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ESTIMATION OF DISTRIBUTION COEFFICIENTS AND LEACHABILITY OF HEXAVALENT CHROMIUM IN 100-D AREA HANFORD FORMATION SEDIMENTS

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ACRONYMS

ASTM	American Society for Testing and Materials
EIP	Environmental Investigation Procedure
ERC	Environmental Restoration Contractor
K_d	distribution coefficient
ORP	oxidation reduction potential
RARA	Radiation Area Remedial Action
RESRAD	RESidual RADioactivity dose model
RPD	relative percent difference

1.0 INTRODUCTION

This document describes bench-scale testing conducted to estimate hexavalent chromium sediment/water distribution coefficients (K_d's) and leachability of hexavalent chromium in the Hanford Site's 100 Area sediments where site-specific information does not currently exist. Samples used for testing were obtained from the 100-D Area.

This document is organized as follows:

- Introduction, including background project information and test objectives
- Scope and design of the testing
- Methods and Materials
- Results and Discussion
- Conclusions
- Data Appendices.

1.1 BACKGROUND

Available literature provides broad and varied descriptions of mechanisms and conditions that affect the mobility of metals in sediments, and as a result, a complex relationship emerges for each metal, pore water and sediment environment. Metals exist within sediment pore waters as either free metal cations, in soluble complexes with inorganic or organic ligands, or associated with mobile inorganic and organic colloidal material. These mobile species can interact with the sediments through either surface adsorption, solubility-precipitation or particulate filtration [for colloids] processes.

Hexavalent chromium is typically present in sediment porewaters as chromate ions $HCrO_4^-$ (pore water pH <6.5) or CrO_4^{2-} (pore water H ≥6.5), or as dichromate ion $Cr_2O_7^{2-}$ (pore water pH ≥6.5) at higher dissolved chromium concentrations (EPA 1992). It is difficult, and perhaps impossible, to measure the speciation of Cr on the sediments directly. BHI identified soils for this test by using SW-846 extraction procedures. Results suggest that there is measurable Cr^{+6} in the sediments as shown in Appendix A.

Because of the anionic nature of hexavalent chromium in groundwater, its association with sediment surfaces is limited to positively charged exchange sites, the number of which decreases with increasing sediment pH. Stollenwerk and Grove (1985) found that hexavalent chromium adsorption was due in part to the presence of iron oxides and hydroxides within alluvial particles, but that hexavalent chromium was readily desorbed with the input of uncontaminated water. Korte et al. (1976) found that hexavalent chromium was mobile in alkaline sediments. In Korte et al.'s work, parameters that correlated with hexavalent chromium immobility were free iron oxides, total manganese, and sediment pH, whereas sediment properties, surface area, and percent clay had no significant effect on hexavalent chromium mobility.

It has been also shown by other studies that organic matter can act as an electron donor in the redox reaction between hexavalent and trivalent chromium (Bartlett and Kimble

1976; Bloomfield and Pruden 1980) and that the reaction rate for the reduction to Cr^{+3} increases with decreasing sediment pH (Cary et al. 1977; Bloomfield and Pruden 1980). However natural Hanford sediments in general contain very little organic carbon (<0.05 to 0.1%) so that we feel organic carbon reduction processes are insignificant in the 100-Area sediments barring the co-disposal of organics in the liquid waste streams.

The interested reader is also pointed to a recent review of contaminant-sediment geochemical literature published by EPA [EPA 1999] and available electronically at http://www.epa.gov/radiation/technology/partition.htm, that contains chapters on Cr geochemistry, and Cr distribution coefficient literature.

The migration potential of metal contaminants through sediments is commonly quantified by the parameter named K_d. The K_d is defined as the ratio of sediment-bound contaminant concentration to the concentration of contaminant in the water at equilibrium. The ratio is calculated using the concentration of contaminant bound to the solid (per gram of solid) divided by the concentration of contaminant in solution (per milliliter of liquid). The K_d represents a number of different mechanisms affecting the distribution of the contaminant, of which only sorption (i.e., adsorption and ion exchange) is typically addressed through short-term testing (ASTM 1993; ASTM 1987).

To date, only K_d (and not leachability) has been used to evaluate groundwater impact using the RESidual RADioactivity dose model (RESRAD). RESRAD also has a computation feature to evaluate groundwater impact from residual vadose sediment contaminant concentrations, utilizing *leachability* parameters, which represent combined dissolution and desorption of contaminated sediments with the introduction of water. Given the multiple mechanisms available for hexavalent chromium adsorption/desorption and/or solubility/precipitation in sediment, as well as the wide range of K_d values currently published in the literature, specific testing of hexavalent chromium mobility in sediment underlying former 100 Areas waste sites is warranted. This conclusion that site-specific Cr(VI) mobility data should be collected at sites requiring clean-up decisions is also the key conclusion promoted by the recent EPA document, EPA (1999).

Contaminated and uncontaminated sediment from the 116-D-7 retention basin site, located north of the 100-DR-1 Operable Unit at the Hanford Site was selected for use in the bench-scale tests reported herein. The basin was an open concrete structure with a vertical concrete wall lengthwise down the middle of the basin and wood and concrete baffles to control water flow through the basin. Between 1944 to 1967, the site received large quantities (the exact amount is unknown) of process effluent water contaminated with radionuclides and water treatment chemicals to allow for thermal cooling and radio decay prior to discharge to the Columbia River. The basin is known to have had extensive leaks throughout its period of usage. Sodium dichromate was used for corrosion control in the reactor cooling water. Cr was used for cleaning activities as chromic acid, a Cr^{+3} form . After operations ceased in 1967, the site was decommissioned as part of the Radiation Area Remedial Action (RARA) Program. The upper portion of the basin's side walls, center structure, and baffles were knocked down into the basin and the entire site was stabilized with 0.6 to 1.2 m (2 to 4 ft) of overburden sediment.

The 116-D-7 site and underlying vadose zone (i.e., unsaturated sediments above the groundwater table) consist of material from the Hanford Formation. The Hanford Formation consists predominantly of medium-dense to dense sand and gravel, with various degrees of silt and cobble-sized material. The long-term groundwater depth beneath the site is estimated at 13.4 m (44 ft) below the bottom of the remedial action excavation. The site is located approximately 190 m (626 ft) from the 100-year flood level of the Columbia River.

The basin is currently being remediated as part of the Group 2 Remedial Action Project. The excavation of previously placed overburden backfill and the removal and disposal of the 116-D-7 engineered structure were completed in 1998. The remaining sediment beneath the removed structure was sampled to determine if remedial action goals had been achieved. Hexavalent chromium was found at concentrations ranging from 0.8 mg/kg to 18 mg/kg (see Appendix A Table A.1 for past results). RESRAD modeling indicates a potential impact to groundwater from these sediments, assuming a hexavalent chromium K_d value of zero. A K_d range for hexavalent chromium from 0 to 1800 mL/g has been found in a literature search but the available K_d data in this reported range is neither specific for the 100-D Area, or the 100 Areas, in general. Thus one major objective of this report was to perform Cr(VI) adsorption tests using 100-Area site specific sediments and waters. Similar elevated hexavalent chromium vadose zone sediment concentrations are anticipated at other 100-D Area sites.

It is also possible that the hexavalent chromium found in Hanford 100 Area contaminated sediment is present as an insoluble precipitate as opposed to being adsorbed on surface exchange sites. At this moment leach rates for Cr(VI) in sediments are not as readily available in the literature and have not been measured for Hanford site-specific sediments. Important decisions affecting the cost and extent of remedial action in the 100 Areas are currently based on very conservative RESRAD predictions. The determination of area-specific K_d and leach rates would provide a more accurate picture of actual potential impacts to groundwater and support future remedial action cleanup goals and planning.

The tests described herein were performed on sediments from the 116-D-7 site at the 100 D Area. Applicability of the results outside of the 116-D-7 site and 100 D Area are to be determined on a case by case basis by the lead regulatory agency. EPA and Ecology have stated that generally there is a potential for *the analogous sediments approach* at three groupings: 100 BC and K Areas; 100 D and H Areas; and 100 F Area.

1.2 TEST OBJECTIVES

The primary objectives of the bench-scale tests reported herein were to:

1. Estimate a K_d for hexavalent chromium specific to Hanford Formation sediments found throughout the 100 Areas.

2. Estimate a leach rate for hexavalent chromium specific to contaminated sediments found in the Hanford Formation throughout the 100 Areas.

To achieve these objectives, the testing utilized a combination of batch equilibrium adsorption tests (with clean sediments exposed to water spiked with hexavalent chromium) and batch and column leach tests (with hexavalent chromium contaminated sediments exposed to uncontaminated groundwater) to generate the necessary data.

A flow-through column tests was used to determine the Cr leach rate of sediment contaminated with hexavalent chromium using a flow rate equivalent to ten times faster than rainfall plus proposed irrigation. The faster flow rate was within the range of most leach and adsorption tests performed in laboratory studies and gave a residence time of 4 days in the column. We feel that this reaction time is long enough for most simple surface adsorption and slightly soluble salt dissolution reactions to reach equilibrium based on 30 years experience performing such tests. Effluent solution samples were taken over designated time intervals to establish the concentration of chromium in the effluent with time and sediment pore volumes eluted. A mass balance analysis was performed using initial concentrations and final concentrations of Cr(VI) in the sediment and in the effluent water. Both total and Cr(VI) were measured in the effluent using two independent analytical methods. A final leach rate will be determined by ERC based on the data collected.

2.0 MATERIALS AND METHODS

2.1 100-D HANFORD SEDIMENT

Two sediment samples, one uncontaminated and one Cr(VI) contaminated were obtained from ERC. The samples were shipped in 5-gal buckets directly from the field. Two 5-gallon buckets of each [clean and contaminated] sediment were obtained. The clean sediment was labeled SW-OA and SW-OB.

An initial weight of 10 kg of uncontaminated sediment was homogenized by cone and quartering to acquire more representative and consistent sub samples for the batch adsorption test. The material used for batch sorption testing was sieved through a # 5 sieve. Particles larger than 4 mm were discarded. The same procedure was used to obtain a sub sample of contaminated sediment to perform the flow-through column and batch [deionized water] leach tests.

General soil chemistry of the sediments was (pH, conductivity, etc.) was measured using an aqueous extract (Sparks, 1996). Initial testing of both the uncontaminated and contaminated sediments included the following:

- Moisture content (initial)
- Wet sieve analysis after initial splitting (percentage of material retained/passing a series of sieves: 1-inch, 5, 10, 18,35, 60, 120, and 230 mesh)
- Moisture content (after passing # 5 sieve)
- Sediment pH (50/50 mix with deionized water after 1 hour of contact)

- Conductivity (50/50 mix with deionized water after 1 hour of contact)
- Alkalinity (50/50 mix with deionized water after 1 hour of contact)
- Oxidation reduction potential (ORP) (50/50 mix with deionized water after 1 hour of contact)
- Major anions (50/50 mix with deionized water after 1 hour of contact)
- Major cations – acid digestion
- Total chromium – acid digestion
- Hexavalent chromium – alkaline extraction.

2.2 UNCONTAMINATED GROUNDWATER

Two water samples were obtained for this work. The first batch of water came from an old Hanford well [well 699-90-45] that was thought to be a background well outside the zone where any Cr(VI) contamination was present. This water was used in the screening batch adsorption tests. During the batch adsorption testing the analyses of the well were obtained and it was found that the water contained high iron contents suggesting some casing corrosion products were present. It was decided to obtain another groundwater sample from a newer well. Thus a second well [199-D5-42] was pumped and this water was used in the batch and flow-through column leach tests.

Initial testing of the unspiked groundwater consisted of the following:

- pH
- Conductivity
- Alkalinity
- ORP
- Total chromium
- Hexavalent chromium
- Major cations
- Major anions.

2.3 BATCH ADSORPTION TESTING METHOD

Batch adsorption testing should be applied only to situations in which sorptive processes (i.e., adsorption and ion exchange) are operable for the species of interest and are considered to be the main mechanisms of concern. Batch testing was used to acquire a minimum of three data points for each Cr(VI) starting solution concentration (i.e., triplicates were run). The data were evaluated to verify that the relationship of the partition coefficient over the range of concentration is independent of starting Cr(VI) concentrations. The resulting K_d factor (assuming a linear relationship) will be reported as a 100 Areas Hanford Formation sediment site-specific value. In the event of a non-linear relationship, the data could be evaluated for consideration of using concentration specific K_d values.

Batch adsorption testing used a measured weight of uncontaminated sediment with a measured quantity of Cr(VI)-spiked groundwater to a standard laboratory container, fully immersing the sediment at a ratio of 1:4 (sediment/water). The sediment or groundwater could contain trace levels of chromium and thus they were measured for natural background levels to allow corrections to the final calculations. The batch test container was continually agitated/mixed to ensure full contact between the sediment particles and groundwater. Samples were taken at two discrete time intervals for analysis of the contaminant of interest. The test was concluded when sample results were relatively unchanged from one time to the next. At this point, the concentration of the contaminant in the sediment is assumed to be at equilibrium with the contaminant in the water. Once the time of equilibrium is established, the remainder of the data for each concentration can be evaluated for linearity. Due to the difficulty and highly variable results of sediment analyses, the sediment Cr(VI) concentrations were calculated by difference based on changes in Cr(VI) concentrations in the water samples before and after contact with the sediments.

The water used typified uncontaminated groundwater of the 100-HR-3 Operable Unit (uncontaminated portion of the groundwater unit underlying the 100-DR-1 Operable Unit). The chosen uncontaminated sediment was first equilibrated two times with unspiked groundwater for periods of 24 hours to acclimate the sediment and groundwater. After equilibration as much of the residual groundwater as possible was removed from the container, [the residual liquid was accurately weighed], and Cr(VI) spiked groundwater was added.

The spiked groundwaters had their pH re-adjusted to return to 8.3 ± 0.1, which is the natural pH of the water. Solutions were allowed to equilibrate for several days prior to use. Just prior to use, the spiked groundwater was filtered through 0.45 μm membranes to remove any fine suspended material. Hanford groundwater has been shown to have a similar composition to vadose zone pore water as determined by saturation extracts and 1:1 water extracts thus the test results should be applicable for the vadose zone sediment/pore water environment. [See Serne et al. 1993 and Serne and Wood 1990 for details on use of groundwater to simulate vadose zone pore waters]. Characterization data for the groundwaters and sediments used in the test are shown either in the Results and Discussion section or Appendices dependent upon their importance to the discussion.

The batch adsorption tests were run using 50 g of oven dry sediment and 200 mL of spiked groundwater in wide-mouth ,250-mL plastic containers known to not adsorb metals (high-density polyethylene). There was also triplicate container blanks (spiked groundwater without sediment) to account for Cr^{+6} stability and container adsorption and triplicate sediment blanks (sediment and deionized water to see if native Cr leached from the sediments).

Three different spike levels [0.1, 1.0 and 10 mg/L] of hexavalent chromium [as sodium dichromate] were used. Tests were run in triplicate for contact times of 4 and 14 days. The uncontaminated sediment [SW-OA] was sieved through a #5 mesh [4.00 mm]. Material larger than 4.00 mm was not used in the batch adsorption test.

We found that the sediments did not leach measurable (<0.01 ppm in leachate) amounts of total or Cr(VI) into the distilled water. Further the spiked groundwater Cr(VI) concentrations remained constant at 0.1, 1.0, or 10.0 mg/L over the 4- and 14-day contact times.

2.4 FLOW-THROUGH COLUMN LEACH TEST

Column testing consisted of packing a vertical column with a measured amount (weight and volume) of sediment and allowing a source of water to flow through the column at a constant rate. The flow was from bottom to top to minimize air entrapment and channeling. The amount of water that percolates through the sediment is measured in terms of pore volumes. The column effluent is sampled at discrete intervals in relation to the number of pore volumes passed through the sediment. The effluent concentration of Cr(VI) can be plotted versus time or volume of water to create a plot showing leach rate or cumulative mass leached.

The flow through column leach tests used the contaminated sediments from buckets P1-0A and P1-OB and uncontaminated groundwater from well 199-D5-42. After homogenization the sediment from each bucket was seived through the #5 mesh screen to obtain material # 4 mm. Two sediment columns were packed. The first column [Column A] was packed with sediment from bucket P1-0A and the second column [Column B] was packed with sediment from bucket P1-0B.

The columns were inert Teflon tubes [41-mm diameter by 244-mm long] with Teflon end caps with one fitting centrally located in each that connected to the inlet and outlet tubing, respectively. A 41-mm diameter by 914-mm tall column represents a volume of 1,207 mL.

Each column was to be was contacted with the volume of groundwater expected to percolate through a representative cross section or area in one year for the irrigation scenario: 914 mm (36 in.) of water, which represents rainfall (6 in.) plus irrigation (30 in.). To get results in a more timely fashion than one year, the laboratory flow rate was selected to be 10 times this rate such that 914 mm of water was pumped and collected in 40 days. Given the dimensions of the column, the residence time for a pore volume of water was 4 days, which is long enough to expect minimal kinetic effects for the leaching of slightly soluble Cr^{+6} salts. The volumetric flow rate was about 33 mL/day.

The column with sediment P1-0A was used first but unfortunately the test was terminated after one effluent aliquot was collected when the inlet line became unattached and the column drained overnight. We felt that the early leach data are the most critical and that the first column test was potentially compromised to such a level that we could not defend the data. The second column, filled with sediment P1-0B, was successfully run for ~40 days.

Column B was packed with 565.93 g wet weight of sediment [528.01 g oven dry] to a bulk density of 1.64 g/ cm^3. Given the volume of the column, dry weight of packed

sediment and a particle density of 2.78 g/cm^3, the porosity was calculated to be 0.41. A calculated pore volume is thus [0.41 * 322.1 = 132.2 cm^3.

Leachate was collected in small aliquots at a minimum of one sample per pore volume. The first pore volume was collected in roughly four equal aliquots. The next four pore volumes were collected using a frequency of 2 samples per pore volume, and the remainder of the samples were collected at a frequency of one sample per pore volume. Samples were filtered prior to analysis with 0.45-micron membrane filters. The filters were shown to have no effect on total or hexavalent chromium concentrations using spiked groundwater.

Each aliquot was analyzed for pH, hexavalent chromium and total Cr by colorimetric techniques and later for total Cr by ICP/MS, a more sensitive analytical method. Several aliquots were also measured for common cations and anions. Final residual sediment concentrations of Cr(VI) were measured by ERC using the SW-846 alkaline digestion method.

At the end of the Column B test, the column was weighed then the sediment oven dried and the pore volume determined gravimetrically to compare with the calculated pore volume.

2.5 WATER EXTRACTS (BATCH LEACH TESTS)

Upon discovering that very little Cr(VI) was leaching from the Column B leach column, we ran batch leach tests on left-over air dried material from bucket P1-OA that had been sieved through #5 screen and small aliquots of moist sediment from bucket P1-OB. For sample P1-OA one test was performed using 50.15 g oven dried material and 75 mL of distilled water. The sediment and water slurry was continuously mixed/shaken for 16 hours. Then the slurry was centrifuged and the supernatant solution decanted and filtered through a 0.45-micron membrane filter.

For P1-OB sediment two separate aliquots of moist sediment [52.78 and 53.32 g] were contacted with 75 mL of distilled water for 16 hours in a similar fashion. The solution was then centrifuged and filtered through a 0.45 μm membrane and Cr (VI) and total Cr measured both by the colorimetric technique and the more sensitive ICP/MS technique that measures total Cr.

We also performed a water extract with a 16 hr contact time for an aliquot of the oven dried sediment P1-0B after leaching for 40 days in the Column B leach test. Cr(VI) and total Cr were measured using the colorimetric and ICP/MS techniques respectively.

