



Project Summary

The Effect of Underground Coal Gasification on Ground Water

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The potential effect of underground coal gasification (UCG) on groundwater has been examined in a combined field and laboratory study. The study was directed at Fruitland Formation subbituminous coal of the San Juan Basin and at the groundwater found in this coal seam. A field site for a possible UCG test was selected and two wells were drilled into the coal seam which lies about 500 feet below the surface. Groundwater samples were collected and used to establish baseline features. Core samples of overburden, underburden and coal were used for baseline characterization of the minerals.

A number of static leaching and sorption studies were performed. Overburden was leached by both acidic and basic water. This material acts as a strong buffer, holding the water at a high pH. The amounts of Cl^- and F^- leached from overburden were about 10 ppm and show little dependence on the pH of the leaching solution.

Ash was generated at several different temperatures. The results of leaching studies of these ashes are reported. The amount of ash dissolved depends upon the ionic strength of the leaching solution in addition to pH. Predominant species dissolved are calcium, aluminum, sulfate, hydroxide and carbonate. Indications are that solubility of the ash decreases with increasing ashing temperature.

Adsorption capacity experiments were conducted in an effort to determine the extent to which mineral matter in Fruitland Formation coal contributes to sorption. Results from the study indicate that coal minerals account for about 95 percent of the sorptive capacity of metal ions while the carbonaceous matter accounts for only about five percent. This sorption appears to be

largely ion exchange with the K^+ and Ca^{+2} cations found on the local clay minerals. Distribution coefficients, K_d , for sorption on coal were determined for the cations and anions under conditions reasonably similar to those in the groundwater of the San Juan Basin. The effect of the natural chelating agent humic acid was generally found to be minimal. Numerical values for the K_d are reported as a function of initial concentration in solution and the data are presented graphically as isotherms. The isotherms indicate multilayer adsorption as initial ion concentration increases and generally fit a modified Langmuir equation well.

Phenol adsorption by clay, raw coal and demineralized coal was studied. It was found that phenol adsorbs strongly to the carbonaceous matter and only slightly to the minerals.

The analytical problem of silicon determination in complex matrices by graphite furnace atomic adsorption spectroscopy techniques has been studied and improved methods are reported here.

This Project Summary was developed by EPA's Industrial Environmental Research Laboratory, Cincinnati, OH, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The subbituminous coal of the San Juan Basin of northwestern New Mexico is one of the largest deposits of the Southwest. Most of the coal lies in deep deposits which will probably only be tapped by underground coal conversion. The most attractive conversion method at the present time is underground coal

gasification (UCG). The principal consideration in the ultimate viability of the UCG process is one of economics; however, environmental factors play a role in the economics of the process.

There are several potentially serious environmental problems with UCG: subsidence, air quality impacts (including SO_x, NO_x, and particulates), and groundwater contamination. The possibility of groundwater contamination is the most substantial and least understood of the three. The purpose of this project was to study the potential for groundwater contamination in the San Juan Basin as a result of UCG. The approach was to establish baseline characteristics of groundwater, coal and rock at a prospective UCG site in the San Juan Basin; to determine solubility and rates of solution of metals from the residue of a UCG burn; and to determine sorptive characteristics of metal ions and organics on the rock, clay and coal.

Baseline Studies

A field site for a possible UCG test was selected about ten miles northwest of Farmington, New Mexico. Fruitland Formation subbituminous coal lies at a depth of 500 feet at the test site and the seam is 16 feet thick. The overburden is part of the Kirtland Shale Formation and the underburden is Pictured Cliffs Sandstone.

Two wells were drilled at the test site and cores were taken from about 15 feet above the principal coal seam to about 15 feet into the underburden.

Water is found in the Kirtland Shale and typically fills wells to within 130 feet of the surface in the vicinity of the test site. The water is part of a confined aquifer which slowly drains in the direction of the San Juan River. The aquifer is charged from exposed sections of Kirtland shale and Fruitland Formation coal at the mesas. The Fruitland Formation coal is water saturated and lies well below the water table. The water migration rate appears to be one to two feet per year, so that little flow occurs through the UCG site. The flow rate suggests that equilibrium will be established between dissolved ions in the water and any adsorption or ion exchange sites in the rock, clay, or coal. Permeability of the coal seam is greater than that of the overburden and underburden, so the flow occurs through the coal seam.

Water samples were collected from the wells in the overburden region and in the coal seam and they were analyzed using standard techniques. Analyses showed that the principal cations in the water are

Na⁺, K⁺, Ca⁺², Mg⁺² and Sr⁺²; the major anions are Cl⁻, SO₄⁻², and HCO₃⁻. These species account for essentially all of the mass observed in the total dissolved solids analyses. The pH of the samples ranged between 7.8 and 10.7.

Baseline determinations of the nature of the Kirtland shale overburden and Pictured Cliffs sandstone underburden were made from rock samples taken from the cores. The rock is composed almost entirely of quartz, feldspar and clay. Clays make up almost 30 percent of the rock with kaolinite and montmorillonite as the principal clay minerals. Cation exchange capacities of 2.7 meg/100 g overburden and 2.2 meg/100 g underburden were determined.

