairmore Group	Beaver Mines
	Bullhead Group	Gething	Gladstone		
		Cadomin	Cadomin		
	Jurassic	Upper	Fernie Group	Fernie Group	
		Middle			Kootenay Group
Lower		Mist Mountain			
Triassic					

Fig. 4. Stratigraphic context and correlation of coal-bearing units in the Rocky Mountains of British Columbia.

Attribute values were derived from about 100 reports submitted over several decades and by many authors. The quality of attribute data varies between reports. Some reports contain detailed information on attributes such as sample, location, laboratory methods used, sample type and seam, while others, especially older reports, contain minimal information.

The database includes different types of samples, including raw exploration samples, run-of-mine, clean composites and bulk samples. Where available, details of the collection method and sample type are captured in the database. Care should be taken when making comparisons between sample types. This public dataset is skewed toward exploration and raw samples over clean; most clean samples remain on Confidential status under the terms of the Coal Act.

Older reports, especially those from before the 1980s, contain few ash chemistry analyses; normally a single sample represents an average clean coal blend product for the entire deposit. In those times the primary goal of ash chemistry analysis was to quantify fouling and slagging potential of the coal. As the importance of ash analysis for predicting coke strength after reaction (CSR) became increasingly recognized, companies commonly obtained numerous analyses for individual seams and for raw, run-of-mine, and clean fractions.

Sample location accuracy for each sample is assigned a

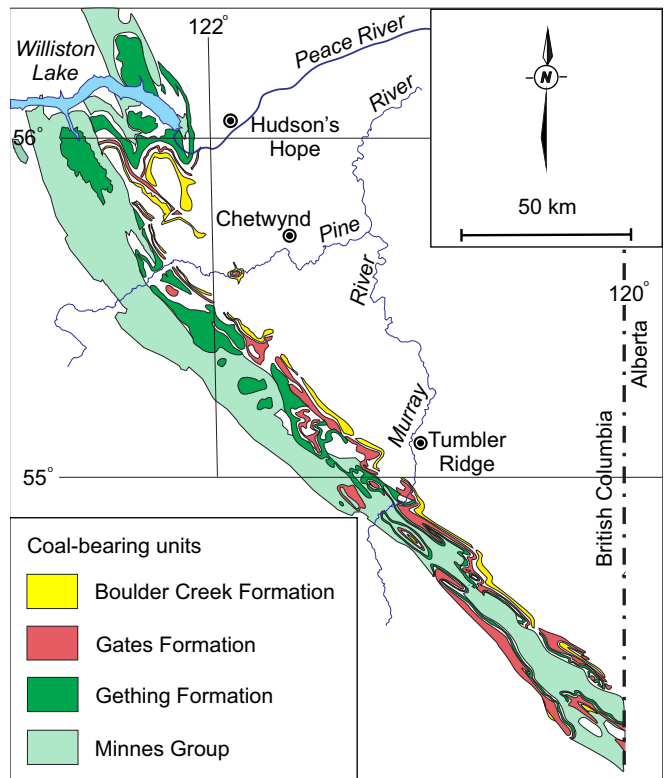


Fig. 5. Distribution of the coal-bearing units of the Peace River coalfields, northeast British Columbia.

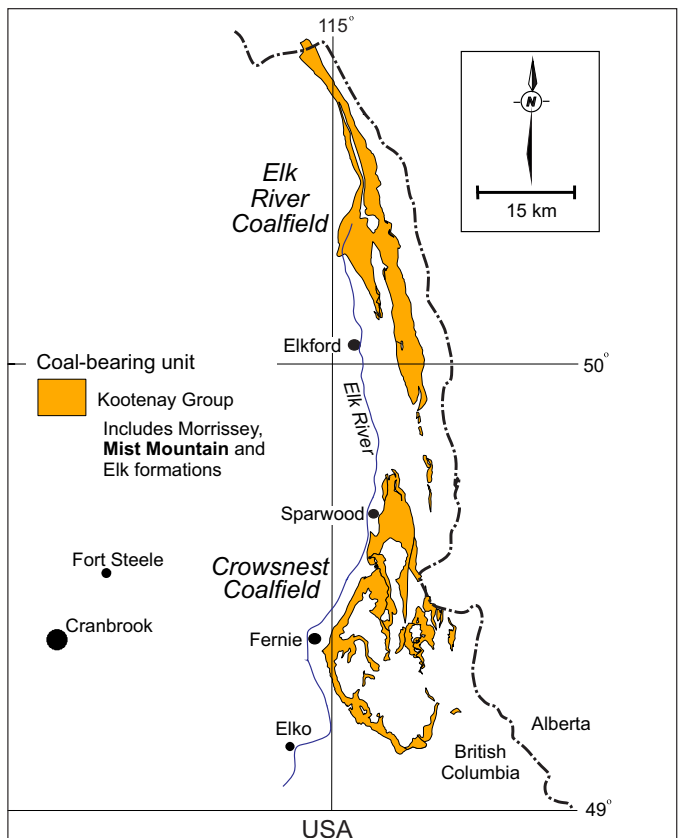


Fig. 6. Distribution of the coal-bearing formation of the Elk River and Crowsnest coalfields, southeast British Columbia.

high, medium or low value. “High” accuracy indicates that the sample location is explicitly provided in the original report. “Medium” indicates that the location is plotted on a map in a report and can be confidently assigned a co-ordinate within 100m or that the sample was collected from a single seam from numerous drill holes or surface sites and a position near the centre of an exploration program was assigned. For “Low” accuracy samples, co-ordinates were not reported and sample is assigned a location near the centre of the property (as designated in MINFILE), or based on other reported information in the report, such as a mention of a geographic location.

