SCATTERSCORE METHOD TO EVALUATE CHANGES IN WATER QUALITY¹

by

Ann G. Kim² and Carol Cardone

Abstract. In Pennsylvania, water quality is monitored at mine sites remediated with coal combustion by-products (CCB), on a quarterly or annual basis. This produces extensive data files including values for 32 parameters that are difficult to evaluate for overall changes in water quality. Tracking a few major parameters, such as pH, Fe, or acidity, produces a complex data set that excludes other significant values. A quantitative measure of estimating if the overall change in water quality is an improvement, no significant change or deterioration should take into account all measured quantities. Since the variation in water quality parameters over time for this data set is not normally distributed, mean and standard deviation are not appropriate statistics. To assess the change in water quality at a site, a scatterscore evaluation was developed. In this reconnaissance method, a score is calculated based on the differences between up gradient (control) versus down gradient (treatment) water quality data sets. All parameters measured over a period of time at two sampling points are compared. The relationships between the range of measured values and the ratio of the medians for each parameter produces a data point that falls into one of four quadrants. Counting the number of values in each quadrant, multiplying by an appropriate weight and normalizing the final value produces a scatterscore that indicates the overall changes in water quality at mine sites where CCB were placed. This evaluation method, indicated that there was slight to moderate improvement in water quality at 30 % of the CCB remediated sites and slight deterioration at 25 % of the sites. The scatterscore at the remaining sites indicated random change in the measured parameters.

Additional Key Words: Acid Mine Drainage, Coal Combustion By-Products

Introduction

The U.S. Department of Energy's National Energy Technology Laboratory (NETL) supports research to promote the increased use of Coal Combustion By-Products (CCB) (DOE, 1994). Treating CCB as a waste material imposes a significant cost on utilities and their customers. Benefits of CCB utilization include conservation of land, energy and natural resources.

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²Ann G. Kim is a Team Leader for By-Product Utilization in the Environmental Science Division of the National Energy Technology Laboratory, U.S. Department of Energy, Pittsburgh PA, 15236-0940. Carol Cardone is a Physical Scientist in the Environmental Science and Technology Division. Increased cost and heightened regulations are also making disposal of CCB an undesirable option (EERC, 1998). To take advantage of the inherent value of the material, CCB can be used in a number of ways, including its use in mine remediation. The scatterscore method, described in this paper, addresses the need to evaluate changes in water quality at mine sites where CCB have been used to control acid mine drainage (AMD).

Acid mine drainage (AMD), a legacy of coal mining in the U.S., has had an impact on surface streams since the eighteenth century. Compliance with discharge standards, required by the Federal Water Pollution Control Act of 1972, the Clean Water Act of 1977, and the Surface Mining Control and Reclamation Act, is largely responsible for a significant improvement in stream water quality over the past 25 years. However, lower cost reagents and preventive measures used during reclamation or closure could further reduce current and future discharges of AMD.

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According to the American Coal Ash Association, in 1998 more than 107 million tons of CCB were produced in the United States by coal-burning electric utility companies, and an estimated 2 pct were used in mining applications (ACAA 1998). The Council of Industrial Boiler Owners estimates that 61 pct. (3.6 million tons) of residues from fluidized bed combustion were used in mine reclamation in 1995 (CIBO 1997). The use of CCB as backfill at mine sites is intended to reduce the generation of AMD. The CCB may have an impact on the discharge of AMD through four possible mechanisms: neutralization, bacterial inhibition, pyrite encapsulation and water diversion (Kim and Cardone, 1997). If the CCB is alkaline, it can neutralize acidic groundwater; and, at a higher pH, bacterial activity is inhibited. A pozzolanic CCB can encapsulate pyrite, isolating it from air and water and preventing the formation of AMD. The deposition of CCB or a CCB grout can also reduce the permeability of mine strata, diverting water away from acid-forming materials. Studies at field sites have indicated limited reduction in the generation of AMD, but have not addressed the overall impact on water quality (Ackman et al 1996; Hawkins et al 1991; Kim and Ackman 1994).

The Environmental Protection Agency (EPA) recently issued a regulatory determination for fossil fuel combustion wastes generated as co-managed wastes (EPA 2000). In their regulatory determination, the EPA retained the hazardous waste exemption under the Resource Conservation and Recovery Act (RCRA) for these materials. However, they also proposed that national regulations are warranted for coal combustion wastes when they are disposed in landfills, surface impoundments, or when used to fill surface or underground mines. These national regulations would also be applied to large volume coal combustion wastes that had been exempted under an earlier regulatory determination. Although no case of environmental damage has been directly attributed to mine backfill with CCB, it has generally been difficult to evaluate water quality changes at mine sites.

