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BRITISH COLUMBIA
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Front cover: Coal core from the Gething Formation, Carbon Creek, northern British Columbia. **Photo by Paul Jago**.

Back cover: Sheared coal from the Gates Formation, northern British Columbia. **Photo by Paul Jago**.

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Evaluation of coal ash chemistry indices for predicting CSR (coke strength after reaction with CO_2) for coking coals of the Rocky Mountains, British Columbia

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Abstract
CSR (coke strength after reaction with CO_2) is a globally accepted measure of coking coal quality. But because obtaining direct CSR measurements is logistically complex, time-consuming, and expensive, numerous indices calculated from standard ash analyses have been developed to serve as predictors of CSR. Based on unpublished proprietary data from 50 samples representing the main coking coal-producing units in the Rocky Mountains of British Columbia (Gates, Gething, and Mist Mountain formations), correlations between measured CSR and the most commonly used predictive index (Base-Acid Ratio or BAR) are moderate to strong. Thus, they can be used to provide a reasonable first-order prediction for CSR. For all three formations, correlations improve slightly by modifying the predictive index by adding P_2O_5. Correlations improved further when the BAR index was modified to correct for calcium in apatite, which is less reactive that calcium in carbonate minerals. Ash chemistry-based predictions are not accurate enough for feasibility studies or product marketing, but they can provide a timely and inexpensive first indication of CSR. The relationships between CSR and other factors (rank, fluidity, and petrographic properties) have much weaker correlations to CSR than ash chemistry. CSR prediction methods that are based on rheological and petrographic properties fail to correlate well with measured CSR values for the British Columbia Rocky Mountain coking coals in this study and appear to have no predictive value.

Keywords: Coke strength after reaction with CO_2 (CSR), coal ash chemistry, Gates Formation, Gething Formation, Mist Mountain Formation, British Columbia, coking coal quality, predictive indices, base-acid ratio (BAR), ash index, correction for calcium in apatite

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1. Introduction

Although CSR (coke strength after reaction with CO_2) is a well-accepted measure of coking coal quality, obtaining direct CSR measurements is logistically complex, time-consuming and expensive. In contrast, collecting samples for ash chemistry is relatively simple and the analyses can be done rapidly and at low cost. Ash chemistry has a strong influence on CSR, and numerous indices calculated from standard coal ash analyses have been developed to serve as CSR proxies (e.g., Price et al., 1992; Ryan and Price, 1992; de Cordova et al., 2016). Where such indices (e.g., Base-Acid Ratio (BAR) and Ash Index (AI) correlate well with CSR, they provide a first-pass prediction of coking coal quality and can serve as a valuable exploration tool (Ryan et al. 1999). The applicability of these indices is not universal, and the effectiveness of CSR prediction methods varies between coal basins (Price and Gransden, 1987; Pearson, 1989; Todoschuck et al., 2004; de Cordova et al., 2006; North et al., 2018). Thus, the reliability of ash chemistry indices needs to be tested basin-by-basin or even unit-by-unit.

Ash chemistry-based predictive methods are based on the principle that under blast furnace conditions (temperatures above 1000 °C and in the presence of CO_2), iron, calcium, sodium, potassium and magnesium catalyze the Boudouard reaction:

$$CO_2 + C \leftrightarrow 2CO \qquad \text{(Eq. 1)}$$

which represents the breakdown of coke (Linstad et al. 2004, Longbottom et al. 2014). When this occurs in a blast furnace, the coke is no longer functional and needs to be replaced (Ryan and Price 1993). The oxides of silicon, aluminum and titanium are relatively inert. Thus, ash chemistry-based indices quantify the relative amounts of catalytic and non-catalytic materials in the ash. The higher the ratio, the lower the CSR that would be expected. Nippon Steel Corporation established a CSR of 57% as a minimum for trouble-free operation of a conventional steel blast furnace (Pearson, 1989). What constitutes acceptable to highly desirable CSR values varies with the steelmaker, depending on how much PCI (pulverized coal injection coal) is used (Ryan et al. 1993), and other differences in blast furnace technology. Pricing schemes based on specifications vary, and change with time (for examples, see S&P Global Platts, 2020; HIS Markit, 2019). At the time of this writing CSRs of greater than 62% are considered good; depending on the buyer, premium prices are offered for coals with CSRs of 67 to 72%.

In this paper, we used CSR and confidential ash chemistry data from 50 samples collected and analyzed by coal exploration companies working in the Rocky Mountains of British Columbia (Fig. 1). The samples are from the three main coking coal-bearing units in the province, the Gates, Gething, Mist Mountain formations (Fig 2). These data are confidential under the terms of the British Columbia Coal Act Regulation, so the data values and identifying information are not included. The data appear on plots, identified only their host formation. The main goal of this study is to test the validity of CSR prediction methods that are based on ash chemistry by comparing measured CSR values to ash chemistry-based indices for these coals. In addition to Base-Acid Ratio and Ash Index we consider new indices that include P_2O_5, and an index that corrects the BAR index for calcium in apatite. We find that measured CSR values from Rocky Mountain coking coals in British Columbia correlate well with all the indices we tested. Although the accuracy of ash chemistry-based predictions is not precise enough for feasibility studies or product marketing, this study indicates that they can provide a timely and inexpensive first indication of CSR for these coals.

2.Geological setting

The 50 samples used in this study are from the Gething, Gates, and Mist Mountain formations (Figs. 1, 2), the three rock units that host economically important deposits of metallurgical coal in British Columbia. These formations are components of three major Mesozoic siliciclastic sequences that are preserved in the Rocky Mountains of Canada (Stott, 1984). Each of these sequences was formed by a major transgressive-regressive cycle and includes marine, prodeltaic, nearshore, deltaic, and alluvial deposits.

The Mist Mountain Formation is part of the lowest sequence, which includes Jurassic marine shales of the Fernie Formation that are overlain in the East Kootenay coalfields by Jurassic to Lower Cretaceous sandstones, siltstones, shales, mudstones, and conglomerates of the Kootenay Group (Fig. 2). Part of the Kootenay Group, the Mist Mountain Formation consists of deltaic and interdeltaic coastal plain deposits, up to 665 m thick, that are overlain by fluvial to alluvial deposits (Grieve, 1993). The Gething and Gates formations are parts of the second cycle, which includes Lower Cretaceous marine and non-marine siliciclastic rocks of the Bullhead and Fort St. John Groups in the Peace River coalfields (Fig. 2). The Gething Formation, a component of the Bullhead Group, includes Hauterivian to earliest Albian conglomerate, coarse- to fine-grained sandstone, siltstone, mudstone, claystone and coal (Gibson, 1992). In the British Columbia Rocky Mountain foothills, its thickness ranges from 120 to 1000 m. The Gates Formation, up to 260 m thick, is an Albian component of the Fort St. John Group, and comprises nearshore-marine sandstones and non-marine strandplain and fluvial deposits (Lamberson et al. 1996). The third sequence includes Upper Cretaceous successions that do not host coking coal.

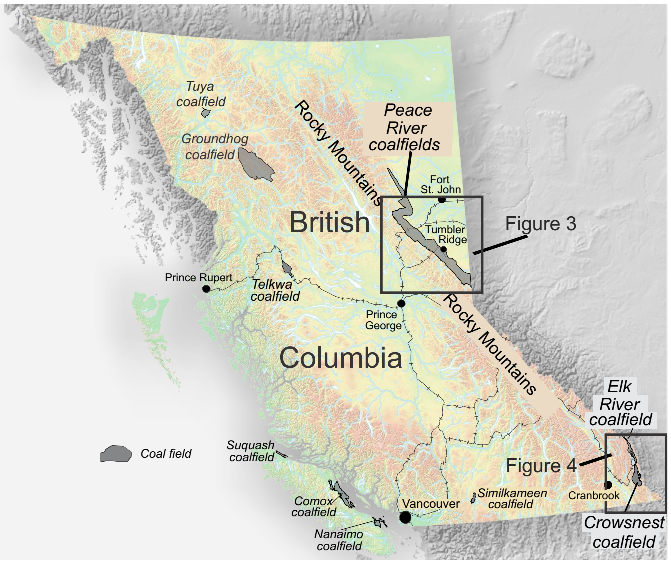


Fig. 1. Coalfields in British Columbia.

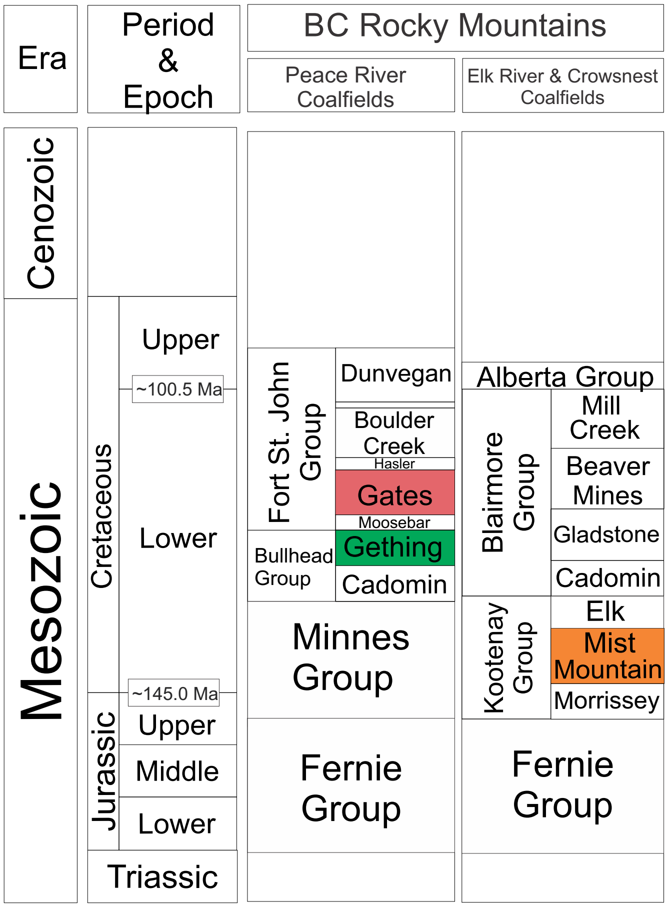


Fig. 2. Coalfield stratigraphy, Rocky Mountains of British Columbia. Analyses of samples from the three main coking-coal producing units (Mist Mountain, Gething, and Gates formations) are used in this study.

Western Canadian Rocky Mountain coking coals are recognized for their favourable ash chemistry, which is a function of their predominantly non-marine depositional setting. Coals that are 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 acidic conditions of peat swamps, 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 production of sulphide and nucleation of pyrite and, possibly, calcite and illite (Teichműller and Teichműller 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 coke that is slower to breakdown in the blast furnace.