5. Discussion

5.1. The uses of ash chemistry analyses

Coal ash chemistry analyses have been used since the early 1980s as a first order indicator of coke strength after reaction (CSR), a measure of coking quality (Pearson, 1989). As a rule of thumb, a base-acid ratio (BAR) value of less than 0.2 is an indicator that the ash chemistry of the sample will not lower the CSR. They are also used to assess slagging and fouling potential (Stach, 1982; Song et al., 2010). Various workers have proposed methods to apply ash analyses to other predictions, such as the phase-mineral assemblages of mineral matter (Ryan and Price, 1993), and depositional environment, tectonic activity during deposition, and subsidence rate (Vassilev et al., 2010).

Major oxide ash analysis is a simple and inexpensive test and is offered by most laboratories, including those that do not specialize in coal analysis. Predictions for CSR based on ash analyses are far less reliable than direct measurements but are a cost-effective way to identify variation within a deposit, formation, or seam, and to make more effective and strategic use of costlier analytical methods. Coal ash chemistry analysis results are not affected by oxidation, so surface samples are adequate. The sample does not have to go through the coking process, so it does not have to be large. Sampling can be done at any stage of exploration, including prospecting.

5.1.1. Indication of coke strength after reaction (CSR)

Coke strength after reaction with CO₂ (CSR) began to be recognized globally as an important measure of coking coal quality in the 1980s. The higher the CSR, the better the coke is expected to perform in the hot CO₂ rich conditions in the blast furnace of a steel mill.

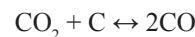
To directly measure CSR, a large coal sample is coked in a laboratory oven. A small sample of the coke is then heated and held at 1100 degrees C under 1 atmosphere pressure of CO₂ for one hour. This is a proxy for conditions in the middle of a blast furnace, but does not replicate them. The resistance of the coke to breakdown under these conditions is quantified by tumbling the resultant coke in a drum test and measuring the % of the coke that remains at greater than 10mm. Steel mills normally require coking coals with CSRs of 57% or higher (Pearson, 1989).

A direct CSR test requires a large sample (250 to 500 kg). Because coking quality is reduced by oxidation of coal

macerals, a fresh, unoxidized sample is required; surface and near-surface samples cannot be used. This is practical during mining and advanced mine development, but not at early exploration stages. The cost of collecting and transporting large samples and the scarcity of laboratories with the appropriate testing facilities limit the numbers of direct CSR tests that are done.

In addition to the base-acid ratio (BAR) of the ash, other factors known to affect the reactivity of coke to CO₂ include the composition of the mineral matter in the coal, the amount of ash, the volatile content (coke from medium volatile coal are less reactive those from high and low volatile coals), coal texture, rank, and the ratio of inert to reactive macerals (Pearson, 1989). Many methods of predicting CSR using these parameters have been proposed to save on the cost of direct CSR testing (Pearson, 1989; Ryan and Price, 1993; Todoschuk et al., 2004; Hu, 2002). However, because every coal basin is different, methods that can be relied upon to produce accurate predictions for coals from all coking coal-producing basins around the world are elusive.

The Boudouard reaction:



occurs in the steel blast furnace and represents the breakdown of coke in the presence of CO₂, after which the coke is no longer functional and needs to be replaced (Ryan and Price, 1993). At temperatures above 1000 degrees C, this reaction is catalysed and proceeds at much higher rates in the presence of iron, calcium, sodium, potassium and magnesium (Linstad et al., 2004; Longbottom et al., 2014). The oxides of silicon, aluminum and titanium are relatively inert. Thus the Base-Acid Ratio

$$\text{BAR} = (\text{Fe}_2\text{O}_3 + \text{CaO} + \text{NaO} + \text{K}_2\text{O} + \text{MgO}) / (\text{SiO}_2 + \text{Al}_2\text{O}_3 + \text{TiO}_2)$$

can be used as a first order predictor of CSR. (Some workers include TiO₂ in the equation, others do not). A coking coal with a lower BAR can be expected to make a coke that will last longer and perform better in the blast furnace. As a rule of thumb, coking coals with a BAR of less than 0.2 have ash chemistry that does not lower CSR. The BAR is a blunt instrument for CSR prediction because it uses ash chemistry only, ignoring other important factors that control CSR: composition of the mineral matter, amount of ash, volatile content/rank, coal texture, and maceral type.

5.1.2. Use of the BAR index to predict slagging and fouling

A low BAR also indicates a higher fusion temperature, which predicts a lower likelihood of slagging and fouling problems (Stach, 1982) in any coal. Slagging and fouling occur when the ash melts in a furnace or boiler and forms hard sticky materials that interfere with the furnace or boiler function. When ash particles come into contact with hot surfaces, they may melt and form slag, which is costly to dispose. Fouling occurs where ash particles soften and adhere to furnace or boiler surfaces such as combustion chambers and gas outlets.