Leachate Studies

Overburden

Overburden samples were pulverized and then the leaching characteristics as a function of pH were studied using a batch technique. Most of the metals (Ag, Ba, Cd, Co, Cr, Cu, Mn, Ni, and Pb) showed no significant leaching at pH higher than five. In general there is a decrease in the amount of metal in solution from a high value near pH 1 to a much lower value as pH increases. Iron, zinc and aluminum show a general decrease in concentration to a minimum in the vicinity of pH 6-7 with increases as the pH approaches 10. Sodium, calcium, magnesium and lithium concentrations decrease as pH increases.

The overburden has considerable buffer capacity. Solutions of all but very high and very low pH were buffered to a final pH of 8.3 to 8.4. This may help explain the groundwater basicity. The concentrations of Cl⁻ and F⁻ in the leachates were very low and showed no trend with pH. The specific conductance of the leachate was significantly higher at the extreme ends of the pH scale indicating that more of the rock was dissolved at very high and low pH's.

Underburden

Samples of the underburden were equilibrated with solutions over the pH range of 1-12. The rock has strong buffer action as evidenced by pH's of the 7.1 to 7.3 for all the leachates. It is not clear why the pH of the underburden leachates is considerably lower than the groundwater pH or the leachates from the overburden. A comparison of the total dissolved solids concentrations of the leachates and initial pH of the leaching solutions shows a minimum total dissolved solids concentration in the vicinity of pH 7 with large amounts of rock dissolving in either

strongly acidic or strongly basic solutions. Sulfate is the most abundant anion with over half of the mass of the total dissolved solids from the pH 7 leach comprised of sulfate. At the extremes of the pH scale sulfate makes up a small fraction of the total dissolved solids mass. Concentrations of Cl⁻, F⁻ and CN⁻ were so low at all pH values that variations are insignificant.

Ash

Coal from the Fruitland Formation was used to prepare a series of ash samples to simulate the material which will be left after an underground coal gasification experiment. Ash for a dynamic leaching study was prepared using ASTM procedure D-3173 (1) which involves a final ashing temperature of 750°C. Distilled-deionized water was gravity-fed through a column filled with the pulverized ash. Analyses at the leachate showed Ca⁺², Na⁺, Mg⁺² and K⁺ present as the principal cations and Hg⁺², Al⁺³, Pb⁺², Zn⁺², Fe⁺³ and Cu⁺² present as trace constituents.

Ashes were also produced using ASTM procedure D-3173(1) modified to give final ashing temperatures between 700°C and 1050°C, in an effort to study the effect of ashing temperature on leaching characteristics. Batch leaching tests using distilled-deionized water and a simulated ground water were performed on each ash. The simulated ground water approximated the characteristics of the San Juan Basin in pH, conductivity and primary ion concentration. A comparison of the two leaching solutions indicates that the simulated ground water dissolves more of the ash than the distilled-deionized water does. This may be due to ionic strength or pH effects. The solubility of the ash is also affected by ashing temperature with solubility decreasing as temperature increases.

Distribution Coefficients (Overburden and Underburden)

Ultimately the rate of migration of an ion is determined by a heterogeneous equilibrium of the ion between the solution and the solid phases. The equilibrium is characterized by a distribution coefficient K_d which is defined as:

$$K_d = \frac{\text{(activity of ion A in the solid phase)}}{\text{(activity of ion A in the liquid phase)}}$$

Since the activities are defined in concentration terms, K_d becomes the ratio of the concentration of the ion (A) in the solid phase to the concentration in the liquid phase. It is inversely proportional to the pollutant transport rate and directly proportional to both the exchange capacity and selectivity of the exchanger.

Distribution coefficients are dependent upon the specific experimental conditions for which the values are obtained. In an effort to understand how some of the experimental factors influence K_d , we measured the K_d of Cd^{+2} on the overburden and underburden as a function of Cd^{+2} concentration and rock particle size.

Samples of Kirtland shale overburden and Pictured Cliffs sandstone underburden were crushed and sorted into three particle size ranges. The samples were equilibrated with solutions containing a range of Cd^{+2} concentrations. The concentrations of Cd^{+2} , Na^+ , K^+ and Mg^{+2} were measured in the equilibrium solutions.

The K_d 's of Cd^{+2} on the overburden as a function of Cd^{+2} concentration and rock particle size is shown in Figure 1. A similar plot was obtained for the underburden. For all of the cases studied, K_d values increase with increasing Cd^{+2} ion concentration to a maximum in the vicinity of 100 mg/l. This is followed by a rather abrupt decrease which may be explained in two ways. Either the maximum indicates saturation of the surface sites by the Cd^{+2} added from the solution or ion exchange occurs between the cadmium ions in solution and the abundant metal ions bound to the clay minerals. If the latter is occurring, the displaced ions (Na^+ , K^+ and Mg^{+2}) should appear in solution. Analyses show that for each Cd^{+2} concentration range the amount of desorbed cation remains low until the concentration of added Cd^{+2} reaches 1000 mg/l, at which point there is an abrupt increase, by a factor of three or more, in the amount of desorbed metal ion.