Pennsylvania Data set

The Pennsylvania Department of Environmental Protection (PADEP) has extensive data on the use of CCB in mine reclamation. The PADEP requires mining companies which place CCB in surface mines to apply for a modification of their mining permit (Module 25) and then submit quarterly and annual reports (PADEP 1993). DOE personnel have been allowed to copy the Module 25 applications and monitoring reports at five PADEP offices. This information included the operator's name and location, the number of acres in the mining permit and the number proposed for placement of CCB. The ash generator(s) was identified, and the volume of ash to be placed daily, monthly or annually was given in the permit application. Water samples were obtained from 593 monitoring points, such as wells, springs, pools, ponds, pits, and discharges.

Parameters to be reported quarterly included pH (field and lab), specific conductivity, alkalinity, acidity, iron, manganese, sulfates, fluoride, chloride, sodium, total dissolved solids, total suspended solids, ammonia nitrogen, nitrate nitrogen, bicarbonate, turbidity, and chemical oxygen demand. The concentrations of aluminum, arsenic, barium, cadmium, calcium, chromium, copper, lead, magnesium, mercury, nickel, selenium, silver and zinc were included in annual reports. Ash composition and leachate data were also submitted on an annual basis. When transcribed into spreadsheets, there are over 6,300 rows of water quality data in the data set. Sampling locations were identified structurally as above (up gradient) or structurally below (down gradient) the ash placement sites. The period for the water monitoring data extended from 1978 to 2000.

To evaluate the effect of using CCB in mine reclamation on water quality required merging data on 32 water quality parameters in the quarterly and annual reports. The number of parameters makes comprehensive evaluation of water quality difficult.

The mine water system is a complex chemical system that involves inputs from meteoritic water and ground water, and chemical reactions between pyrite, spoil, overburden, and the CCB. The volume of water in the system, the rate of infiltration and evaporation, and the type of sampling points are also independent variables.

In addition to the number of variables, there were other difficulties in trying to analyze the PADEP data. At several sites, it was not clear whether missing data indicated a value below the analytical detection limit or no analysis. Also, the date CCB were placed was not available for some sites, or could only be estimated as some point within a given year. The amount of ash and the placement schedule were generally not available. In many cases, it was difficult to match up gradient and down gradient sampling points, and limiting the number of variables evaluated required a qualitative decision on the importance of each water quality parameter. Even tracking a few major parameters, such as pH, Fe, Al, and Mn, produces a complex data set that is not easy to evaluate.

The measured concentrations are a function of both the chemical reaction rate and the amount of water in the system. Precipitation, snow melt, groundwater discharge and recharge, and possible changes in the flow path affect the volume of water in the system. Since the reports do not include flow rates or data on water volume, the concentration values cannot be normalized to an objective standard such as daily or annual load. Also, relationships between variables may be a function of the geologic conditions and mineralogical characteristics of the CCB, which vary for each site.

Changes in the value of each variable are related to additions to the system (solubility, reaction), removals from the system (precipitation, adsorption, reaction), and changes in the volume of water and in the various reaction rates. In the absence of simple or obvious relationships, each water quality parameter is considered an independent variable.

Based on previous evaluations of the data, the distribution of values cannot be assumed to be normal (Kim and Cardone 1997a; Kim and Cardone 1997b). Therefore, statistical tests of significance that apply to normally distributed data sets, e.g., t-test, should not be used to compare the water quality data. Also, the data sets are relatively small, sometimes fewer than 10 values, and the central limit theorem (the sample mean equals the population mean when n is large) does not necessarily apply.

Water Quality Evaluation Methods

There are a number of methods used to analyze water quality data. Methods vary based on informational goals, the type of samples, and the size of the sampling area. Research in this area has been extensive as indicated by the number of methods proposed or developed since 1970 (Dixon and Chiswell 1996). According to Fetter (1994) relatively simple methods such as the Piper Plot, StiffDiagram, Schoeller Diagram, Durov and Langlier-Ludwig plots are visual representations of the concentrations of major cations (usually calcium, magnesium and sodium) and anions (usually chloride, bicarbonate and sulfate). They are most useful for quick visual comparison of the composition of waters from different sources.

A Water Quality Index (WQI) was developed by the National Sanitation Foundation in 1970 (Brown et al 1970). A panel of 142 water quality scientists selected 9 parameters (dissolved oxygen, fecal coliform, pH, biochemical oxygen demand, temperature, total phosphate, nitrate, turbidity and total solids) and then developed a Q value from 0 to 100 based on the raw data for each parameter. Each Q value is multiplied by a weighting factor based on that parameter's importance in water quality. The summation of the weighted Q values equals the WQI, and possible values between 0 and 100 fall into one of five ranges defined as very bad, bad, medium, good and excellent.