5.1.3. The origin of mineral matter in coal

Mineral matter in coal can be phytogenic, detrital, or authigenic. Phytogenic minerals are components of some plants (for example silica in horsetails and grasses). Detrital minerals are introduced by water, wind, or groundwater, and authigenic minerals form during coalification and can be deposited in cracks by descending or ascending solutions (Mackowsky, 1975; Diessel, 1992).

Coals that were overlain by non-marine sedimentary deposits tend to have mineral assemblages that produce favourable base-acid ratio chemistry for the CSR of coking coals. Fresh-water cover preserves the acidic conditions of the peat swamp, which discourages bacterial action and favours the nucleation of kaolinite, resulting in coal with a mineral matter component consisting mainly of a kaolinite-quartz assemblage. A marine cover introduces additional sulphur and changes the pH from acidic to alkaline conditions, encouraging bacterial action, which reduces sulfate to H_2S . These conditions lead to the production of sulphide and nucleation of pyrite and, possibly, calcite and illite (Teichmüller and Teichmüller, 1975; Mackowsky, 1975; Pearson 1980). The quartz-kaolinite assemblage is richer in the non-reactive cations (Si, Al) and relatively poorer in the reactive ones (Fe, Ca, Na, Mg and K), resulting in a lower BAR and a less reactive coke.

Experiments by Price et al. (1992) showed that of the minerals commonly found in coal, those damaging to CSR are pyrite, siderite, bauxite, calcite, gypsum, lime and magnesium oxide. Minerals that are neutral or positive for CSR are quartz, apatite, kaolinite, feldspars and muscovite.

5.2. The ash chemistry character of British Columbia Rocky Mountain bituminous coals.

The data summarized herein (Tables 2-5; Figs. 7-11) include all types of samples, from exploration grab samples, to channel, to run-of-mine, to bulk samples and clean composites. They were not pre-selected to represent the clean product coals of these coalfields. The averages and the variability of quality parameters represent the entirety of coals sampled during exploration and development in the Rocky Mountain coalfields. Exploration samples commonly include seams and sub-members that would not be included in run-of-mine or bulk samples, and coals that may not coke. This public dataset is skewed toward exploration and raw samples over clean because most clean samples remain on confidential status under the terms of the British Columbia Coal Act Regulation. The database structure allows for sorting and separation of types of samples for analytical applications.

The major Rocky Mountain coal-bearing formations were deposited mainly in non-marine environments (Stott, 1968, 1975; Carmichael, 1982; Leckie and Kalkreuth, 1990; Legun, 1990; Grieve, 1993). Consequently, the quartz-kaolinite assemblage with low sulphur is the most common mineralogy (Pearson, 1980; Grieve et al., 1996). Of 69 raw run-of-mine samples from the Mist Mountain and Gates formations in a low-temperature ash (LTA) survey (Grieve et al., 1996), only four

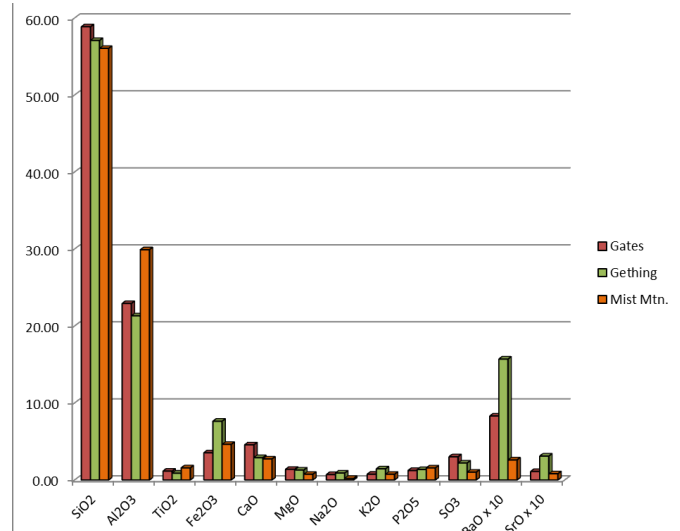


Fig. 7. Mean coal ash oxide values, in percent of ash, for the Gates, Gething, and Mist Mountain formations.

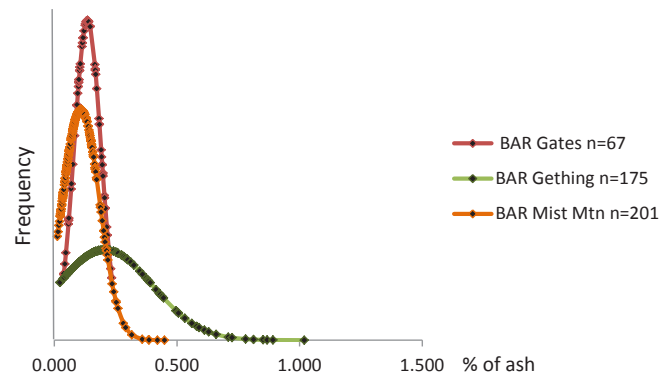


Fig. 8. Frequency distribution curves for base-acid ratios for the Gates, Gething and Mist Mountain formations

lack quartz and kaolinite as the two most abundant minerals.