When the number of moles of Cd^{+2} absorbed is compared with the total number of moles of Mg^{+2} , Na^+ and K^+ released, a ten-fold increase in Cd^{+2} only increases the moles of Mg^{+2} , Na^+ and K^+ released by a factor of five. At the same time K_d decreases dramatically. This suggests that ion exchange is the dominant sorption mechanism. As the Cd^{+2} concentration reaches very high levels the readily accessible ions in the clay matrix become saturated and the amount of ion exchange does not keep up with the increased Cd^{+2} concentration.

Sorption Studies on Coal

Sorption Capacities

An adsorption capacity experiment was conducted in an effort to determine the extent to which the mineral matter in Fruitland Formation coal contributes to sorption. The experiment was designed in

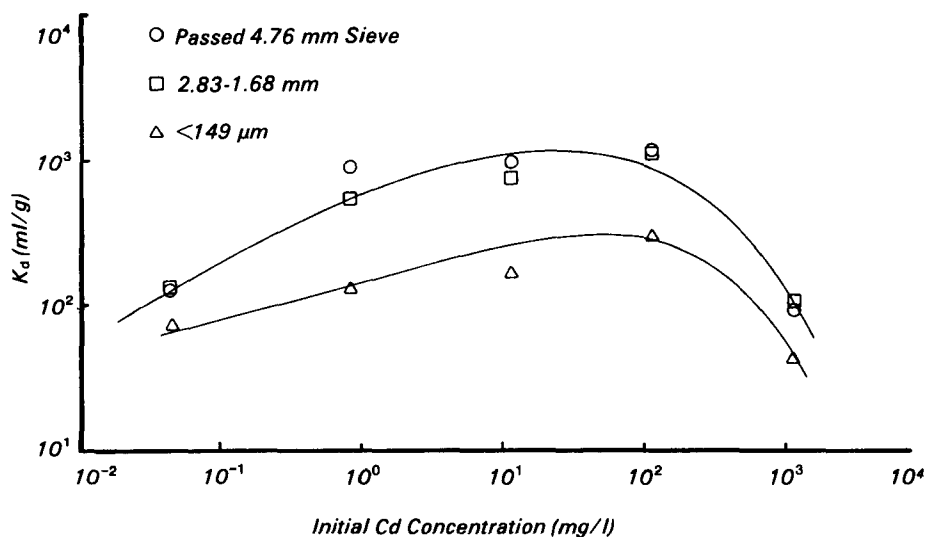


Figure 1. K_d for Cd^{+2} on Pictured Cliffs sandstone as a function of initial concentration of Cd^{+2} .

such a way as to distinguish between ion exchange and simple solution.

The coal was demineralized by digestion in a series of acids. This coal typically contained 0.5 percent ash. The exchangeable ion sites on the demineralized coal and on the raw coal were loaded with Na^+ by equilibrating the coal with a sodium chloride solution. Sorption capacities were determined by equilibrating the Na -loaded coals with a solution of 1 N ferrous ammonium sulfate. The solutions were analyzed for Fe^{+2} , Na^+ and Ca^{+2} .

After blank correction for leachable Na^+ , ion exchange and sorption capacities were calculated for both raw and demineralized coal. The total amount of Na^+ and Ca^{+2} released into solution was interpreted as the ion exchange capacity of the coal, while the total sorptive capacity was taken to be the amount of Fe^{+2} adsorbed by the coal, calculated by subtracting the final Fe^{+2} concentration from the initial concentration. The difference between

total sorption and sorption due to ion exchange is simply called adsorption.

Table 1 shows that inorganic matter accounts for approximately 95 percent of the sorptive capacity of Fruitland Formation coal while the carbonaceous material contributes only about five percent to the adsorption of iron. It can also be seen that from one-third to one-half of the sorptive capacity for iron may be directly attributed to ion exchange.

Distribution Coefficients

Since distribution coefficients are influenced by such factors as the composition of the liquid phase, the chemical nature of the solid phase and pH, we tried to approximate field conditions when we determined the K_d 's. The K_d 's for each ion were determined in the presence of all the other ions selected for study and the background ionic strength was adjusted to a constant value with the predominant

Table 1. Sorption Capacities of Raw and Acid-Washed Fruitland Coal

	Raw Coal	Acid-Washed Coal
Total Sorption Capacity	155±15 meq Fe^{+2} /kg	8.1±0.8 meq Fe^{+2} /kg
Ion-Exchange Capacity*	55±5 meq Na^+ /kg	2.2±0.2 meq Na^+ /kg
	10±meq Ca^{+2} /kg	0.5±0.1 meq Ca^{+2} /kg
	65±4 meq/kg	2.7±0.2 meq/kg
Adsorption Capacity (by diff.)	90±11 meq Fe^{+2} /kg	5.4±0.6 meq Fe^{+2} /kg

*Small amounts of trace elements, such as K^+ or Mg^{+2} , not replaced by Na^+ may have been displaced by Fe^{+2} . Therefore, reported ion-exchange capacities are considered to be minimum values.

cationic and anionic constituents of the local groundwater. An attempt was made to use realistic concentration ranges of the ions of interest (Mn^{+2} , Fe^{+3} , Zn^{+2} , Cd^{+2} , Al^{+3} , Cr^{+3} , Co^{+2} , Ni^{+2} , Cu^{+2} , Hg^{+2} , Pb^{+2} , Be^{+2} , CN^- , F^- , MoO_4^{-2} , SeO_3^{-2} and AsO_4^{-3}).