3.0 RESULTS AND DISCUSSION

3.1 SEDIMENT AND GROUNDWATER CHARACTERISTICS

Both the uncontaminated and contaminated sediments are coarse grained as shown in Table 3.1. The uncontaminated sediment is is 71% gravel-25% sand-4% silt/clay and the P1-OA contaminated sediment is 62% gravel-35% sand –3% silt/clay.

Table 3.1 Particle Size Distribution of Hanford Sediment from 116-D-7

SW-0A (Clean Sediment)			
Sieve	Size (mm)	g retained	Wt %
1 inch	25.40	1110.88	50.39
#5	4.00	464.03	21.05
#10	1.68	69.95	3.17
#18	1.00	148.41	6.73
#35	0.50	225.46	10.23
#60	0.25	69.61	3.16
#120	0.125	28.63	1.30
#230	0.063	27.69	1.26
Pan	<0.063	59.78	2.71
Total		2204.44	100.00
P1-0A (Chrome Contaminated Sediment)			
Sieve	Size (mm)	g retained	Wt %
1 inch	25.40	598	33.90
#5	4.00	501	28.40
#10	1.68	190	10.77
#18	1.00	329	18.65
#35	0.50	66	3.74
#60	0.25	16	0.91
#120	0.125	11	0.62
#230	0.063	17	0.96
Pan	<0.063	36	2.04
Total		1764	100.00

The moisture content and chemical composition of the 1:1 water extract for the two sediments are shown in Table 3.2. The contaminated sediment has a higher moisture content and leachable anions, lower pH, alkalinity and slightly lower Eh than the uncontaminated sediment. The data suggest that there is residual moisture from the liquid waste disposal and that the liquid waste disposed had a slightly lower pH than native porewater and higher content of chloride and sulfate.

Table 3.2 Chemical Description of Water Extracts of the Sediments

Constituent	Clean Soil	Contaminated Soil
Moisture	2.6	6.7
Soil pH	8.9	8.12
Conductivity -uS/cm	173	263
Alk-in mg/L CO3	23.1	12
Redox-in mv	252	221
Anions (mg/L)		
Fluoride	0.12	<0.1
Chloride	8.94	58.86
Nitrite	<0.1	<1
Bromide	<0.08	0.32
Nitrate	2.08	3.88
Phosphate	<0.2	<0.2
Sulfate	1.51	16.76

The acid extracts of the two sediments allows one to estimate the total metal concentrations in the sediments. It is clear from the data shown in Table 3.3 that the contaminated sediment [P1-OA] contains higher levels of several metals such as Al, Ba, Cr, Fe, and Mg.

Table 3.3 Acid Extractable Metals in 116-D-7 Sediments (mg/kg)

Constituent	Clean Soil mg/kg	Contaminated Soil mg/kg
Al	6635	14483
Sb	<2	<4.7
As	<1	<1
Ba	88	228
Be	<0.3	<0.7
Cd	<0.03	<0.03
Ca	6788	6802
Cr	22	177
Co	14	19
Cu	20	28
Fe	30467	38617
Pb	<3	<5
Mg	5910	8372
Mn	371	430
Ni	11	11
K	<1000	<1080
Se	<0.4	<0.4

Constituent	Clean Soil mg/kg	Contaminated Soil mg/kg
Ag	<0.1	<0.1
Na	284	393
Tl	<5.3	5.4
V	77	97
Zn	55	71

Three aliquots of the #5 mesh sieved sediments of the clean sediment [SW-OA] and the two contaminated buckets [P1-OA and P1-OB] were submitted by ERC to their analytical contract lab for Cr(VI) analysis by the SW-846 alkaline extract procedure. At the end of the flow-through column leach test three aliquots of the oven dried leached sediment were submitted to the analytical lab that had determined the total Cr(VI) in the original sediments. In a separate effort PNNL performed its own SW-846 digestion of the leached sediment and submitted the solution for total Cr analysis using ICP-MS as opposed to the colorimetric method specific for Cr(VI) that was used by the ERC analytical lab subcontractor. The results for 6 replicate analyses for the ERC lab and three for the PNNL lab are shown in Table 3.4.

Table 3.4 Cr(VI) Content in the Clean, Uncontaminated, and Leached Sediment

Sediment	Description	Cr(VI) mg/kg	std. dev. (+/-)
SW-OA	Clean	0.851	0.070
P1-OA	Contaminated	6.332	0.428
P1-OB	Contaminated	5.946	0.300
P1-OB	Column Leached	6.788	0.544
P1-OB(PNNL)	Column Leached	5.020	0.845

The clean sediment appears to have 0.85 ppm of Cr(VI) and as shown in Table 3.3 it has 22 ppm of total Cr. The contaminated sediment P1-OA has 6.3 ppm Cr(VI) and as shown in Table 3.3 the sediment contains 177 ppm of total Cr.

The average Cr(VI) concentration in the leached sediment from the flow-through column B as measured by the EPA SW-846 protocol was 6.788 ± 0.544 mg/kg. The PNNL results were 5.02 ± 0.84 mg/kg. Note that the ERC value for the leached sediment is larger than the average for the unleached sediment. In practical terms this means that the amount of Cr(VI) leached from the sediment during the flow-through column test was insignificant. The Cr(VI) content of the sediments also is a small percentage of the total Cr in the sediments being ~4% in each case.

The chemical composition of groundwater from well 199-D5-42 is shown in Table 3.5. The chemical composition is quite similar to most groundwater samples taken in the 100-Areas. The water is predominantly a calcium-magnesium bicarbonate-sulfate dominated water with some nitrate contamination. The pH and Eh suggest that the water

is in equilibrium with carbon dioxide and oxygen from the air and calcite in the sediments. No analyses of the water from well 699-90-45 was performed. Historical data in the HEIS data base indicated that the well had atypical iron and other metals associated with corrosion.

Table 3.5 Chemical Composition of Water From Well 199-D5-42

	Average	std. Dev
pH	8.10	0.020
Conductivity-uS/cm	428	13
Alk-in mg/L CO3	54.1	1.9
Redox-in mv	212	2.5
Total Cr-ppm	0	0
Cr VI-ppm	0	0
Anions(mg/L)		
Fluoride	0.17	0.01
Chloride	7.8	0.1
Nitrite	0.68	0.04
Bromide	0.095	0.008
Nitrate	27.2	0.1
Phosphate	<0.2	
Sulfate	82.5	0.2
Cations(mg/L)		
Al	0.01	
Ca	49.46	
Cr	0.00	
Fe	0.07	
K	1.71	
Mg	14.58	
Mn	0.17	
Na	13.19	
Si	16.48	

3.2 BATCH ADSORPTION TESTS

The results of the batch adsorption tests for the 4 and 14 day contacts are shown in Tables 3.6 and 3.7, respectively. For one Cr(VI) spike concentration, the 1.0 mg/L solution, triplicate adsorption tests were also run at a solution to solid ratio of 2:1 or 200 ml to 100 g. After 14 days of contact the K_d values for Cr(VI) and total Cr were 0.0 ± 0.0 and 0.1 ± 0.0 ml/g, respectively. These results suggest that varying the solution to sediment ratio over the range 4:1 to 2:1 has no effect on the K_d. There should not be any effect if the adsorption isotherm is linear, which is the desired outcome.

Table 3.6. 4-Day Contact Time Kd Data for Cr(VI) Adsorption

4-Day Contact Time				
Cr(VI) Concentration (mg/L)	Kd for Cr(VI) ML/g	Std. Dev. ML/g	Kd for Total Cr mL/g	Std. Dev. mL/g
0.1	0.3	0.1	0.0	0.3
1.0	0.0	0.0	0.2	0.3
10.0	0.0	0.05	0.3	0.3

Table 3.7. 14-Day Contact Time Kd Data for Cr Adsorption

14-Day Contact Time				
Cr(VI) Concentration (mg/L)	Kd for Cr(VI) ML/g	Std. Dev. ML/g	Kd for Total Cr mL/g	Std. Dev. mL/g
0.1	0.2	0.1	0.0	0.1
1.0	0.0	0.0	0.1	0.1
10.0	0.0	0.0	-0.2	0.1

Taken at face value the results suggest that there is a small amount of adsorption of Cr(VI) at the lowest Cr(VI) spiked concentration. However, we feel that the measured K_d is just as likely an artifact of running tests very close to the detection limit for the colorimetric method used to measure Cr(VI). Further, when one desires to measure the Kd for a poorly adsorbing species such as Cr(VI) one should use the flow-through column method and measure the breakthrough curve (see EPA 1999 Vol 1 for more discussion). Batch adsorption methods that rely upon measuring a starting and ending concentration in solution, are not accurate for poorly adsorbing analytes. You end up taking two numbers that are very close to being the same and taking their difference to calculate the K_d. The small error in each measurement can be as large or larger than the calculated difference. Propagation of errors analyses corroborate this statement. Thus when attempting to measure the K_d of a very weakly adsorbing species some other technique than the batch method is advised. Flow-through column tests are recommended.

The K_d for total Cr after 4 days appears to show some adsorption for the two higher spiked concentrations but the standard deviations are large. If surface adsorption is the controlling mechanism one would expect that the K_d would remain constant or drop as solution Cr concentration increased. It does not make sense to see a higher K_d for the highest starting Cr concentration. Because the Hanford sediment is a heterogeneous mix of surface adsorption sites one would expect the K_d to be highest at low concentrations of Cr as the most preferred sites fill. Then the remaining solution Cr would interact with less preferred sites, etc. There is a mechanism that would allow the calculated K_d to increase as the solution concentration of Cr was increased. The mechanism is precipitation of a Cr containing compound. Usually, if precipitation is the mechanism

controlling the fate of a contaminant there will be a very dramatic increase in the calculated K_d as the solution concentration is increased above the solubility limit .

We consider the total Cr K_d data in Tables 3.6 and 3.7 to simply reflect variances in the analytical values for the spiked waters and the sediment effluents. We do not believe that the K_d values represent surface adsorption. The K_d for total Cr measured after 14 days contact suggests that there is no adsorption occurring. The total chromium in these batch adsorption tests was measured using the colorimetric procedure and also represents Cr(VI) because there was no natural Cr in any valence state in the groundwater. The specific colorimetric results for the Cr(VI) in the solution blanks shows that the spiked Cr remained stable in the +6 valence state, thus the total Cr measurements are just a repeat of the specific Cr(VI) measurements. The slight variation in the measured values between Cr(VI) and total Cr on the same solutions represents analytical variability. We thus remain firm in our conclusion that there is no significant Cr(VI) adsorption onto the Hanford Formation sediments. The original test plan called for a much more comprehensive batch adsorption test activity should this screening effort show that the K_d for Cr(VI) was equal to or larger than 0.5 mL/g. Based on the screening results we did not perform the more comprehensive testing activity documented in the test plan.

3.3 FLOW-THROUGH COLUMN LEACH TEST

The effluent concentrations of Cr(VI) measured by the colorimetric technique for Column B are shown in Table 3.8. Time, volume of effluent and cumulative pore volumes are also tabulated. We had to dilute the first few samples that came out of the column because the aliquot size was too small to run with no dilution. The colorimetric procedure requires a set sample size [50 mL] to conduct the test. We also did not have adequate volume to run total Cr but suggest that all leachable Cr would have been Cr(VI) based on the insolubility of Cr(III) in slightly alkaline waters.

The column effluent Cr(VI) data are shown in Figure 1. It would appear that P1-0B sediment has either very little Cr(VI) in it or that the Cr is not leaching into the groundwater at appreciable concentrations. We elected to take some of the remaining effluent samples and we re-measured Cr using the ICP/MS technique that has a much lower detection limit than the colorimetric technique. Table 3.9 shows both sets of results.

Table 3.8 Column B Details for Cr(VI) Elution

Time (days)	Cum.Vol. Collected (ml)	Cumulative Pore Volumes	Dilution Factor	Instrument Reading (ppm)	Recovery %	Cr(VI) Conc. (ppm)
1	34.8	0.30	25	0.00	95	<0.263
2	65.1	0.56	2.5	0.00	95	<0.026
3	96.6	0.83	2.5	0.00	95	<0.026
4	127.8	1.10	1.67	0.00	95	<0.018
6	189.8	1.64	1.0	0.01	95	0.011
8	225.4	1.94	1	0.01	95	0.011

Time (days)	Cum.Vol. Collected (ml)	Cumulative Pore Volumes	Dilution Factor	Instrument Reading (ppm)	Recovery %	Cr(VI) Conc. (ppm)
10	314.1	2.71	1	0.01	95	0.011
12	376.3	3.24	1	0.01	95	0.011
14	435.7	3.76	1	0.01	95	0.011
16	500.3	4.31	1	0.01	95	0.011
18	563.8	4.86	1	0.01	90	0.011
21	656.7	5.66	1	0.01	90	0.011
24	750.2	6.47	1	0.01	90	0.011
28	875.8	7.55	1	0.01	90	0.011
32	999.7	8.62	1	0.00	95	<0.011
36	1123.8	9.69	1	0.01	95	0.011
39	1218.8	10.51	1	0.01	95	0.011
43	1342.1	11.57	1	0.01	95	0.011

Table 3.9. Comparison of Cr Measurements of Column B Effluents Using Two Methods

Sample ID Column Effluent (PV)	ICP/MS Total Cr ug/L	Original Colorimetric mg/L	Original Colorimetric ug/L
0.3	1.81	<0.263	<263
0.56	4.60	<0.026	<26
0.83	1.87	<0.026	<26
1.1	30.89	<0.018	<18
1.64	4.86	0.011	11
1.94	2.91	0.011	11
2.71	2.61	0.011	11
3.24	2.00	0.011	11
3.76	3.73	0.011	11
4.31	2.75	0.011	11
4.86	2.16	0.011	11
5.66	2.58	0.011	11
6.47	1.99	0.011	11
7.55	2.85	0.011	11
8.62	2.69	<0.011	<11
9.69	1.92	0.011	11
10.51	1.55	0.011	11
11.57	1.63	0.011	11

Note that the first 4 data points in Figure 1 for the colorimetric data are really "less than" values but we could not plot them as such in the figure. The Y-axis for the colorimetric method data reflects Cr(VI) while the ICP-MS data represent total dissolved Cr. As mentioned before the total Cr is undoubtedly Cr(VI) also because Cr(III) is very insoluble

and unstable at the pH and Eh conditions present. It is obvious that not much Cr is leached from the sediment and the solution concentration appears to reach a steady state concentration that is quite low after the first two pore volumes. Figure 2 shows the Column B leach data plotted as cumulative percent of Cr leached versus pore volumes.

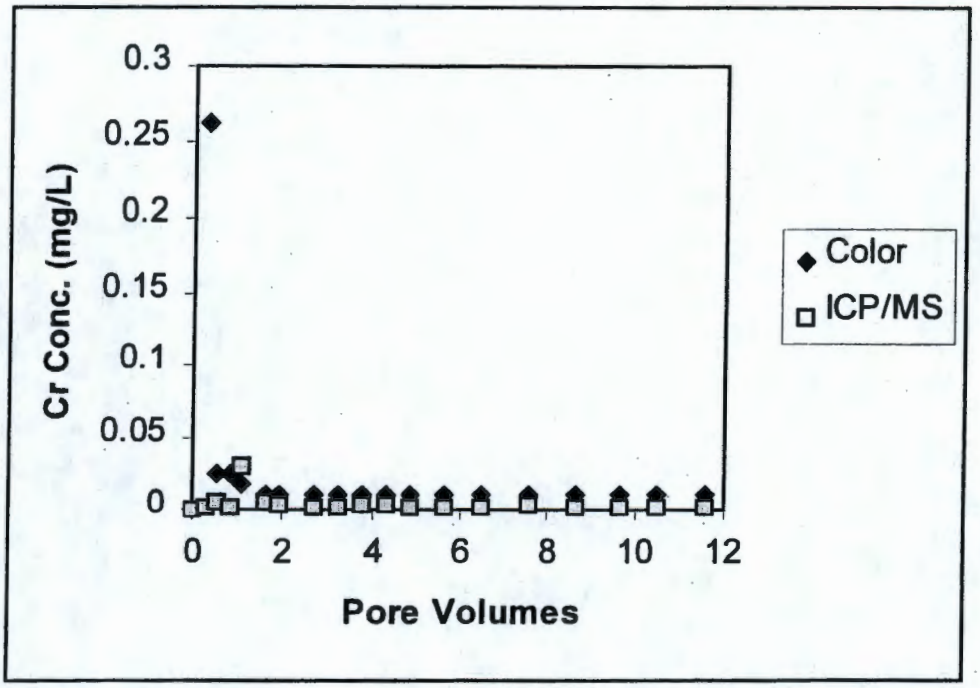

Figure 1. Effluent Cr [assumed to be Cr(VI)] Concentrations [mg/L] vs Pore Volumes

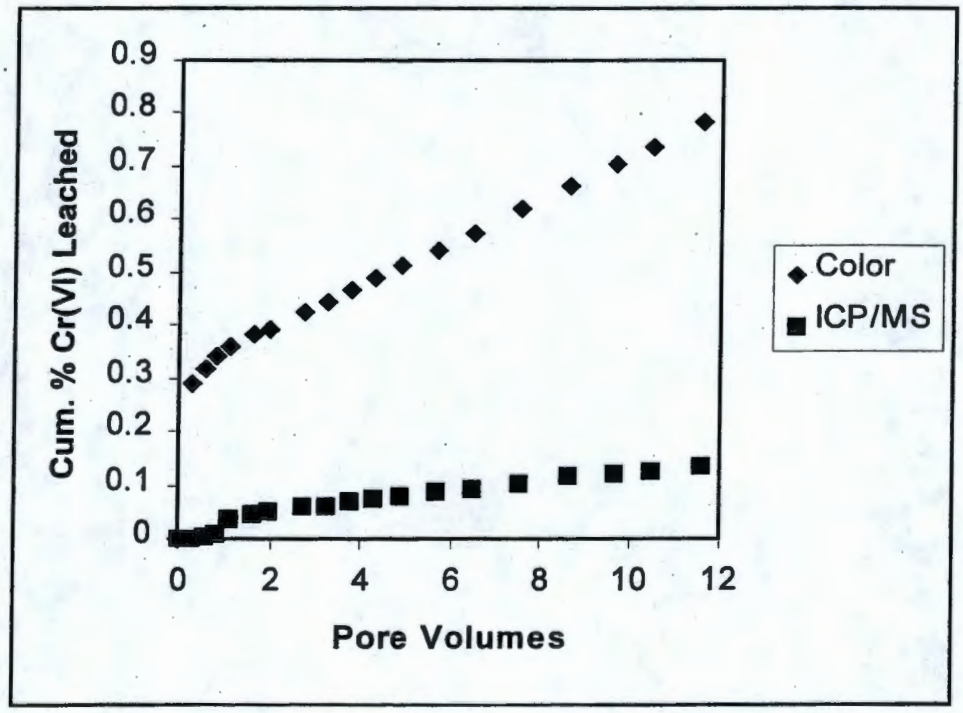

Figure 2. Cumulative % Cr(VI) Leached From Column B Determined by Two Techniques

From Figure 2 we can bound the release of Cr(VI) using the colorimetric measurements and or total soluble Cr using the ICP-MS data and assuming that the first four Cr(VI) values measured by the colorimetric technique are not detection limit values. However as we just stated the first four data points measured colorimetrically detection limit values. Thus the ICP-MS data although not a direct measure of Cr(VI) itself more realistically describes the fate of soluble Cr in this test.