British Columbia Rocky Mountain bituminous coking coal products are recognized for their favourable ash chemistry and good CSR values (Pearson, 1980, 1989; Grieve et al., 1996). Only five samples in the database have coke strength after reaction CSR tests; two from the Mist Mountain Formation and three from the Gething Formation. All BAR values presented herein were calculated including TiO_2 in the BAR equation. Not all Rocky Mountain coals are non-marine; marine transgressions are preserved the Gates, Gething and Mist Mountain formations, distinguishable by total sulphur values that are anomalously high relative to the rest of the dataset. High values for Fe_2O_3 may flag the presence of pyrite (FeS_2) or siderite ($FeCO_3$), both of which have a negative effect on CSR.

Thirty-five samples were not included in Tables 2 to 5 and Figures 7 to 11, but they remain in the database. Samples from the Boulder Creek Formation and Minnes Group are too few for meaningful comparisons and were not tabulated. Anomalously rusty, calcareous and bony coals were also excluded (i.e., where $Fe_2O_3 > 32\%$, $CaO > 25\%$, $SiO_2 < 20\%$, and ash $> 40\%$).

Table 2. Oxides and BAR means and medians.

	Major oxides										Minor oxides		BAR	
	SiO ₂	Al ₂ O ₃	TiO ₂	Fe ₂ O ₃	CaO	MgO	Na ₂ O	K ₂ O	P ₂ O ₅	SO ₃	BaO	SrO		
All samples	56.88	25.38	1.21	5.70	3.08	1.05	0.50	1.02	1.42	1.83	0.60	0.16	.151	mean
	56.80	25.87	1.15	3.72	2.26	0.80	0.38	0.74	1.09	1.06	0.40	0.08	.112	median
	443	443	409	443	443	435	439	439	417	416	48	51	443	samples
Gates	58.86	22.92	1.15	3.53	4.56	1.38	0.70	0.75	1.23	3.01	0.83	0.11	.135	mean
	58.70	22.93	1.12	3.30	4.39	1.37	0.66	0.58	1.04	2.98	0.71	0.08	.130	median
	67	67	67	67	67	67	67	67	67	67	10	10	67	samples
Gething	57.08	21.41	0.88	7.78	2.90	1.28	0.90	1.44	1.35	2.20	1.57	0.31	.206	mean
	57.80	19.65	0.83	4.48	2.18	0.91	.067	1.33	0.96	1.32	1.56	0.31	.127	median
	175	175	172	175	175	175	175	174	170	174	5	5	175	samples
Mist Mtn.	56.05	29.66	1.57	4.62	2.73	0.73	0.20	0.73	1.56	1.01	0.39	0.15	.108	mean
	56.14	29.90	1.56	3.70	2.00	0.46	0.10	0.60	1.20	0.60	0.26	0.08	.091	median
	201	201	171	201	201	193	197	198	180	175	33	36	201	samples