Ideally the pH of the solutions would also be comparable to that of San Juan Basin groundwater. However, when the pH was adjusted to a realistic value (9.4-10), many of the metal ions formed insoluble hydroxides resulting in metal concentrations much lower than found in the actual groundwater samples. Therefore, the experiments were done without pH adjustment (between six and seven).

One explanation for the solubility of the metal ions in San Juan Basin groundwater may be the presence of soluble metal chelates. Humic substances are ubiquitous constituents of soil, peat, coal and natural water and they are known to complex metal ions. Because humic material influences the distribution of aqueous metal ions via chemical complexation, we decided to determine the distribution coefficients in the presence and absence of humic acid.

Distribution coefficients for all of the cations were determined with the background ionic strength adjusted to a constant value with Na^+ , Ca^{+2} , K^+ and Mg^{+2} ; the principal cations released as a result of UCG. Chloride ions were employed to represent the anionic constituents of the natural water.

Distribution coefficients for the anions were determined with the ionic strength adjusted to a constant value with Cl^- and SO_4^{-2} . Potassium ions were used to represent the cationic species in the water.

Since local groundwater movement in the San Juan Basin is only one-two feet per year, we used the assumption that equilibrium will be established between the ions in solution and the coal surfaces. All of the K_d 's were determined by the batch method. This method involved adding a known amount of contaminant solution to a measured quantity of solid material and agitating the mixture until equilibrium was reached. The distribution between solid and liquid phases was calculated by comparing the initial ion concentration with the final concentration. Table 2 summarizes the experimental conditions.

The results of the adsorption experiments are listed in Tables 3 and 4. The data show that Fruitland Formation coal has a high affinity for Al^{+3} , Hg^{+2} , Fe^{+3} and Cu^{+2} ; a moderate affinity for Pb^{+2} , Zn^{+2} , and Cr^{+3} ; and a lower affinity for Cd^{+2} , Mn^{+2} , Co^{+2} , Ni^{+2} and Be^{+2} . The replace-

Table 2. Experimental Conditions Used to Determine Distribution Coefficients of Anions and Cations on Coal

Variable	Value	Variable	Value
Weight of Coal	50.0g	pH	6-7
Particle Size	0.25-1.40mm	Temperature	Room Temp.
Sample Volume	200 ml	Equilibrium Time	5 days
Humic Acid Conc'n.	5.00 mg/l	Agitation	2 x daily
Adjustment of Background Ionic Strength			
Experiment Set	Ionic Strength Adjuster	Salt Used	Ion Concentration (mg/l)
For Cations	Na^+	NaCl	1000
	Mg^{+2}	$MgCl_2 \cdot 6H_2O$	100
	K^+	KCl	100
	Ca^{+2}	$CaCl_2 \cdot 2H_2O$	500
For Anions	Cl^-	KCl	2000
	SO_4^{-2}	K_2SO_4	1000

Initial Concentrations of Anions and Cations Under Study

Ion	Salt Used	Initial Concentration Range (mg/l)
Fe^{+3}	$FeCl_2 \cdot 4H_2O$	1-100
Al^{+3}	$AlCl_3 \cdot 6H_2O$	0.2 - 160
Mn^{+2}	$MnCl_2 \cdot 4H_2O$	0.2 - 20
Zn^{+2}	$ZnCl_2$	0.2 - 20
Hg^{+2}	$HgCl_2$	12 - 100
Cr^{+3}	$CrCl_3 \cdot 6H_2O$	0.2 - 16
Co^{+2}	$CoCl_2 \cdot 6H_2O$	2 - 16
Ni^{+2}	$NiCl_2 \cdot 6H_2O$	1.6 - 14
Cu^{+2}	$CuCl_2 \cdot 2H_2O$	2 - 16
Cd^{+2}	$CdCl_2 \cdot 2.5H_2O$	0.03 - 0.50
Pb^{+2}	$PbCl_2$	5 - 40
Be^{+2}	$BeSO_4$	1 - 8
CN^-	KCN	1 - 12
F^-	$KF \cdot 2H_2O$	20 - 160
SeO_3^{-2}	H_2SeO_3	17 - 176
MoO_4^{-2}	$(NH_4)_6Mo_7O_{24} \cdot 4H_2O$	21 - 182
AsO_4^{-3}	K_3AsO_4	21 - 164

ment power of the anions has been found to be: $CN^- > F^- > MoO_4^{-2} > SeO_3^{-2} > AsO_4^{-3}$.