3. Samples and analytical data

3.1 Data sources

The CSR, ash chemistry and rank data used in this study were obtained from assessment reports submitted as part of the statutory reporting requirements for maintaining coal tenure in the province. Under the terms of the British Columbia Coal Act Regulation, results from almost all the samples (48) will remain confidential indefinitely. The data are presented here on plots and tables without identifying information other than formation. Forty-nine of the samples are clean coking coals; one Gething Formation sample is raw, albeit with very low ash content (3.62%). Most (43) are of medium volatile bituminous rank (mvb); five are low volatile bituminous (lvb) and two are high volatile bituminous (hvb).

Nineteen of the 50 samples are from five deposits in the Gates Formation, which hosts coal along the Rocky Mountain Foothills from north of Tumbler Ridge to the British Columbia-Alberta border (Fig. 3) and has produced more than 175 million tonnes of steelmaking coal (British Columbia Ministry of Energy, Mines and Petroleum Resources 2018a) from the Sukunka, Bullmoose, Quintette, Wolverine, and Trend mines. The Wolverine mine currently produces about between 1 and 2 million tonnes of Gates Formation coal per year.

Twelve samples are from three deposits in the Gething Formation, which hosts coal along the Rocky Mountain Foothills from near Hudson's Hope to Tumbler Ridge (Figs. 2, 3). Gething Formation coal is currently mined at the Brule and Willow Creek mines and is marketed as pulverized coal injection (PCI) product. The Gething Formation also hosts coking coal. Several tens of thousands of tonnes of coal were produced in the early to middle 20th century from the King Gething and Bullhead Mountain mines, and from the Sukunka mine in the 1970s (British Columbia Ministry of Energy, Mines and Petroleum Resources 2018a).

A further 19 samples are from six deposits in the Mist Mountain Formation (Figs. 2, 4), the unit from which most of the coal mined in British Columbia's history has been derived; more than 830 million tonnes since the end of the 19th century (British Columbia Geological Survey 2018b). Currently, 25 to 30 million tonnes are mined each year from the Fording River, Greenhills, Line Creek and Elkview mines.

3.2 Analytical laboratories

CSR determinations were carried out at the CANMET Lab in Ottawa, Ontario (44), the ALS Lab in Richmond, British Columbia (4), and Coal Tech in Murrysville, Pennsylvania (2). Moveable wall oven testing is the definitive method. However, this method is expensive because it requires a large sample

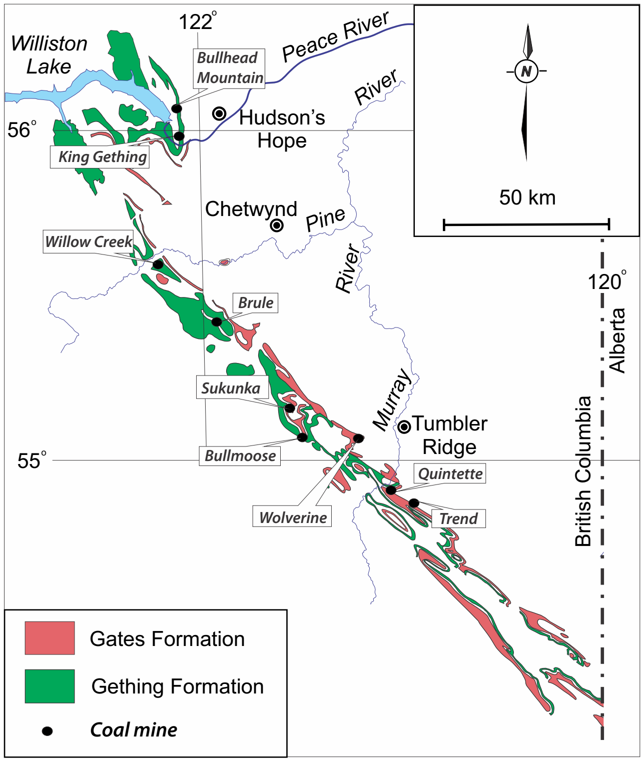


Fig. 3. The Peace River coalfields in northeast British Columbia. Coal is produced from the Gething and Gates formations (Lower Cretaceous).

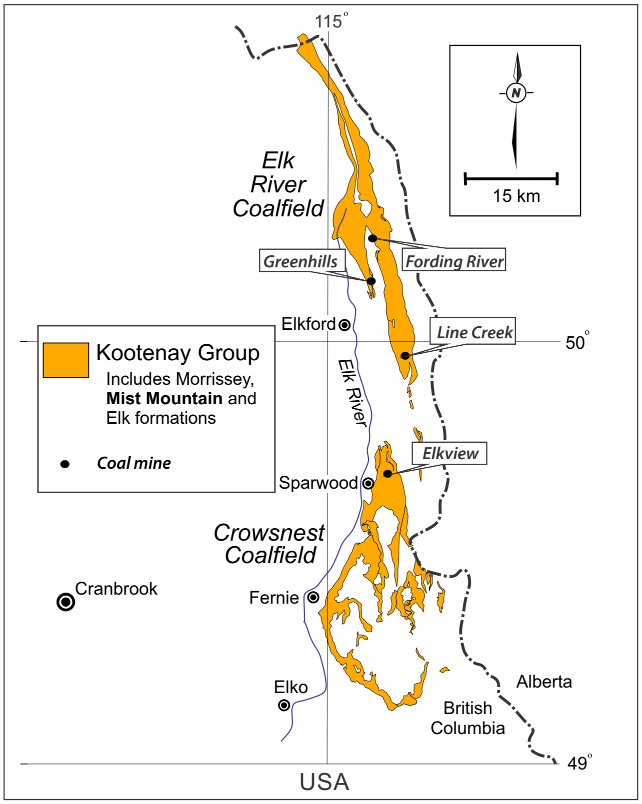


Fig. 4. The Elk River and Crowsnest coalfields of southeastern British Columbia. Coal is produced from the Mist Mountain Formation, Kootenay Group (Jura-Cretaceous).

(ca. 350 kg), and many CSR measurements in the dataset were taken using smaller sole-heated ovens. The sole-heated oven method (MacPhee et al., 2012) uses a smaller sample (ca.15 kg) and was developed to bring down the cost of obtaining a CSR measurement. Our dataset contains 19 moveable wall oven tests and 31 sole-heated oven tests. Where samples were analysed by both methods, we used the moveable wall oven data. Coking conditions used in the two methods are not identical, thus data points from the two methods are represented on figures by different symbols.

Most (37 of 50) standard ash analyses in the dataset were analysed at GWIL Birtley Labs in Calgary. The remainder were analysed at ALS in Richmond BC, EVES in the Elk Valley, Coal Tech Lab in Murrysville Pennsylvania, and CANMET in Ottawa. Most (33 of 50) of the proximate analyses, which determined the relative amounts of moisture, ash, volatile matter and fixed carbon expressed as a percentage of the total mass of the sample, were conducted at GWIL Birtley Labs in Calgary, Alberta. The remainder were done at CANMET Labs in Ottawa, Ontario, EVES lab in the Elk Valley, British Columbia, and Coal Tech Lab in Murrysville, Pennsylvania. The procedures for producing the clean coals for the 50 samples were not captured in the database, it should be assumed that they were not identical.

3.3 Characteristics of the sample set

3.3.1 Ash percentage, rank as measured by volatile matter, and CSR

The mean values and ranges of some important coal quality characteristics are presented in Table 1. The Gates Formation samples have the narrowest range of values for ash percentage (Fig. 5), and volatile matter (Fig. 6) and have the largest range of CSR values (Fig. 7). The Mist Mountain Formation CSR values are generally higher than those of the other two formations.

3.3.2 CSR vs individual oxides

The correlation matrix for CSR and major oxides (Table 2) provides insight as to which ash elements are most damaging to CSR. Iron has a moderately to strongly negative correlation to CSR in all three formations. Calcium, magnesium, and sulphur show a strongly negative effect on CSR in Gates Formation samples, whereas the influence of silicon, aluminum, titanium, and phosphorous is positive. In the Gething Formation, aluminum has a moderate positive correlation with CSR and iron has a strong negative correlation. The only element with a significant influence on CSR in the Mist Mountain formation samples is iron, and that effect is negative. There is no significant correlation between potassium in ash and CSR in any of the three formations.

Table 1. Coal quality parameter ranges for the Gates, Gething and Mist Mountain formations.

	Gates Formation		Gething Formation		Mist Mountain Formation	
Characteristic	Mean	Range	Mean	Range	Mean	Range
Ash %, dry basis	8.3	6.1-9.8	5.4	1.8–14.2	8.6	5.9-11.0
Volatile matter % (dry, ash-free basis)	26.1	25.4-28.4	26.3	20.6-34.5	25.4	19.6-34.8
Vitrinite reflectance % (RoMax)	1.18	1.01-1.36	1.21	0.94-1.49	1.35	1.00-1.60
CSR %	55.5	35.7-71.0	57.7	42.3-68.5	66.0	42.3-76.7

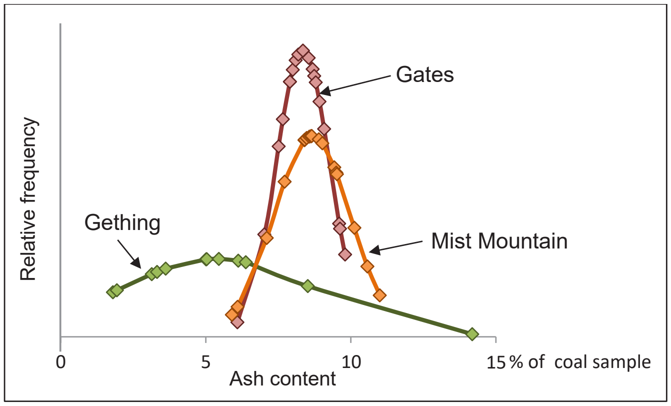


Fig. 5. Ash content ranges in the sample set, by formation

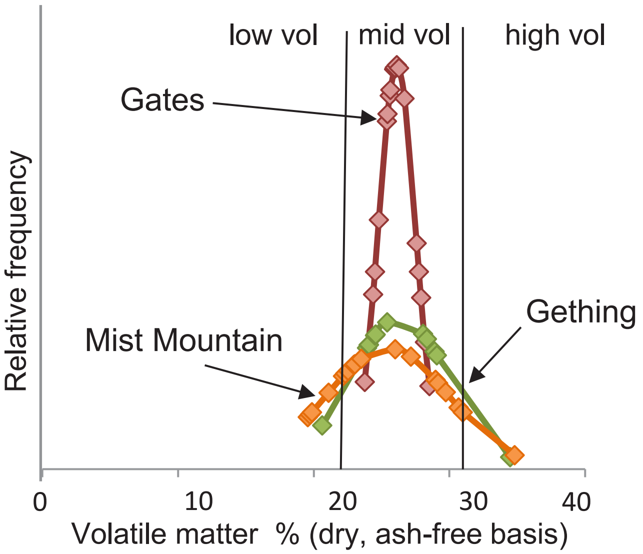


Fig. 6. Volatile matter ranges, by formation. All 19 Gates Formation samples are in the mid-volatile range.