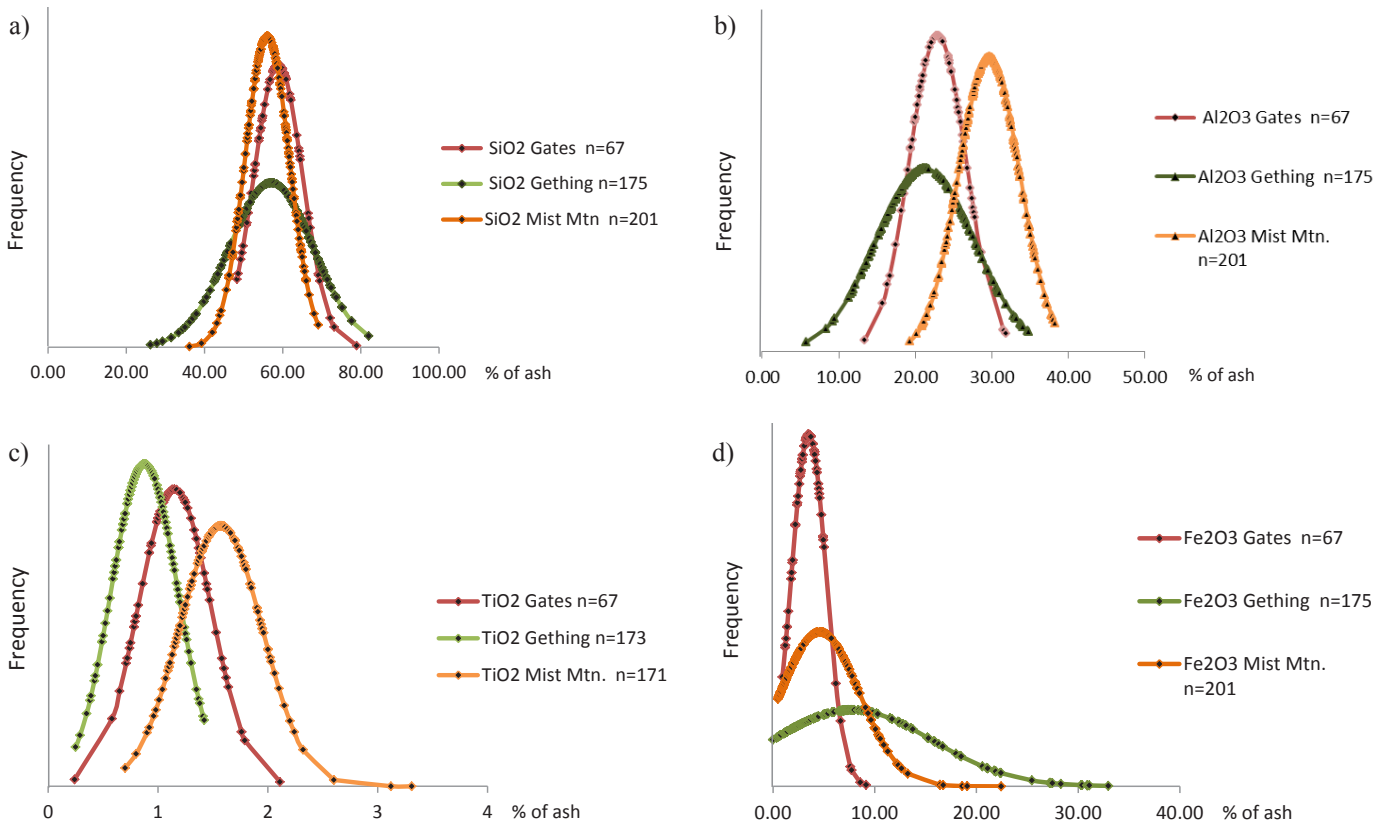


Fig. 9. Frequency distribution curves for major oxides for the Gates, Gething and Mist Mountain formations. **a)** SiO₂ **b)** Al₂O₃; **c)** TiO₂; **d)** Fe₂O₃; **e)** CaO; **f)** MgO; **g)** Na₂O; **h)** K₂O; **i)** P₂O₅; **j)** SO₃.

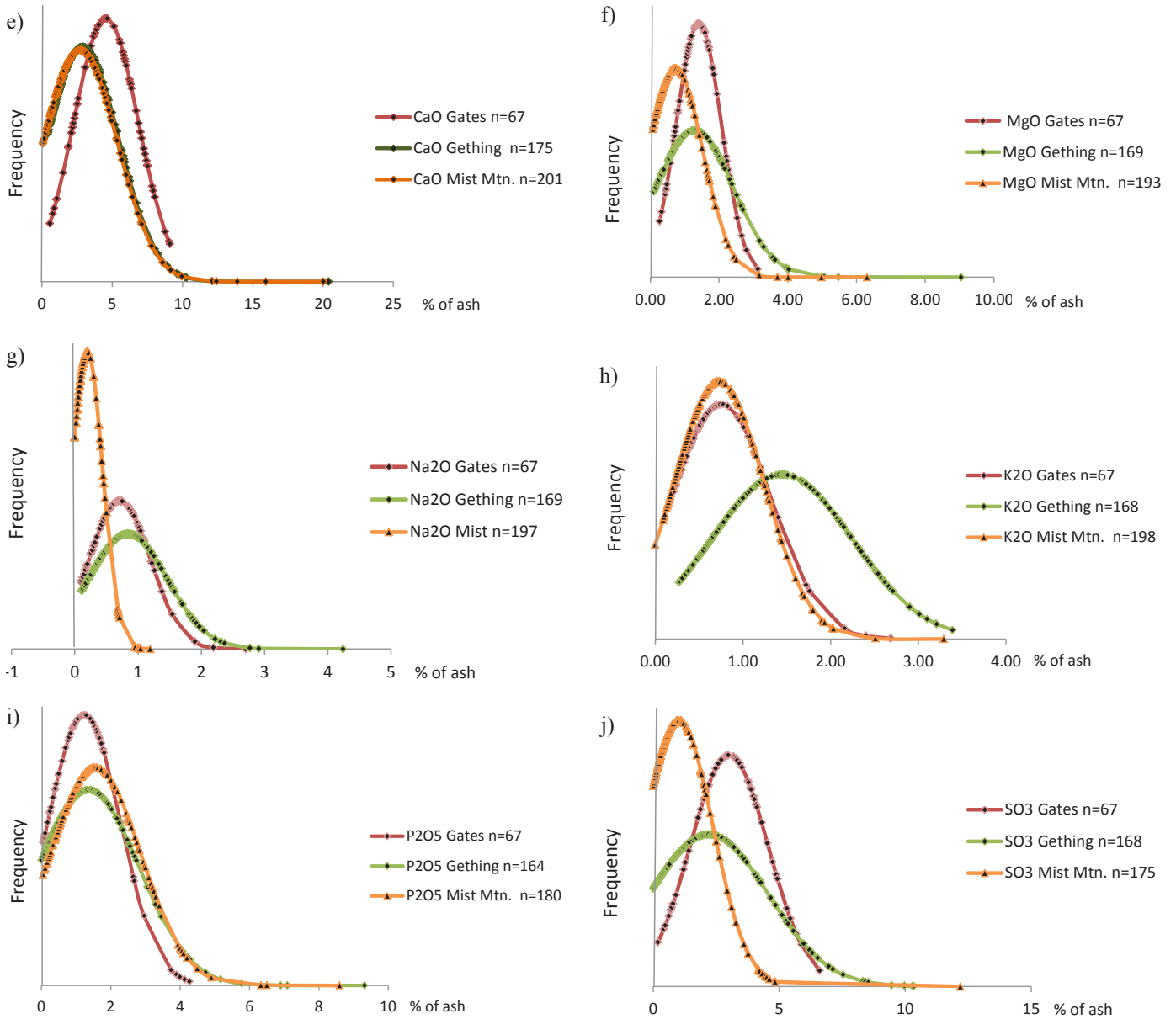


Fig. 9.continued.