The shape of the cadmium isotherm, shown in Figure 2, is representative of the shape of the fluoride and molybdate isotherms. The isotherm of lead, shown in Figure 3, is unique in shape compared to the other ions which were studied. Figure 4 shows the shape of the isotherms for the remainder of the ions studied.

Theoretically, chelation of a trace element by humic material decreases the amount of free ion available for adsorption. Since a greater quantity of trace element remains in solution, K_d values should decrease when chelation by humic substances occurs. Our data generally show small increases in the solubility of the metal ions in the presence of humic acid. Over the rather limited range of conditions explored, the effect is not large. In the cases of Cd^{+2} and Pb^{+2} there may even be a slight increase in K_d with the addition of humic acid.

The effect of coal particle size on the adsorption of trace metal ions was also

investigated. A simulated contaminant solution consisting of Fe, Al, Mn and Zn ions was prepared with the background ionic strength adjusted to 800 ppm using Ca^{+2} and Na^+ . The coal was separated into four particle size ranges. Coal from each size range was equilibrated with a known amount of the contaminant solution and then the solution was analyzed for the metals of interest.

Table 5 shows the results. The particle size effects bear a close resemblance to exponential functions, that is, K_d appears to decrease exponentially with increasing mean particle size. The data could not be made to fit any function which was proportional to r^2 where r is the mean particle radius (r^2 will be directly proportional to surface area whether the particle is a sphere or irregular figure). We conclude, therefore, that some of the adsorption occurs at surface sites and that there are additional sites inside the coal molecular network that become more accessible as the particle size decreases.

Table 3. The Adsorption of Selected Cations on Fruitland Formation Coal

Trace Element	No Humic Acid				Humic Acid, 5 ppm			
	C _o (mg/l)	Amt in Soln (mg/l)	Amt Ads (mg/kg)	K _d	C _o (mg/l)	Amt in Soln (mg/l)	Amt Ads (mg/kg)	K _d
Mn	0.186	0.093	0.372	4.0±0.22	0.187	0.093	0.376	4.0±0.22
	0.963	0.560	1.61	2.9±0.22	0.963	0.590	1.49	2.5±0.22
	5.00	2.24	11.04	4.9±0.22	5.03	2.24	11.2	5.0±0.22
	21.1	11.4	38.8	3.4±0.22	21.4	12.0	37.6	3.1±0.22
Fe	1.08	0.015	4.26	280±23	1.18	0.015	4.66	310±23
	5.72	0.080	22.6	280±23	5.67	0.080	22.4	280±23
	27.3	0.520	107	210±23	26.3	0.520	103	200±23
	103	3.68	397	110±23	106	5.67	401	70±23
Zn	0.210	<0.02 ^a	0.840	∞	0.210	<0.02 ^a	0.840	∞
	1.07	<0.02 ^a	4.28	∞	1.07	<0.02 ^a	4.28	∞
	4.74	0.305	17.7	58±3.7	4.75	0.282	17.9	63±3.7
	20.6	4.36	65.0	15±3.7	20.8	4.48	65.3	15±3.7
Cd	0.032	<7x10 ^{-4a}	0.128	∞	0.032	<7x10 ^{-4a}	0.128	∞
	0.063	0.006	0.228	38±3	0.063	0.019	0.176	9±3
	0.123	0.045	0.312	7±3	0.123	0.071	0.208	3±3
	0.490	0.134	1.42	11±3	0.490	0.142	1.39	10±3
Al	20.2	<0.04	80.8	∞	20.2	<0.04	80.8	∞
	39.3	<0.04	157	∞	39.3	<0.04	157	∞
	75.3	5.48	279	51±3	69.3	4.85	258	53±3
	154	34.6	479	14±3	153	28.6	498	17±3
Cr	2.52	0.127	9.57	75±4.4	2.36	0.127	8.83	70±5.5
	4.48	0.339	16.6	49±4.4	4.42	0.324	16.4	50±4.4
	9.10	0.981	32.5	33±4.4	4.94	0.876	32.3	37±4.4
	17.35	3.88	53.9	14±4.4	17.6	2.93	58.7	20±4.4
Co	2.16	0.363	7.19	20±5.9	2.08	0.248	7.33	30±5.9
	4.21	1.00	12.8	13±5.9	4.22	0.722	14.0	19±5.9
	8.16	3.16	20.8	6.3±0.37	8.10	2.93	20.7	7.1±0.37
	16.45	9.75	26.8	2.8±0.48	16.9	8.77	32.5	3.7±0.48
Ni	1.60	0.247	5.41	22±5.8	1.50	0.101	5.60	55±5.8
	3.10	0.902	8.79	10±3.9	3.06	0.611	9.80	16±3.9
	6.36	2.83	14.1	5.0±0.96	6.40	2.58	15.3	5.9±0.96
	13.6	8.26	21.4	2.6±0.89	13.8	7.47	25.3	3.4±0.89
Cu	2.02	<0.003	4.08	∞	2.03	<0.003	8.12	∞
	4.08	0.071	16.0	230±17	4.11	0.084	16.1	190±17
	8.12	0.179	31.8	120±11	8.03	0.178	31.4	180±11
	16.5	1.08	61.7	60±11	16.6	0.908	62.8	70±11
Hg	11.7	<0.2	46.8	∞	11.4	<0.2	45.6	∞
	23.5	0.60	91.6	153±4.3	23.1	0.6	90.0	150±4.3
	49.4	2.60	187	72±4.3	48.9	2.4	186	78±4.3
	97.7	13.3	338	25±4.3	95.8	11.5	337	29±4.3
Pb	6.85	1.98	19.5	10±2.4	6.85	1.75	20.4	12±2.4
	11.9	2.43	37.9	16±2.4	11.9	2.21	38.8	18±2.4
	21.6	2.87	74.9	26±2.4	21.8	2.87	75.7	26±2.4
	40.8	3.76	148	39±2.4	41.4	4.19	149	36±2.4
Be	0.64	<0.002	2.46	∞	0.64	<0.002	2.56	∞
	1.12	0.14	3.92	28±2.5	1.18	0.17	4.04	24±2.5
	2.31	0.81	6.00	7.4±0.4	2.38	0.78	6.40	8.2±0.4
	4.31	2.33	7.92	3.4±0.1	4.18	2.30	7.52	3.3±0.1