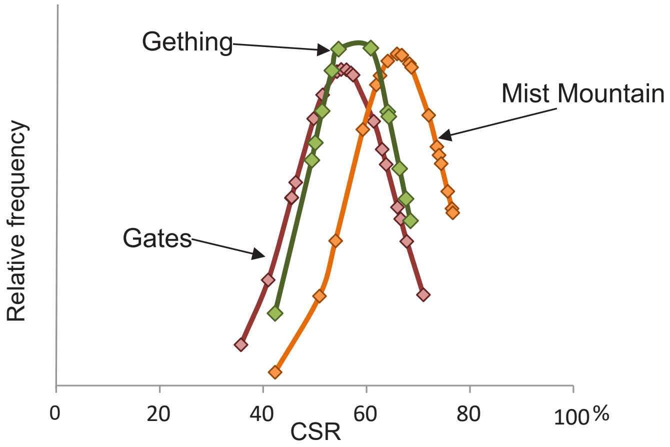


Fig. 7. CSR ranges, by formation.

Table 2. Correlation matrix, CSR vs major ash oxides, by formation.

	SiO_2	Al_2O_3	TiO_2	Fe_2O_3	CaO	MgO	Na_2O	K_2O	P_2O_5	SO_3
CSR Gates n=19	0.776	0.684	0.585	-0.722	-0.842	-0.773	-0.580	0.157	0.602	-0.880
CSR Gething n=12	0.308	0.648	0.151	-0.515	-0.374	-0.463	-0.301	-0.209	0.418	-0.422
CSR Mist Mountain n=19	0.455	0.304	0.267	-0.631	-0.212	-0.179	-0.130	-0.178	0.237	-0.387

3.3.3 CSR vs rank

Plots of measured CSR versus rank as measured by volatile matter (Fig. 8) for the three formations show distributions that are best fit with non-linear solutions. These plots are consistent with the observation that the best coking coals are most commonly of mid-volatile rank (Price and Gransden, 1987; Ryan and Price, 1993); low-volatile and high-volatile coals tend to have lower CSRs. The rank range in the Gates Formation sample set is narrow (between 25-29 % volatile matter, dry mineral-matter-free basis), so the data do not provide a meaningful illustration of the effect of rank difference on CSR. The Gething Formation plot shows a parabolic distribution, with the best CSR values in the mid-volatile range. However, all the best CSR values also have favourable ash chemistry, so the relative importance of rank is not clearly illustrated. The Mist Mountain Formation plot is unusual in that the highest CSR values are associated with higher rank coals outside of the mid-volatile range. In this case, the samples with the lowest BARs have the best CSRs, regardless of rank, so it appears that favourable ash chemistry is the stronger influence. However, in the entire dataset, no sample with VMdaf higher than 31% has an acceptable (>57%) CSR value.

3.3.4 CSR vs ash content

A negative relationship between CSR and ash content was expected, assuming that inert material (mineral matter and inert macerals) decreases fluidity, which in turn reduces coke quality (Price and Gransden 1987, Price et al.1992) and that the higher the ash, the higher the amount of inert material. However, a scatter plot of CSR vs ash content (Fig. 9) does not support such a correlation, except for a weak negative correlation for the Gething Formation. Instead, it shows a weak positive correlation between ash and CSR for the entire sample set (Fig. 9a). The Gates Formation samples (Fig. 9b) show no correlation, and the Mist Mountain Formation samples (Fig. 9d) show a moderate positive correlation. The reasons for these observations are unclear, but they may reflect an ash mineralogy predominated by quartz and kaolinite which, in contrast to most ash minerals, have been shown by Price et al. (1992) to have a slightly positive effect on fluidity. The plots suggest that, at least for the range of ash content of the clean coals in this study (maximum 14%), increased ash content does not have a significant negative effect on CSR. Although ash chemistry is important to CSR in these coals, the amount of ash in the clean coal is not.

4. Predictive indices

The BAR (base-acid ratio) index and all the other BAR-based indices evaluated in this paper are calculated from standard ash analysis values, which include the major oxides (SiO_2, Al_2O_3, TiO_2, Fe_2O_3, CaO, Na_2O, K_2O, MgO, P_2O_5, SO_3) as a percentage of the ash residue after a sample is combusted.

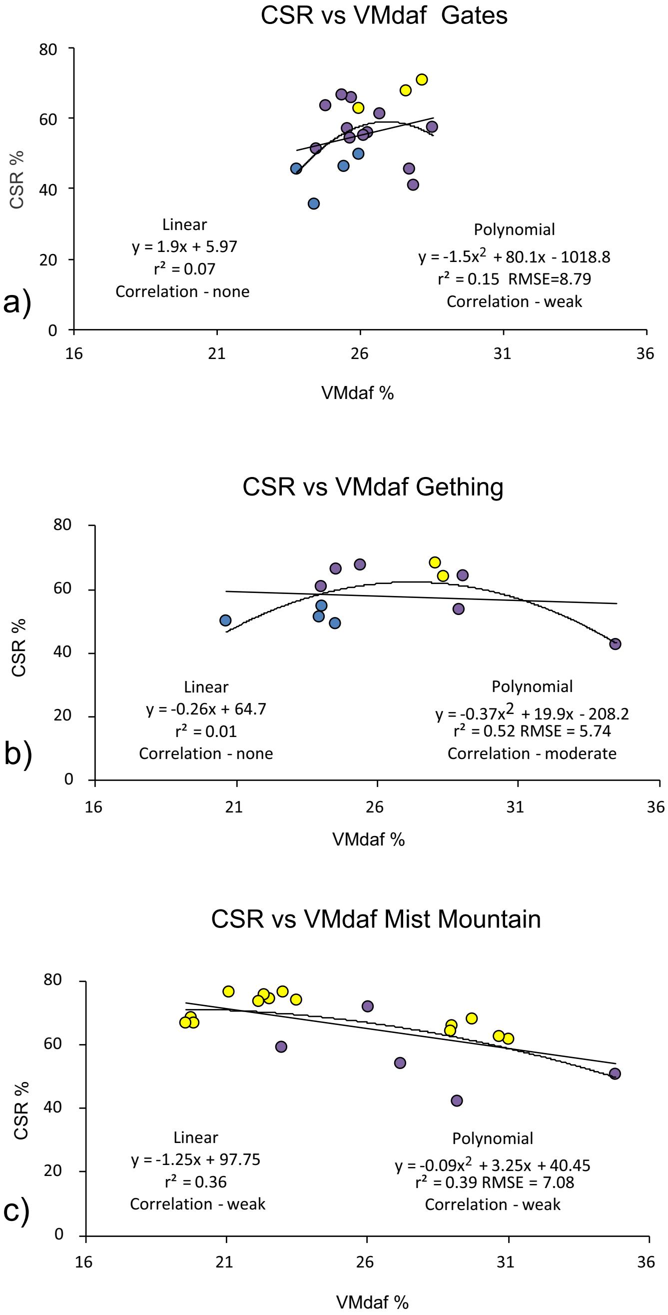


Fig. 8. CSR vs volatile matter (daf = dry ash-free basis), **a)** Gates Formation, **b)** Gething Formation, **c)** Mist Mountain Formation. Data from the Gates and Gething formations lack a linear correlation; the polynomial parabolic fit is marginally better (weak and moderate), which may suggest an 'ideal rank' for CSR in these units. For the Mist Mountain Formation, the parabolic fit is only slightly better than the linear fit but the correlations for both are weak. Yellow dots have BAR less than 0.1, purple dots have BAR between 0.1 and 0.2, blue dots have BAR greater than 0.2.

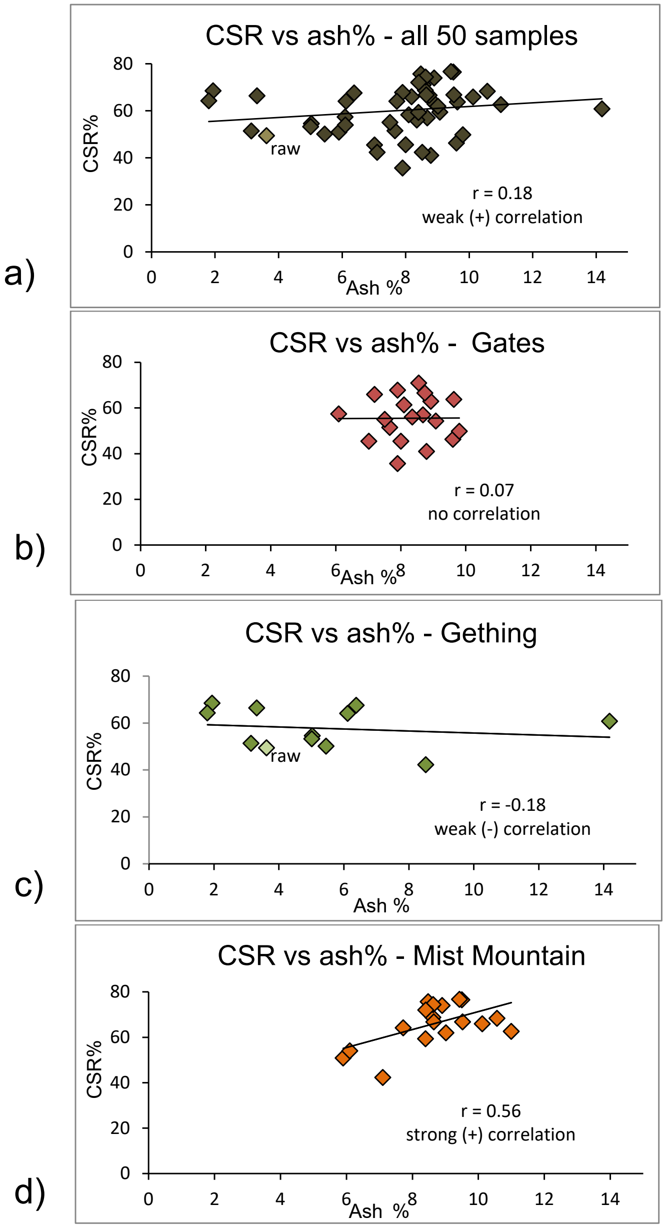


Fig. 9. CCSR vs ash content. **a)** All 50 samples, weak positive correlation. **b)** Gates Formation, no correlation. **c)** Gething Formation, weak negative correlation. **d)** Mist Mountain Formation, strong positive correlation.