BAR values for British Columbia Rocky Mountain bituminous coals tend to be low, less than 0.2 (Table 2), which favours good CSR values for coking coals. The BAR values for Gates and Mist Mountain formations show narrow ranges of values; the range of values is notably higher for the Gething Formation creating a flatter wider curve, skewed to the high side (Fig. 8).

The values for the oxides of SiO₂ and Al₂O₃ form symmetrical bell-shaped distribution curves for all three formations. All other distributions, with the exception of CaO for the Gates, form right-skewed curves, caused by a handful of strongly anomalous high-side values (Fig. 9). The Gething Formation curves for the oxides are markedly wider and flatter than those of the Gates and Mist Mountain for most of the analytes (SiO₂, Al₂O₃, Fe₂O₃, MgO and Na₂O). This is consistent with the reputation of the Gething Formation coal having markedly

heterogeneous coal properties along trend and even within seams (Ryan, 1997; Ryan and Lane, 2006), and accounts for the greater range of values for the BAR for the Gething. The Gething includes some marine-influenced seams coal seams which may have pyrite, which can add to the skew of the Fe₂O₃ curve to the right (Fig. 9d). The median value of the BAR for the Gething is 1.25, much less than the mean of 2.15 (Table 2), and is more representative of the formation as a whole. BAR values correlate with Fe₂O₃ values most strongly in the Gething Formation (Table 5). CaO values are markedly higher and correlate better with BAR values in the Gates formation than they do in the Gething and Mist Mountain formations (Figure 9e, Table 5).

Some reports include analyses for the minor oxides BaO and SrO (Fig. 10). These data are used to improve understanding of potential environmental contaminants, and can also serve as

Table 3. Oxides, BAR and AI means broken down by coking clean, coking raw, and non-coking coals.

	Major oxides										Indices			
	SiO ₂	Al ₂ O ₃	TiO ₂	Fe ₂ O ₃	CaO	MgO	Na ₂ O	K ₂ O	P ₂ O ₅	SO ₃	BAR	AI	Ash	
Gates Coking Clean (FSI >3)	56.94	22.90	1.19	4.18	4.80	1.65	0.90	0.72	1.10	3.17	.153	1.58	8.0	mean
	58.00	23.18	1.10	3.73	4.34	1.50	0.90	0.62	1.14	2.98	.139	1.65	7.9	median
	15	15	15	15	15	15	15	15	15	15	15	6	12	samples
Gates Coking Raw and unspecified (FSI >3)	58.85	24.02	1.21	3.22	4.09	1.25	0.60	0.82	1.47	2.73	.122	1.73	14.5	mean
	58.70	24.51	1.17	2.72	3.47	1.28	0.50	0.60	1.20	2.70	.106	1.40	11.3	median
	34	34	34	34	34	34	34	34	34	34	34	34	34	samples
Gates Non-coking	61.24	20.35	1.10	3.46	5.18	1.38	0.70	0.73	0.81	3.29	.143	3.80	26.4	mean
	59.00	20.00	1.07	3.48	6.88	1.58	0.73	0.50	0.95	3.43	.165	4.51	25.8	median
	13	13	13	13	13	13	13	13	13	13	13	13	13	samples
Gething Coking Clean (FSI >3)	53.20	25.90	0.93	7.84	3.21	1.31	0.80	1.06	1.56	2.41	.206	2.61	14.6	mean
	54.10	27.50	0.88	6.02	2.26	0.85	0.66	0.76	0.89	1.37	.112	1.30	11.1	median
	26	26	23	26	26	26	26	26	23	26	26	26	26	samples
Gething Coking Raw and unspecified (FSI >3)	55.43	19.92	0.86	9.26	3.11	1.52	0.90	1.59	1.47	2.43	.240	2.46	11.8	mean
	55.40	17.90	0.77	7.36	2.60	0.94	0.66	1.47	0.74	2.05	.201	1.51	10.5	median
	54	54	54	54	54	54	54	54	52	54	54	54	54	samples
Gething Non-coking	58.87	21.47	0.87	6.64	2.60	1.10	0.80	1.47	1.29	2.00	.180	1.77	11.1	mean
	61.61	20.10	0.84	2.90	1.88	0.86	0.71	1.41	1.00	1.10	.107	0.94	8.03	median
	93	93	93	93	93	93	93	92	93	93	93	85	85	samples
Mist Mtn. Coking Clean (FSI >3)	55.79	29.25	1.72	5.91	2.03	0.49	0.10	0.66	1.57	0.68	.109	0.74	8.2	mean
	55.02	29.40	1.60	5.40	1.80	0.40	0.08	0.60	1.18	0.60	.096	0.72	7.9	median
	51	51	37	51	51	51	51	51	51	37	51	37	37	samples
Mist Mtn. Coking Raw and unspecified (FSI >3)	56.04	30.07	1.58	5.11	1.75	0.73	0.20	0.85	1.21	0.88	.102	1.20	12.9	mean
	55.30	30.30	1.50	4.23	1.60	0.64	0.10	0.66	0.80	0.64	.090	0.90	9.8	median
	38	38	36	38	38	34	36	36	33	33	38	38	38	samples
Mist Mtn. Non-coking	54.25	29.62	1.51	4.32	4.20	1.25	0.30	0.82	1.34	1.46	.136	1.72	14.6	mean
	54.90	29.30	1.50	2.76	3.03	0.73	0.17	0.68	0.87	0.70	.116	1.28	14.0	median
	56	56	49	56	56	55	55	55	47	50	56	56	55	samples

Table 4. Total sulphur: means, medians and ranges of values, by formation.