^aThe symbol < indicates the concentrations were below the given detection limit.

Adsorption of Organics

The potential for release of large quantities of both inorganic and organic contaminants is one of the principal environmental concerns associated with UCG. A large number of organics are generated during the pyrolysis stage of UCG; these are transported in the vapor phase to the region surrounding the burn

where they then enter the groundwater. Comparison with wastewater effluents from surface coal processing plants has produced the estimate that concentrations of phenolic compounds alone could reach levels of 1000-3000 mg/l. On this basis, we have chosen to use phenol as a model organic and perform a study of the interaction of phenol with the UCG surroundings.

The adsorption of phenol on standard clay (Na-Montmorillonite), overburden, coal and demineralized coal was studied by equilibrating these substances with solutions of varying phenol concentration. The liquid was separated from the suspended matter and analyzed for phenol.

The adsorption characteristics of phenol on Na-Montmorillonite were

Table 4. The Adsorption of Selected Anions on Fruitland Formation Coal

Trace Element	No Humic Acid				Humic Acid, 5 ppm			
	C ₀ (mg/l)	Amt in Soln (mg/l)	Amt Ads (mg/kg)	K _d	C ₀ (mg/l)	Amt in Soln (mg/l)	Amt Ads (mg/kg)	K _d
CN ⁻	1.25	<0.03 ^a	4.96	>1500	1.20	<0.03 ^a	4.80	>1500
	2.58	<0.03 ^a	10.3	>1500	2.48	<0.03 ^a	9.92	>1500
	5.63	<0.03 ^a	22.5	>1500	5.25	<0.03 ^a	21.0	>1500
	11.2	<0.03 ^a	44.8	>1500	10.7	<0.03 ^a	42.8	>1500
F	48.4	24.0	97.6	4.1±0.23	47.6	22.6	100	4.4±0.23
	75.4	41.0	138	3.4±0.23	74.6	41.0	134	3.3±0.23
	121	67.0	216	3.2±0.23	120	68.0	208	3.1±0.23
	203	90.0	452	5.0±0.23	202	92.0	440	4.8±0.23
Se	16.9	12.8	12.8	0.93±0.02	16.9	13.7	12.8	0.93±0.02
	42.1	38.0	16.4	0.43±0.02	42.5	38.4	16.4	0.43±0.02
	77.2	72.8	17.6	0.24±0.02	76.4	71.7	19.2	0.27±0.02
	176	155	84.0	0.52±0.02	172	151	84.0	0.56±0.02
Mo	21.4	16.4	20.0	1.2±0.60	22.0	18.4	14.4	0.78±0.06
	44.3	29.5	59.2	2.0±0.60	43.6	33.9	38.8	1.1±0.60
	95.4	51.4	176	3.4±0.60	90.6	52.9	151	2.8±0.60
	182	145	150	1.0±0.60	180	149	125	0.8±0.60
As	21	19	≈0	≈0	21	21	≈0	≈0
	45	46	≈0	≈0	45	48	≈0	≈0
	86	86	≈0	≈0	91	88	≈0	≈0
	164	164	≈0	≈0	163	160	≈0	≈0

^aBelow the detection limit.

examined because montmorillonite makes up approximately half of the clay minerals found in the overburden and San Juan Basin groundwater contains a large concentration of monovalent cations. Adsorption on Na-Montmorillonite conforms to the linearized Langmuir isotherm over the equilibrium phenol concentration range of 50-1000 ppm. The observed adsorption capacity is 3.52 mg phenol per gram of clay. At concentrations greater than 1000 ppm the amount of phenol adsorbed increases substantially; the amount adsorbed accelerating for some magnitude beyond this concentration. This behavior is characteristic of physical adsorption described by the Brunauer-Emmett-Teller (BET) equation which takes into account multiple layer formation of physically adsorbed molecules (2).