4.1. Base Acid Ratio (BAR)

The Base-Acid Ratio (BAR) uses values from a standard coal ash analysis to generate a ratio of reactive components over inert components.

$$BAR = \frac{Fe_2O_3 + CaO + Na_2O + K_2O + MgO}{SiO_2 + Al_2O_3 + TiO_2} \qquad \text{(Eq. 2)}$$

4.2. Ash Index (AI)

The Ash Index (AI) incorporates the amount of ash (determined by proximate analysis) into the BAR calculation.

$$AI = (\%\ Ash) * \frac{Fe_2O_3 + CaO + Na_2O + K_2O + MgO}{SiO_2 + Al_2O_3 + TiO_2} \qquad \text{(Eq. 3)}$$

4.3. Experimental indices incorporating P_2O_5

To test if standard predictive indices might be improved, we incorporated P_2O_5 into the BAR (BAR_p) and AI (AI_p) indices. P_2O_5 correlates positively with CSR in all three formations, and so was added to the denominator.

$$BAR_p = \frac{Fe_2O_3 + CaO + Na_2O + K_2O + MgO}{SiO_2 + Al_2O_3 + TiO_2 + P_2O_5} \qquad \text{(Eq. 4)}$$

$$AI_p = (\%\ Ash) * \frac{Fe_2O_3 + CaO + Na_2O + K_2O + MgO}{SiO_2 + Al_2O_3 + TiO_2 + P_2O_5} \qquad \text{(Eq. 5)}$$

4.4. Experimental indices correcting for calcium in apatite

Another experimental predictive method follows the suggestion of Ryan and Ng (2015) to correct the BAR for calcium in apatite. As discussed further below (section 6.2), Price et al. (1992) demonstrated that elements vary in their ability to degrade coke depending on which mineral they are in. For example, calcium in apatite is less damaging to CSR than if in calcite, because apatite is more resistant to breakdown and release of calcium in hot, CO_2-rich conditions.

The first step in this method is to determine how much CaO in the ash analysis is likely to be in apatite. Apatite ($Ca_5(PO_4)_3(OH,F,Cl)$) is the most common phosphorous mineral in coal, but crandallite ($CaAl_3(PO_4)_2(OH)_5{\bullet}(H_2O)$), gorceixite ($BaAl_3(PO_4)(PO_3OH)(OH)_6$), and goyazite ($SrAl_3(PO_4)_2(OH)_5{\bullet}(H_2O)$) also occur. Crandallite can be flagged by a high proportion of P_2O_5 to CaO (P_2O_5/CaO in crandallite = 2.53; in contrast, P_2O_5/CaO in apatite = 0.759). The presence of gorceixite can be flagged by anomalously high amounts of BaO; goyazite can be flagged by high SrO. In samples lacking crandallite, gorceixite or goyazite, all phosphorous is assumed to be in apatite, and the correction can be applied. The reactivity of crandallite, gorceixite and goyazite in blast furnace conditions are unknown, so where their presence in a sample is indicated, no correction is made. Where it can be assumed that all phosphorous in the sample is in apatite, the corresponding amount of CaO is subtracted from the CaO in the sample's ash analysis, and the remaining CaO is assumed to be in a reactive mineral (for example, calcite or dolomite) and remains in the base acid ratio for calculation of BAR-Capatite. Apatite is 55.07% CaO and 41.82% P_2O_5 a ratio of 0.759. Thus, the amount of CaO in the BAR-Capatite is CaO – (P2O5 /0.759). Where the amount is negative, the CaO is assigned a zero value.

Anomalous values of BaO and SrO were defined for the formations in this study as greater than the mean plus 2 standard deviations of samples from the database of Riddell and Tian

(2017), which are for: the Gates Formation BaO > 1.56% and SrO >0.22%; the Gething Formation BaO >2.87% and SrO >0.60%; and the Mist Mountain Formation BaO: >0.90% and SrO >0.65%.

For a hypothetical example (Table 3), the uncorrected BAR is: (4.90 + 7.66 + 2.22 + 0.68 + 0.48) / (55.49 + 20.22 + 0.97) = 0.202. To check for presence of crandallite, determine the P_2O_5/CaO ratio. In this example P_2O_5/CaO = 1.69/7.66 = 0.22. This is well below the P_2O_5/Cao ratio of crandallite (2.53), so it can be assumed that crandallite is absent. Because BaO is 0.20%, not anomalously high, the sample is unlikely to contain gorceixite. Similarly, SrO is only 0.20%, which indicates that the sample lacks goyazite. Because P_2O_5 appears to be in apatite, the correction can be applied: CaO(corrected) = CaO - (P2O5/0.759) = 7.66 - (1.69/0.759) = 5.43. Substituting this value of 5.43 into the BAR equation, BAR-Capatite = (4.90 + 5.43 + 2.22 + 0.68 + 0.48) / (55.49 + 20.22 + 0.97) = 0.179.

Table 3. Hypothetical chemistry to apply calcium in apatite correction.

SiO_2	Al_2O_3	TiO_2	Fe_2O_3	CaO	MgO	Na_2O	K_2O	P_2O_5	SO_3	BaO	SrO
55.49	20.22	0.97	4.90	7.66	2.22	0.68	0.48	1.69	5.30	0.20	0.20%

One sample in the present study has a P_2O_5/CaO ratio high enough to indicate the presence of crandallite; none has anomalously high values of BaO or SrO so gorceixite and goyazite are assumed to be absent. Thus, the BAR-Capatite correction was applied to 49 of the 50 samples in the dataset.

4.5. Other CSR prediction methods

Many methods for predicting CSR have been devised, and the origin, evolution, applicability, and pitfalls of these methods have been detailed elsewhere (see Ryan et al., 1992; Diez et al., 2002; Todoschuk et al. 2004; Dash et al., 2012; de Cordova et al. 2016; North et al., 2018). Before the 1980s, steelmakers made models empirically using locally available coals. As local supplies dwindled and global trading increased, it was found that predictive methods used for a local coal or coal blend were not always useful for coals sourced from elsewhere. For example, models that rely on fluidity and/or the ratio of reactive macerals to inerts (inert macerals plus mineral matter) predicted that western Canadian coking coals would have poor coking quality. However, by the 1980s it was recognized that this was not necessarily true (Pearson, 1989; Ryan et al. 1993; Coin and Broome, 1997; Ryan et al., 1998).

Where the required data were available, we applied the BHP Australia equation, the Kobe Steel equation, and the Nippon Steel method to our dataset, and compared predictions to the measured CSRs. The BHP Australia equation (cited in Pearson, 1989, and Ryan et al., 1993) predicts CSR by an equation derived from regression analysis of coals from New South Wales and Queensland, and includes ash chemistry, rank as measured by volatile matter, fluidity, and the percentage of inert macerals and minerals:

$$\text{CSR} = 133.8 - (15.56*\text{BAR}) - (3.1*\text{VM}) + (8.5*\log \text{fluidity}) - (0.22*\text{per cent inert macerals}) \quad \text{(Eq. 6)}$$

The Kobe Steel equation (cited in Ryan et al., 1993) predicts CSR by an equation derived from regression analysis of coals used by Kobe Steel of Japan before 1984. It includes rank as measured by vitrinite reflectance, fluidity, and ash chemistry:

$$\text{CSR} = (70.9*\text{RoMax}) + (7.8*\log \text{fluidity}) - (89*\text{BAR}) - 32 \quad \text{(Eq. 7)}$$

The Nippon Steel method as adapted by Pearson (1989), predicts CSR by plotting vitrinite reflectance against percent inerts, and comparing the co-ordinate location to iso-CSR lines on the chart (Fig. 10). The lines were derived empirically by contouring CSR values for coals that the steelmaker used before 1980, which included Japanese domestic coals and, as those sources were depleted, increasing amounts of Australian and American coals.

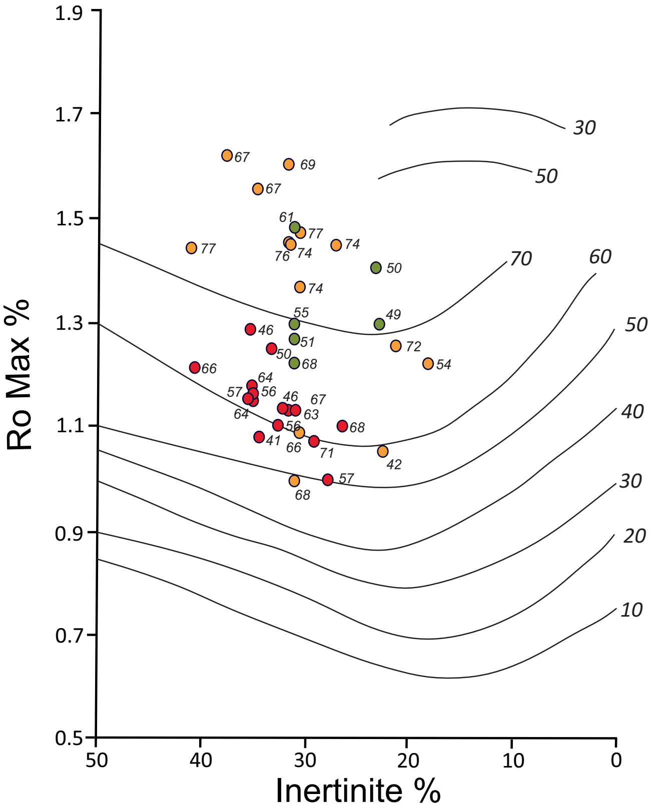


Fig. 10. The Nippon Steel CSR prediction method. The iso-CSR contours on the chart were derived empirically by contouring CSR values for coals that the steelmaker used before 1980. From Pearson (1989). The thirty-eight of the 50 samples in this study that have reflectance (RoMax%) and inertinite % data are plotted. Measured CSR values for the samples appear beside data points. Colours: Gates Formation in red, Gething Formation in green, Mist Mountain Formation in orange.

5. Results

As expected, a strong linear negative correlation is apparent on a plot of CSR values against the BAR index for all 50 samples (Fig. 11), confirming that coal ash chemistry is important in the Gates, Gething, and Mist Mountain formations, at least for the rank range represented by the dataset (i.e. VMdaf between 19.6 and 31.0%. The two samples with VMdaf greater than 31% have low CSR despite having favourable ash chemistry (Fig. 6.) Scatter plots of measured CSR vs Base-Acid Ratio (BAR), Ash Index (AI), and experimental indices incorporating

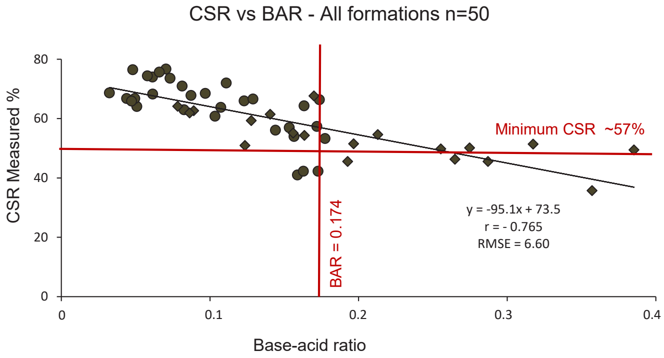


Fig. 11. Measured CSR values vs. the base-acid ratio (BAR) for all 50 samples. The strong linear negative correlation confirms that coal ash chemistry is an important factor to CSR for the coals in this sample set.