Using the colorimetric data and using the detection limit values allows one to describe the leaching as essentially an instantaneous release of <0.3% of the Cr(VI) followed by a constant additional mass release as a function of pore volume or time. After nearly 12 pore volumes of leachate collected over 43 days of leaching the total mass of Cr(VI) removed from the sediment was <0.8 per cent per the colorimetric method data. These data could be used as an upper bound of the Cr(VI) leach rate.

If we consider only the ICP/MS data that has much better sensitivity, we do not get the instantaneous wash-off event and the final % of Cr leached is 0.1 % or expressed as a fraction 0.001.

The slopes of the almost straight lines on Figure 2 can be used as the leach rate input for RESRAD analysis. Since the ICPMS has a much better sensitivity, the slope of the lower curve is a more accurate estimate of the leach rate for these sediments. In either case greater than 99 % of the Cr(VI) remains attached to the sediment after leaching with 12 pore volumes of solution (the equivalent of more than one year's recharge for the irrigation scenario).

The first column test [Column A] that was aborted after collecting one aliquot gave an initial result similar to the data presented in Table 3.8 and Figures 1 and 2. After running for 16 hours 78 ml of effluent were collected and an aliquot[1ml] was analyzed for Cr(VI) using the colorimetric technique. The aliquot was diluted 50-fold to obtain adequate solution for the test and the instrument reading was 0.01 mg/L Cr(VI). This value was near the detection limit of the colorimetric test and when corrected for dilution the sample contained 0.5 mg/L Cr(VI). This value equates to the removal of ~1.2% of the total Cr(VI) that was in the sediment P1-0A. However this value is a bit uncertain because of the low sensitivity of the colorimetric technique and the 50-fold dilution. We had expected to find a significant wash-off effect and planned accordingly, but did not observe the effect.

We have found very little Cr(VI) or total soluble Cr leaching from the contaminated sediments P1-0A or P1-OB from 100-D-7 Area. We expected that the first pore volume would leach significant amounts of Cr from the sediment such that we could collect small volumes of effluent (break the first pore volume up into 4 aliquots or more) and still find measurable Cr. We had to dilute the first few samples to analyze for Cr out of the column because the aliquot size was too small to run with no dilution. We also did not have adequate volume to run total Cr but suggest that all leachable Cr would have been Cr(VI). As mentioned in the introduction, initial leaching of U from contaminated 300 Area sediments and many contaminants from grouted waste shows a significant fraction goes into solution to cause the "instantaneous" wash-off phenomenon. We designed the 100-Area Cr(VI) leach tests assuming we would observe such wash-off.

The Column B flow-through test was stopped after ~10 pore volumes of leachate were collected. The column was dismantled and the sediment dried and weighed to get an accurate value for the bulk density and porosity.

Our first suspicion was that the sediment in bucket P1-0B was not contaminated. We thus went ahead and performed the SW-846, method 3060A, test for total Cr(VI) in the sediment that had been leached in the flow-through column. An aliquot of this sediment was also given to ERC for their independent analysis. We took 50 mL of treatment solution, [contained 1 M NaOH, 0.25 M NaCO3 and a 1 M buffer of potassium phosphate (mono- and dibasic)], contacted it with 2.5 g of sediment from the leached column material that originally came from bucket 1P-0B and heated the slurry for 2 hours. Next, we neutralized the solution to a pH of 7.5 and analyzed the total Cr by ICP/MS. The results are presented in Appendix A. We found 5.02 ± 0.845 mg/kg Cr(VI) in the leached sediment. ERC found 6.79 ± 0.54 mg/kg using the exact SW-846 procedure where final Cr measurements use the colorimetric technique that is specific for Cr(VI) whereas the ICP/MS technique measures total Cr.

The original sediment from bucket P1-OB that had not been leached contained 5.95 ± 0.30 mg/kg based on ERC generated data. A comparison of the results suggests that the 43 day leaching test did not remove a statistically meaningful amount of Cr(VI) present in the sediments. This is consistent with the effluent solution data that shows between 0.1 and 0.7% of the Cr(VI) was leachable.

3. 4 BATCH LEACH TEST

Upon discovering that very little Cr(VI) was leaching from either column of contaminated sediment, we ran quick batch leach tests on left-over air dried material from bucket P1-OA that had been sieved through #5 screen and small aliquots of moist sediment from bucket P1-OB. For sample P1-OA one test was performed using 50.15 g oven dried material contacting 75 mL of distilled water for 16 hours. For P1-OB two separate aliquots of moist sediment [52.78 and 53.32 g] were contacted with 75 mL of distilled water for 16 hours. The sediment/water slurries were shaken on a linear shaker table for the entire contact period. The slurry was then centrifuged and filtered through 0.45 μm membranes and Cr (VI) measured. Two separate analyses of the leachate from sample P1-OA gave a leachate Cr(VI) concentration of 0.03 ppm by the colorimetric technique and 0.0224 ppm by ICP-MS. Upon correcting for solution to solid ratio used this is equivalent to 0.0335[ICP-MS] to 0.045 [Colorimetric] μg of leachable Cr (VI) per gram of sediment. The total Cr(VI) in the sediment from bucket P1-OA is 6.332 mg/kg and thus the leachable Cr(VI) is 0.53% or 0.0053 fraction by ICP-MS and 0.71% or 0.0071 fraction by the colorimetric technique.

For the two leachates from contacting sediment from bucket P1-OB there was no detectable Cr (VI) leached when the colorimetric technique was used that has a detection limit of 0.01 ppm and 0.0017 and 0.0021 mg/L when using the ICP-MS technique. Given our detection limit of 0.01 ppm for the colorimetric method and assuming a moisture content of the moist sediment of ~5% by weight, we can state that sediment P1-

OB contains less than 0.015 μg of leachable Cr(VI) per gram of sediment. The Cr(VI) content of the P1-OB material was determined to be 5.95 mg/kg. These data equate to leaching <0.3% or 0.003 fraction of the estimated Cr(VI) content. When using the more sensitive ICP-MS analyses of the amount leached from the sediment P1-OB is between 0.04 to 0.05% or 0.0004 to 0.0005 fraction.

A second sample of oven dry sediment from P1-OB was subjected to the overnight 1:1 water extract with 50 ml of deionized water. Triplicate tests were run and the leachates analyzed by ICP-MS for total Cr. The triplicate tests showed 0.039, 0.037, and 0.040 mg/L Cr in solution. This equates to leaching between 0.0062 to 0.0067 fraction or 0.62 to 0.67% of the Cr(VI) present in the sediment.

On two separate occasions sediment left over at the end of the flow-through leach column was subjected to an additional 1:1 water extract for a time period of ~16 hours (overnight). In total 5 aliquots were leached and the solutions contained 0.027, 0.034, 0.049, 0.044, and 0.041 mg/L Cr as measured by ICP-MS.

3.5 LEACH RATE DISCUSSION

Figure 3 presents the flow-through column test data plotted versus time for convenience for the modelers. Here time is actual contact time and not the year's long period that the irrigation scenario would take for the equivalent flux of water to percolate. The data based on colorimetric analyses of the effluent plot the Cr(VI) release assuming that the first four aliquots contained Cr(VI) at the detection limit for the samples. The plot overestimates Cr(VI) release because of the dilutions required and any rate calculated from this curve represents an upper bound. The curve based on the ICP-MS data should be considered more realistic.

Figure 4 shows all the data collected from the successful column leach test, the aborted column test and all the batch leach tests. We leave it to the modelers to determine how to use the information to bound their risk calculations. The batch leach test sampled the effluent solution for either Cr(VI) [analyzed by colorimetric techniques] or total soluble Cr [analyzed by ICP-MS] after ~16 hours of slurry mixing using a linear shaker table. The effluents were filtered to remove large [>0.4 micron suspended particles] prior to analysis. In Figure 4 the x-axis is cumulative leach time and the y-axis is cumulative % of the Cr(VI) present in the sediments that has leached at each time period.

The data in Figure 4 can be used to develop alternative conceptual Cr(VI) leach models to the one recommended from Figure 3. Figure 4 shows that the initial release of Cr(VI) found in column test when using the colorimetric measurement technique may be mostly an artifact of not having enough solution to measure Cr(VI). Recall that we had to dilute the samples with deionized water in order to get enough sample to run. Seeing as we got detection limit (less than values) on the diluted samples we can only present the cumulative leach data as a less than what is reported. The more sensitive ICP-MS data show no evidence [see Figure 3] of an early larger release of Cr. Many other tests wherein contaminated Hanford sediments or solidified waste forms have been leached do show the "wash-off" phenomenon for other contaminants (see for example Serne et al.

1994, Serne et al. 1992, Criscenti and Serne 1990, and Serne 1990). We are somewhat surprised that the Cr data do not show this common trend. The batch sediment-water leach tests that were performed overnight (~16 hr) show variation between the two contaminated sediment samples and some difference between the measured values when two techniques were used to measure leached Cr. The one data point for the aborted column test shows the largest % release of Cr at a value of 1.2% in the first aliquot. All the data support the idea that Cr(VI) in the 116-D-7 sediments is not readily leached by Hanford vadose zone pore waters or groundwater.

There are inconsistent indications that there might be some "instantaneous washoff" of Cr but more long-term leaching using either the flow-through column or the sequential batch extraction procedure as described in EPA 1311 (see Serne et al. 1994 for details) could be performed to generate enough data to resolve this question.

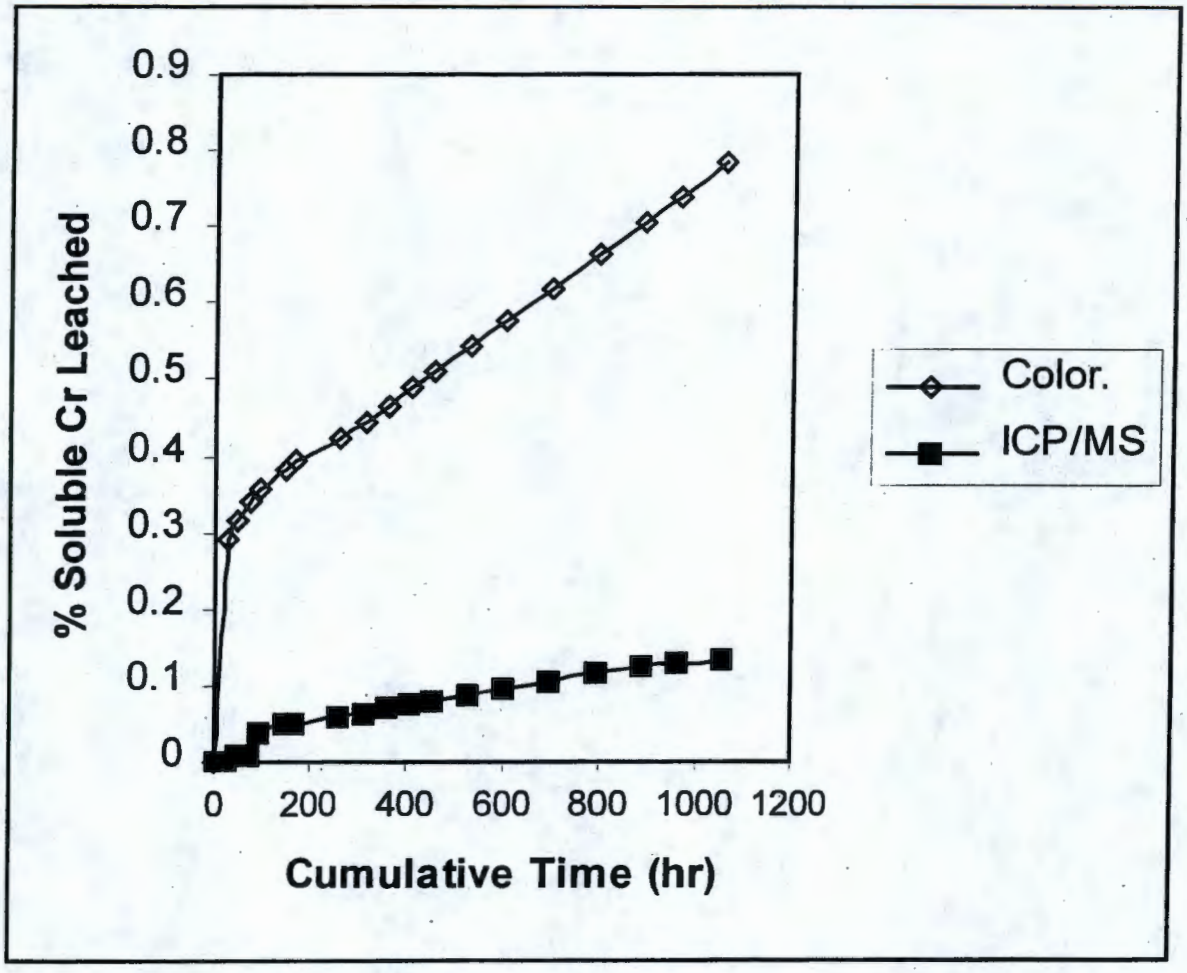

Figure 3. Release Rate of Soluble Cr in Column B Flow-Through Test. (% Calculated Assuming Only Sediment Cr(VI) Leaches)

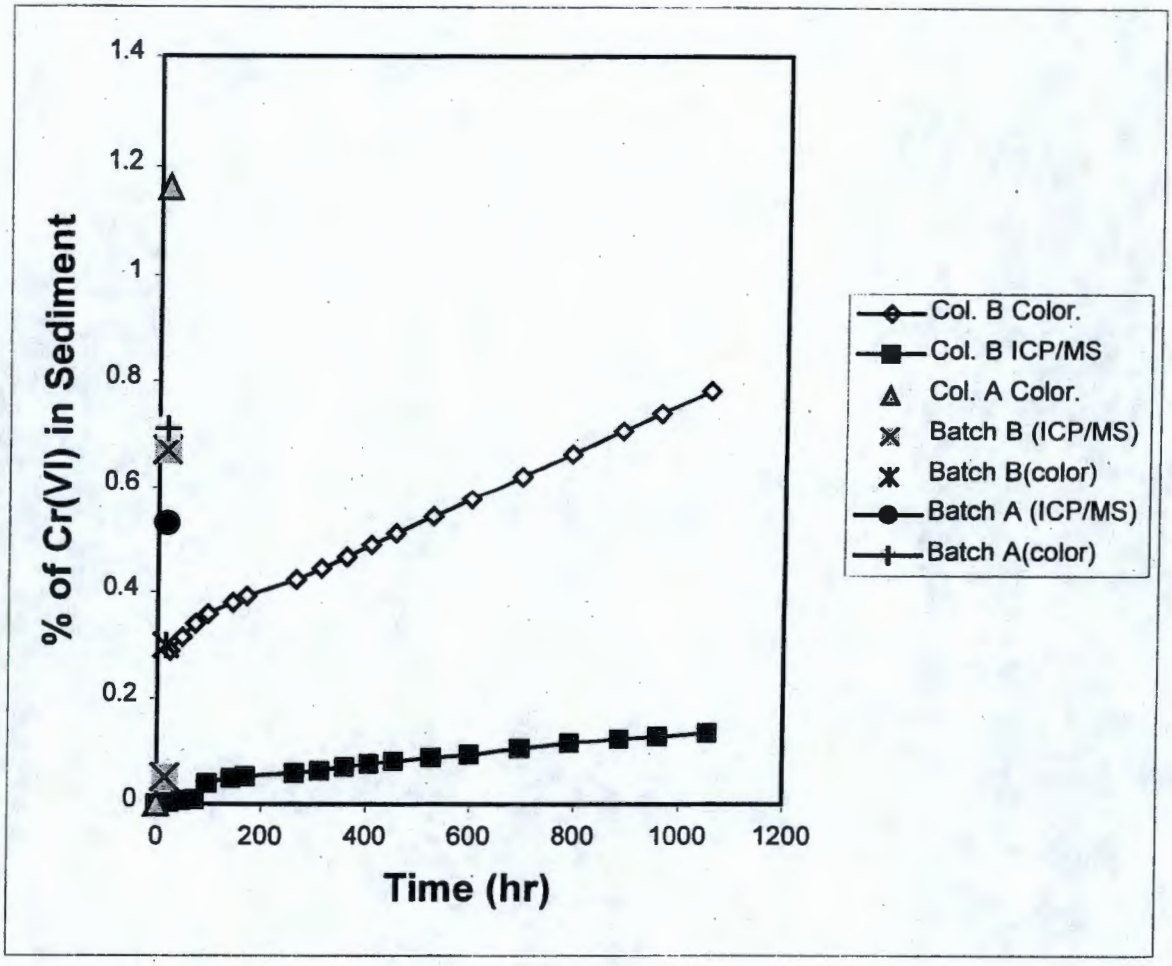

Figure 4. Plot of All the Soluble Cr Leach Data as a Function of Time. Soluble Cr is Assumed To Be Cr(VI) and Time is Actual Duration of the Lab Tests.

3.6 SOLUBILITY CONSIDERATIONS

The nearly constant column effluent concentrations exhibited in Table 3. 9 suggest that a Cr(VI) bearing solid with a low solubility may be controlling the release of Cr. The geochemical code MINTEQA2/PRODEFA2 [see EPA 1999 or Allison et al. 1991] was used to determine what the equilibrium concentration of Cr would be in a effluent solution with the chemical composition of that found at the beginning of the column leach test and near the end of the column leach test. In the latter case the chemical composition was essentially the same as the groundwater reported in Table 3.5.

The chemical composition of the column effluent as a function of pore volume is shown in the Appendix.

The MINTEQA2 data base contains only two Cr(VI) bearing solids with commonly occurring sediment components that would appear to be a plausible solubility control.

The one solid is barium chromate [$BaCrO_4$]. Another plausible solid would be ferric chromate [$Fe_2(CrO_4)_3$]. Unfortunately no thermodynamic data for this compound is in MINTEQA2 and it was beyond the scope of this project to scour the literature and Cr(VI) soil chemist experts throughout the world. We also know from past geochemical studies of the Hanford groundwater that most groundwaters at Hanford are in equilibrium with barite [$BaSO_4$].

For this simple geochemical modeling exercise we also assumed that the sediment/water system was at equilibrium with atmospheric levels of carbon dioxide and the mineral calcite [$CaCO_3$]. A water with the composition of the initial column effluent (contains high concentrations of leachable Cl, sulfate, calcium, magnesium and a pH of 7.8 the solution would contain 3.2 mg/L Cr(VI) and 4.1 mg/L Ba if barium chromate was controlling the Cr and Ba solution concentrations. If we assume that barite controls the amount of Ba in the solution and that barium chromate controls the Cr, then the equilibrium solution would contain 111 mg/L Cr and 0.12 mg/L Ba. The Cr solution concentration increases dramatically because barite is much more insoluble and it removes Ba from solution allowing the Cr to increase while still maintaining both minerals in equilibrium.

For the column effluent at the end of the flow-through column leach test there is no elevated concentrations of other common elements that leach from the sediment and the water is the same as the groundwater used in the tests. The pH increases slightly to 8.1 and we maintained the equilibrium with carbon dioxide and calcite. When we assume that barium chromate is the controlling solid for both Cr(VI) and Ba the equilibrium concentrations are 2.35 mg/L and 3.02 mg/L, respectively. When we assume that the Ba in solution is controlled by barite, then the equilibrium solution would contain 65.4 mg/L Cr(VI) and 0.11 mg/L Ba.

In all cases the Cr(VI) predicted solution concentrations are much higher (by at least 2 orders of magnitude) than what we found in the laboratory tests. Thus we either need to find an alternate Cr(VI) bearing solid with a lower solubility or we need to consider Cr(VI) replacing some other anion such as sulfate in barite to form a solid solution where trace quantities of one species substitutes into the crystalline structure of an insoluble compound thus lowering the solution concentration of the trace constituent well below values predicted for pure compounds.