Phenol adsorption on Kirtland Shale overburden is quite similar to adsorption on Na-Montmorillonite. Adsorption follows the Langmuir equation up to about 1000 ppm phenol solution with an adsorption capacity of 4.82 mg phenol per gram of overburden. This implies that sorption sites on the overburden are likely of the same nature as those in clays; in fact, sorption on the Kirtland Shale is probably due to sorption on the clay components of the shale. Sorption appears to be physical adsorption with multilayer effects showing up at high phenol concentration.

For adsorption on coal there are two linear segments to the Langmuir isotherm

followed by the rapid increase in adsorption of equilibrium phenol concentrations in excess of 4500 ppm. In the case of raw coal the overall adsorption data may be interpreted as a sum of contributions from overburden clay minerals in the coal plus that from the organic matter of coal. The adsorption capacity of the organic component has a substantially higher value than the clay minerals. The signifi-

cance of this is that a large quantity of phenol can be adsorbed on coal so that the coal remaining in the aquifer down-dip from the burn site should retard phenol migration quite effectively.

Conclusions

From many points of view northwest New Mexico represents a very good site for an underground coal gasification

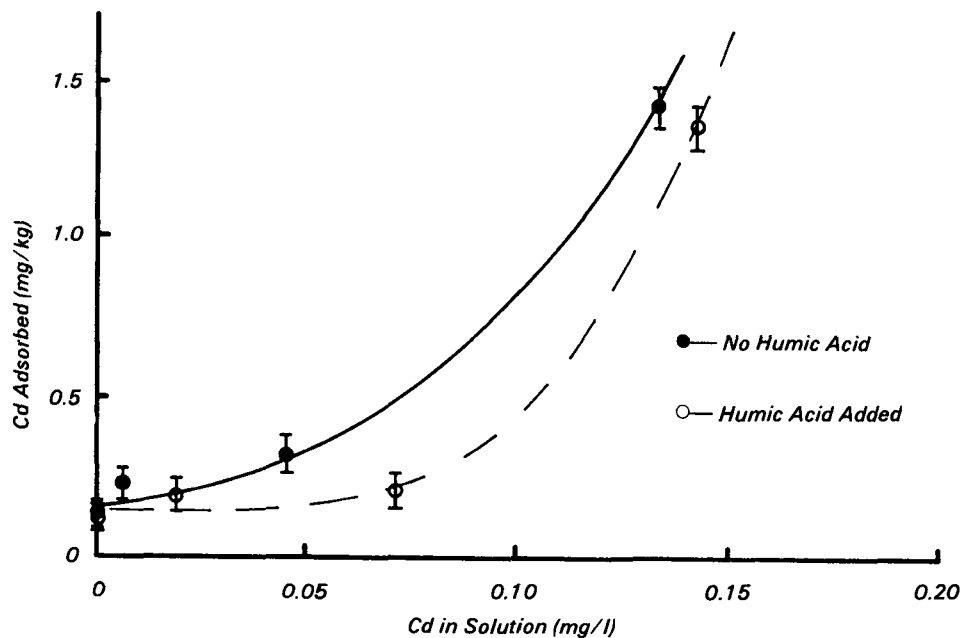


Figure 2. Sorption isotherm of cadmium.

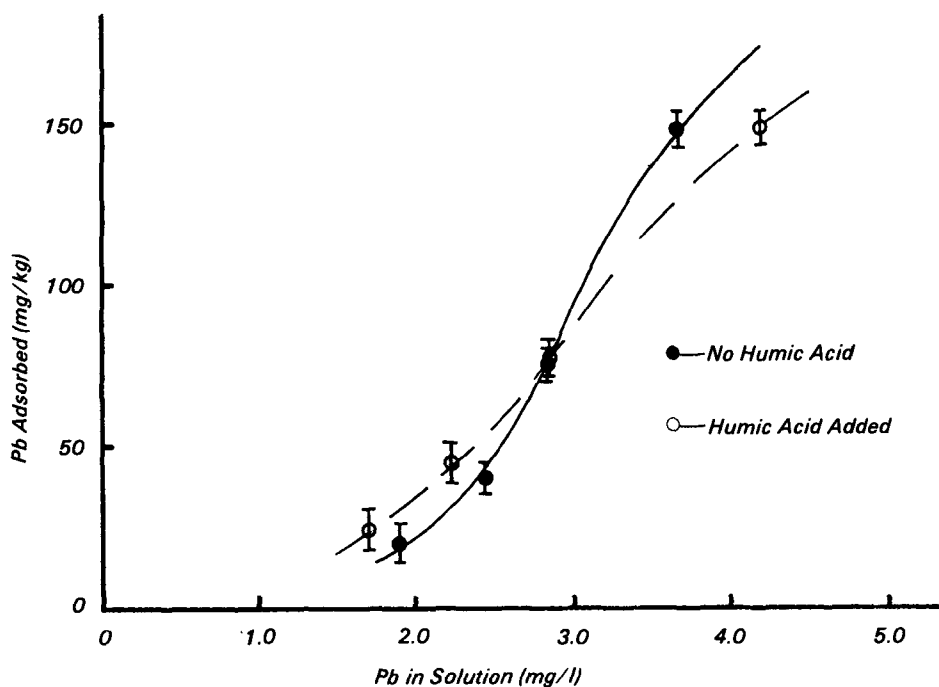


Figure 3. Sorption isotherm of lead.