P_2O_5 (BAR_p, and AI_p) and correcting for calcium in apatite (BAR-Capatite), for each of the three formations, are illustrated in Figures 12-14 and tabulated in Table 4. Correlation coefficients (r), root mean square errors (RMSEs), and equations for best fit lines were calculated in Excel.

5.1. Gates Formation

Gates Formation sample plots show strong linear correlations between CSR and all indices (Fig. 12, Table 4). The BAR index corrected for calcium in apatite index (BAR-Capatite) produces the best correlation, with a correlation coefficient of -0.872. The root mean square error (RMSE) is 4.78%.

CSRs for the Gates Formation samples correlate well because, as shown in Table 2, all the oxides in the numerators of these indices, except for K_2O, correlate well and negatively with CSR, and the oxides in the denominators correlate wel and positively with CSR.

The importance of the ash oxides for the Gates Formation in terms of negative correlation with CSR (Table 2), from worst to best, are $CaO>MgO>Fe_2O_3>Na_2O>K_2O$.

5.2. Gething Formation

Gething Formation sample plots (Fig. 13, Table 4) show the weakest correlations of the three units, but all are linear, and moderate to strong (all r values are stronger than -0.59). The AIp index displays the best correlation coefficient (-0.704) and has an RMSE of 5.86%. Both the BAR and the AI correlations with CSR are improved by adding phosphorous to the denominator.

Table 4. Relationships between measured CSR and predictive indices, by formation. The index with the best correlation for each formation, and the corresponding predictive equations as derived by linear regression, are in bold type.

Relationship	Correlation coefficient r	RMSE	Linear equation
Gates Formation n=19			
CSR/BAR	-0.852	4.99	CSR=74.83-(112.81*BAR)
CSR/AI	-0.822	5.43	CSR=73.58-(12.77*AI)
CSR/BARp	-0.855	4.94	CSR=74.62-(133.12*BARp)
CSR/AIp	-0.831	5.31	CSR=73.63-(12.99*AIp)
CSR/BAR-Capatite	**-0.872**	**4.78**	**CSR=70.96-(102.31*BAR-Capatite)**
Gething Formation n=12			
CSR/BAR	-0.592	6.65	CSR=67.94-(53.52*BAR)
CSR/AI	-0.700	5.89	CSR=69.39-(12.54*AI)
CSR/BARp	-0.595	6.63	CSR=67.89-(54.54*BARp)
CSR/AIp	**-0.704**	**5.86**	**CSR=69.38-(12.82*AIp)**
CSR/BAR-Capatite	-0.634	6.38	CSR=67.31-(58.26*BAR-Capatite)
Mist Mountain Formation n=19			
CSR/BAR	-0.779	5.70	CSR=81.2-(185.34*BAR)
CSR/AI	-0.648	6.92	CSR=82.24-(23.90*AI)
CSR/BARp	-0.782	5.67	CSR=81.20-(188.89*BARp)
CSR/AIp	-0.653	6.89	CSR=82.33-(24.53*AIp)
CSR/BAR-Capatite	**-0.802**	**5.43**	**CSR=77.36-(192.28*BAR-Capatite)**

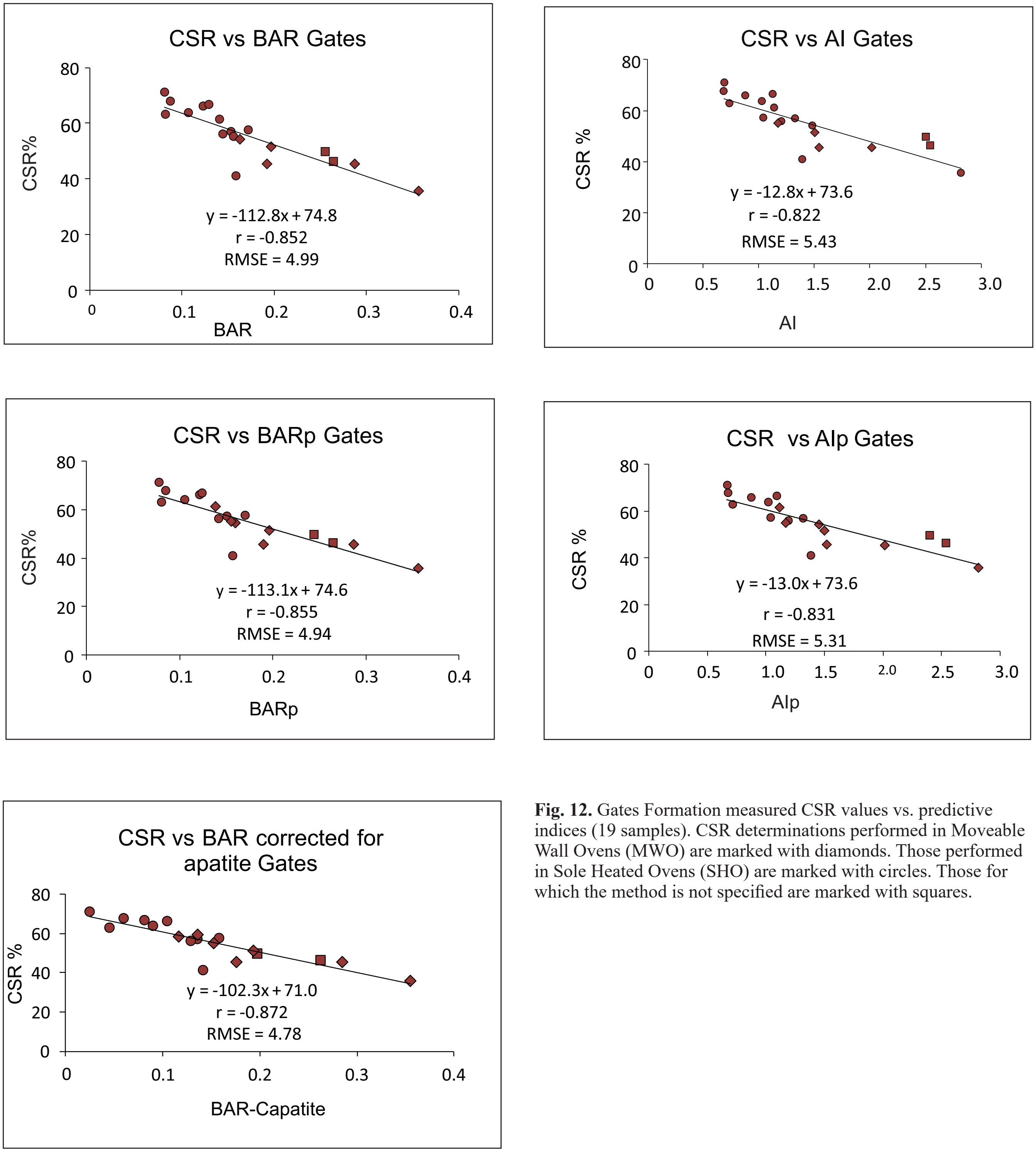
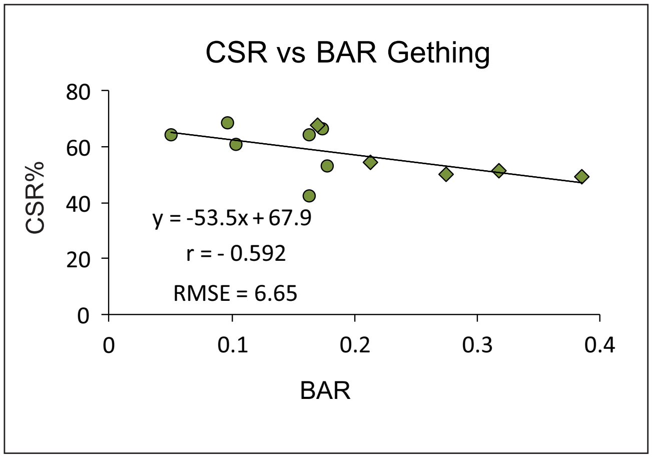


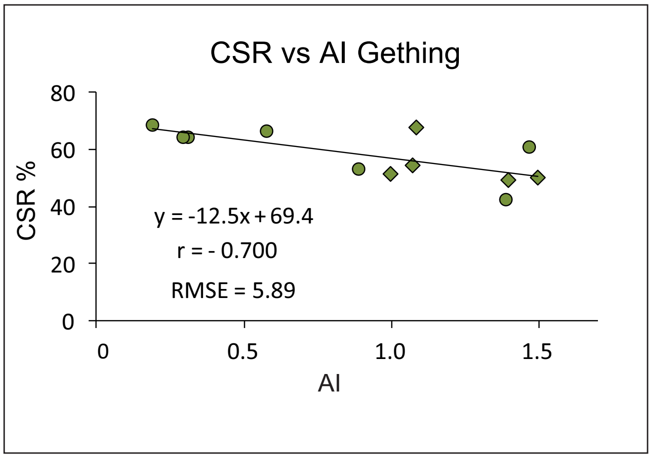
Fig. 12. Gates Formation measured CSR values vs. predictive indices (19 samples). CSR determinations performed in Moveable Wall Ovens (MWO) are marked with diamonds. Those performed in Sole Heated Ovens (SHO) are marked with circles. Those for which the method is not specified are marked with squares.

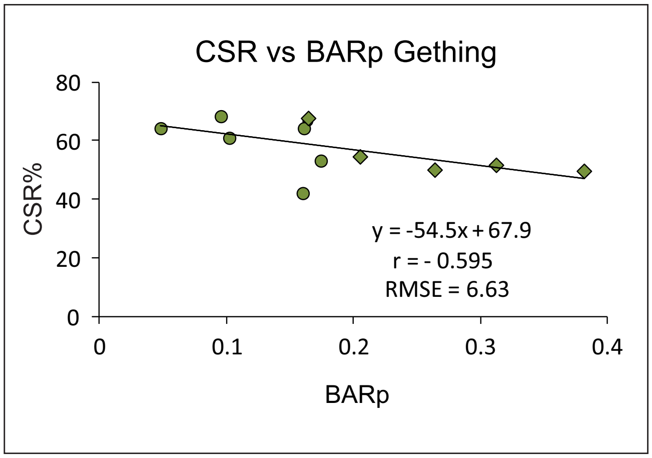
In the Gething Formation sample set, the only oxides with significant correlations to CSR are Al_2O_3 (positive) and Fe_2O_3 (negative). The Gething Formation is the only one of the three units for which the AI index correlates better with CSR than does BAR. This is likely because the Gething Formation has the widest range of ash content values and is the only unit for which CSR has a negative (albeit weak) correlation with ash content. The importance of the metallic and alkali oxides for the Gething Formation in terms of negative correlation with CSR (Table 2), from worst to best, are Fe_2O_3>MgO>CaO>Na_2O>K_2O.

