DEVELOPMENT AND VERIFICATION OF A KINETIC

MODEL OF POLLUTANT DESORPTION

FROM DREDGE SEDIMENT AND SEWAGE SLUDGE

FINAL REPORT

by

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OVERVIEW

This final report encompasses a two phase research effort. The initial direction was toward the development and verification of a kinetic model of heavy metal desorption from dredge sediment and sewage sludge. The second phase used the insights and results gained from that effort to begin an investigation of the toxicity of cadmium in sediments. This change of direction was agreed upon by both the Manhattan College and EPA Narragansett Laboratory researchers and was reflected in the renewal application for the second year of funding. The report is divided into distinct parts, reflecting each topic.

The first part reports on the role of solid phase sulfide in determining the toxicity of cadmium in sediments. For marine sediments the importance of sulfide and the possibility of the formation of insoluble metal sulfides has often been pointed out. We have shown that acid volatile sulfide - solid phase amorphous FeS(s) and MnS(s) which are soluble in cold acid - is the dominant sediment property that controls the cadmium binding capacity of marine sediments and provides the proper normalization for establishing the toxicity of cadmium in a variety of marine sediments. This is a major finding of our research project. The results are presented as a paper which is being submitted for publication. An additional Appendix II is included which presents all the experimental data in tabular form.

The second part of this report presents the results of the development of the methodology that was needed for preforming the experiments and measurements to assess the toxicity of cadmium in sediments. The experimental calibration of the cadmium electrode and the design and testing of a diffusional sampler is presented. Also a validation experiment for the Acid Volatile Sulfide extraction method is presented.

The third part of this report presents the results of the sludge and sediment desorption experiments. These data confirm that the original model proposed for this reaction was correct. A three phase model is appropriate: A reversibly sorbed component; a metal sulfide component that is released via oxidation; and a refractory component that is not released within the time scale of the experiment.

ACKNOWLEDGEMENT

TOXICITY OF CADMIUM IN SEDIMENTS:

THE ROLE OF ACID VOLATILE SULFIDE

by

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INTRODUCTION

The toxicity of chemicals in sediments is strongly influenced by the extent to which the chemical binds to the sediment. This modifies the chemical potential to which the organisms are subjected. As a consequence different sediment types will exhibit different degrees of toxicity for the same total quantity of chemical. These differences have been reconciled by relating organism response to the chemical concentration in the interstitial water of the sediments [see the review in EPA, 1989]. As a consequence the relevant sediment properties are those which influence the distribution of chemical between the solid and aqueous phases.

The varying toxicity of non-ionic organic chemicals in different sediments has been found to be primarily determined by the organic carbon content of the sediments [EPA, 1989]. The purpose of this paper is to establish the importance of another sediment phase: the acid volatile sulfide phase - the sediment sulfides that are soluble in cold acid - in determining the toxicity of cadmium in sediments. By implication, this phase is likely to be important for all metals which form insoluble sulfides. Most freshwater and marine sediments - completely aerobic sediments are the exception - contain sufficient acid volatile sulfide for this phase to be the predominant determinant of toxicity.

METHODS AND MATERIALS

A. Exposure System Design

Sediment dwelling amphipods were exposed for 10 days to control and cadmium-spiked sediments in a 900 mL flow-through chamber with 200 mL of sediment (3.5 cm depth) and 600 mL of overlying seawater. Lighting was continuous to inhibit the amphipods' swimming behavior. Filtered air and seawater flow (10 volume replacements/day) ensured acceptable dissolved oxygen concentrations and cadmium free overlying water.

A diffusion sampler ("peeper") [Hesslein, 1976; Carignan et al.,1984; 1985], designed to fit within the exposure chamber and sample the interstitial and overlying water concentrations, was constructed of Plexiglas G grade unshrunk cast acrylic sheet: 6 × 3 × 2 in. deep with 6 rows of 3 3/4 in. diameter 1 1/2 in. deep holes, each of which has a volume of about 5 mL. The open side of the

peeper is covered by a sheet of 1 micron polycarbonate membrane (Nucleopore), followed by a 30 mil low density polyethylene gasket and a 1/2 inch Plexiglas cover plate, both of which have the same hole pattern as the body and secured with PVC-1 cap screws and nuts. Equilibration time was measured to be less than one day.