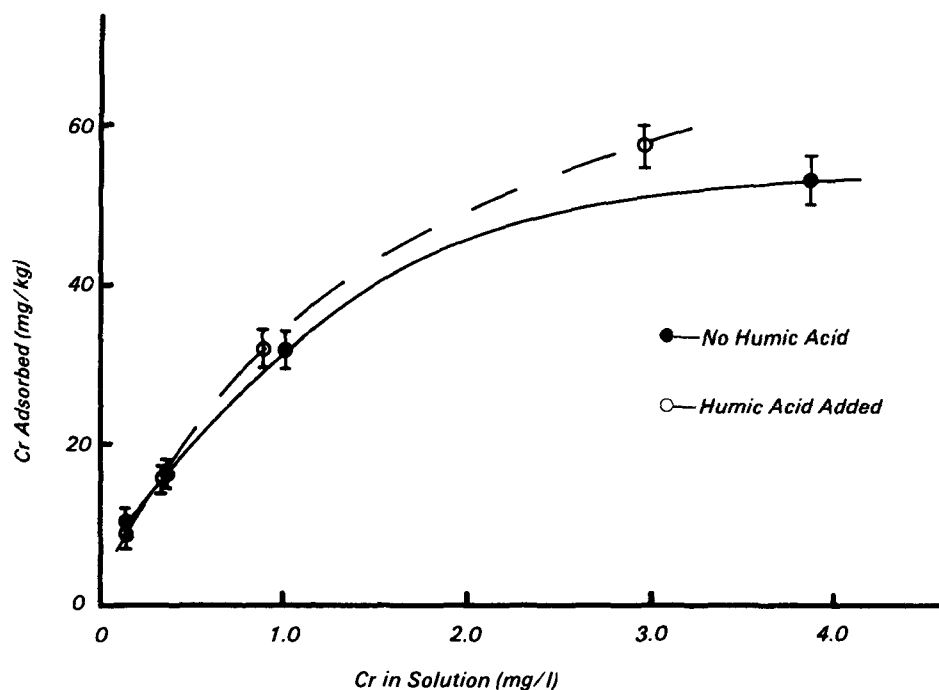


Figure 4. Sorption isotherm of chromium.

(UCG) project. The proximity of major power plants and a power distribution network, as well as extremely large, deep coal deposits make such a project attractive. The environment of the locale is high desert and therefore characterized by low human and animal populations and sparse vegetation. Background studies indicate the groundwater is brackish. The combination of these factors allow one to project a minimum environmental impact of such a site.

Static leaching of overburden and underburden indicates that pH is a very important variable, with large quantities of rock dissolving at very high and very low pH. Baseline studies show that the groundwater is strongly alkaline and the most abundant dissolved anion is sulfate. Trace metal measurements indicate that only at low pH values are significant amounts extracted. The distribution coefficients determined here for several metals were found to be functions of initial concentration of metal and particle size and when presented as isotherms the data fit the Freundlich equation.

Sorption studies on coal indicate that the inorganic matter in the coal accounts for approximately 95% of the adsorption of trace metals. The amounts of metals adsorbed onto the coal and the distribution function for the process have been measured in the presence of humic acid. The results indicate that the affinity of humic acid for the trace metals studies is: $Fe^{+2} > Al^{+3} > Pb^{+2} > Cr^{+3} > Ni^{+2} > Mn^{+2} > Cd^{+2} > Be^{+2}$. By fitting the sorption results to a Langmuir isotherm the sorption capacity of Fruitland Formation coal was found to be 1.5 g/kg for cations and 2.7 g/kg for anions.

Table 5. Effect of Particle Size on Adsorption

Trace Element	C_0 (mg/l)	Particle size range, mm	K_d
Al	50	<0.250	∞
		0.250-1.397	10 ± 1.5
		1.397-3.327	8 ± 1.5
Mn	13	<0.250	2.3 ± 0.22
		0.250-1.397	0.9 ± 0.22
		1.397-3.327	0.5 ± 0.22
Fe	120	<0.250	160 ± 23
		0.250-1.397	36 ± 5.2
		1.397-3.327	1.4 ± 0.20
Zn	10	<0.250	32 ± 3.7
		0.250-1.397	10 ± 1.2
		1.397-3.327	1.5 ± 0.17
Σ	193	<0.250	56 ± 13.4
		0.250-1.397	24 ± 3.1
		1.397-3.327	2.3 ± 0.76
		3.327-6.680	1.8 ± 0.76

References

1. "Standard Methods of Laboratory Sampling and Analysis of Coal and Coke," D-3173, American Society for Testing and Materials, 1976.
2. A.W. Adamson, *Physical Chemistry of Surfaces*, 3rd Edn., John Wiley and Sons, New York, 1976, Chapter IX.

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The complete report, entitled "The Effect of Underground Coal Gasification on Ground Water," (Order No. PB 84-220 318; Cost: \$13.00, subject to change) will be available only from:

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