An alternate water quality index (WQM) has been developed to evaluate the cumulative effect of combined factors (Alcock 2000). This water quality index attempts to include the joint effect of multiple factors. The end result is a 100 point scale based on manipulation of the same factors used in the WQI. A similar method defines a water quality index that includes other parameters with other ranges related to quality indices between 0 and 16 with weights between 6 and 16 (Stambuk-Giljanovic 1999). Dividing this index by the maximum admissible concentration, WQE_{MAC} , produces a value relative to the amount of water pollution. A similar method increases the number of parameters to 20, and includes a subjective constant based on the visual impression of contamination (Pesce and Wunderlin 2000).

Trend analysis has been used to explain some of the variability in monthly water quality data (Hirsch et al 1982). The technique is appropriate for data collected by systematic monthly sampling. The collection of ancillary data, such as time of day, water temperature, and discharge, are also recommended.

The Environmental Protection Agency has developed two commonly used water quality models. The Enhanced Stream Water Quality Model (QUAL2E) is a steady state model for conventional pollutants in branching streams and well mixed lakes. It can be used to study the impact of waste loads on in stream water quality. The MINTEQA2 model is an equilibrium speciation model that can be used to calculate the equilibrium composition of dilute aqueous solutions. Both models are DOS based and can be downloaded from EPA's website (EPA 2000b).

Water quality monitoring programs should first address technical and information goals, and also define the meaningful indicators. The assessment of ambient conditions, the detection of trends, and exceeding regulatory limits may require different approaches. Determining time dependent trends in water quality requires information on seasonal changes in flow, and usually require evenly spaced observations. The number of parameters, the different sampling frequency and the need to compare water quality at discreet sampling points were limitations that precluded the use of typical methods to evaluate the PADEP data.

The purpose of placing CCB at mine sites is to either prevent the formation of AMD or to reduce the impact of mine water on receiving streams. The purposes of monitoring water quality are to evaluate the effectiveness of the CCB treatment and to determine that no elements have been leached from the CCB by the mine water. There are several comparisons that can be used for this type of evaluation.

The first method is comparison to an objective standard, such as primary drinking water, or groundwater criteria or an appropriate index. This comparison is limited to particular elements that are perceived to have particular health or environmental impacts. It is unusual if the standard includes all elements in the water analysis. However, it may include parameters that are not appropriate for the particular sample. This approach is most useful for determining regulatory compliance. Comparing a discharge sample to an objective standard does not indicate that values of water quality variables are related to the treatment applied, in this case, the presence of CCB at the mine site.

Water quality at a single sampling point evaluated on a Before and After basis is most appropriate for a short duration limited event, for example the effect of a storm on discharge. If applied to longer term monitoring, the Before data should be accumulated for a long enough period of time to encompass all conditions that will affect the After data. For systems such as a mine pool or a stream, there is no one-to-one correspondence of Before and After samples, and time is not a primary factor controlling concentration. Before and After comparisons are more accurate when concentration values can be converted to daily load which reduces the impact of precipitation, infiltration or runoff.

Another comparison can be made with In versus Out samples. This requires a controlled system in which it can be determined with certainty that In and Out are directly connected through the treatment area and that there are no extraneous additions to or deletions from the system. In water quality evaluations, this would require a relatively small distance and a short time interval. These conditions may be met in limited surface water systems, but are rarely met in groundwater systems.

Similar to the In and Out methods, but applied to a

broader scale, is the Control versus Treatment approach. It is assumed that the Control (background or baseline) samples and Treatment samples were originally similar and that all factors that affect the Control sampling point have an equivalent effect on the Treatment sampling point. It is not necessary that the Control and Treatment sampling points be connected, and this approach accommodates sampling on a broader (quarterly or annual) time scale. It is applicable to mine pool samples where the volume of water is unknown and where the response time of the system is relatively long.

The appropriate approach to water quality monitoring is dependent on the goal, whether regulatory compliance, evaluation of time dependent changes, comparison to other sampling points or systems, or determining the effectiveness of some treatment method. The sampling period, the sampling protocol, and the number of parameters measured will also have an impact on the quality and usefulness of the resultant data. Given the inherent variability of a water system, the sampling period will constrain which approach is most applicable.

Scatterscore Method

In evaluating the PADEP data, the simple goal was to determine if the water affected by the placement of CCB was better or at least no worse than unamended samples. Given the nature and scope of most mine water systems, Control versus Treatment was considered the most viable approach. The Before and After approach could also be applied at down gradient sampling points.