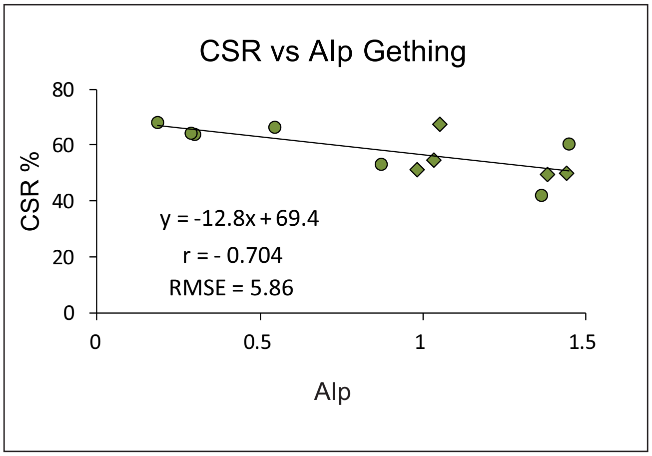
5.3. Mist Mountain Formation

Mist Mountain Formation sample plots (Fig. 14, Table 4) show good linear correlations with all indices tested (all r values are stronger than -0.64). The BAR-Capatite index gives the best correlation, with an r of -0.802, and an RMSE of 5.43%. The









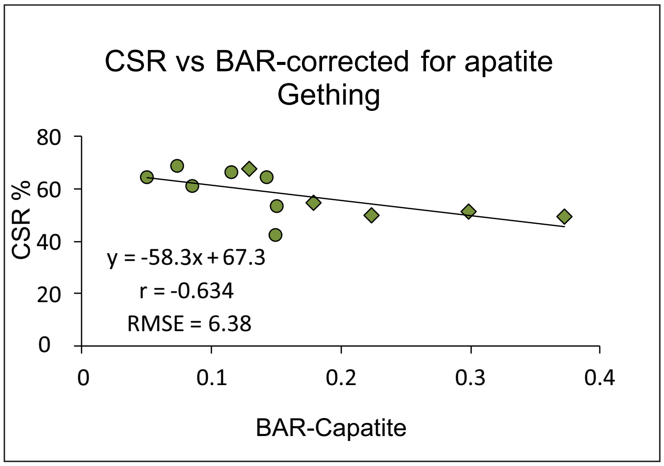


Fig. 13. Gething Formation measured CSR values vs. predictive indices (12 samples). CSR determinations performed in Moveable Wall Ovens (MWO) are marked with diamonds. Those performed in Sole Heated Ovens (SHO) are marked with circles.

only oxide from the BAR with a significant CSR correlation is that of iron, and it is negative (Table 2). The importance of the metallic and alkali oxides for the Mist Mountain Formation in terms of negative correlation with CSR (Table 2), from worst to best, are Fe_2O_3>>CaO>MgO>K_2O>Na_2O.

5.4 Results of other predictive methods

Table 5 shows the measured CSR values from the dataset, along with the predicted CSRs for the same samples using the BHP, Kobe, and Nippon prediction methods. The results are graphically illustrated in Figure 15, where the red lines represent a one-to-one correlation between the real value and

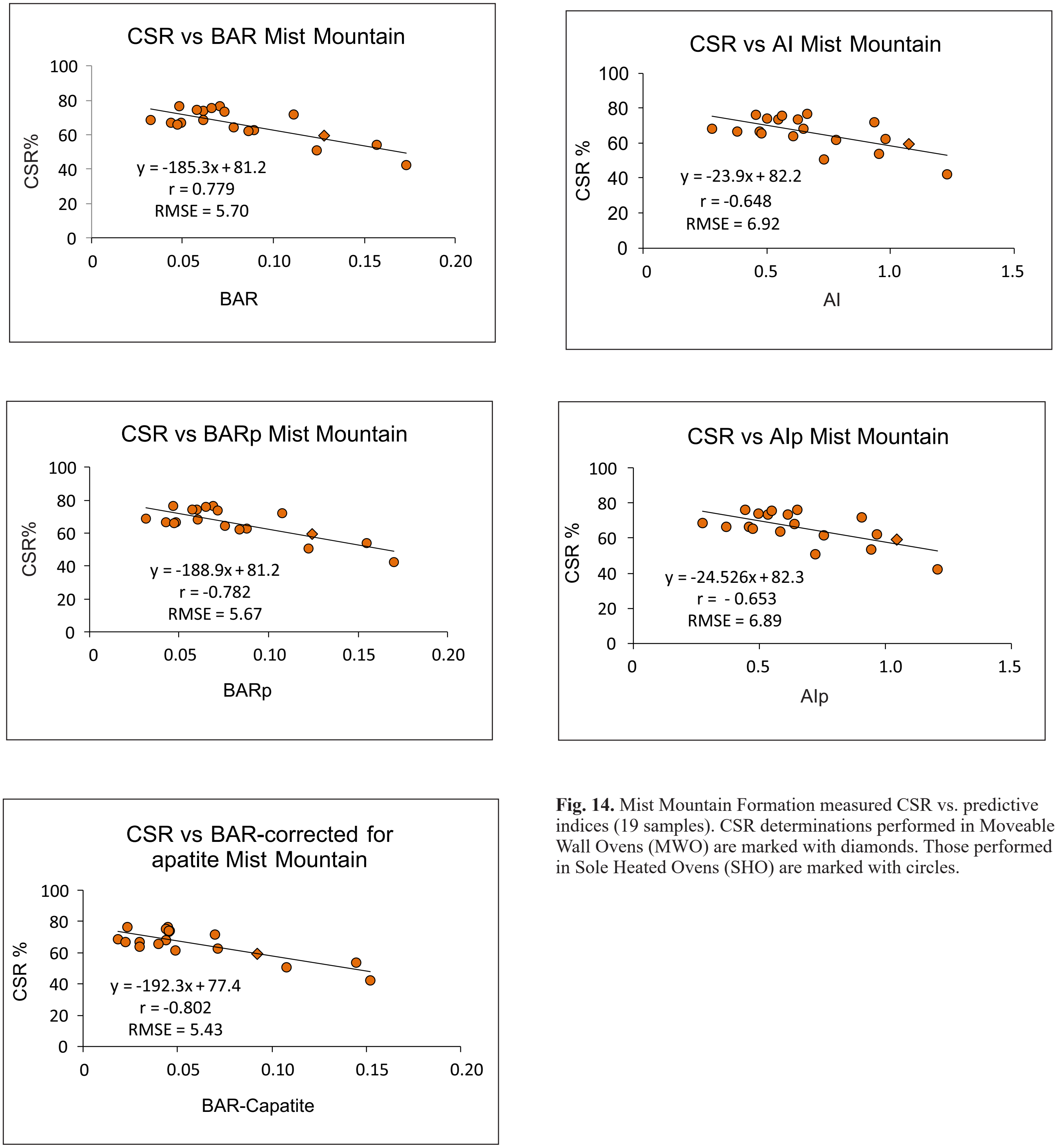


Fig. 14. Mist Mountain Formation measured CSR vs. predictive indices (19 samples). CSR determinations performed in Moveable Wall Ovens (MWO) are marked with diamonds. Those performed in Sole Heated Ovens (SHO) are marked with circles.

the prediction. These methods performed very poorly for predicting the CSR values in this dataset, even though the BHP and Kobe methods include an ash chemistry component.

6. Discussion

6.1 Strength of correlations

Moderate to strong (r >0.5) correlations exist between the 50 measured CSR values and the predictive indices calculated from ash chemistry (Figs. 11-14, Table 4), especially those from the Gates Formation. The strength of these correlations indicates that ash chemistry is an important factor controlling CSR in these coals. Outliers may be accounted for by factors such as relative proportions of inert and reactive macerals, mineralogy, grain size, dispersion of minerals, and coke-making processes, which influence CSR include in other coals such as shown by Price and Gransden (1992), Ryan et al. (1999), Todoschuk et al. (2004), and Zhang et al. (2019).

Table 5. Measured CSRs and CSRs predicted by the BHP Australia equation, the Kobe Steel equation, and the Nippon Steel method.

CSR measured	CSR predicted by BHP Australia equation	CSR predicted by Kobe Steel equation	CSR predicted by Nippon method
46	65	56	65
50	64	55	66
46	38	31	63
71	52	49	50
41	42	36	52
63	52	46	58
57	48	40	62
66	44	35	60
56	56	44	55
68	52	53	60
64	59	39	49
57	47	43	60
67	51	41	60
58	49	48	65
59	58	62	72
36	No data	No data	70
46	No data	No data	65
52	No data	No data	70
55	No data	No data	66
55	62	51	68
64	No data	No data	66
42	No data	No data	60
53	No data	No data	71
66	No data	No data	72
69	No data	No data	72
64	No data	No data	73
61	No data	No data	73
49	57	58	45
51	60	62	40
68	59	68	75
50	69	69	40
77	64	54	68
77	69	46	46
74	59	46	50
74	68	45	50
76	68	56	65
69	73	No data	No data
67	72	No data	No data
74	83	No data	No data
67	73	No data	No data
72	71	No data	No data
51	51	No data	No data
64	51	No data	No data
63	38	No data	No data
62	51	No data	No data
68	48	No data	No data
66	50	No data	No data
59	65	No data	No data
42	55	No data	No data