The input files for the four predictions [two water compositions that bracket the column effluent composition and two solubility controls (barium chromate only and barium chromate and barite coexisting)] are found in the appendix as well as abbreviated versions of the output files. Complete output files are available from the authors.

4.0 SUMMARY AND CONCLUSIONS

The adsorption tests using uncontaminated 100-Area sediment and spiked groundwater with Cr(VI) starting concentrations between 0.1 and 10 mg/L suggest there may be a small amount of adsorption at the lowest Cr(VI) concentration. The average K_d for Cr(VI) after between 4 and 14-days of contact is 0.2 ± 0.1 mL/g. At higher Cr(VI) concentrations the K_d was found to be 0. However, we feel that the measured K_d for the lowest Cr(VI) concentrations is just as likely an artifact of running tests very close to the detection limit for the colorimetric method used to measure the Cr(VI). Further, when one desires to measure the Kd for a poorly adsorbing species such as Cr(VI) one should use the flow-through column method and measure the breakthrough curve (see EPA 1999 Vol. 1 for more discussion).

Based on the batch adsorption screening results showing that the Cr(VI) K_d was less than 0.5 mL/g we did not perform the more comprehensive adsorption testing activity documented in the test plan.

Geochemical principles for the adsorption of anionic species, such as Cr(VI), onto sediments that have a net negative residual surface charge, such as the Hanford sediments, suggest that simple ion exchange processes should not be significant. The large CrO_4^- plumes in the Hanford groundwater suggest that Cr(VI) adsorption onto Hanford sediments is very small. We recommend that a K_d value of 0 ml/g continue to be used for future predictive modeling of the fate of Cr(VI) in the 100 Areas.

However the leach testing of contaminated Hanford sediments from the 100-Area show that Cr(VI) bound to the sediments does not readily leach into pore waters with the typical composition of Hanford groundwater. One column leach test run for 43 days showed that less than 1% of the Cr(VI) present in the sediments could be removed in ~12 pore volumes of solution. The volume of water that was percolated through the sediment represents the total amount of water that would flush through the vadose zone in one year for a scenario that allowed 914 mm (36 in.) of water, [rainfall (6 in.) plus irrigation (30 in.)]. Additional 1:1 water extracts of the contaminated sediments showed that less than 1% of the Cr(VI) was leached after 16 hours of vigorous shaking, the exact amounts removed varied from 0.04 to 0.71% dependent on which analytical technique was used to measure Cr.

A direct mass balance measurement of the Cr(VI) in the sediment before leaching and after 43 days of leaching in the column test showed no measurable loss of Cr(VI). Within analytical error both sediment samples gave the same result. This fact corroborates the solution analyses that found less than 1% of the Cr(VI) was removed from the sediment.

The fact that sediment that was removed from the column leach test and subjected to another vigorous water extract test yielded a solution Cr(VI) concentration in the same range as sediment that was not pre-leached suggests that a very insoluble Cr(VI) bearing precipitate may be present. All solutions generated by mixing the contaminated sediments with uncontaminated Hanford groundwater had concentrations in the range of

0.002 to 0.05 mg/L. The column effluents also reached a steady state Cr solution concentration of either 0.003 or 0.01 mg/L dependent on analytical technique used. Because the flow rate was held constant and we felt that the residence time for the solution in the column was adequate to reach local equilibrium, the steady-state solution concentration fits a solubility controlled conceptual model. We recommend that future predictions of the fate of Cr(VI) in the contaminated sediments from the 100-Area consider using such a constant leach rate model. The data in Figure 2 (slope of the column B plot ICPMS results could form the basis for deriving the constant leach rate that the RESRAD computer code can utilize. To be conservative and to bound predictions (calculate "worst-case" leach values one could also use some instantaneous wash-off value judiciously chosen from the batch extract tests described in section 3. X and shown in Figure 3.

MINTEQA2 geochemical predictions suggest that either an unidentified Cr(VI) bearing solid is present or that the Cr(VI) present in the 100-D-7 sediments is not present as a pure Cr(VI) solid but rather substituted as a trace constituent in some other mineral. Chromate would thus substitute into the crystal lattice for some other common anion such as sulfate.

Another possibility is that the Cr present in the sediment is not present as Cr(VI) despite the SW-846 alkaline leach method suggesting that there is some Cr(VI) present in the sediment. Perhaps the SW-846 alkaline leach procedure yields a small false positive when a large amount of Cr(III) is present in the solid. Recall that the SW-846 alkaline leach results show that the Cr(VI) content in the sediments is only ~4% of the total Cr that is leachable in strong acid regardless if the total Cr value is 22 or 177 mg/kg, the values found for the uncontaminated and contaminated samples. One might expect that if the contaminated sediment at 116-D-7 actually had Cr(VI) contamination in it that the % versus the total Cr measured in the SW-846 alkaline leach process would be larger than 4%. There is less doubt that the colorimetric technique is measuring Cr(VI) in solution as opposed to giving a false positive for Cr(III) in solution. Alternatively, the alkaline leach procedure used on the sediments may actually allow some leached Cr(III) to oxidize to Cr(VI) during the digestion/extraction. It would be useful to take varying amounts of pure Cr(III) solids and run them through the SW-846 alkaline leach procedure to see if the results do yield a value of near zero for the Cr(VI) content. Perhaps a pure Cr_2O_3 could be used.

It would also be prudent to perform a few more column leach tests with other contaminated sediments from the 100-Area, especially ones with higher Cr(VI) levels, at several flow rates, especially rates slower than the 10x value used in this work for the irrigation scenario.

An effort to find what the controlling Cr(VI)-bearing solid is within the contaminated sediment should be discussed but may be a significant research challenge.

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APPENDIX A

SUPPORT DATA

Table A-1. 116-D-7 Hexavalent Chromium and Total Chromium Analytical Results From Past ERC Work.

Sample Location	Sample Number	Cr^{+6} (mg/kg)	Total Chromium (mg/kg)	Notes
A1	B0PK25	1.3	117	
A2	B0PK19	2.9	153	
A3	B0PK24	0.80 U	144	
B4	B0PK17	0.80 U	226	
B5	B0PK23	8.5	339	
B6	B0PK21	0.80 U	131	
C7	B0PK26	1.4	117	
C7	B0PK27	3.0	142	Duplicate of B0PK26
C7	B0PK16	5.89	209	Split of B0PK26
C8	B0PK20	18.0	152	
C9	B0PK18	3.8	90.9	

U = not detected

The ratio of the Cr(VI) to total Cr in these sediments averages 3.5 % for those samples with measurable Cr(VI) and 2.7% if we include the samples where Cr(VI) concentrations are less than the detection limit of 0.8 ppm. As mentioned in the text, the contaminated sediment P1-OA and P1-OB contained on average Cr(VI) to total Cr ratios of 4%. This fairly constant ratio for various samples of contaminated sediment should be compared to other Cr contaminated areas. If the ratio remains constant we would suggest that the SW-846 test methodology be checked to see if the presence of high total Cr [assumed to be Cr(III)] gives a small signal for Cr(VI). That is, all the measured Cr in the sediment MAY BE Cr(III) and natural processes may be slowly oxidizing and leaching very low amounts out of the sediments.

Table A-2 Sediment Data for SW-OA and P1-OA						
SW-OA (Clean Sediment)						
	1:1 Water Extract					
Sample #	1	2	3	4	5 Rerun	Average
Moisture	2.4	2.8	2.7			2.6
Soil pH	8.87	8.96	8.9	9.03	8.9	8.93
Conductivity-uS/cm	349	117	115		111	173
Alk-in mg/L CO3	20.9	14	34.5			23
Redox-in mv	306.4	258.2	190.4			252
Fluoride	0.13	0.14	0.10	0.12		0.12
Chloride	8.11	8.82	9.03	9.80		8.94
Nitrite	<0.1	<0.1	<0.1	<0.1		<0.1
Bromide	<0.08	<0.08	<0.08	<0.08		<0.08
Nitrate	1.90	1.70	2.66	2.06		2.08
Phosphate	<0.2	<0.2	<0.2	<0.2		<0.2
Sulfate	1.55	1.49	1.42	1.57		1.51
Oxalate	<0.2	<0.2	<0.2	<0.2		<0.2
P1-OA (Cr Contaminated Sediment)						
	1:1 Water Extract					
	1	2	3	4		Average
Moisture	6.8	6.6	6.6			6.7
Soil pH	8.1	8.2	8.2	8.1		8.12
Conductivity-uS/cm	bad point	286	257	247		263
Alk-in mg/L CO3	10.5	10.5	10.5	17.4		12
Redox-in mv	215.1	223.7	218.8	225.1		221
Fluoride	Bad sample	<0.1	<0.1	<0.1		<0.1
Chloride		66.19	58.10	52.30		58.86
Nitrite	<1	<1	<1	<1		<1
Bromide		0.34	0.31	0.33		0.32
Nitrate		4.00	3.82	3.82		3.88
Phosphate		<0.2	<0.2	<0.2		<0.2
Sulfate		16.89	16.61	16.79		16.76
Oxalate		<0.2	<0.2	<0.2		<0.2
			Moisture Content % (Weight)			
			P1-OA		SW-OA	
	Field Sample		3.32		2.36	
	< 2mm (rep A)		6.82		2.78	
	< 2mm (rep B)		6.55		2.72	
	< 2mm (rep C)		6.61			
	<2 mm (Ave.)		6.66		2.75	
	< 4mm (rep A)		6.80		2.40	
	< 4mm (rep B)		6.60		2.80	
	< 4mm (rep C)		6.60		2.70	
	<4 mm (Ave.)		6.67		2.63	

Table A.3 Sieve Samples for Hexavalent Chromium Analysis

Sample	Sieve Size	Size mm	mg/kg Hex Chrome	Wt. In Eash Size Grams	Weight Percent of Total	mg Cr(VI) in split	Wt. % Cr(VI) in Each Size
BOWCF 4	pan	0.062	3.31	36	2.04	0.11916	3.59
BOWCF 3	#230	0.063	3.81	17	0.96	0.06477	1.95
BOWCF 6	#120	0.125	4.13	11	0.62	0.04543	1.37
BOWCF 5	#60	0.25	5.75	16	0.91	0.092	2.78
BOWCF 7	#35	0.5	8.23	66	3.74	0.54318	16.39
BOWCF 8	#18	1	5.23	329	18.65	1.72067	51.91
BOWCF 9	#10	2	3.71	190	10.77	0.7049	21.26
BOWCH 0	#5	4	0.04	501	28.40	0.02004	0.60
BOWCH 1	1 inch	25.4	0.008	598	33.90	0.004784	0.14
			Totals	1764		3.314934	100
total in <4 mm sizes(calc)			**4.98**				
total for P1-OA			6.33				
total for P1-OB			5.95				

This is the value one would get if only the <4 mm material was submitted. This was what was done for P1-OA and P1-OB. Calculated value is a little low.

Table A.4 Characteristics of Groundwater Used in Batch Adsorption Test					
Well-699-90-45					
Constituent	1	2	3	4	Average
pH	8.31	8.31	8.32	8.31	8.3
Conductivity-uS/cm	475	460	465	469	467.3
Alk- mg/L CO3	66.1	66.1	48	62.8	60.8
Redox-in mv	216.1	189.9	208.5	189.3	201.0
Total Cr-ppm	0.01	0	0.02	0.01	0.01
Cr VI-ppm	0	0	0	0	0.0
Total Cr-ppm-wash	0	0	0	0	0.0
Cr VI-ppm-wash	0	0	0	0	0.0
Cations	in ppm				
Al	0.06	0.01	0.01	0.04	0.03
Ca	40.70	41.38	42.09	39.33	40.87
Cr-ICP/MS	0.001	0.001	0.001	0.001	0.001
Fe	0.08	0.09	0.09	0.09	0.08
K	2.47	3.64	5.89	8.08	5.02
Mg	14.43	14.67	14.97	14.11	14.54
Mn	0.03	0.04	0.04	0.04	0.03
Na	25.10	24.63	20.54	19.38	22.41
Si	16.97	16.78	17.15	16.11	16.75
Anions	in ppm				Average
Fluoride	0.43	0.44	0.44	0.45	0.44
Chloride	16.02	16.55	16.27	16.62	16.36
Nitrite	<0.1	<0.1	<0.1	<0.1	<0.1
Bromide	0.12	0.11	0.11	0.11	0.11
Nitrate	8.47	8.68	8.58	8.60	8.58
Phosphate	<0.2	<0.2	<0.2	<0.2	<0.2
Sulfate	62.17	64.33	64.69	64.70	63.97
Oxalate	<0.2	<0.2	<0.2	<0.2	<0.2

Table A.5 Characteristics of Groundwater Used in Flow-through Column Leach Test						
Well 199-D5-42						
Constituent	Sample 1	Sample 2	Sample 3	Sample 4	Average	
pH	8.125	8.084	8.087	8.087	8.1	
Conductivity-uS/cm	445	429	419	419	428.0	
Alk-in mg/L CO3	53	56.3	53		54.1	
Redox-in mv	209.1	212.8	213.9		211.9	
Total Cr-ppm	0	0	0	0	0.0	
Cr VI-ppm	0	0	0	0	0.0	
Cations	in ppm					
Al	0.00	0.00	0.00	0.02	0.01	
Ca	49.19	49.34	49.72	49.58	49.46	
Cr-ICP/MS	0.000	0.000	0.000	0.000	0.00	
Fe	0.07	0.07	0.07	0.07	0.07	
K	4.87	0.65	0.00	1.31	1.71	
Mg	14.42	14.60	14.71	14.58	14.58	
Mn	0.14	0.18	0.17	0.17	0.17	
Na	14.90	14.44	12.43	10.97	13.19	
Si	16.19	16.38	16.79	16.56	16.48	
Anions	in ppm					
Fluoride	0.18	0.16	0.18	0.17	0.17	
Chloride	8.01	7.73	7.81	7.77	7.83	
Nitrite	0.71	0.72	0.64	0.66	0.68	
Bromide	0.08	0.09	0.10	0.10	0.10	
Nitrate	27.20	27.14	27.05	27.26	27.16	
Phosphate	<0.2	<0.2	<0.2	<0.2	<0.2	
Sulfate	82.77	82.24	82.55	82.48	82.51	
Oxalate	<0.2	<0.2	<0.2	<0.2	<0.2	

Table A.6 Details on Batch Kd Tests									corrected			corrected
Bottle #	Concentration	Soil to water	Bottle Wt	Soil wt	Residual	solution wt.	Total Cr	dilution	Total	Cr VI		Cr-VI
	mg/L				Water wt		mg/L		Cr-mg/L	mg/L		mg/L
4 Days												
1	0.1	1 to 4	36.977	50.02	98.188	287.008	Not enough sample available			0.08	1	0.08
2	0.1	1 to 4	36.686	50.03	97.850	287.046	0.07	1	0.13	0.08	1	0.08
3	0.1	1 to 4	38.651	49.98	99.592	287.162	0.05	1	0.09	0.09	1	0.09
4	1.0	1 to 4	36.62	50.08	97.322	287.068	0.52	2	1.04	0.45	2	0.90
5	1.0	1 to 4	37.033	49.95	97.388	287.150	0.36	2	0.72	0.45	2	0.90
6	1.0	1 to 4	38.791	49.93	99.047	287.184	0.39	2	0.78	0.45	2	0.90
7	10	1 to 4	38.865	50.00	98.551	287.031	0.30	20	6	0.52	20	10.40
8	10	1 to 4	37.301	50.00	98.265	287.003	0.38	20	7.6	0.47	20	9.40
9	10	1 to 4	39.141	50.03	100.471	287.048	0.37	20	7.4	0.47	20	9.40
14 Days												
10	0.1	1 to 4	39.167	49.92	98.955	287.026	0.09	1	0.09	0.09	1	0.09
11	0.1	1 to 4	39.13	50.00	99.060	294.172	0.11	1	0.11	0.08	1	0.08
12	0.1	1 to 4	37.26	49.91	97.007	287.068	0.11	1	0.11	0.09	1	0.09
13	1.0	1 to 4	38.807	50.09	97.930	287.043	0.44	2	0.88	0.46	2	0.92
14	1.0	1 to 4	38.809	49.99	99.010	287.051	0.08	2	0.16	0.45	2	0.9
15	1.0	1 to 4	38.846	49.97	99.795	287.012	0.48	2	0.96	0.45	2	0.9
16	10	1 to 4	36.859	49.99	98.651	287.013	0.51	20	10.2	0.45	20	9
17	10	1 to 4	38.714	49.98	99.111	287.043	0.6	20	12	0.47	20	9.4
18	10	1 to 4	36.876	50.06	95.942	287.104	0.55	20	11	0.46	20	9.2
									total			Cr-VI
31	0.1	Ao	37.264				0.105	1	0.105	0.1	1	0.11
32	1.0	Ao	37.245				0.48	2	1.02	0.51	2	0.96
33	10	Ao	39.193				0.485	20	9.7	0.44	20	9.70
37	1.0	1 to 2	36.863	100.00	158.532	330.039	0.41	2	0.82	0.45	2	0.9
38	1.0	1 to 2	39.025	100.03	158.859	330.083	0.42	2	0.84	0.45	2	0.9
39	1.0	1 to 2	37.174	99.99	154.280	330.028	0.43	2	0.86	0.45	2	0.9
41	Blank	1 to 2	36.866	100.01	157.522	330.063	0	1	0	0	1	0

Table A.6 (continued) Details on Batch Kd Tests										
Bottle #	Concentration	Resid	corrected		Kd		corrected		Kd-CrVI	Ave.
	mg/L	water	init. Conc		total		init conc.			std. Dev.
1	0.1	11.191					0.10		0.35	0.3
2	0.1	11.134	0.10		-0.29	-0.1	0.10		0.35	0.10
3	0.1	10.961	0.10		0.12	0.3	0.10		0.19	
4	1.0	10.622	0.97		-0.08	0.2	0.91		0.01	0.0
5	1.0	10.405	0.97		0.41	0.26	0.91		0.01	0.00
6	1.0	10.326	0.97		0.28		0.91		0.01	
7	10	9.686	9.23		0.62	0.3	9.23		-0.13	-0.1
8	10	10.964	9.17		0.25	0.29	9.17		-0.03	0.05
9	10	11.300	9.15		0.05		9.15		-0.06	
10	0.1	9.868	0.10		0.13	0.0	0.10		0.19	0.2
11	0.1	9.930	0.10		-0.11	0.1	0.10		0.36	0.1
12	0.1	9.837	0.10		-0.11		0.10		0.18	
13	1.0	9.033	0.97		0.12	0.1	0.92		0.00	0.0
14	1.0	10.211	0.97			0.1	0.91		0.01	0.0
15	1.0	10.979	0.96		0.00		0.91		0.01	
16	10	11.802	9.13		-0.13	-0.2	9.13		0.02	0.0
17	10	10.417	9.19		-0.28	0.1	9.19		-0.03	0.0
18	10	9.006	9.26		-0.17		9.26		0.01	
31	0.1									
32	1.0									
33	10									
37	1.0	21.669	0.905584		0.1	0.1	0.9		0.0	0.0
38	1.0	19.804	0.914256		0.1	0.0	0.9		0.0	0.0
39	1.0	17.116	0.929479		0.1		0.9		0.0	
41	Blank									