In order to keep the evaluation simple, several conditions were imposed on the selection of a method. First, all parameters in the data set would be included; there would be no evaluation of the relative importance of different variables. Data manipulations would be performed in a spreadsheet with minimal editing requirements. There would be no absolute or relative data conversions; concentrations would be evaluated in mg/L and pH in standard units. Since the sampling intervals were not consistent, no attempt was made to match Because water quality parameters are samples. essentially different in surface and underground environments, comparisons are considered valid only between samples from similar sources, i.e., stream samples would not be compared to well samples.

The evaluation would be based on the difference between values at control and treatment sampling points for all variables. These would be aggregated to a single score indicative of overall change. An average of all possible comparisons (Controls versus Treatments, Befores versus Afters) would be the final score, a single mathematical value indicative of the change in water quality related to placement of the CCB.

At each site there is at least one up gradient sampling point (Control) and one down gradient sampling point (Treatment). An example of the quarterly sample data is given in Table 1 and annual data in Table 2. Values based on differences between parameters at up and down gradient sampling points were plotted on a scattergram and a scatterscore was calculated. This approach was also applied to water samples obtained at the down gradient sites for before and after placement of CCB.

Range Comparison

At each sampling point all values, for each parameter, fall within a range with maximum and minimum values. When compared, if treatment has a positive effect, the range of the down values will be equal to or lower than the range of the up values. There are seven possible relationships between ranges defined by high or low values at the up and down sampling points (Fig.1). The Up range is on the right and the Down range is on the left. The top bar represents the maximum value and the lower bar the minimum value. The ranges may be equal, partially overlap or contain no similar values.



Figure 1. Relationship between up and down gradient ranges.

The up range (R_U) is defined as the maximum parameter value measured at the up gradient sampling point minus the minimum parameter value for the same sampling point. The down range (R_D) is the same for the down gradient sampling point.

$$R_U = (Max_U - Min_U)$$
 (1)

$$R_D = (Max_D - Min_D)$$
 (2)

The range total (R_t) is equal to maximum, up or down minus minimum, up or down. The sum of the ranges (ΣR) then is equal to the sum of the difference between the maximum and minimum values for up and down ranges. The range value (R_t) equals the range total divided by the sum of the ranges. This measures the degree of overlap between the ranges.

$$R_{t} = Max_{U:D} - Min_{U:D} \quad (3)$$

$$\Sigma R = R_{U} + R_{D} \quad (4)$$

$$R_{v} = \frac{R_{t}}{\Sigma R} \quad (5)$$

The difference, Δ Max, between the maximum value of the up set and the maximum value of the down set would be positive if the maximum up is greater, and negative if the maximum up is less than maximum down. Dividing Δ Max by its absolute value yields values of 1 or -1.

$$\Delta Max = Max_{U} - Max_{D} \qquad (6)$$

Combining these factors produces the range comparison (RC)

$$RC = R_v * \Delta Max_{abs}$$
 (7)

For example, in Figure 2, if all the up values are between 80 and 50 and the down values are between 75 and 40, the range total for all values would be 80 minus 40. It does not matter which set is higher or lower.