	Number of samples	Total sulphur mean %	Total sulphur median %	Range %
All samples	351	0.571	0.500	0.14 – 2.55
Gates	65	0.433	0.420	0.14 – 0.84
Gething	163	0.758	0.710	0.28 – 2.55
Mist Mtn.	123	0.395	0.370	0.14 – 0.87

flags for identifying the mineralogy of phosphatic minerals in the coal (i.e., Ba for gorcoixite and Sr for goyazite), or indicate tonsteins in the seam.

Table 3 shows mean and median values broken down by formation and into clean coking, raw coking and non-coking categories. The amount of ash and the ash index (AI; ash percentage multiplied by BAR) are also tabulated. Non-coking coals are defined for this table as those with FSI values of 3 or lower. This table gives some indication of the effect of coal washing on the BAR and AI values. Clean Gates Formation coking coals have higher a mean BAR than the raw coking coals, but a lower AI, indicating that washing is effective at reducing total ash levels, but less effective at removing the minerals that produce reactive oxides in the ash. The opposite effect is seen in the Mist Mountain Formation data, where the BAR is similar for clean and raw coking coals, but the AI is

significantly lower for the clean coals; possibly indicating that washing processes more effectively remove the reactive components. The AI numbers for the Gething Formation are complicated by a quirk of the dataset: the clean coking samples all have higher ash content than the raw coking samples. All 26 of the clean samples in the Gething dataset are from the Bri-Dowling and Peace River deposits near Williston Lake, which happen to have higher mean ash values than the raw coking and the non-coking samples in the dataset. Comparisons about the differences in ash chemistry in coking vs raw Gething coals from this dataset are unlikely to be meaningful.

Total sulphur values for non-marine coals from the Canadian Rockies and from Australian Gondwana coals tend to be below 1%, in contrast to marine-influenced Illinois Basin and Appalachian coals, which have total sulphur values as high as 5% (Pearson, 1980). This shows up in the ash analyses as relatively high mean SiO₂ and Al₂O₃ values and relatively low mean Fe₂O₃ values (Table 2; Fig. 9). Of the 350 samples in this database that have total sulphur analyses reported, the mean value is low, at 0.571% (Table 4). Maximum values for the Gates and Mist Mountain formations are less than 1%; values in the Gething Formation range as high as 2.55%.

Sulphur forms analyses identify how much of the sulphur in a sample occurs in organic form, how much as pyrite, and how much as sulphate. The dataset includes sulphur forms analyses from 191 samples. The relative amounts of the sulphur forms are plotted on ternary diagrams (Fig. 11). In the Gates, Gething and Mist Mountain formations, organic sulphur is the predominant form, pyrite is less common, and sulphate is negligible or below detection. This can help identify the minerals in the coal. For example, if a sulphur form analysis for a sample with high Fe₂O₃ shows that there is very little pyrite (FeS₂) in the sample, the iron must be in a different mineral, such as siderite (FeCO₃).

Table 5. Correlation coefficients for base-acid ratios and major oxides, by formation.

	SiO ₂	Al ₂ O ₃	TiO ₂	Fe ₂ O ₃	CaO	MgO	Na ₂ O	K ₂ O	P ₂ O ₅	SO ₃	
Gates BAR	-0.739	-0.171	-0.010	0.744	0.872	0.794	0.401	-0.178	0.172	0.628	Correlation coefficient
	67	67	67	67	67	67	67	67	67	67	Samples
Gething BAR	-0.759	-0.427	-0.414	0.935	0.634	0.564	-0.036	-0.234	-0.097	0.738	Correlation coefficient
	175	175	172	175	175	175	175	174	170	174	Samples
Mist Mtn. BAR	-0.724	-0.514	-0.154	0.747	0.665	0.677	0.078	0.138	0.160	0.474	Correlation coefficient
	201	201	170	201	201	193	197	198	180	175	samples