Table A.7 Cation Composition of Effluents from Column Flow-Through Leach Test											
				Color	ICP/MS						
Sample ID	Pore	Al	Ca	Cr(VI)	Cr	Fe	K	Mg	Mn	Na	Si
	Volume	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
6/22/99	0.3	0.01	248.71	<0.263	0.002	0.79	4.88	86.84	0.01	38.66	3.49
6/23/99	0.56	0.07	159.02	<0.026	0.005	0.80	191.85	43.38	0.01	29.72	3.63
6/24/99	0.83	0.05	110.74	<0.026	0.002	0.32	43.39	32.80	0.01	25.00	3.87
6/25/99	1.1	0.04	75.83	<0.018	0.031	0.19	0.44	21.18	0.01	15.63	3.70
6/27/99	1.64	0.18	109.83	0.011	0.005	0.31	1.24	16.45	0.02	15.14	3.76
6/28/99	1.94	0.30	95.50	0.011	0.003	0.25	6.19	16.02	0.02	11.69	4.37
7/1/99	2.71	0.10	59.71	0.011	0.003	0.09	0.00	16.06	0.01	17.26	4.01
7/3/99	3.24	0.15	91.10	0.011	0.002	0.15	0.00	16.23	0.01	14.59	3.87
7/5/99	3.76	0.27	81.13	0.011	0.004	0.31	0.00	15.40	0.01	11.99	3.88
7/7/99	4.31	0.10	64.43	0.011	0.003	0.14	0.00	16.27	0.00	17.26	3.99
7/9/99	4.86	0.22	63.42	0.011	0.002	0.24	0.00	16.55	0.02	16.90	4.88
7/12/99	5.66	0.16	61.24	0.011	0.003	0.16	0.00	16.32	0.01	18.92	4.27
7/15/99	6.47	0.06	62.28	0.011	0.002	0.13	0.00	16.34	0.00	18.48	4.34
7/19/99	7.55	0.09	67.58	0.011	0.003	0.15	13.41	19.33	0.00	24.04	4.66
7/23/99	8.62	0.78	67.24	<0.011	0.003	0.35	7.63	18.23	0.07	20.22	6.18
7/27/99	9.69	0.04	62.75	0.011	0.002	0.13	0.00	17.78	0.00	19.06	4.30
7/30/99	10.51	0.03	61.31	0.011	0.002	0.12	0.00	17.46	0.00	17.83	4.30
8/3/99	11.57	0.07	69.29	0.011	0.002	0.14	0.00	20.72	0.00	20.22	4.79

Table A.8 Flow-through Column Effleunt pH, EC, and Anions

Time			Color			Anions	ppm						
(Days)	Cum. Vol.	PV	Cr(VI)	pH	EC	F	Cl	NO2	Br	NO3	PO4	SO4	CO3
1	34.8	0.3	<0.263	7.82	not measured								
2	65.1	0.56	<0.026	7.99	887	<1	322	<1	1.1	32.6	<0.4	157.92	35.45
3	96.6	0.83	<0.026	8.03	872								
4	127.8	1.1	<0.018	8.15	630	<1	25.4	<0.6	<0.6	26.47	<0.4	110.73	51.94
6	189.8	1.64	0.011	8.32	502								
8	225.4	1.94	0.011	8.32	462	<1	8.5	<0.2	<0.2	25.88	<0.4	94.05	52.91
10	314.1	2.71	0.011	8.38	456								
12	376.3	3.24	0.011	8.27	447	<1	7.7	<0.2	<0.2	26.28	<0.4	89.46	48.93
14	435.7	3.76	0.011	8.19	440								
16	500.3	4.31	0.011	8.27	435								
18	563.8	4.86	0.011	8.45	not measured								
21	656.7	5.66	<0.011	8.54	436	<1	8.8	<0.2	<0.2	26.10	<0.4	86.69	53.09
24	750.2	6.47	0.011	8.55	442								
28	875.8	7.55	0.011	8.54	548								
32	999.7	8.62	<0.011	8.460	598								
36	1123.8	9.69	0.011	8.537	435	<1	10.2	<0.2	<0.2	27.24	<0.4	85.95	59.77
39	1218.8	10.51	0.011	8.545	421								
43	1342.1	11.57	0.011	8.554	420								

Table A-9 Performance Check on ICP-MS Using Known Standards and Water Extracts of Cr Contaminated Sediment and Previously Leached Sediment from Column B

solutions	Value ppb	Matrix spikes	Amount of soln used ml	Amount of Spike added ml	Expected Value ppb	% Recovery
Standards						
5 ppb	6.06				5	121%
10 ppb	11.29				10	113%
50 ppb	59.29				50	119%
100 ppb	115.07				100	115%
200 ppb	214.70				200	107%
5 ppb-Acidified	6.17				5	123%
10 ppb-Acidified	7.04				10	70%
100 ppb-Acidified	120.17				100	120%
200 ppb-Acidified	209.98				200	105%
DI water	0.82					
DI water-acidified	1.06					
Batch Leach Extracts						
1:1 extract-unused sediment-A	38.94					
1:1 extract-unused sediment-B	37.08					
1:1 extract-unused sediment-C	39.99					
unused sediment-A(matrix spike)	42.20	50 ppb spike	2	1	45.72	108%
unused sediment-B(matrix spike)	42.09	50 ppb spike	2	1	44.48	106%
unused sediment-C(matrix spike)	42.69	50 ppb spike	2	1	46.42	109%
Leached Column Sediment Extract						
1:1 extract-column sediment-A	49.04					
1:1 extract-column sediment-B	43.52					
1:1 extract-column sediment-C	40.86					
1:1 extract-column sediment-A	44.45	50 ppb spike	2	1	52.46	118%
1:1 extract-column sediment-B	56.01	50 ppb spike	2	1	48.77	87%
1:1 extract-column sediment-C	46.76	50 ppb spike	2	1	47.00	101%

Table A.10 Cation Composition of Batch Leach Extract of Contaminated Sediment										
Sample ID	Al	Ca	Cr(VI) color.	Cr	Fe	K	Mg	Mn	Na	Si
	ppm									
P1-OA-1	0.71	15.03	<0.01	0.022	0.04	0.00	2.10	0.00	1.83	1.81
P1-OB-2	0.09	10.75	<0.01	0.002	0.03	0.00	2.32	0.00	1.48	1.70
P1-OB-3	0.16	9.69	nm	0.002	0.03	0.00	2.09	0.00	2.96	1.70

Table A.11 0.45 micrometer filter check				
	Instrument Reading	Dilution Factor	Concentration ppm	% Recovery
500X unfiltered	0.02	500	10	100
500X filtered	0.02	500	10	100
40X unfiltered	0.22	40	8.8	88
40X filtered	0.22	40	8.8	88
Note: All solutions diluted from 10ppm Cr^{6+} stock solution				

Table A.12 Procedure Check on Colorimetric Cr(VI) Measurement

Solution	Result	% Recovery
DI Water Blank	0.00	---
DI + 0.01 ppm Std.	0.01	100
DI + 0.025 ppm Std.	0.030	120
DI + 0.05 ppm Std.	0.04	80
DI + 0.10 ppm Std.	0.08	80
DI + 0.10 ppm Std.	0.12	120
DI + 0.50 ppm Std.	0.53	106
DI + 0.50 ppm Std.	0.51	102
Well 199-D5-42	0.00	---
Well + 0.01 ppm Std.	0.02	200
Well + 0.10 ppm Std.	0.11	110
Well + 0.50 ppm Std.	0.47	94
Well + 0.50 ppm Std.	0.55	110

APPENDIX B

PC MINTEQA2 OUTPUT FILE

THIS IS THE OUTPUT FILE FOR THE FIRST EFFLUENT FROM THE COLUMN LEACH TEST ASSUMING THAT ONLY BARIUM CHROMATE IS CONTROLLING CR AND BA.

PART 1 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:31: 2

Hexchrome solubility for ERC
Will use groundwater composition and vary Cr(VI) solids

Temperature (Celsius): 25.00
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

This is the input information!

330	0.000E-01	-7.90	
732	1.580E+02	-2.78	
410	1.920E+02	-2.31	
140	3.600E+01	-3.22	
180	3.220E+02	-2.04	
492	3.300E+01	-3.27	y
150	2.490E+02	-2.21	y
500	3.900E+01	-2.77	y
460	8.600E+01	-2.45	y
770	1.400E+01	-3.84	y
281	8.000E-01	-4.84	y
212	1.000E-02	-7.06	y
100	2.500E-01	-5.74	y

H2O has been inserted as a COMPONENT

3 3		
3301403	21.6600	-0.5300
3021201	9.6681	-6.3900
330	7.9000	0.0000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	1.259E-08	-7.900	0.000E-01
732	SO4-2	1.660E-03	-2.780	1.580E+02
410	K+1	4.898E-03	-2.310	1.920E+02
140	CO3-2	6.026E-04	-3.220	3.600E+01
180	Cl-1	9.120E-03	-2.040	3.220E+02
492	NO3-1	5.370E-04	-3.270	3.300E+01
150	Ca+2	6.166E-03	-2.210	2.490E+02

500	Na+1	1.698E-03	-2.770	3.900E+01
460	Mg+2	3.548E-03	-2.450	8.600E+01
770	H4SiO4	1.445E-04	-3.840	1.400E+01
281	Fe+3	1.445E-05	-4.840	8.000E-01
212	CrO4-2	8.710E-08	-7.060	1.000E-02
100	Ba+2	1.820E-06	-5.740	2.500E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED

Sum of CATIONS= 2.618E-02 Sum of ANIONS = 1.412E-02

PERCENT DIFFERENCE = 2.993E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

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|  IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION: |
|       SO4-2        Log activity guess:    -2.78      |
|       CO3-2        Log activity guess:    -5.86      |
|       H4SiO4       Log activity guess:    -3.84      |
|       Fe+3         Log activity guess:   -15.40      |
|       CrO4-2       Log activity guess:    -7.10      |
|                                                      |
-------------------------------------------------------
```

PART 3 of OUTPUT FILE

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
5002120	NaCrO4-	1.170E-07	9.939E-08	-7.00267	0.84948	0.767
4102120	KCrO4-	4.286E-07	3.641E-07	-6.43882	0.84948	0.870
3300020	OH-	9.389E-07	7.976E-07	-6.09821	0.84948	-13.927
3307700	H3SiO4 -	1.600E-06	1.359E-06	-5.86684	0.84948	-9.858
3307701	H2SiO4 -2	4.253E-10	2.215E-10	-9.65467	0.52073	-21.333
4603300	MgOH +	2.684E-07	2.280E-07	-6.64214	0.84948	-11.713
4601400	MgCO3 AQ	2.285E-06	2.300E-06	-5.63830	1.00672	2.977
4601401	MgHCO3 +	8.870E-06	7.535E-06	-5.12291	0.84948	11.466
4607320	MgSO4 AQ	1.759E-04	1.771E-04	-3.75182	1.00672	2.247
1503300	CaOH +	7.183E-08	6.102E-08	-7.21455	0.84948	-12.527
1501400	CaHCO3 +	1.378E-05	1.171E-05	-4.93146	0.84948	11.416
1501401	CaCO3 AQ	5.931E-06	5.971E-06	-5.22394	1.00672	3.150
1507320	CaSO4 AQ	3.514E-04	3.537E-04	-3.45134	1.00672	2.306
5001400	NaCO3 -	4.330E-08	3.678E-08	-7.43439	0.84948	1.339
5001401	NaHCO3 AQ	2.983E-07	3.003E-07	-6.52239	1.00672	10.077
5007320	NaSO4 -	4.838E-06	4.110E-06	-5.38618	0.84948	0.771
4107320	KSO4 -	1.962E-05	1.666E-05	-4.77822	0.84948	0.918
2813300	FeOH +2	3.520E-10	1.833E-10	-9.73679	0.52073	-1.907
2817320	FeSO4 +	1.996E-15	1.696E-15	-14.77058	0.84948	3.991
2811800	FeCl +2	1.602E-16	8.342E-17	-16.07873	0.52073	1.763
2811801	FeCl2 +	3.388E-18	2.878E-18	-17.54089	0.84948	2.201
2811802	FeCl3 AQ	2.208E-21	2.223E-21	-20.65304	1.00672	1.127
2813301	FeOH2 +	5.673E-06	4.819E-06	-5.31700	0.84948	-5.599
2813302	FeOH3 AQ	4.466E-06	4.496E-06	-5.34721	1.00672	-13.603

2813303	FeOH4 -	4.202E-06	3.569E-06	-5.44742	0.84948	-21.529
2817321	Fe(SO4)2 -	3.600E-17	3.058E-17	-16.51458	0.84948	5.491
2813304	Fe2(OH)2+4	1.230E-17	9.045E-19	-18.04359	0.07353	-1.816
2813305	Fe3(OH)4+5	5.377E-20	9.108E-22	-21.04059	0.01694	-4.529
1003300	BaOH +	6.329E-11	5.376E-11	-10.26952	0.84948	-13.287
3301400	HCO3 -	4.367E-04	3.710E-04	-3.43065	0.84948	10.400
3301401	H2CO3 AQ	1.042E-05	1.049E-05	-4.97921	1.00672	16.678
3307320	HSO4 -	8.202E-10	6.967E-10	-9.15694	0.84948	2.058
2123300	HCrO4 -	6.652E-07	5.651E-07	-6.24789	0.84948	6.580
2123301	H2CrO4 AQ	9.809E-16	9.874E-16	-15.00549	1.00672	5.648
2123302	Cr2O7 -2	2.124E-11	1.106E-11	-10.95627	0.52073	14.840
2121800	CrO3Cl -	4.081E-16	3.466E-16	-15.46013	0.84948	7.379
2127320	CrO3SO4-2	2.380E-15	1.239E-15	-14.90688	0.52073	9.277

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	7.676E-05	-4.115	0.000	0.000
330	H+1	-6.759E-04	-3.170	7.900	0.000
3301403	CO2 (g)	1.196E-04	-3.922	21.660	-0.530
3021201	BACRO4	-2.783E-05	-4.555	9.668	-6.390

PART 4 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:31: 3

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

CrO4-2

95.7	PERCENT BOUND IN SPECIES #	212	CrO4-2
1.5	PERCENT BOUND IN SPECIES #4102120		KCrO4-
2.4	PERCENT BOUND IN SPECIES #2123300		HCrO4 -

SO4-2

66.5	PERCENT BOUND IN SPECIES #	732	SO4-2
10.7	PERCENT BOUND IN SPECIES #4607320		MgSO4 AQ
21.3	PERCENT BOUND IN SPECIES #1507320		CaSO4 AQ
1.2	PERCENT BOUND IN SPECIES #4107320		KSO4 -

K+1

99.6	PERCENT BOUND IN SPECIES #	410	K+1

Fe+3

39.6	PERCENT BOUND IN SPECIES #2813301	FeOH2 +
31.1	PERCENT BOUND IN SPECIES #2813302	FeOH3 AQ

	29.3	PERCENT BOUND IN SPECIES #2813303	FeOH4 -
Cl-1			
	100.0	PERCENT BOUND IN SPECIES # 180	Cl-1
NO3-1			
	100.0	PERCENT BOUND IN SPECIES # 492	NO3-1
Ca+2			
	94.0	PERCENT BOUND IN SPECIES # 150	Ca+2
	5.6	PERCENT BOUND IN SPECIES #1507320	CaSO4 AQ
Na+1			
	99.7	PERCENT BOUND IN SPECIES # 500	Na+1
Mg+2			
	94.7	PERCENT BOUND IN SPECIES # 460	Mg+2
	5.0	PERCENT BOUND IN SPECIES #4607320	MgSO4 AQ
H4SiO4			
	98.9	PERCENT BOUND IN SPECIES # 770	H4SiO4
	1.1	PERCENT BOUND IN SPECIES #3307700	H3SiO4 -
CO3-2			
	1.8	PERCENT BOUND IN SPECIES #4601401	MgHCO3 +
	2.9	PERCENT BOUND IN SPECIES #1501400	CaHCO3 +
	1.2	PERCENT BOUND IN SPECIES #1501401	CaCO3 AQ
	90.8	PERCENT BOUND IN SPECIES #3301400	HCO3 -
	2.2	PERCENT BOUND IN SPECIES #3301401	H2CO3 AQ
H+1			
	2.0	PERCENT BOUND IN SPECIES #4601401	MgHCO3 +
	3.2	PERCENT BOUND IN SPECIES #1501400	CaHCO3 +
	100.0	PERCENT BOUND IN SPECIES #3301400	HCO3 -
	4.8	PERCENT BOUND IN SPECIES #3301401	H2CO3 AQ
H2O			
	2.2	PERCENT BOUND IN SPECIES #3300020	OH-

26.5 PERCENT BOUND IN SPECIES #2813301 FeOH2 +

31.3 PERCENT BOUND IN SPECIES #2813302 FeOH3 AQ

39.2 PERCENT BOUND IN SPECIES #2813303 FeOH4 -

Ba+2

100.0 PERCENT BOUND IN SPECIES # 100 Ba+2

PART 5 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:31: 3

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
212	CrO4-2	2.792E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
732	SO4-2	1.647E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	4.916E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.434E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
180	Cl-1	9.093E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
492	NO3-1	5.328E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	6.220E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.698E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.541E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
770	H4SiO4	1.458E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	4.810E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	4.368E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	4.283E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	2.965E-05	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED
Sum of CATIONS = 2.508E-02 Sum of ANIONS 1.234E-02
PERCENT DIFFERENCE = 3.404E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 2.907E-02

EQUILIBRIUM pH = 7.900

PART 6 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:31: 3

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]
6015000	ANHYDRITE	-1.123	[1.000] 150 [1.000] 732

5015000	ARAGONITE	-0.041	[1.000]	150	[1.000]	140					
5046000	ARTINITE	-5.177	[-2.000]	330	[2.000]	460	[1.000]	140			
			[5.000]	2							
6010000	BARITE	1.921	[1.000]	100	[1.000]	732					
2046000	BRUCITE	-3.750	[1.000]	460	[2.000]	2	[-2.000]	330			
5015001	CALCITE	0.098	[1.000]	150	[1.000]	140					
2077000	CHALCEDONY	-0.315	[-2.000]	2	[1.000]	770					
8646000	CHRYSOTILE	-0.738	[-6.000]	330	[3.000]	460	[2.000]	770			
			[1.000]	2							
8246000	CLINOENSTITE	-2.134	[-1.000]	2	[1.000]	460	[1.000]	770			
			[-2.000]	330							
2077001	CRISTOBALITE	-0.251	[-2.000]	2	[1.000]	770					
8215000	DIOPSIDE	-1.236	[-2.000]	2	[1.000]	150	[1.000]	460			
			[2.000]	770	[-4.000]	330					
5015002	DOLOMITE	0.005	[1.000]	150	[1.000]	460	[2.000]	140			
6046000	EPSOMITE	-3.863	[1.000]	460	[1.000]	732	[7.000]	2			
8646003	SEPIOLITE(C)	-1.343	[-0.500]	2	[2.000]	460	[3.000]	770			
			[-4.000]	330							
2028100	FERRIHYDRITE	3.362	[-3.000]	330	[1.000]	281	[3.000]	2			
2028103	Fe(OH)3 soil	5.553	[-3.000]	330	[1.000]	281	[3.000]	2			
4128100	FEOH)2.7CL.3	8.289	[-2.700]	330	[1.000]	281	[2.700]	2			
			[0.300]	180							
6028100	FE2(SO4)3	-44.205	[2.000]	281	[3.000]	732					
8046000	FORSTERITE	-6.052	[-4.000]	330	[2.000]	460	[1.000]	770			
2028102	GOETHITE	7.753	[-3.000]	330	[1.000]	281	[2.000]	2			
6015001	GYPSUM	-0.913	[1.000]	150	[1.000]	732	[2.000]	2			
4150000	HALITE	-6.536	[1.000]	500	[1.000]	180					
3028100	HEMATITE	20.514	[-6.000]	330	[2.000]	281	[3.000]	2			
5015003	HUNTITE	-4.263	[3.000]	460	[1.000]	150	[4.000]	140			
5046001	HYDRMAGNESIT	-12.665	[5.000]	460	[4.000]	140	[-2.000]	330			
			[6.000]	2							
6050000	JAROSITE NA	2.929	[-6.000]	330	[1.000]	500	[3.000]	281			
			[2.000]	732	[6.000]	2					
6041002	JAROSITE K	6.990	[-6.000]	330	[1.000]	410	[3.000]	281			
			[2.000]	732	[6.000]	2					
6028101	JAROSITE H	-1.229	[-5.000]	330	[3.000]	281	[2.000]	732			
			[7.000]	2							
8450000	MAGADIITE	-7.507	[-1.000]	330	[-9.000]	2	[1.000]	500			
			[7.000]	770							
3028101	MAGHEMITE	10.120	[-6.000]	330	[2.000]	281	[3.000]	2			
5046002	MAGNESITE	-0.589	[1.000]	460	[1.000]	140					
6050001	MIRABILITE	-7.816	[2.000]	500	[1.000]	732	[10.000]	2			

ID #	NAME	Sat. Index	Stoichiometry in [brackets]							
3050000	NATRON	-10.236	[2.000]	500	[1.000]	140	[10.000]	2		
5046003	NESQUEHONITE	-2.998	[1.000]	460	[1.000]	140	[3.000]	2		
2077002	QUARTZ	0.168	[-2.000]	2	[1.000]	770				
8646004	SEPIOLITE(A)	-4.210	[-0.500]	2	[2.000]	460	[3.000]	770		
			[-4.000]	330						
2077003	SIO2(A,GL)	-0.820	[-2.000]	2	[1.000]	770				
2077004	SIO2(A,PT)	-1.128	[-2.000]	2	[1.000]	770				
8646002	TALC	0.720	[-4.000]	2	[3.000]	460	[4.000]	770		
			[-6.000]	330						
6050002	THENARDITE	-8.749	[2.000]	500	[1.000]	732				
5050001	THERMONATR	-11.670	[2.000]	500	[1.000]	140	[1.000]	2		
8215001	TREMOLITE	4.529	[-8.000]	2	[2.000]	150	[5.000]	460		
			[8.000]	770	[-14.000]	330				
5010000	WITHERITE	-2.087	[1.000]	100	[1.000]	140				
2015000	LIME	-19.514	[-2.000]	330	[1.000]	150	[1.000]	2		
2015001	PORTLANDITE	-9.392	[-2.000]	330	[1.000]	150	[2.000]	2		
2046001	PERICLASE	-8.468	[-2.000]	330	[1.000]	460	[1.000]	2		
3046001	MAG-FERRITE	12.783	[-8.000]	330	[1.000]	460	[2.000]	281		
			[4.000]	2						
8215002	WOLLASTONITE	-3.550	[-1.000]	2	[-2.000]	330	[1.000]	770		
			[1.000]	150						
8215003	P-WOLLSTANIT	-4.400	[-1.000]	2	[-2.000]	330	[1.000]	770		
			[1.000]	150						
8015001	CA-OLIVINE	-14.920	[-4.000]	330	[1.000]	770	[2.000]	150		
8015002	LARNITE	-16.412	[-4.000]	330	[1.000]	770	[2.000]	150		
8015007	CA3SIO5	-37.854	[-6.000]	330	[1.000]	770	[3.000]	150		
			[1.000]	2						
8015003	MONTICELLITE	-7.784	[-4.000]	330	[1.000]	770	[1.000]	150		
			[1.000]	460						
8015005	AKERMINITE	-15.538	[-1.000]	2	[-6.000]	330	[2.000]	770		
			[2.000]	150	[1.000]	460				
8015004	MERWINITE	-23.326	[-8.000]	330	[2.000]	770	[1.000]	460		
			[3.000]	150						
3028102	LEPIDOCROCIT	6.882	[-3.000]	330	[1.000]	281	[2.000]	2		
3021201	BACRO4	0.000	[1.000]	212	[1.000]	100				
3021205	K2CRO4	-9.626	[1.000]	212	[2.000]	410				
3021206	K2CR2O7	-14.604	[2.000]	212	[2.000]	410	[2.000]	330		
			[-1.000]	2						
3021208	MGCRO4	-12.995	[1.000]	212	[1.000]	460				
3021210	NA2CRO4	-13.803	[1.000]	212	[2.000]	500				
3021211	NA2CR2O7	-21.302	[2.000]	212	[2.000]	500	[2.000]	330		
			[-1.000]	2						
2021200	CrO3	-17.446	[1.000]	212	[2.000]	330	[-1.000]	2		
3015000	CaCrO4	-5.107	[1.000]	150	[1.000]	212				

THIS IS THE OUTPUT FILE FOR THE FIRST EFFLUENT FROM THE COLUMN LEACH TEST ASSUMING THAT BOTH BARIUM CHROMATE AND BARITE ARE CONTROLLING CR AND BA SOLUTION CONCENTRATIONS.

PART 1 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:51:48

Hexchrome solubility for ERC
First liquid out of column fix Barite and Ba chromate and CO2

Temperature (Celsius): 25.00
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E-01	-7.90	
732	1.580E+02	-2.78	
410	1.920E+02	-2.31	
140	3.600E+01	-3.22	
180	3.220E+02	-2.04	
492	3.300E+01	-3.27	y
150	2.490E+02	-2.21	y
500	3.900E+01	-2.77	y
460	8.600E+01	-2.45	y
770	1.400E+01	-3.84	y
281	8.000E-01	-4.84	y
212	1.000E-02	-7.06	y
100	2.500E-01	-5.74	y

H2O has been inserted as a COMPONENT

3 4		
3301403	21.6600	-0.5300
3021201	9.6681	-6.3900
6010000	9.9760	-6.2800
330	7.9000	0.0000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	1.259E-08	-7.900	0.000E-01
732	SO4-2	1.660E-03	-2.780	1.580E+02
410	K+1	4.898E-03	-2.310	1.920E+02
140	CO3-2	6.026E-04	-3.220	3.600E+01
180	Cl-1	9.120E-03	-2.040	3.220E+02
492	NO3-1	5.370E-04	-3.270	3.300E+01
150	Ca+2	6.166E-03	-2.210	2.490E+02
500	Na+1	1.698E-03	-2.770	3.900E+01

460	Mg+2	3.548E-03	-2.450	8.600E+01
770	H4SiO4	1.445E-04	-3.840	1.400E+01
281	Fe+3	1.445E-05	-4.840	8.000E-01
212	CrO4-2	8.710E-08	-7.060	1.000E-02
100	Ba+2	1.820E-06	-5.740	2.500E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED

Sum of CATIONS= 2.618E-02 Sum of ANIONS = 1.412E-02

PERCENT DIFFERENCE = 2.993E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

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| IMPROVED ACTIVITY GUESSES PRIOR TO FIRST ITERATION: |
|      SO4-2       Log activity guess:    -2.78       |
|      CO3-2       Log activity guess:    -5.86       |
|      H4SiO4      Log activity guess:    -3.84       |
|      Fe+3        Log activity guess:   -15.40       |
|      CrO4-2      Log activity guess:    -7.10       |
|                                                     |
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PART 3 of OUTPUT FILE

Type I - COMPONENTS AS SPECIES IN SOLUTION

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
330	H+1	1.485E-08	1.259E-08	-7.90000	0.84748	0.072
732	SO4-2	4.529E-04	2.336E-04	-3.63146	0.51585	0.287
410	K+1	4.893E-03	4.147E-03	-2.38229	0.84748	0.072
140	CO3-2	2.675E-06	1.380E-06	-5.86021	0.51585	0.287
180	Cl-1	9.093E-03	7.706E-03	-2.11318	0.84748	0.072
492	NO3-1	5.328E-04	4.516E-04	-3.34529	0.84748	0.072
150	Ca+2	6.052E-03	3.122E-03	-2.50561	0.51585	0.287
500	Na+1	1.692E-03	1.434E-03	-2.84347	0.84748	0.072
460	Mg+2	3.456E-03	1.783E-03	-2.74890	0.51585	0.287
770	H4SiO4	1.442E-04	1.452E-04	-3.83796	1.00696	-0.003
281	Fe+3	1.583E-15	3.571E-16	-15.44726	0.22551	0.647
212	CrO4-2	9.203E-04	4.747E-04	-3.32356	0.51585	0.287
100	Ba+2	8.769E-07	4.523E-07	-6.34454	0.51585	0.287

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
5002120	NaCrO4-	3.992E-06	3.383E-06	-5.47073	0.84748	0.768
4102120	KCrO4-	1.462E-05	1.239E-05	-4.90685	0.84748	0.871
3300020	OH-	9.412E-07	7.976E-07	-6.09821	0.84748	-13.926
3307700	H3SiO4 -	1.604E-06	1.359E-06	-5.86675	0.84748	-9.857
3307701	H2SiO4 -2	4.294E-10	2.215E-10	-9.65458	0.51585	-21.329

4603300	MgOH +	2.746E-07	2.327E-07	-6.63323	0.84748	-11.712
4601400	MgCO3 AQ	2.331E-06	2.348E-06	-5.62939	1.00696	2.977
4601401	MgHCO3 +	9.076E-06	7.691E-06	-5.11399	0.84748	11.467
4607320	MgSO4 AQ	7.356E-05	7.407E-05	-4.13036	1.00696	2.247
1503300	CaOH +	7.380E-08	6.254E-08	-7.20382	0.84748	-12.526
1501400	CaHCO3 +	1.416E-05	1.200E-05	-4.92073	0.84748	11.417
1501401	CaCO3 AQ	6.078E-06	6.121E-06	-5.21321	1.00696	3.150
1507320	CaSO4 AQ	1.475E-04	1.486E-04	-3.82807	1.00696	2.306
5001400	NaCO3 -	4.327E-08	3.667E-08	-7.43568	0.84748	1.340
5001401	NaHCO3 AQ	2.974E-07	2.994E-07	-6.52368	1.00696	10.077
5007320	NaSO4 -	1.981E-06	1.679E-06	-5.77493	0.84748	0.772
4107320	KSO4 -	8.034E-06	6.809E-06	-5.16693	0.84748	0.919
2813300	FeOH +2	3.548E-10	1.830E-10	-9.73747	0.51585	-1.903
2817320	FeSO4 +	8.188E-16	6.939E-16	-15.15872	0.84748	3.992
2811800	FeCl +2	1.611E-16	8.309E-17	-16.08044	0.51585	1.767
2811801	FeCl2 +	3.375E-18	2.860E-18	-17.54361	0.84748	2.202
2811802	FeCl3 AQ	2.189E-21	2.204E-21	-20.65679	1.00696	1.127
2813301	FeOH2 +	5.678E-06	4.812E-06	-5.31768	0.84748	-5.598
2813302	FeOH3 AQ	4.458E-06	4.489E-06	-5.34789	1.00696	-13.603
2813303	FeOH4 -	4.205E-06	3.564E-06	-5.44810	0.84748	-21.528
2817321	Fe(SO4)2 -	6.049E-18	5.127E-18	-17.29018	0.84748	5.492
2813304	Fe2(OH)2+4	1.273E-17	9.017E-19	-18.04493	0.07081	-1.800
2813305	Fe3(OH)4+5	5.677E-20	9.065E-22	-21.04261	0.01597	-4.503
1003300	BaOH +	1.858E-12	1.575E-12	-11.80275	0.84748	-13.286
3301400	HCO3 -	4.377E-04	3.710E-04	-3.43065	0.84748	10.401
3301401	H2CO3 AQ	1.042E-05	1.049E-05	-4.97921	1.00696	16.678
3307320	HSO4 -	3.369E-10	2.855E-10	-9.54440	0.84748	2.059
2123300	HCrO4 -	2.276E-05	1.929E-05	-4.71466	0.84748	6.581
2123301	H2CrO4 AQ	3.348E-14	3.371E-14	-13.47226	1.00696	5.648
2123302	Cr2O7 -2	2.498E-08	1.289E-08	-7.88981	0.51585	14.845
2121800	CrO3Cl -	1.393E-14	1.181E-14	-13.92793	0.84748	7.380
2127320	CrO3SO4-2	3.360E-14	1.733E-14	-13.76111	0.51585	9.281

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	7.494E-05	-4.125	0.000	0.000
330	H+1	-6.960E-04	-3.157	7.900	0.000
3301403	CO2 (g)	1.178E-04	-3.929	21.660	-0.530
6010000	BARITE	9.626E-04	-3.017	9.976	-6.280
3021201	BACRO4	-9.616E-04	-3.017	9.668	-6.390