DATE	FIELD	LAB	SPECIÉ.	ALK.	ACID.	IRON	MANGANESE	SULFAT	TDS	TSS	AMMON	NITRAT	BICAR	TURBIDIT	COD	FLUORIO		SODILIM
	_11	-14						E			IA	E	В	Y	002	Ę	E	000.00
SAMPLED	рн	рн	COND,	as CaCO3	as CaCO3	(Fe)	(Mn)	(SO4)			(NH3-N)	(NO3-				(F)	(C))	(Na)
												N)	(CaCO					
GW-1A																		
Feb-91	5.16	5.18	441.00	2.00	8.00	7.31	24,04	153.10	319.00		0.00	1.45	2.00	40.00		<u>an n</u>	0.30	7 07
Feb-92	6,17	6.18	620.00	2.00	9.00	0.38	0.12	202.00	424.00		0.00	1 47	2 00	2 10		0.00	0.30	1.97
Feb-93	6.24	5.86	476.00	4.00	4.00	0.49	0.24	199.42	275.00		0.00	1.09	0.00	4 70		0.00	0.40	6 10
May-93	6.08	5.69	406.00	4.00	6.00	0.22	0,07	170.20	270,00		0.00	1.54	0.00	3.30		0.00	1.82	3.66
Aug-93	6.90	6,83	398.00	16.00	0.00	0.06	0.05	133.80	294.00		0,00	1.03	16.00	2.20		0.00	4 31	6.50
Nov-93	6.10	5.73	502.00	9.00	. 6.00	0.81	0.21	172.20	261.00		0.00	0.85	9.00	5.20		0.00	1.97	5.90
Nov-94	6.07	6.15	348.00	5.60	2.47	0.30	0.10	140.60	215.00	2.00	0.00	1.41	5.60	5,20	29.00	0.00	0.00	5.00
02/15/95	4.80	6.16	355,00	9.14	0.00	0,64	0.10	160.30	313,00	3.00	0.00	1.20	9.14	3.10	0,00	0.00	2.25	3,80
03/03/93	7.70	5,15	318.00	0.00	11,06	4.25	0.38	174.42	320.00	65.00	0.00	0.94	0.00	17.00	0.00	0.00	0.00	4.40
11/15/95	5,00	5.20	494,00	2.90	6.00	5.24	0.20	168.00	247,00	5.00	0.00	0,94	2.90	1.80	209.00	0.00	1.78	5.46
02/21/06	5.52	5.04	401.00	4.80	1.70	1.35	0.12	145.00	250,00	35.00	0.00	1,94	4.60	14.00	20.40	0.00	0,00	4.70
05/20/96	5.04	5.01	433,00	2.10	8.79	0.35	0.04	150.00	253.00	5.00	0.00	1.15	2.10	4,30	0.00	0.00	5,34	4.00
08/20/96	5.80	3.65	432.00	9.22	13.60	0,05	0.15	157.00	215,00	6.00	0.00	1,60	4.22	0.45	46.60	0.00	1.29	3,60
11/12/96	5.51	5.86	312.00	6.83	3.98	0.80	0.12	190,00	200.00	7.00	0.00	0.00	0.00	2.00	26.00	0.00	0.00	4.30
02/12/97	5.57	5.90	320.00	3.88	2.07	0.33	0.04	123.00	102.00	2.00	0.00	1.43	0,63	4.40	0.00	0.00	0.00	4.20
05/29/97	5.50	5.64	334.00	2.04	4.26	0.35	0.05	141.00	201.00	79.00	0.00	1.18	3.66	2,30	0.00	0.00	1,94	3.40
03/02/98	5,52	6.08	282.00	9,70	0.00	0.00	0.00	129.00	278.00	4.00	0.00	1.33	2.04	40,00	49.10	0.00	2,48	2.90
05/14/98	6.06	7.03	276,00	14.B0	0.00	0.43	0.00	115.00	196.00	0.00	0.00	1.04	14.90	0.00	20.00	0.00	0.00	3.20
08/12/98	6.00	6,40	372.00	6.50	0.00	1.59	0,13	146.00	241.00	60.00	0.00	1 16	6.50	9.00	41 10	0.00	0.00	2.15
11/18/98	8,19	6.32	271.00	9.60	0.40	0,72	0.05	131.00	250.00	24.00	1.00	0.90	9.60	6 20	29.70	0.00	0.00	4 66
06/01/99	6.19	6.18	354.00	4.02	0.00	0.17	0.02	150.00	344.00	2.00			0.00	0.20	20.70	0.00	0.00	4.00
0141.01																		
GVV-ZA																		
Feb-91	6.10	6.09	169.00	14.00	0.00	17.48	1.09	49.60	133.00		0.00	0.00	44.00	60.00				
Feb-92	6.39	6.41	381.00	37.00	0.00	76.40	2.07	110 70	231.00		0,00	0.00	14.00	105.00		0.06	0.30	3.01
Feb-93	5.76	5.59	794.00	4.00	12.00	94.60	4.86	356.80	504.00		0.00	0.00	0.00	03.00		0,00	1.10	5.71
May-93	5,47	5.31	918.00	6.00	13.00	10.59	4.16	459 30	707.00		0.00	0.40	0.00	30.00		0.00	0.42	4.91
Aug-93	5.94	5.67	802.00	0.00	19.00	21.20	6,10	360.40	855.00		0.00	0.00	0,00	90.00		0.00	4.02	5.70
Nov-93	5.51	5.0B	1131.00	2.00	22,00	11.95	5.45	492.90	910.00		0.00	0.14	2.00	43.00		0.00	8.26	5.80
Nov-94	4.99	5.01	1578.00	1.45	22.36	14.84	7,35	714.90	992.00	20.00	0.00	0.10	1.45	45.00	41.08	0.00	15.03	6.30
02/15/1995	4.66	4.60	1175.00	0.00	13.55	11.71	72.70	778,30	1198.00	18.00	0.00	0.30	0.00	24.00	0.00	0.00	13.40	6 20
05/09/95	4.52	4.19	1258.00	0.00	27.10	51.50	8.08	795.21	1245.00	130.00	0.00	0.89	0.00	65.00	33,54	0.00	21.31	8,90
08/14/95	5.28	4.73	1265.00	0.00	35.20	60.60	9.05	600.00	900.00	77.00	0.00	0.00	0.00	110.00	140.00	0.00	16.00	10,65
11/15/95	5.02	4,90	138.00	0.00	18.00	28.50	8.25	670.00	969.00	87.00	0.00	0.07	0,00	86.00	46,60	0.00	12.00	7,40
02/21/96	4.75	4.68	1522.00	0.00	19,71	17.40	10.20	600.00	1065.00	28,00	0.00	0.00	0.00	28,00	0.00	0,00	22.41	7.00
05/20/95	5.03	4.79	1873.00	0.00	22.00	15.40	6.00	753.00	1066.00	39.00	0.00	0.09	0.00	35.00	24.50	0.00	0.07	5.80
00/20/90	4.82	4.32	1517.00	0.00	12.70	27.60	6.80	995.00	1288.00	72.00	0.00	0.08	0.00	60.00	49.50	0.00	14.90	B.10
11/12/90	4.47	4.75	1374,00	0.00	24.80	9.06	8,50	775.00	1038.00	48.00	0.00	0.08	0,00	66.00	0,00	0.00	8,95	6.60
02/ (2/9/	4.19	4.49	1511.00	0,00	31.40	20.60	/.39	890.00	1138.00	87.00	0.00	0.04	0,00	27.00	20,30	0.00	14.80	8.20
03/02/98	4.01	4.24	950.00	0.00	∠0,8U 5.45	0,49	8.17	878,00	1106.00	34.00	0.00	0,00	0.00	50.00	0.00	0.00	17.30	6,30
05/14/08	4 60	4.90	1117 00	2.00	0,15	24.04	3.67	505.00	842.00 910.00	24.00	0.00	0.04	0.97	35.00	68.00	0.00	4.13	4.50
08/12/98	4 33	4 24	1843.00	2.00	27.40	∠4.94 17.65	3,04	393.00 977.00	1385.00	152.00	0,00	0.05	2,00	/2.00	0.00	0.00	4.97	4.66
11/18/96	7.45	4.38	1442.00	0.00	40.80	21 50	8.50	764.00	1220.00	66.00	0.00	0.00	0.00	01.00	05.70	0.00	25.50	8.90
08/01/99	4,64	4,48	1663.00	0.00	31,91	25.40	7,79	1084.00	1486.00	86.00	0.00	0.00	0.00	40.00	00.00	0.00	17,90	13,70