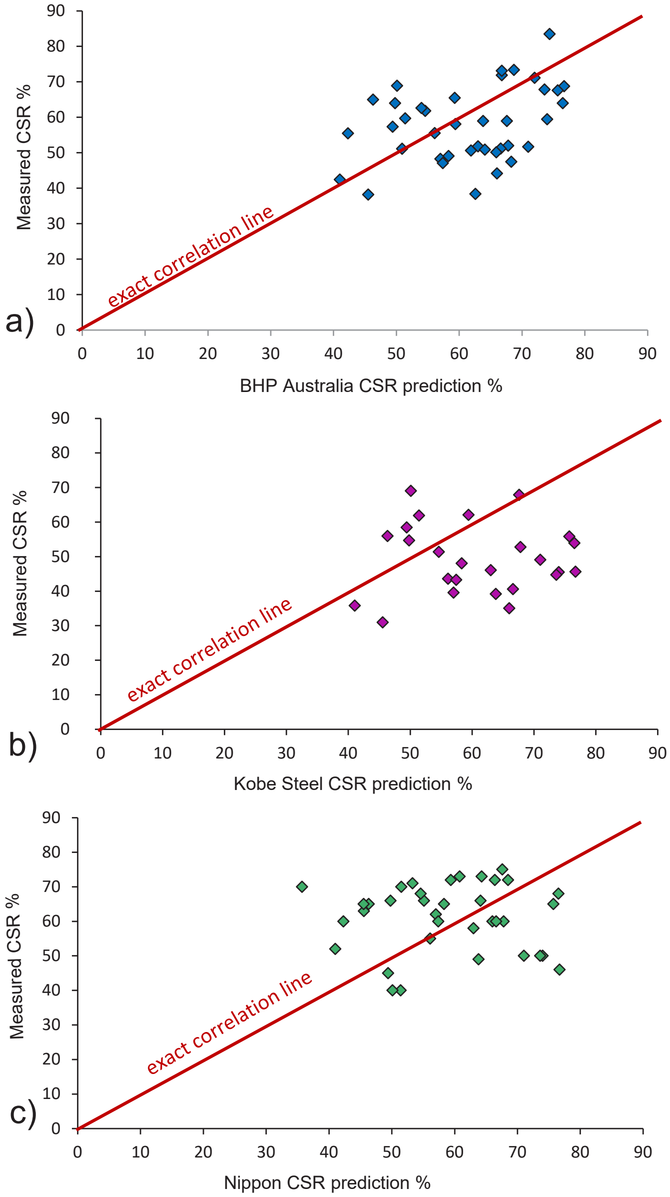


Fig. 15. Measured CSRs vs. those predicted by the BHP Australia equation, the Kobe Steel equation, and the Nippon Steel method. The red lines represent exact correlation between the measured and predicted CSR values.

6.2 The effect of mineralogy on CSR

The differences between the three formations in how well CSR correlates with ash chemistry indices may be a function of differences in mineralogy and texture. Price et al. (1992) demonstrated that elements vary in their ability to degrade coke depending on which mineral they are in. These differences are not accounted for in ash chemistry indices. The minerals commonly found in coal that damage CSR include (from most to least damaging) pyrite, hematite, siderite, bauxite, calcite, gypsum, lime and magnesium oxide. Minerals that are neutral or positive for CSR are quartz, apatite, kaolinite, feldspars and muscovite (Price et al., 1992). Furthermore, Zhang et al. (2019) have shown that fine-grained particles are more damaging to CSR than coarse-grained particles of the same mineral.

Grieve et al. (1996) identified the most common minerals from coals from the Mist Mountain (61 samples) and Gates (8 samples) formations using X-ray diffraction analysis on material left after the organic material was removed by low-temperature ashing (LTA) using an oxygen plasma stream. Quartz and kaolinite are the two most abundant minerals in both units. In the Gates Formation, quartz and kaolinite are followed in abundance by illite, siderite, calcite and dolomite; ankerite and anatase are sparse. In the Mist Mountain Formation, quartz and kaolinite are followed in abundance by siderite, illite, apatite; calcite, muscovite and dolomite. Gorciexite and ankerite are rare. Trace pyrite was positively identified in 22 of the 69 samples. Mineralogical data from the Gething Formation are scarce. But because the ash chemistry of the Gething coals is similar to the Gates and Mist Mountain formations, silica- and alumina-rich (Riddell and Tian 2017), it is likely that it too contains quartz and kaolinite as the most abundant minerals.

As discussed below, the correlation matrix for the ash oxides with one another and CSR (Table 6) provides clues to the identities of minerals that formed the ashes. Strong correlations

Table 6. Correlation matrix, ash chemistry oxides and CSR, by formation. Strong (0.70 or -0.70 or greater) correlations are highlighted in green. Moderate correlations (>0.5 to <0.70, or >-0.5 to <0.70) are highlighted in yellow.

Gates	SiO_2	Al_2O_3	TiO_2	Fe_2O_3	CaO	MgO	Na_2O	K_2O	P_2O_5	SO_3	BaO	SrO	CSR
SiO_2	—												
Al_2O_3	0.45	—											
TiO2	0.44	0.36	—										
Fe_2O_3	-0.77	-0.68	-0.45	—									
CaO	-0.89	-0.75	-0.51	0.81	—								
MgO	-0.67	-0.60	-0.23	0.68	0.72	—							
Na_2O	-0.42	-0.69	-0.12	0.65	0.54	0.74	—						
K_2O	0.03	0.49	0.15	-0.34	-0.33	-0.06	0.31	—					
P_2O_5	0.19	0.70	0.35	-0.60	-0.45	-0.49	-0.59	0.48	—				
SO_3	-0.82	-0.80	0.49	0.77	0.90	0.68	0.55	-0.24	-0.54	—			
BaO	-0.30	0.27	0.22	-0.19	0.02	-0.07	-0.05	0.53	0.65	-0.10	—		
SrO	0.27	0.25	0.26	-0.55	-0.25	-0.31	-0.44	0.11	0.59	-0.47	0.52	—	
CSR	0.78	0.68	0.58	-0.72	-0.84	-0.77	-0.58	0.16	0.60	-0.88	0.20	0.70	—

Gething	SiO_2	Al_2O_3	TiO_2	Fe_2O_3	CaO	MgO	Na_2O	K_2O	P_2O_5	SO_3	BaO	SrO	CSR
SiO_2	—												
Al_2O_3	0.41	—											
TiO2	0.56	0.24	—										
Fe_2O_3	-0.43	-0.52	-0.27	—									
CaO	-0.87	-0.64	-0.42	0.35	—								
MgO	-0.91	-0.60	-0.55	0.37	0.87	—							
Na_2O	0.09	0.13	0.17	0.38	-0.38	-0.08	—						
K_2O	0.50	0.05	-0.09	-0.27	-0.44	-0.21	0.04	—					
P_2O_5	0.25	0.13	0.19	-0.25	-0.26	-0.44	-0.30	-0.30	—				
SO_3	-0.90	-0.59	-0.50	0.28	0.89	0.96	-0.15	-0.35	-0.42	—			
BaO	0.41	-0.17	-0.28	-0.31	0.27	0.38	-0.40	-0.06	0.22	0.48	—		
SrO	-0.63	-0.36	-0.41	-0.03	0.59	0.64	-0.30	-0.19	0.30	0.60	0.46	—	
CSR	0.31	0.65	0.15	-0.52	-0.37	-0.46	-0.30	-0.21	0.42	-0.42	-0.06	0.09	

Mist Mtn.	SiO_2	Al_2O_3	TiO_2	Fe_2O_3	CaO	MgO	Na_2O	K_2O	P_2O_5	SO_3	BaO	SrO	CSR
SiO_2	—												
Al_2O_3	-0.33	—											
TiO2	-0.12	0.20	—										
Fe_2O_3	-0.23	-0.26	-0.23	—									
CaO	-0.58	-0.17	0.01	-0.31	—								
MgO	-0.51	-0.30	-0.21	-0.05	0.80	—							
Na_2O	-0.35	-0.25	-0.30	-0.06	0.60	0.45	—						
K_2O	0.42	-0.87	-0.23	0.13	0.02	0.22	0.3	—					
P_2O_5	-0.19	-0.08	0.57	-0.44	0.43	-0.11	0.17	-0.21	—				
SO_3	-0.57	-0.28	-0.11	-0.12	0.88	0.93	0.63	0.20	0.05	—			
BaO	-0.44	-0.16	0.67	-0.50	0.53	0.42	0.20	0.04	0.45	0.59	—		
SrO	0.16	0.03	0.73	-0.36	-0.12	-0.34	-0.37	0.07	0.53	-0.14	0.63	—	
CSR	0.46	0.30	0.27	-0.63	-0.21	-0.18	-0.13	-0.18	0.24	-0.39	-0.32	0.31	—

(0.70 or -0.70 or stronger) are highlighted in green, strong correlations (0.5 or -0.5 to weaker than 0.70 or -0.70) are highlighted in yellow.

6.2.1. Iron minerals

Iron minerals commonly found in coal include: pyrite (FeS_2); hematite (Fe_2O_3); magnetite (Fe_3O_4); siderite $FeCO_3$); illite [(K, H, 3O) (Al, Mg, Fe)$_2$ (Si,Al)$_4$ 10(OH)$_2$, (H2O)]; ilmenite ($FeTiO_3$) and ankerite [CaFe(CO_3)$_2$]. British Columbia Rocky Mountain coals characteristically have low pyrite content (Gransden et al. 1979; Price and Gransden, 1987; Grieve et al., 1996). Only in the Gates Formation is there a strong positive correlation between Fe_2O_3 and SO_3 which might indicate the presence of pyrite. However, Ryan et al. (2015) cautioned that correlations between the base and metal oxides and SO_3 may be misleading, because they may represent sulphates formed from organic sulphur bonding with cations and oxygen during ashing, rather than from original minerals.

Table 2 shows that presence of iron oxide in ash correlates negatively with CSR in all three formations, but most strongly in the Gates Formation. This may indicate that the iron minerals in the Gates Formation are more damaging to CSR than those in the other 2 units. This is consistent with the observation of Grieve et al. (1996) that pyrite is in five out of eight Gates Formation samples they tested (albeit in trace amounts), that siderite and illite are present in subequal amounts in the Gates Formation, whereas illite (the least damaging of the iron minerals) is the most abundant iron mineral in the Mist Mountain Formation, followed by siderite. Traces of pyrite were found in 17 of 61 Mist Mountain Formation samples.

Data on the mineralogy of the Gething Formation coals are sparse, but the correlation matrix of ash oxides (Table 6) provides clues to their identity. The negative correlation between CSR and Fe_2O_3 for the Gething Formation is the lowest of the three formations, suggesting that it contains iron in minerals that are less deleterious to CSR. Also, the correlation between iron and sulphur oxides is weak. Together, these observations suggest that pyrite is not abundant in the Gething Formation. This may be an artifact of sampling bias; pyrite-bearing samples are easy to identify in the field, and geologists would tend to avoid collecting them for CSR testing. Similarly, the correlation between calcium oxide and iron oxide is not strong, arguing against the abundance of ankerite. Probably most of the iron is in illite, and some is in siderite.

Correlation between Fe_2O_3 and TiO_2 is negative in all three formations, so iron is unlikely to be present as ilmenite. Grieve et al. (1996) found a trace of a mineral tentatively identified as ilmenite in one Mist Mountain Formation sample.