PART 4 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:51:48

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

Fe+3

39.6 PERCENT BOUND IN SPECIES #2813301 FeOH2 +

31.1 PERCENT BOUND IN SPECIES #2813302 FeOH3 AQ

29.3 PERCENT BOUND IN SPECIES #2813303 FeOH4 -

SO4-2

66.2	PERCENT BOUND IN SPECIES #	732	SO4-2
10.8	PERCENT BOUND IN SPECIES #4607320		MgSO4 AQ
21.6	PERCENT BOUND IN SPECIES #1507320		CaSO4 AQ
1.2	PERCENT BOUND IN SPECIES #4107320		KSO4 -

K+1

99.5	PERCENT BOUND IN SPECIES #	410	K+1

H4SiO4

98.9	PERCENT BOUND IN SPECIES #	770	H4SiO4
1.1	PERCENT BOUND IN SPECIES #3307700		H3SiO4 -

Cl-1

100.0	PERCENT BOUND IN SPECIES #	180	Cl-1

NO3-1

100.0	PERCENT BOUND IN SPECIES #	492	NO3-1

Ca+2

97.3	PERCENT BOUND IN SPECIES #	150	Ca+2
2.4	PERCENT BOUND IN SPECIES #1507320		CaSO4 AQ

Na+1

99.6	PERCENT BOUND IN SPECIES #	500	Na+1

Mg+2

97.6	PERCENT BOUND IN SPECIES #	460	Mg+2
2.1	PERCENT BOUND IN SPECIES #4607320		MgSO4 AQ

CO3-2

1.9	PERCENT BOUND IN SPECIES #4601401		MgHCO3 +
2.9	PERCENT BOUND IN SPECIES #1501400		CaHCO3 +
1.3	PERCENT BOUND IN SPECIES #1501401		CaCO3 AQ
90.7	PERCENT BOUND IN SPECIES #3301400		HCO3 -
2.2	PERCENT BOUND IN SPECIES #3301401		H2CO3 AQ

H+1

2.0	PERCENT BOUND IN SPECIES	#4601401	MgHCO3 +
3.1	PERCENT BOUND IN SPECIES	#1501400	CaHCO3 +
95.1	PERCENT BOUND IN SPECIES	#3301400	HCO3 -
4.5	PERCENT BOUND IN SPECIES	#3301401	H2CO3 AQ
4.9	PERCENT BOUND IN SPECIES	#2123300	HCrO4 -

H2O

2.2	PERCENT BOUND IN SPECIES	#3300020	OH-
26.5	PERCENT BOUND IN SPECIES	#2813301	FeOH2 +
31.2	PERCENT BOUND IN SPECIES	#2813302	FeOH3 AQ
39.3	PERCENT BOUND IN SPECIES	#2813303	FeOH4 -

CrO4-2

95.7	PERCENT BOUND IN SPECIES	# 212	CrO4-2
1.5	PERCENT BOUND IN SPECIES	#4102120	KCrO4-
2.4	PERCENT BOUND IN SPECIES	#2123300	HCrO4 -

Ba+2

100.0	PERCENT BOUND IN SPECIES	# 100	Ba+2

PART 5 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:51:48

EQUILIBRATED MASS DISTRIBUTION

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
281	Fe+3	1.434E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
732	SO4-2	6.840E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	4.916E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
770	H4SiO4	1.458E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
180	Cl-1	9.093E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
492	NO3-1	5.328E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	6.219E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	1.698E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	3.541E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	4.828E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	4.605E-04	100.0	0.000E-01	0.0	0.000E-01	0.0

2	H2O	4.281E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
212	CrO4-2	9.617E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	8.769E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 2.563E-02 Sum of ANIONS 1.287E-02

PERCENT DIFFERENCE = 3.313E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 3.014E-02

EQUILIBRIUM pH = 7.900

PART 6 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 11:51:48

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]							
6015000	ANHYDRITE	-1.500	[1.000]	150	[1.000]	732				
5015000	ARAGONITE	-0.030	[1.000]	150	[1.000]	140				
5046000	ARTINITE	-5.159	[-2.000]	330	[2.000]	460	[1.000]	140		
			[5.000]	2						
6010000	BARITE	0.000	[1.000]	100	[1.000]	732				
2046000	BRUCITE	-3.741	[1.000]	460	[2.000]	2	[-2.000]	330		
5015001	CALCITE	0.109	[1.000]	150	[1.000]	140				
2077000	CHALCEDONY	-0.315	[-2.000]	2	[1.000]	770				
8646000	CHRYSOTILE	-0.711	[-6.000]	330	[3.000]	460	[2.000]	770		
			[1.000]	2						
8246000	CLINOENSTITE	-2.125	[-1.000]	2	[1.000]	460	[1.000]	770		
			[-2.000]	330						
2077001	CRISTOBALITE	-0.251	[-2.000]	2	[1.000]	770				
8215000	DIOPSIDE	-1.216	[-2.000]	2	[1.000]	150	[1.000]	460		
			[2.000]	770	[-4.000]	330				
5015002	DOLOMITE	0.025	[1.000]	150	[1.000]	460	[2.000]	140		
6046000	EPSOMITE	-4.242	[1.000]	460	[1.000]	732	[7.000]	2		
8646003	SEPIOLITE(C)	-1.325	[-0.500]	2	[2.000]	460	[3.000]	770		
			[-4.000]	330						
2028100	FERRIHYDRITE	3.361	[-3.000]	330	[1.000]	281	[3.000]	2		
2028103	Fe(OH)3 soil	5.552	[-3.000]	330	[1.000]	281	[3.000]	2		
4128100	FEOH)2.7CL.3	8.288	[-2.700]	330	[1.000]	281	[2.700]	2		
			[0.300]	180						
6028100	FE2(SO4)3	-45.369	[2.000]	281	[3.000]	732				
8046000	FORSTERITE	-6.034	[-4.000]	330	[2.000]	460	[1.000]	770		
2028102	GOETHITE	7.752	[-3.000]	330	[1.000]	281	[2.000]	2		
6015001	GYPSUM	-1.289	[1.000]	150	[1.000]	732	[2.000]	2		
4150000	HALITE	-6.539	[1.000]	500	[1.000]	180				
3028100	HEMATITE	20.513	[-6.000]	330	[2.000]	281	[3.000]	2		
5015003	HUNTITE	-4.225	[3.000]	460	[1.000]	150	[4.000]	140		
5046001	HYDRMAGNESIT	-12.621	[5.000]	460	[4.000]	140	[-2.000]	330		
			[6.000]	2						
6050000	JAROSITE NA	2.151	[-6.000]	330	[1.000]	500	[3.000]	281		
			[2.000]	732	[6.000]	2				
6041002	JAROSITE K	6.212	[-6.000]	330	[1.000]	410	[3.000]	281		

			[2.000]	732	[6.000]	2				
6028101	JAROSITE H	-2.006	[-5.000]	330	[3.000]	281	[2.000]	732		
			[7.000]	2						
8450000	MAGADIITE	-7.507	[-1.000]	330	[-9.000]	2	[1.000]	500		
			[7.000]	770						
3028101	MAGHEMITE	10.119	[-6.000]	330	[2.000]	281	[3.000]	2		
5046002	MAGNESITE	-0.580	[1.000]	460	[1.000]	140				
6050001	MIRABILITE	-8.206	[2.000]	500	[1.000]	732	[10.000]	2		
3050000	NATRON	-10.238	[2.000]	500	[1.000]	140	[10.000]	2		
5046003	NESQUEHONITE	-2.989	[1.000]	460	[1.000]	140	[3.000]	2		
2077002	QUARTZ	0.168	[-2.000]	2	[1.000]	770				
8646004	SEPIOLITE(A)	-4.192	[-0.500]	2	[2.000]	460	[3.000]	770		
			[-4.000]	330						
2077003	SIO2(A,GL)	-0.820	[-2.000]	2	[1.000]	770				
2077004	SIO2(A,PT)	-1.128	[-2.000]	2	[1.000]	770				
8646002	TALC	0.747	[-4.000]	2	[3.000]	460	[4.000]	770		
			[-6.000]	330						
6050002	THENARDITE	-9.139	[2.000]	500	[1.000]	732				
5050001	THERMONATR	-11.672	[2.000]	500	[1.000]	140	[1.000]	2		
8215001	TREMOLITE	4.596	[-8.000]	2	[2.000]	150	[5.000]	460		
			[8.000]	770	[-14.000]	330				
5010000	WITHERITE	-3.620	[1.000]	100	[1.000]	140				
2015000	LIME	-19.503	[-2.000]	330	[1.000]	150	[1.000]	2		
2015001	PORTLANDITE	-9.381	[-2.000]	330	[1.000]	150	[2.000]	2		
2046001	PERICLASE	-8.459	[-2.000]	330	[1.000]	460	[1.000]	2		
3046001	MAG-FERRITE	12.791	[-8.000]	330	[1.000]	460	[2.000]	281		
			[4.000]	2						
8215002	WOLLASTONITE	-3.539	[-1.000]	2	[-2.000]	330	[1.000]	770		
			[1.000]	150						
8215003	P-WOLLSTANIT	-4.389	[-1.000]	2	[-2.000]	330	[1.000]	770		
			[1.000]	150						
8015001	CA-OLIVINE	-14.898	[-4.000]	330	[1.000]	770	[2.000]	150		
8015002	LARNITE	-16.390	[-4.000]	330	[1.000]	770	[2.000]	150		
8015007	CA3SIO5	-37.822	[-6.000]	330	[1.000]	770	[3.000]	150		
			[1.000]	2						
8015003	MONTICELLITE	-7.764	[-4.000]	330	[1.000]	770	[1.000]	150		
			[1.000]	460						
8015005	AKERMINITE	-15.508	[-1.000]	2	[-6.000]	330	[2.000]	770		
			[2.000]	150	[1.000]	460				
8015004	MERWINITE	-23.285	[-8.000]	330	[2.000]	770	[1.000]	460		
			[3.000]	150						
3028102	LEPIDOCROCIT	6.881	[-3.000]	330	[1.000]	281	[2.000]	2		
3021201	BACRO4	0.000	[1.000]	212	[1.000]	100				
3021205	K2CRO4	-8.095	[1.000]	212	[2.000]	410				
3021206	K2CR2O7	-11.540	[2.000]	212	[2.000]	410	[2.000]	330		
			[-1.000]	2						
3021208	MGCRO4	-11.453	[1.000]	212	[1.000]	460				
3021210	NA2CRO4	-12.272	[1.000]	212	[2.000]	500				
3021211	NA2CR2O7	-18.239	[2.000]	212	[2.000]	500	[2.000]	330		
			[-1.000]	2						
2021200	CrO3	-15.913	[1.000]	212	[2.000]	330	[-1.000]	2		
3015000	CaCrO4	-3.563	[1.000]	150	[1.000]	212				

THIS IS THE OUTPUT FILE FOR THE EQUILIBRIUM EFFLUENT (ENDING STEADY STATE COMPOSITION) FROM THE COLUMN LEACH TEST ASSUMING THAT ONLY BARIUM CHROMATE IS CONTROLLING CR AND BA.

PART 1 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 12:15:33

Hexchrome solubility for ERC
Equilibrium liquid out of column fix Ba chromate and CO2

Temperature (Celsius): 25.00
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E-01	-8.40	
732	8.600E+01	-2.78	
410	5.000E+00	-2.31	
140	5.410E+01	-3.22	
180	1.000E+01	-2.04	
492	2.700E+01	-3.27	y
150	6.490E+01	-2.21	y
500	1.700E+01	-2.77	y
460	1.500E+01	-2.45	y
770	1.400E+01	-3.84	y
281	1.000E-01	-4.84	y
212	1.000E-02	-7.06	y
100	2.500E-01	-5.74	y

H2O has been inserted as a COMPONENT

3 3		
3301403	21.6600	-0.5300
3021201	9.6681	-6.3900
330	8.4000	0.0000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.981E-09	-8.400	0.000E-01
732	SO4-2	1.660E-03	-2.780	8.600E+01
410	K+1	4.898E-03	-2.310	5.000E+00
140	CO3-2	6.026E-04	-3.220	5.410E+01
180	Cl-1	9.120E-03	-2.040	1.000E+01
492	NO3-1	5.370E-04	-3.270	2.700E+01
150	Ca+2	6.166E-03	-2.210	6.490E+01
500	Na+1	1.698E-03	-2.770	1.700E+01
460	Mg+2	3.548E-03	-2.450	1.500E+01
770	H4SiO4	1.445E-04	-3.840	1.400E+01
281	Fe+3	1.445E-05	-4.840	1.000E-01
212	CrO4-2	8.710E-08	-7.060	1.000E-02
100	Ba+2	1.820E-06	-5.740	2.500E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED

Sum of CATIONS= 5.350E-03 Sum of ANIONS = 4.313E-03

PERCENT DIFFERENCE = 1.074E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
5002120	NaCrO4-	5.118E-08	4.679E-08	-7.32984	0.91418	0.735
4102120	KCrO4-	1.121E-08	1.025E-08	-7.98937	0.91418	0.838
3300020	OH-	2.760E-06	2.523E-06	-5.59804	0.91418	-13.959
3307700	H3SiO4 -	4.576E-06	4.183E-06	-5.37848	0.91418	-9.890
3307701	H2SiO4 -2	3.087E-09	2.156E-09	-8.66630	0.69844	-21.461
4603300	MgOH +	1.795E-07	1.641E-07	-6.78490	0.91418	-11.745
4601400	MgCO3 AQ	5.227E-06	5.235E-06	-5.28107	1.00165	2.979
4601401	MgHCO3 +	5.933E-06	5.424E-06	-5.26567	0.91418	11.434
4607320	MgSO4 AQ	3.681E-05	3.687E-05	-4.43335	1.00165	2.249
1503300	CaOH +	7.149E-08	6.535E-08	-7.18472	0.91418	-12.559
1501400	CaHCO3 +	1.372E-05	1.254E-05	-4.90163	0.91418	11.384
1501401	CaCO3 AQ	2.019E-05	2.022E-05	-4.69412	1.00165	3.152
1507320	CaSO4 AQ	1.094E-04	1.096E-04	-3.96028	1.00165	2.308
5001400	NaCO3 -	1.886E-07	1.724E-07	-6.76351	0.91418	1.307
5001401	NaHCO3 AQ	4.444E-07	4.451E-07	-6.35151	1.00165	10.079
5007320	NaSO4 -	1.927E-06	1.762E-06	-5.75406	0.91418	0.739
4107320	KSO4 -	4.672E-07	4.271E-07	-6.36948	0.91418	0.886
2813300	FeOH +2	2.538E-12	1.773E-12	-11.75131	0.69844	-2.034
2817320	FeSO4 +	5.189E-18	4.744E-18	-17.32387	0.91418	3.959
2811800	FeCl +2	1.219E-20	8.516E-21	-20.06976	0.69844	1.636
2811801	FeCl2 +	1.073E-23	9.812E-24	-23.00826	0.91418	2.169
2811802	FeCl3 AQ	2.527E-28	2.531E-28	-27.59675	1.00165	1.129
2813301	FeOH2 +	1.613E-07	1.475E-07	-6.83135	0.91418	-5.631
2813302	FeOH3 AQ	4.344E-07	4.351E-07	-6.36140	1.00165	-13.601
2813303	FeOH4 -	1.195E-06	1.093E-06	-5.96144	0.91418	-21.561
2817321	Fe(SO4)2 -	8.561E-20	7.826E-20	-19.10646	0.91418	5.459
2813304	Fe2(OH)2+4	3.555E-22	8.460E-23	-22.07262	0.23797	-2.327
2813305	Fe3(OH)4+5	2.456E-26	2.606E-27	-26.58398	0.10612	-5.326
1003300	BaOH +	1.851E-10	1.693E-10	-9.77147	0.91418	-13.319
3301400	HCO3 -	1.284E-03	1.174E-03	-2.93048	0.91418	10.369
3301401	H2CO3 AQ	1.048E-05	1.049E-05	-4.97904	1.00165	16.680
3307320	HSO4 -	2.205E-10	2.016E-10	-9.69553	0.91418	2.026
2123300	HCrO4 -	1.964E-07	1.796E-07	-6.74578	0.91418	6.548
2123301	H2CrO4 AQ	9.906E-17	9.923E-17	-16.00338	1.00165	5.651
2123302	Cr2O7 -2	1.598E-12	1.116E-12	-11.95221	0.69844	14.713
2121800	CrO3Cl -	1.272E-18	1.163E-18	-17.93453	0.91418	7.348
2127320	CrO3SO4-2	1.631E-16	1.139E-16	-15.94353	0.69844	9.150

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-4.673E-04	-3.330	0.000	0.000
330	H+1	-3.952E-04	-3.403	8.400	0.000
3301403	CO2 (g)	-4.579E-04	-3.339	21.660	-0.530
3021201	BACRO4	-2.018E-05	-4.695	9.668	-6.390

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

CrO4-2

98.7	PERCENT BOUND IN SPECIES #	212	CrO4-2

SO4-2

83.4	PERCENT BOUND IN SPECIES #	732	SO4-2
4.1	PERCENT BOUND IN SPECIES #	4607320	MgSO4 AQ
12.2	PERCENT BOUND IN SPECIES #	1507320	CaSO4 AQ

K+1

99.6	PERCENT BOUND IN SPECIES #	410	K+1

Fe+3

9.0	PERCENT BOUND IN SPECIES #	2813301	FeOH2 +
24.3	PERCENT BOUND IN SPECIES #	2813302	FeOH3 AQ
66.7	PERCENT BOUND IN SPECIES #	2813303	FeOH4 -

Cl-1

100.0	PERCENT BOUND IN SPECIES #	180	Cl-1

NO3-1

100.0	PERCENT BOUND IN SPECIES #	492	NO3-1

Ca+2

91.1	PERCENT BOUND IN SPECIES #	150	Ca+2
1.2	PERCENT BOUND IN SPECIES #	1501401	CaCO3 AQ
6.8	PERCENT BOUND IN SPECIES #	1507320	CaSO4 AQ

Na+1

99.6	PERCENT BOUND IN SPECIES #	500	Na+1

Mg+2

92.2	PERCENT BOUND IN SPECIES #	460	Mg+2
6.0	PERCENT BOUND IN SPECIES #	4607320	MgSO4 AQ

H4SiO4

96.9	PERCENT BOUND IN SPECIES #	770	H4SiO4
3.1	PERCENT BOUND IN SPECIES #3307700		H3SiO4 -

CO3-2

1.5	PERCENT BOUND IN SPECIES #	140	CO3-2
1.0	PERCENT BOUND IN SPECIES #1501400		CaHCO3 +
1.5	PERCENT BOUND IN SPECIES #1501401		CaCO3 AQ
94.4	PERCENT BOUND IN SPECIES #3301400		HCO3 -

H+1

1.0	PERCENT BOUND IN SPECIES #1501400		CaHCO3 +
97.9	PERCENT BOUND IN SPECIES #3301400		HCO3 -
1.6	PERCENT BOUND IN SPECIES #3301401		H2CO3 AQ

H2O

29.3	PERCENT BOUND IN SPECIES #3300020		OH-
1.9	PERCENT BOUND IN SPECIES #4603300		MgOH +
3.4	PERCENT BOUND IN SPECIES #2813301		FeOH2 +
13.8	PERCENT BOUND IN SPECIES #2813302		FeOH3 AQ
50.8	PERCENT BOUND IN SPECIES #2813303		FeOH4 -

Ba+2

100.0	PERCENT BOUND IN SPECIES #	100	Ba+2

PART 5 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 12:15:33

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED MOL/KG	DISSOLVED PERCENT	SORBED MOL/KG	SORBED PERCENT	PRECIPITATED MOL/KG	PRECIPITATED PERCENT
212	CrO4-2	2.027E-05	100.0	0.000E-01	0.0	0.000E-01	0.0
732	SO4-2	8.955E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.279E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
281	Fe+3	1.791E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
180	Cl-1	2.821E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
492	NO3-1	4.356E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.620E-03	100.0	0.000E-01	0.0	0.000E-01	0.0

THIS IS THE OUTPUT FILE FOR THE EQUILIBRUM EFFLUENT FROM THE COLUMN LEACH TEST ASSUMING THAT BOTH BARIUM CHROMATE AND BARITE ARE CONTROLLING CR AND BA SOLUTION CONCENTRATIONS.

PART 1 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 12:14:20

Hexchrome solubility for ERC
Equilibrium liquid out of column fix Barite and Ba chromate and CO2

Temperature (Celsius): 25.00
Units of concentration: MG/L
Ionic strength to be computed.
If specified, carbonate concentration represents total inorganic carbon.
Do not automatically terminate if charge imbalance exceeds 30%
Precipitation is allowed only for those solids specified as ALLOWED
in the input file (if any).
The maximum number of iterations is: 200
The method used to compute activity coefficients is: Davies equation
Intermediate output file

330	0.000E-01	-8.40	
732	8.600E+01	-2.78	
410	5.000E+00	-2.31	
140	5.410E+01	-3.22	
180	1.000E+01	-2.04	
492	2.700E+01	-3.27	y
150	6.490E+01	-2.21	y
500	1.700E+01	-2.77	y
460	1.500E+01	-2.45	y
770	1.400E+01	-3.84	y
281	1.000E-01	-4.84	y
212	1.000E-02	-7.06	y
100	2.500E-01	-5.74	y

H2O has been inserted as a COMPONENT

3 4		
3301403	21.6600	-0.5300
3021201	9.6681	-6.3900
6010000	9.9760	-6.2800
330	8.4000	0.0000

INPUT DATA BEFORE TYPE MODIFICATIONS

ID	NAME	ACTIVITY GUESS	LOG GUESS	ANAL TOTAL
330	H+1	3.981E-09	-8.400	0.000E-01
732	SO4-2	1.660E-03	-2.780	8.600E+01
410	K+1	4.898E-03	-2.310	5.000E+00
140	CO3-2	6.026E-04	-3.220	5.410E+01
180	Cl-1	9.120E-03	-2.040	1.000E+01
492	NO3-1	5.370E-04	-3.270	2.700E+01
150	Ca+2	6.166E-03	-2.210	6.490E+01
500	Na+1	1.698E-03	-2.770	1.700E+01

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                                    [  6.000]   2
6050000 JAROSITE NA      -2.021     [ -6.000] 330  [  1.000] 500  [  3.000] 281
                                    [  2.000] 732  [  6.000]   2
6041002 JAROSITE K        0.817     [ -6.000] 330  [  1.000] 410  [  3.000] 281
                                    [  2.000] 732  [  6.000]   2
6028101 JAROSITE H       -6.349     [ -5.000] 330  [  3.000] 281  [  2.000] 732
                                    [  7.000]   2
8450000 MAGADIITE        -7.419     [ -1.000] 330  [ -9.000]   2  [  1.000] 500
                                    [  7.000] 770
3028101 MAGHEMITE         8.091     [ -6.000] 330  [  2.000] 281  [  3.000]   2
5046002 MAGNESITE        -0.232     [  1.000] 460  [  1.000] 140
6050001 MIRABILITE       -8.512     [  2.000] 500  [  1.000] 732  [ 10.000]   2