Table 1. Example of Quarterly Data for one Control (GW-1A) and one Treatment (GW-2A)Sampling Point

Table 2. Example of Annual Data for one Control (GW-1A) and one Treatment (GW-2A)Sampling Point.

DATE	Aluminu	Arsenic	Bariu	Cadmium	Calciu	Chromiu	Copper	Lea	Magnesiu	Mercury	Nickel	Selenium	SILVE	ZINC
	'n		m		m	m		d	m				R	
SAMPLED	(Al)	(As)	(Ba)	(Cd)	(Ca)	(Cr)	(Cu)	(Pb)	(Mg)	(Hg)	(Ni)	(Se)	(Ag)	(Zn)
GW-1A														
02/01/91	3.05	0.02	0.23	0.01		0.00	0.00	0.23	24.04	0.00	0.00	0.02	0.10	0.10
02/01/92	0.23	0.00	0.00	0.00		0.00	0.00	0.13	37.90	0.00	0.05	0.01	0.00	0.28
02/01/93	0.39	0.01	0.14	0.00		0.01	0.02	0.09	24.60	0.00	0.00	0.01	0.00	0.24
02/15/95	0.23	0.00	0.00	0.00	29.50	0.00	0.05	0.00	25.48	0.00	0.00	0.01	0.00	0,10
02/21/96	0.15	0.00	0.00	0.01	70.00	0.00	0.00	0.18	19.00	0.00	0.00	8.00	0.00	0.08
02/12/97	0.13	0.00	0.00	0.00	19.00	0.00	0.00	0.00	20.80	. 0.00	0.00	0.00	0.00	0.00
03/02/98	0.50	0.00	0.00	0.01	22.00	0.00	0.00	0.00	23.00	0.00	0,00	0.00	0.00	0.00
GW-2A														
02/01/91	2.94	0.03	0.23	0.01		0.00	0.00	0.15	5.59	0.00	0.00	0.00	0.00	0.06
02/01/92	162.60	0.04	1.60	0.00		0.03	0.13	0.18	55.50	0.00	0.13	0.01	0.00	0.27
02/01/93	15.08	0.01	1.01	0.00		0.01	0.09	0.42	37.40	0.00	0.12	0.02	0.00	0.43
02/15/95	1.64	0.00	0.00	0.00	214.51	0.00	0.04	0.12	70.90	0.00	0.25	0.00	0.00	0.57
02/21/96	1.81	0.00	0.00	0.01	190.00	0.00	0.09	0.17	59.60	0.00	0.18	6.00	0.00	0.56
02/12/97	3.80	0.00	0.00	0.00	215.00	0.00	0.09	0.23	· 64.50	0.00	0.26	0.00	0.00	0.62
03/02/98	1.51	0.00	0.14	0.01	150.00	0.00	0.05	0.00	44.00	0.00	0.14	0.00	0.00	0.26