6.2.2. Calcium minerals

Calcium minerals commonly found in coal include: ankerite $[CaFe(CO_3)_2]$; calcite ($CaCO_3$); dolomite $[CaMg(CO_3)_2]$; apatite $[Ca_5(PO_4)3(Cl/F/OH)]$; crandallite $[CaAl_3(PO_4)(PO_3OH)(OH)_6]$, and gypsum ($CaSO_4.2H_2O$). Price et al. (1992) showed that calcite, dolomite and gypsum are the most damaging to CSR, and apatite causes little damage (crandallite and ankerite were not tested). This is consistent with our finding that the BAR_p and the BAR-Capatite improve correlations with CSR. Grieve et al. (1996) found apatite in 25 of 61 Mist Mountain Formation samples and trace amounts in two of eight Gates Formation samples, and that dolomite was the most abundant mineral in one of eight Gates Formation samples and was present in smaller amounts in six more. In the Mist Mountain Formation, Grieve et al. (1996) found dolomite in small to trace amounts in eight of 61 samples, calcite in small amounts in eight of 61; one Gates Formation sample contained dolomite. They found ankerite in small to trace amounts in five of 61 Mist Mountain samples and five of eight Gates samples. Neither gypsum nor crandallite was detected in any samples.

We found a positive correlation between CaO and P_2O_5 in the Mist Mountain (Table 6), whereas the correlation is negative in the Gates Formation, consistent with the finding of Grieve et al. (1996) that apatite is the more abundant calcium-bearing mineral in the Mist Mountain Formation than in the Gates Formation. This may explain why the BAR-Capatite index works better to improve the correlation with CSR in the Mist Mountain than it does for the Gates for Gething formations.

The mineral correction approach could theoretically be applied with other elements. As this attempt demonstrates, it works well for calcium in apatite because: 1) the number of commonly occurring phosphate minerals in coal is limited, and the flags indicating which are present are obvious, so establishing that apatite is the phosphorous-bearing mineral can be done with confidence; and 2) there is a known and high contrast in reactivity between the two most common types of calcium-bearing mineral types (carbonates vs apatites).

The correlation between CaO and MgO is strong and positive in all three formations, indicating dolomite. The correlation between CaO and Fe_2O_3, which may signal ankerite, is strong and positive in the Gates Formation, but negative in the Mist Mountain. By looking at the same relationships, but without any mineral studies to confirm, we might expect to see dolomite, some ankerite, and little apatite in the Gething Formation.

6.2.3. The effect of sulphur

In all three formations, SO_3 in ash correlates negatively with CSR (Table 6), but only strongly so in the Gates Formation. Correlations between the base and metal oxides and SO_3 may be misleading, because they may in part represent new sulphates formed from cations, oxygen, and non-crystalline organic sulphur during ashing rather than from original minerals. This may explain why SO_3 correlates positively and strongly with CaO in all three formations even though gypsum was not detected in any of the samples studied by Grieve et al. (1996). It may also explain why little pyrite was detected in the Gates Formation despite a strong positive correlation between Fe_2O_3 and SO_3.

British Columbia Rocky Mountain coking coals are known for their low sulphur content. Evidence from sulphur forms analyses show that for all three formations, organic sulphur is more abundant than in sulphate or pyritic form in all three formations (Riddell and Tian 2017).

6.3 Other coking coal quality prediction methods

The BHP Australia equation, Kobe Steel equation and the Nippon Steel plot performed poorly and appear to be of little value for predicting CSR for the British Columbia Rocky Mountain coking coals. The tradition of paying attention to the inert/reactive maceral ratio and the fluidity of the coal in predicting coke quality stems from the experience of steelmakers that these factors are useful for predicting cold strength (i.e. strength after coking, but before exposure to high heat and high CO_2 levels) for coals from much of the world (Pearson, 1980; Pearson, 1989; Ryan et al., 1998). Cold strength is best for global coals with fluidities in the range of 200 to 1000 dial divisions per minute (ddpm), mid-volatile rank, and low inerts (<30%; Gransden et al., 1991). British Columbia Rocky Mountain coals are predominantly in the mid-volatile range, but commonly have low fluidities (<50ddpm) and high inerts (30-45%). Before the 1980s, when the importance of ash chemistry to hot strength was recognized, these Rocky Mountain coals were considered inferior to higher fluidity, low-inert coals (Pearson, 1989). However, low fluidity and high inerts content do not appear to be detrimental to CSR in samples with favourable ash chemistry in Rocky Mountain coking coals (Figs. 16, 17).

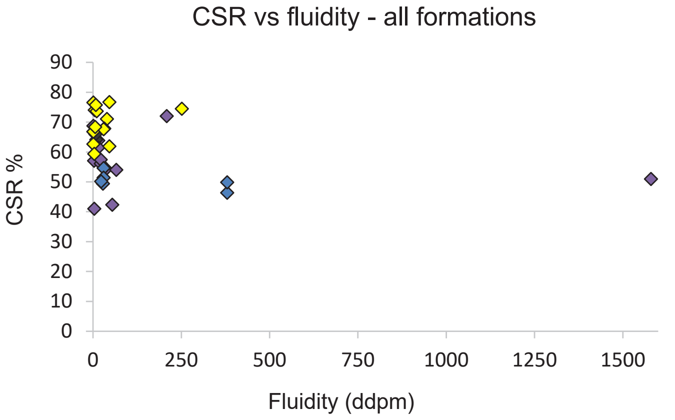


Fig. 16. CSR vs. fluidity for samples from all 3 formations, 38 samples. Samples with very low fluidities of under 200 dial diameters per minute (ddpm) produced cokes with good CSRs. The samples with the favourable ash chemistry (yellow) tend to have higher CSR, regardless of fluidity. Data points are colour coded by BAR: Yellow with BAR less than 0.1, purple with BAR between 0.1 and 0.2, blue with BAR greater than 0.2.

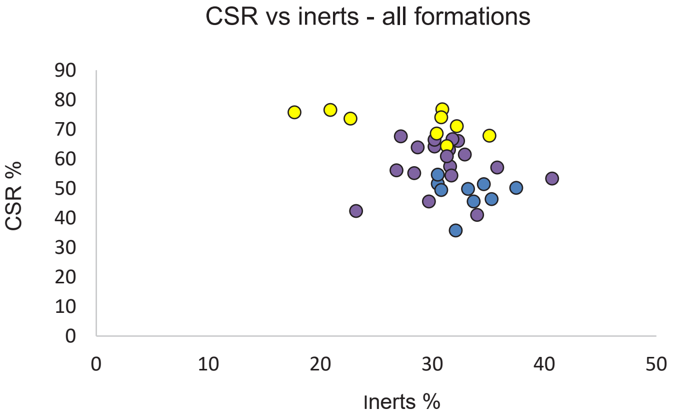


Fig. 17. CSR vs % inerts for samples from all three formations, 36 samples. Samples with inerts as high as 35% produced cokes with good CSRs. The samples with the favourable ash chemistry (yellow) tend to have higher CSR, regardless of inerts content. Data points are coded by BAR: Yellow dots have BAR less than 0.1, purple dots have BAR between 0.1 and 0.2, blue dots have BAR greater than 0.2.

6.4 Limitations of coke quality predictions

Predicting coking quality for a coal is difficult because of the factors that affect it are numerous, some of the factors are interrelated and others independent, and because many of the relationships between factors are non-linear. The success of a prediction method may be an artifact produced when many of the factors in the sample set have uniform values (as in the example of the Gates Formation in this study, where the ranges of rank and of ash content are narrow). Ash chemistry is a relatively simple and inexpensive way to understand one aspect of a coal's coking quality, but it ignores a lot of complexity. In the case of the western Canadian coking coals of the Gates, Gething and Mist Mountain formations, predictions using ash chemistry appear to provide a reliable first-order indication of their coking quality as measured by CSR. These predictions have value, especially at early exploration and development stages before CSR measurements are feasible due to cost and the logistical requirements of collecting good samples for coke oven testing.

7. Conclusions

- Measured CSR values from Rocky Mountain coking coals in British Columbia correlate well (correlation coefficients better than -0.59) with indices calculated from ash chemistry tested in this study. The best correlations are from the Gates Formation, the weakest are from the Gething Formation.

- All samples in this dataset with BAR values >0.174 had CSRs (<57%). In other words higher BAR values in the ash guaranteed lower CSR but ash with a low BAR did not necessarily guarantee a higher CSR. The implication is that although other factors affect CSR, bad ash chemistry cannot be overcome by favourable rheological, petrographic or other properties.

- Because coking coals are generally blended with other coals to take advantage of the best qualities of each, rather than being used individually, a low-CSR coal is not without value. However, it will likely fetch a lower price.

- Plots of CSR vs rank as measured by volatile matter (dry ash free) are consistent with observations that the best coking coals are most commonly of mid-volatile rank; low-volatile and high-volatile coals tend to have lower CSRs. However, parabolic fits of CSR vs VMdaf are weaker than linear fits for plots of CSR vs ash chemistry indices. Ash chemistry appears to have a stronger influence.

- Increased ash content seems to lack a significant negative effect on CSR in this sample set, suggesting that ash chemistry is more important than the amount of ash in the clean coal. This implies that for British Columbia Rocky Mountain coking coals, extra efforts to wash to lower ash contents may not meaningfully improve CSR in coals with good ash chemistry and might not be worth the risks of losing other, potentially beneficial, properties of the lost coal.

- The importance of the ash oxides in terms of negative correlation with CSR varies between formations.

- For the Gates and Mist Mountain formations, the index that produced the best correlation between measured and predicted CSR was the Base-Acid Ratio with the correction for calcium in apatite (BAR-Capatite). For the Gates Formation, this index produces a fit with a correlation coefficient of -0.872 and a root mean square error of 4.78. For the Mist Mountain Formation, this index produces a fit with a correlation coefficient of -0.802 and a root mean square error of 5.43.

- The predictive index that produced the best correlation between real and predicted CSR for the Gething Formations was the Ash Index modified by including phosphorous into the index. This index produces a fit with has a correlation coefficient of -0.704 and a root mean square error of 5.86.

- The applicability of the predictive indices derived in this study depends on the tolerance for the error for its use. Estimates with root mean square errors of 4.5 to 5.5 % are useful during exploration phases, to provide a timely and inexpensive first indication of CSR, identify problematic seams, and help the geologist design blends for oven testing that will better characterize potential product coals. During mining, ash chemistry analysis can provide a working estimate of CSR months before oven test results are available. However, these RMSEs would not be adequate for feasibility studies or product marketing. Ash chemistry-based predictions of CSR cannot replace oven test measurements.

- The success of the BAR-Capatite correction at improving correlation with CSR gives credence to the approach of correcting ash chemistry indices based on knowledge of the minerals that potentially reactive elements occur in. Wider application of such methods may be possible by: 1) better understanding the mineralogy of the non-coal components; 2) developing reliable methods for determining the mineralogy of the non-coal components from ash chemistry or other inexpensive means; and 3) improving knowledge about the reactive behaviour of more of the common coal minerals under blast furnace conditions.

- Prediction methods that use fluidity and inerts content of coals without considering ash chemistry do not produce reliable CSR predictions for British Columbia coking coals.

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