3050000 NATRON           -9.892     [  2.000] 500  [  1.000] 140  [ 10.000]   2
5046003 NESQUEHONITE     -2.640     [  1.000] 460  [  1.000] 140  [  3.000]   2
2077002 QUARTZ            0.156     [ -2.000]   2  [  1.000] 770
8646004 SEPIOLITE(A)     -3.531     [ -0.500]   2  [  2.000] 460  [  3.000] 770
                                    [ -4.000] 330
2077003 SIO2(A,GL)       -0.832     [ -2.000]   2  [  1.000] 770
2077004 SIO2(A,PT)       -1.140     [ -2.000]   2  [  1.000] 770
8646002 TALC              1.744     [ -4.000]   2  [  3.000] 460  [  4.000] 770
                                    [ -6.000] 330
6050002 THENARDITE       -9.447     [  2.000] 500  [  1.000] 732
5050001 THERMONATR      -11.328     [  2.000] 500  [  1.000] 140  [  1.000]   2
8215001 TREMOLITE         7.280     [ -8.000]   2  [  2.000] 150  [  5.000] 460
                                    [  8.000] 770  [-14.000] 330
5010000 WITHERITE        -1.088     [  1.000] 100  [  1.000] 140
2015000 LIME            -18.984     [ -2.000] 330  [  1.000] 150  [  1.000]   2
2015001 PORTLANDITE      -8.862     [ -2.000] 330  [  1.000] 150  [  2.000]   2
2046001 PERICLASE        -8.111     [ -2.000] 330  [  1.000] 460  [  1.000]   2
3046001 MAG-FERRITE      11.112     [ -8.000] 330  [  1.000] 460  [  2.000] 281
                                    [  4.000]   2
8215002 WOLLASTONITE     -3.032     [ -1.000]   2  [ -2.000] 330  [  1.000] 770
                                    [  1.000] 150
8215003 P-WOLLSTANIT     -3.882     [ -1.000]   2  [ -2.000] 330  [  1.000] 770
                                    [  1.000] 150
8015001 CA-OLIVINE      -13.872     [ -4.000] 330  [  1.000] 770  [  2.000] 150
8015002 LARNITE         -15.364     [ -4.000] 330  [  1.000] 770  [  2.000] 150
8015007 CA3SIO5         -36.277     [ -6.000] 330  [  1.000] 770  [  3.000] 150
                                    [  1.000]   2
8015003 MONTICELLITE     -6.909     [ -4.000] 330  [  1.000] 770  [  1.000] 150
                                    [  1.000] 460
8015005 AKERMINITE      -14.145     [ -1.000]   2  [ -6.000] 330  [  2.000] 770
                                    [  2.000] 150  [  1.000] 460
8015004 MERWINITE       -21.403     [ -8.000] 330  [  2.000] 770  [  1.000] 460
                                    [  3.000] 150
3028102 LEPIDOCROCIT      5.868     [ -3.000] 330  [  1.000] 281  [  2.000]   2
3021201 BACRO4            0.000     [  1.000] 212  [  1.000] 100
3021205 K2CRO4          -12.729     [  1.000] 212  [  2.000] 410
3021206 K2CR2O7         -18.706     [  2.000] 212  [  2.000] 410  [  2.000] 330
                                    [ -1.000]   2
3021208 MGCRO4          -13.636     [  1.000] 212  [  1.000] 460
3021210 NA2CRO4         -14.459     [  1.000] 212  [  2.000] 500
3021211 NA2CR2O7        -22.957     [  2.000] 212  [  2.000] 500  [  2.000] 330
                                    [ -1.000]   2
2021200 CrO3            -18.444     [  1.000] 212  [  2.000] 330  [ -1.000]   2
3015000 CaCrO4           -5.576     [  1.000] 150  [  1.000] 212
*******************************************************************************
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500	Na+1	7.397E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	6.172E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
770	H4SiO4	1.457E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.360E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.311E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	9.419E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	2.200E-05	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 5.019E-03 Sum of ANIONS 3.586E-03

PERCENT DIFFERENCE = 1.665E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 7.157E-03

EQUILIBRIUM pH = 8.400

PART 6 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 12:15:33

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]			
6015000	ANHYDRITE	-1.632	[1.000] 150	[1.000] 732		
5015000	ARAGONITE	0.489	[1.000] 150	[1.000] 140		
5046000	ARTINITE	-4.462	[-2.000] 330	[2.000] 460	[1.000] 140	
			[5.000] 2			
6010000	BARITE	1.880	[1.000] 100	[1.000] 732		
2046000	BRUCITE	-3.393	[1.000] 460	[2.000] 2	[-2.000] 330	
5015001	CALCITE	0.628	[1.000] 150	[1.000] 140		
2077000	CHALCEDONY	-0.327	[-2.000] 2	[1.000] 770		
8646000	CHRYSOTILE	0.310	[-6.000] 330	[3.000] 460	[2.000] 770	
			[1.000] 2			
8246000	CLINOENSTITE	-1.788	[-1.000] 2	[1.000] 460	[1.000] 770	
			[-2.000] 330			
2077001	CRISTOBALITE	-0.263	[-2.000] 2	[1.000] 770		
8215000	DIOPSIDE	-0.373	[-2.000] 2	[1.000] 150	[1.000] 460	
			[2.000] 770	[-4.000] 330		
5015002	DOLOMITE	0.892	[1.000] 150	[1.000] 460	[2.000] 140	
6046000	EPSOMITE	-4.544	[1.000] 460	[1.000] 732	[7.000] 2	
8646003	SEPIOLITE(C)	-0.664	[-0.500] 2	[2.000] 460	[3.000] 770	
			[-4.000] 330			
2028100	FERRIHYDRITE	2.348	[-3.000] 330	[1.000] 281	[3.000] 2	
2028103	Fe(OH)3 soil	4.539	[-3.000] 330	[1.000] 281	[3.000] 2	
4128100	FEOH)2.7CL.3	6.682	[-2.700] 330	[1.000] 281	[2.700] 2	
			[0.300] 180			
6028100	FE2(SO4)3	-49.350	[2.000] 281	[3.000] 732		
8046000	FORSTERITE	-5.349	[-4.000] 330	[2.000] 460	[1.000] 770	
2028102	GOETHITE	6.739	[-3.000] 330	[1.000] 281	[2.000] 2	
6015001	GYPSUM	-1.421	[1.000] 150	[1.000] 732	[2.000] 2	
4150000	HALITE	-8.342	[1.000] 500	[1.000] 180		
3028100	HEMATITE	18.485	[-6.000] 330	[2.000] 281	[3.000] 2	
5015003	HUNTITE	-2.661	[3.000] 460	[1.000] 150	[4.000] 140	
5046001	HYDRMAGNESIT	-10.878	[5.000] 460	[4.000] 140	[-2.000] 330	

460	Mg+2	3.548E-03	-2.450	1.500E+01
770	H4SiO4	1.445E-04	-3.840	1.400E+01
281	Fe+3	1.445E-05	-4.840	1.000E-01
212	CrO4-2	8.710E-08	-7.060	1.000E-02
100	Ba+2	1.820E-06	-5.740	2.500E-01
2	H2O	1.000E+00	0.000	0.000E-01

Charge Balance: UNSPECIATED

Sum of CATIONS= 5.350E-03 Sum of ANIONS = 4.313E-03

PERCENT DIFFERENCE = 1.074E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

PART 3 of OUTPUT FILE

Type II - OTHER SPECIES IN SOLUTION OR ADSORBED

ID	NAME	CALC MOL	ACTIVITY	LOG ACTVTY	GAMMA	NEW LOGK
5002120	NaCrO4-	1.416E-06	1.293E-06	-5.88848	0.91282	0.736
4102120	KCrO4-	3.102E-07	2.832E-07	-6.54793	0.91282	0.839
3300020	OH-	2.764E-06	2.523E-06	-5.59804	0.91282	-13.958
3307700	H3SiO4 -	4.583E-06	4.183E-06	-5.37847	0.91282	-9.889
3307701	H2SiO4 -2	3.106E-09	2.156E-09	-8.66630	0.69428	-21.458
4603300	MgOH +	1.858E-07	1.696E-07	-6.77063	0.91282	-11.744
4601400	MgCO3 AQ	5.401E-06	5.410E-06	-5.26679	1.00171	2.979
4601401	MgHCO3 +	6.141E-06	5.605E-06	-5.25140	0.91282	11.435
4607320	MgSO4 AQ	1.388E-05	1.390E-05	-4.85696	1.00171	2.249
1503300	CaOH +	7.438E-08	6.789E-08	-7.16816	0.91282	-12.558
1501400	CaHCO3 +	1.427E-05	1.303E-05	-4.88507	0.91282	11.385
1501401	CaCO3 AQ	2.098E-05	2.101E-05	-4.67755	1.00171	3.152
1507320	CaSO4 AQ	4.146E-05	4.153E-05	-4.38160	1.00171	2.308
5001400	NaCO3 -	1.885E-07	1.721E-07	-6.76424	0.91282	1.308
5001401	NaHCO3 AQ	4.436E-07	4.444E-07	-6.35224	1.00171	10.079
5007320	NaSO4 -	7.030E-07	6.417E-07	-6.19268	0.91282	0.740
4107320	KSO4 -	1.704E-07	1.556E-07	-6.80802	0.91282	0.886
2813300	FeOH +2	2.551E-12	1.771E-12	-11.75180	0.69428	-2.032
2817320	FeSO4 +	1.894E-18	1.729E-18	-17.76224	0.91282	3.960
2811800	FeCl +2	1.223E-20	8.494E-21	-20.07090	0.69428	1.638
2811801	FeCl2 +	1.070E-23	9.771E-24	-23.01004	0.91282	2.170
2811802	FeCl3 AQ	2.512E-28	2.517E-28	-27.59919	1.00171	1.129
2813301	FeOH2 +	1.614E-07	1.473E-07	-6.83184	0.91282	-5.630
2813302	FeOH3 AQ	4.339E-07	4.346E-07	-6.36188	1.00171	-13.601
2813303	FeOH4 -	1.196E-06	1.092E-06	-5.96193	0.91282	-21.560
2817321	Fe(SO4)2 -	1.140E-20	1.041E-20	-19.98272	0.91282	5.460
2813304	Fe2(OH)2+4	3.633E-22	8.441E-23	-22.07360	0.23234	-2.316
2813305	Fe3(OH)4+5	2.541E-26	2.598E-27	-26.58544	0.10223	-5.310
1003300	BaOH +	6.700E-12	6.116E-12	-11.21356	0.91282	-13.318
3301400	HCO3 -	1.286E-03	1.174E-03	-2.93048	0.91282	10.369
3301401	H2CO3 AQ	1.048E-05	1.049E-05	-4.97904	1.00171	16.680
3307320	HSO4 -	8.057E-11	7.355E-11	-10.13342	0.91282	2.027
2123300	HCrO4 -	5.444E-06	4.970E-06	-5.30368	0.91282	6.549
2123301	H2CrO4 AQ	2.741E-15	2.746E-15	-14.56128	1.00171	5.651
2123302	Cr2O7 -2	1.232E-09	8.550E-10	-9.06802	0.69428	14.716
2121800	CrO3Cl -	3.520E-17	3.213E-17	-16.49308	0.91282	7.348
2127320	CrO3SO4-2	1.656E-15	1.150E-15	-14.93932	0.69428	9.152

Type III - SPECIES WITH FIXED ACTIVITY

ID	NAME	CALC MOL	LOG MOL	NEW LOGK	DH
2	H2O	-4.711E-04	-3.327	0.000	0.000
330	H+1	-3.956E-04	-3.403	8.400	0.000
3301403	CO2 (g)	-4.617E-04	-3.336	21.660	-0.530
6010000	BARITE	5.652E-04	-3.248	9.976	-6.280
3021201	BACRO4	-5.641E-04	-3.249	9.668	-6.390

PART 4 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 12:14:20

PERCENTAGE DISTRIBUTION OF COMPONENTS AMONG
TYPE I and TYPE II (dissolved and adsorbed) species

Fe+3

9.0	PERCENT BOUND IN SPECIES #2813301	FeOH2 +
24.2	PERCENT BOUND IN SPECIES #2813302	FeOH3 AQ
66.8	PERCENT BOUND IN SPECIES #2813303	FeOH4 -

SO4-2

83.0	PERCENT BOUND IN SPECIES # 732	SO4-2
4.2	PERCENT BOUND IN SPECIES #4607320	MgSO4 AQ
12.6	PERCENT BOUND IN SPECIES #1507320	CaSO4 AQ

K+1

99.6	PERCENT BOUND IN SPECIES # 410	K+1

H4SiO4

96.9	PERCENT BOUND IN SPECIES # 770	H4SiO4
3.1	PERCENT BOUND IN SPECIES #3307700	H3SiO4 -

Cl-1

100.0	PERCENT BOUND IN SPECIES # 180	Cl-1

NO3-1

100.0	PERCENT BOUND IN SPECIES # 492	NO3-1

Ca+2

95.3	PERCENT BOUND IN SPECIES # 150	Ca+2
1.3	PERCENT BOUND IN SPECIES #1501401	CaCO3 AQ
2.6	PERCENT BOUND IN SPECIES #1507320	CaSO4 AQ

Na+1

99.6	PERCENT BOUND IN SPECIES #	500	Na+1

Mg+2

95.9	PERCENT BOUND IN SPECIES #	460	Mg+2
2.2	PERCENT BOUND IN SPECIES #	4607320	MgSO4 AQ

CO3-2

1.5	PERCENT BOUND IN SPECIES #	140	CO3-2
1.0	PERCENT BOUND IN SPECIES #	1501400	CaHCO3 +
1.5	PERCENT BOUND IN SPECIES #	1501401	CaCO3 AQ
94.3	PERCENT BOUND IN SPECIES #	3301400	HCO3 -

H+1

1.1	PERCENT BOUND IN SPECIES #	1501400	CaHCO3 +
97.5	PERCENT BOUND IN SPECIES #	3301400	HCO3 -
1.6	PERCENT BOUND IN SPECIES #	3301401	H2CO3 AQ

H2O

29.3	PERCENT BOUND IN SPECIES #	3300020	OH-
2.0	PERCENT BOUND IN SPECIES #	4603300	MgOH +
3.4	PERCENT BOUND IN SPECIES #	2813301	FeOH2 +
13.8	PERCENT BOUND IN SPECIES #	2813302	FeOH3 AQ
50.7	PERCENT BOUND IN SPECIES #	2813303	FeOH4 -

CrO4-2

98.7	PERCENT BOUND IN SPECIES #	212	CrO4-2

Ba+2

100.0	PERCENT BOUND IN SPECIES #	100	Ba+2

PART 5 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 12:14:20

---------- EQUILIBRATED MASS DISTRIBUTION ----------

IDX	NAME	DISSOLVED	SORBED	PRECIPITATED

		MOL/KG	PERCENT	MOL/KG	PERCENT	MOL/KG	PERCENT
281	Fe+3	1.791E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
732	SO4-2	3.304E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
410	K+1	1.279E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
770	H4SiO4	1.457E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
180	Cl-1	2.821E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
492	NO3-1	4.356E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
150	Ca+2	1.620E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
500	Na+1	7.397E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
460	Mg+2	6.172E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
140	CO3-2	1.363E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
330	H+1	1.319E-03	100.0	0.000E-01	0.0	0.000E-01	0.0
2	H2O	9.431E-06	100.0	0.000E-01	0.0	0.000E-01	0.0
212	CrO4-2	5.642E-04	100.0	0.000E-01	0.0	0.000E-01	0.0
100	Ba+2	7.997E-07	100.0	0.000E-01	0.0	0.000E-01	0.0

Charge Balance: SPECIATED

Sum of CATIONS = 5.156E-03 Sum of ANIONS 3.722E-03

PERCENT DIFFERENCE = 1.615E+01 (ANIONS - CATIONS)/(ANIONS + CATIONS)

EQUILIBRIUM IONIC STRENGTH (m) = 7.425E-03

EQUILIBRIUM pH = 8.400

PART 6 of OUTPUT FILE

PC MINTEQA2 v3.10 DATE OF CALCULATIONS: 18-OCT-99 TIME: 12:14:20

Saturation indices and stoichiometry of all minerals

ID #	NAME	Sat. Index	Stoichiometry in [brackets]						
6015000	ANHYDRITE	-2.054	[1.000]	150	[1.000]	732			
5015000	ARAGONITE	0.506	[1.000]	150	[1.000]	140			
5046000	ARTINITE	-4.433	[-2.000]	330	[2.000]	460	[1.000]	140	
			[5.000]	2					
6010000	BARITE	0.000	[1.000]	100	[1.000]	732			
2046000	BRUCITE	-3.379	[1.000]	460	[2.000]	2	[-2.000]	330	
5015001	CALCITE	0.645	[1.000]	150	[1.000]	140			
2077000	CHALCEDONY	-0.327	[-2.000]	2	[1.000]	770			
8646000	CHRYSOTILE	0.353	[-6.000]	330	[3.000]	460	[2.000]	770	
			[1.000]	2					
8246000	CLINOENSTITE	-1.774	[-1.000]	2	[1.000]	460	[1.000]	770	
			[-2.000]	330					
2077001	CRISTOBALITE	-0.263	[-2.000]	2	[1.000]	770			
8215000	DIOPSIDE	-0.342	[-2.000]	2	[1.000]	150	[1.000]	460	
			[2.000]	770	[-4.000]	330			
5015002	DOLOMITE	0.923	[1.000]	150	[1.000]	460	[2.000]	140	
6046000	EPSOMITE	-4.967	[1.000]	460	[1.000]	732	[7.000]	2	
8646003	SEPIOLITE(C)	-0.635	[-0.500]	2	[2.000]	460	[3.000]	770	
			[-4.000]	330					
2028100	FERRIHYDRITE	2.347	[-3.000]	330	[1.000]	281	[3.000]	2	
2028103	Fe(OH)3 soil	4.538	[-3.000]	330	[1.000]	281	[3.000]	2	
4128100	FEOH)2.7CL.3	6.681	[-2.700]	330	[1.000]	281	[2.700]	2	

			[0.300]	180							
6028100	FE2(SO4)3	-50.665	[2.000]	281	[3.000]	732					
8046000	FORSTERITE	-5.321	[-4.000]	330	[2.000]	460	[1.000]	770			
2028102	GOETHITE	6.738	[-3.000]	330	[1.000]	281	[2.000]	2			
6015001	GYPSUM	-1.843	[1.000]	150	[1.000]	732	[2.000]	2			
4150000	HALITE	-8.343	[1.000]	500	[1.000]	180					
3028100	HEMATITE	18.484	[-6.000]	330	[2.000]	281	[3.000]	2			
5015003	HUNTITE	-2.602	[3.000]	460	[1.000]	150	[4.000]	140			
5046001	HYDRMAGNESIT	-10.807	[5.000]	460	[4.000]	140	[-2.000]	330			
			[6.000]	2							
6050000	JAROSITE NA	-2.899	[-6.000]	330	[1.000]	500	[3.000]	281			
			[2.000]	732	[6.000]	2					
6041002	JAROSITE K	-0.061	[-6.000]	330	[1.000]	410	[3.000]	281			
			[2.000]	732	[6.000]	2					
6028101	JAROSITE H	-7.227	[-5.000]	330	[3.000]	281	[2.000]	732			
			[7.000]	2							
8450000	MAGADIITE	-7.420	[-1.000]	330	[-9.000]	2	[1.000]	500			
			[7.000]	770							
3028101	MAGHEMITE	8.090	[-6.000]	330	[2.000]	281	[3.000]	2			
5046002	MAGNESITE	-0.218	[1.000]	460	[1.000]	140					
6050001	MIRABILITE	-8.951	[2.000]	500	[1.000]	732	[10.000]	2			
3050000	NATRON	-9.894	[2.000]	500	[1.000]	140	[10.000]	2			
5046003	NESQUEHONITE	-2.626	[1.000]	460	[1.000]	140	[3.000]	2			
2077002	QUARTZ	0.156	[-2.000]	2	[1.000]	770					
8646004	SEPIOLITE(A)	-3.502	[-0.500]	2	[2.000]	460	[3.000]	770			
			[-4.000]	330							
2077003	SIO2(A,GL)	-0.832	[-2.000]	2	[1.000]	770					
2077004	SIO2(A,PT)	-1.140	[-2.000]	2	[1.000]	770					
8646002	TALC	1.787	[-4.000]	2	[3.000]	460	[4.000]	770			
			[-6.000]	330							
6050002	THENARDITE	-9.886	[2.000]	500	[1.000]	732					
5050001	THERMONATR	-11.329	[2.000]	500	[1.000]	140	[1.000]	2			
8215001	TREMOLITE	7.384	[-8.000]	2	[2.000]	150	[5.000]	460			
			[8.000]	770	[-14.000]	330					
5010000	WITHERITE	-2.531	[1.000]	100	[1.000]	140					
2015000	LIME	-18.967	[-2.000]	330	[1.000]	150	[1.000]	2			
2015001	PORTLANDITE	-8.845	[-2.000]	330	[1.000]	150	[2.000]	2			
2046001	PERICLASE	-8.097	[-2.000]	330	[1.000]	460	[1.000]	2			
3046001	MAG-FERRITE	11.125	[-8.000]	330	[1.000]	460	[2.000]	281			
			[4.000]	2							
8215002	WOLLASTONITE	-3.016	[-1.000]	2	[-2.000]	330	[1.000]	770			
			[1.000]	150							
8215003	P-WOLLSTANIT	-3.866	[-1.000]	2	[-2.000]	330	[1.000]	770			
			[1.000]	150							
8015001	CA-OLIVINE	-13.839	[-4.000]	330	[1.000]	770	[2.000]	150			
8015002	LARNITE	-15.331	[-4.000]	330	[1.000]	770	[2.000]	150			
8015007	CA3SIO5	-36.227	[-6.000]	330	[1.000]	770	[3.000]	150			
			[1.000]	2							
8015003	MONTICELLITE	-6.878	[-4.000]	330	[1.000]	770	[1.000]	150			
			[1.000]	460							
8015005	AKERMINITE	-14.098	[-1.000]	2	[-6.000]	330	[2.000]	770			
			[2.000]	150	[1.000]	460					
8015004	MERWINITE	-21.339	[-8.000]	330	[2.000]	770	[1.000]	460			
			[3.000]	150							
3028102	LEPIDOCROCIT	5.867	[-3.000]	330	[1.000]	281	[2.000]	2			
3021201	BACRO4	0.000	[1.000]	212	[1.000]	100					
3021205	K2CRO4	-11.289	[1.000]	212	[2.000]	410					
3021206	K2CR2O7	-15.823	[2.000]	212	[2.000]	410	[2.000]	330			
			[-1.000]	2							

3021208	MGCRO4	-12.179	[1.000]	212	[1.000]	460			
3021210	NA2CRO4	-13.019	[1.000]	212	[2.000]	500			
3021211	NA2CR2O7	-20.074	[2.000]	212	[2.000]	500	[2.000]	330	
			[-1.000]	2					
2021200	CrO3	-17.002	[1.000]	212	[2.000]	330	[-1.000]	2	
3015000	CaCrO4	-4.117	[1.000]	150	[1.000]	212			