Figure 2. Example of range comparison

Defined Ranges based on Fig 2.

$$R_{U} = (Max_{U} - Min_{U}) \quad (80 - 50 = 30)$$

$$R_{D} = (Max_{D} - Min_{D}) \quad (75 - 40 = 35)$$

$$R_{t} = Max_{U:D} - Min_{U:D} \quad (80 - 40 = 40)$$

$$\Sigma R = R_U + R_D$$
 (40+35=75)

$$R_v = \frac{R_t}{\Sigma R} = \frac{40}{75} = .53$$

$$\Delta Max = Max_U - Max_D \qquad (80 - 75 = 5)$$

$$RC = R_v * \Delta Max_{Abs}$$
 (.53 * 1 = .53)

$$\Delta Max_{abs} = \frac{\Delta Max}{ABS(\Delta Max)} \quad (\frac{5}{5} = +1)$$

Table 3 is a summary of the possible relationships between the up and down ranges. Based on those factors, the RC can have values of greater than 0 or less than 0. If the down range is lower, the RC will be between 0 and 1. If there is no overlap in the up and down ranges, the RC will be greater than 1 if the down range of values is lower.

Median Ratio

The range comparison does not completely describe the data set. Therefore, in addition to the ranges, the medians were evaluated. Since the data were not normally distributed, the median is the appropriate statistical descriptor for this type of data, and a ratio of up and down medians was included.

Table 3. Possible Values of Range Parameters

Type ¹	$R_t: \Sigma R$	R	ΔMax	RC
1	2	.5	0	0
2	$R_t < \Sigma R$	<1	+1	<0,1>
3	$R_i < \Sigma R$	<1	-1	<0,- 1>
4	$R_t < \Sigma R$	<1	-1	<0,- 1>
5	$R_i < \Sigma R$	<1	+1	<0,1>
6	$R_t > \Sigma R$	>1	+1	>1
7	$R_i > \Sigma R$	>1	-1	<-1

¹ Type refers to figure 1.

The median ratio (MR) is the up median divided by the down median and can have values in 2 ranges, between 0 and 1 or greater than 1. The MR is greater than 1 if the median for the up values is larger than that of the down values. A value between 0 and 1 indicated the median of the down values is greater. A value of 1 indicates the medians are equal. In the example of figure 2, the up median (65) is greater and the value of MR is greater than 1.

$$MR = \frac{Med_U}{Med_D} \qquad \frac{65}{50} = 1.3$$

<u>Scatterscore</u>

The values of RC and MR are calculated for all variables in the data set. Using these values, one point for each parameter in a data set will be placed in one quadrant of a scattergram (Fig. 3). Each quadrant will represent improvement, mixed results or no improvement. Points in quadrant one indicate that there was improvement in the range but not in the median. Points in Quadrant 2 represent improvement in both the range and the median. In Quadrant 3, there is no improvement in the median or range. In Quadrant 4, there is improvement in the median but not in the range. The quadrant values are summarized in Table 4.

Table 4.	Quadrant	Values	for	Scattergram
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Q	RC	MR	Evaluation	Weigh t
1	>0	<0,1 >	Positive Range	0.5
2	>0	>1	Positive	0.75
3	<0	<0,1 >	Negative	0.25
4	<0	>1	Positive Median	0.5

Counting the number of points in each quadrant and multiplying them by the appropriate weight produces an initial scatterscore (SS_i) , a number that is a semiquantitative evaluation of changes at a site.

$$SS_{i} = 75Q_{2} + 5(Q_{1} + Q_{4}) + 25Q_{3}$$
 (8)

In this data set, there are 32 possible variables, and the distribution of points in the quadrants is normalized to 32 to calculate the scatterscore. If all variables improved, all points would be in quadrant 2; and the scatterscore would be 24. If all the points were in quadrant 3, indicating a deterioration in water quality, the score would be 8. If one quarter of the points were in each quadrant, indicating random change, the scatterscore would be 16. To more readily interpret the values of the scatterscore, the initial scatterscore is converted to a positive or negative value on a scale of -100 to 100 (Fig.4), in which a zero value indicates random distribution of points; positive values indicate improvement and negative values indicate deterioration in water quality.

$$S S = \frac{(S S i - 1 6)}{8} * 1 0 0$$
 (9)

At least 2 scatterscores would normally be calculated for each site, one for up versus down and one for before versus after, at a down sampling point. In many cases, more comparisons could be made, depending on the number of sampling points. Table 5 shows the 20 mine sites with the number of up and down comparisons and also the before and after comparisons. The first column indicates the site number followed by the up and down SS_N values for those sites. Site number 1 has 2 up (U) and 3 down (D) comparisons with 3 down before (Db) and after (Da) CCB comparisons. Independent of the number of comparisons, an average score was calculated for each site. Figure 4 shows the average scores for 20 mine sites where CCB were placed.