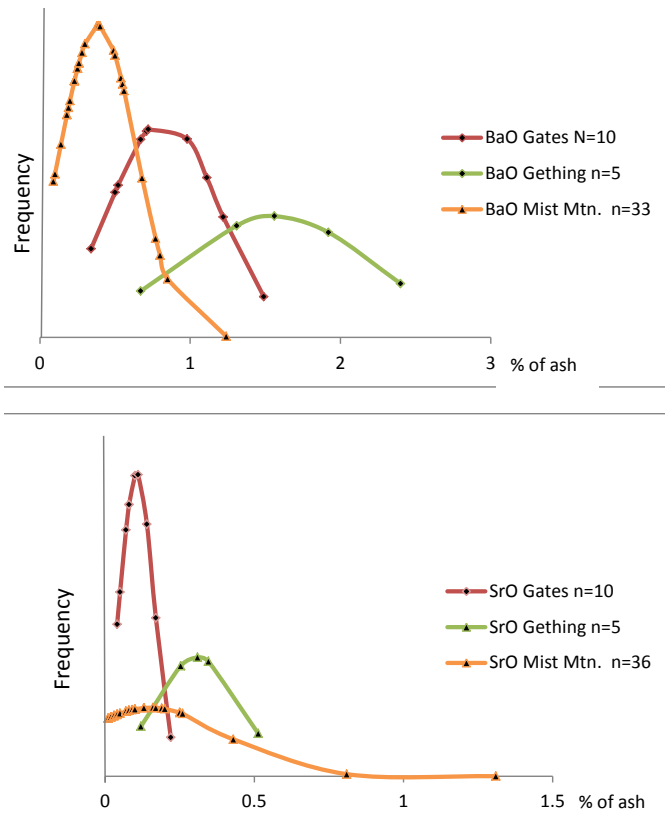


Fig. 10. Distribution curve comparisons by formation for BaO and SrO.

6. Summary

The coal ash chemistry database contains analyses of 478 samples of British Columbia Rocky Mountain bituminous coals. The data were captured from BC COALFILE and other public sources. The three major coking coal-bearing formations of the British Columbia Rocky Mountain coalfields, the Gates, Gething and Mist Mountain formations are recognized for their favourable ash chemistry and good coke strength after reaction (CSR) values. Most seams in British Columbia Rocky Mountain coalfields have predominantly low sulphur, quartz-kaolinite mineral assemblages, which are typical of non-marine depositional environments. This assemblage is richer in the non-reactive elements (silicon and aluminum), and poorer in the undesirable reactive elements (iron, calcium, magnesium, sodium, potassium), which catalyze reactions that erode coke under blast furnace conditions.

The data from the Gething Formation shows the most variability, having greater ranges of values for ash oxides, especially Fe_2O_3 and K_2O , and to a lesser extent, SiO_2 , Al_2O_3 , MgO , SO_3 and BaO . Mean values of Fe_2O_3 , K_2O and BaO are markedly higher in the Gething Formation compared to the Gates and Mist Mountain formations. The mean value of CaO is notably higher for the Gates Formation than for the Gething or Mist Mountain formations.

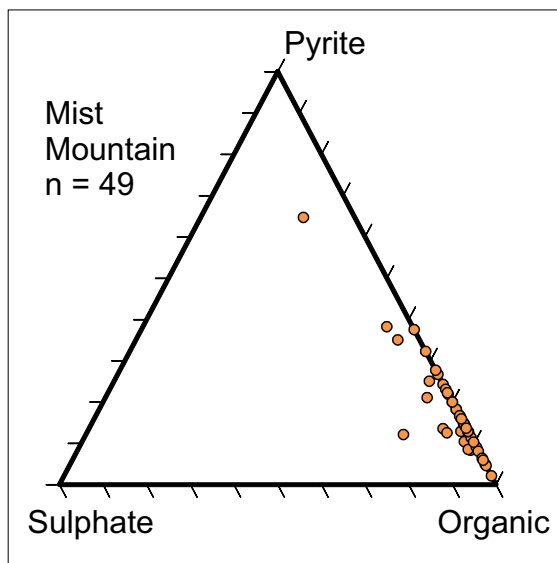
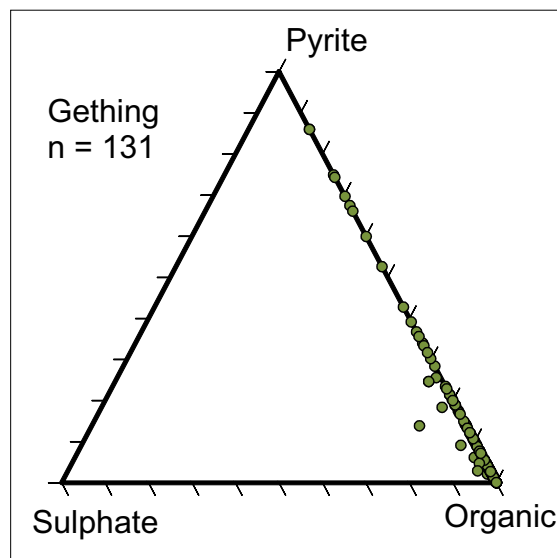
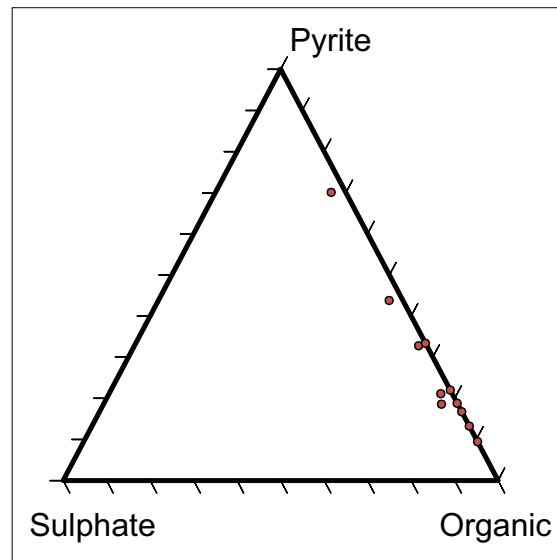


Fig. 11. Sulphur forms of the Gates, Gething and Mist Mountain formations.

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