Figure 3. Scattergram defined by values of RC and MR



Figure 4. Relationship between initial scatterscore and scatterscore on-100 to 100 scale.

Sit #	e U1vsD1	U2vsD1	U1vsD2	U2vsD3	3 U1vsD3	U2vsD2	D1bvsD1a	D2bvsD2a	D3bvsD3a	Average SS
	1 -45	-50					13			-20 ¹
	23	ł	63				15	28	1	27
	38	-7	28	62	2 46	-4	-52	24	-50	13
	4 32						26			29
•	5 50						-22			14
I	6 59		26		22			7	,	29
	7 -21						44			12
i	80						-11			-5
ļ	9 -7						-48			-27
1	0 -15		-64							-40
1	1 -29						-50			-40
1	2 -31		-14		-29		-27			-25
1:	3 -16		39		0		-37	-5	J	-4
1	4 14						-48			-17
1	5 21	-56	-6	-73	-58	-43	-52	-14	-7	-20
1	6 63	-7	20	54	31	19	4	0	-42	23
1	7 46						-63			-8
1	8 -45						20			-12
1	9 -25						-23			-24
2	06						4			

Table 5. Co	mparison	of	Scatterscores	for	Mine	Site	Water	Ouality
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'Site #1 also included a stream comparison that had a SS of 0

Site #3 has 2 up gradient and 3 down gradient sampling points, allowing for 9 comparisons. The highest scatterscore for this site is 62 (moderate improvement) and the lowest is - 52, moderate deterioration. The average scatterscore for this site is 13, indicating overall random change in water quality. Of the average scatterscores, 14 indicate overall random change; 3 scores indicate slight deterioration in water quality and 3 average scores indicate slight improvement.

Average scatterscores for the up gradient versus down gradient comparisons indicate the water quality at 6 sites (30 %) showed slight to moderate improvement due to placement of the CCB (Fig. 5). Five scores (25%) indicated slight deterioration in water quality. The other scores (45 %) indicated random change.

When the before and after scatterscores are averaged for all down gradient sampling points, 2 of the sites (10%) show slight improvement in water quality (Fig.6). Three of the sites (15%) show slight deterioration and one site (5%) moderate deterioration in water quality. The change in water quality at the down gradient sampling points is apparently random.







Figure 6. Average scatterscores for before and after comparisons at down gradient poits.

Based on this type of evaluation in which all parameters are included, it seems that the placement of CCB at mine sites generally has no effect on water quality. There are several factors that make this result the most likely conclusion. First, the data set contains a large number of variables that are unlikely to be affected by the CCB. For example, chemical oxygen demand is a function of the oxidation of organic matter; changes in this parameter are probably not influenced by reaction with the inorganic CCB. Also, parameters that are measured annually are more likely to show random variation. It also should be recognized that there may be no hydrologic connection between the up gradient and down gradient sampling points and that there is no certainty that the water at the down gradient point has been in contact with the CCB. All of these factors would bias the scatterscore toward a random value.



Figure 7 Average scatterscores for up gradient versus down gradient comparisons of water quality.

However, this does not mean that the scatterscore is without value. Random or positive values indicate that the placement of CCB at mine sites probably poses no threat to the environment. Negative values indicate that the water quality data should be examined more closely. The method highlights the problem comparisons, and determining which parameters fall in quadrant 2 of the scattergram targets the parameters of interest.

Summary

The scatterscore is a very general indicator of changes in water quality. It is based on all the available data, but does not include any qualitative evaluation of site characteristics or the adequacy of the data set. Specifically, it does not place greater emphasis on any one parameter or set of parameters. It is simply an attempt to base an evaluation on all parameters over a variable period of time.

A more accurate evaluation of changes in water quality might focus on key parameters or monitor changes at a sampling point over time, if changes in flow or volume could be factored into the evaluation. As given, the data for these sites are not easily treated with such an approach. Therefore, a reconnaissance method, such as the scatterscore, can be used to track general changes and to serve as an indication that a more thorough evaluation is necessary. Using this method, the scatterscores indicated definite water improvement in over 40% of the evaluated sites. Based on this approach, the data from the PADEP indicated no adverse changes in water quality at the mine sites where coal combustion by-products were placed as a backfill.

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