B. Organism Collection and Holding

Ampelisca abdita were collected from tidal flats in the Pettaquamscutt (Narrow) River, a small estuary flowing into Narragansett Bay, RI, transferred to the laboratory within one half hour, and sieved through a 0.5mm mesh screen. *Ampelisca* were collected with a dip net after flotation on the air/water interface. *Rhepoxynius hudsoni* were collected in shallow water at Ninigret Pond, RI. Adult animals were sieved from the sediment through a 1 mm mesh screen in the field, transported to the laboratory within an hour, sieved again and transferred to holding containers. The amphipods were maintained in presieved uncontaminated collection site sediment and flowing filtered seawater, and acclimated to the assay temperature at the rate of 1 to 3°C per day. During acclimation, the *Ampelisca* were fed, *ad libitum*, the laboratory cultured diatom *Phaeodactylum tricornutum*. *Rhepoxynius* were not fed.

C. Sediment Acid Volatile Sulfide

The principal property of concern of the sediments used in these experiments was the acid volatile sulfide (AVS) concentration. It is the solid phase sulfide in the sediment that is soluble in cold acid. The measurement technique is to convert the sulfides to H_2S(aq), purge it with a gas, and trap it [see Morse et al., 1987 for a review]. A 500 mL Erlenmeyer flask reaction vessel fitted with a three-hole stopper is followed by three sequentially connected 250 mL Erlenmeyer flask trapping vessels. The first is a chloride trap with 200 mL of pH 4 buffer (0.05M potassium hydrogen phthlate) to prevent chloride carry over. The second and third traps contain 200 mL of a 0.1M silver nitrate solution for trapping H_2S. The four flasks are connected with airtight appropriately shaped glass and Tygon tubing.

A nitrogen gas flow allows continuous purging of the system. In order to prevent oxidation the gas flows through an oxygen-scrubbing system consisting of a vanadous chloride solution in the

first scrubbing tower and the matrix of the analyte (seawater) in the second tower. Vanadous chloride is prepared using four grams of ammonium metavanadate boiled with 50 mL of concentrated hydrochloric acid and diluted to 500 mL. Amalgamated zinc, prepared by taking about 15 grams of zinc, covering it with deionized water and adding 3 drops of concentrated hydrochloric acid before adding a small amount of mercury to complete the amalgamation, is then added to the vanadous chloride solution.

The sediment sample (10-15 grams of wet sediment) or standard to be analyzed is placed in the reaction vessel after the entire system has been purged with nitrogen for about an hour. The system is again purged for 5-10 minutes, and deaerated 6M hydrochloric acid is added from a thistle tube to achieve a final concentration in the vessel of 0.5M. The system is run at room temperature for one hour which has been found to be sufficient to complete the extraction. The nitrogen gas flows at a bubble rate of about four per second. The sample vessel is swirled every five or ten minutes. At completion all hydrogen sulfide produced has been converted to silver sulfide in the first silver nitrate trap and no precipitate is found the second trap. The suspension in the first silver nitrate trap is passed through a 1.2 micron GF fiber filter, dried at 102°C, and weighed.

Standards prepared from appropriate quantities of iron(II) sulfate and sodium sulfide (the latter being added from a solution standardized against lead perchlorate), typically gave yields of 95-103%. Silver sulfide precipitates were usually in the range 20-30 mg. When a blank was run (sample without acid), about 0.9 mg silver sulfide was obtained. When the acid was run without a sample, about 0.6 mg silver chloride was obtained. This corresponds to a detection limit of ~ 0.5 μmol/g.

D. Sediment Characterization and Spiking Procedure

Sediments of three different acid-volatile sulfide concentrations were used in the toxicity tests. The LI Sound sediment, with a high AVS concentration, was collected from an uncontaminated site in central Long Island Sound (40°7.95'N and 72°52.7'W) with a Smith-MacIntyre grab sampler, returned to the laboratory, press sieved wet through a 2 mm mesh stainless steel screen, homogenized, and stored at 4°C. *A. abdita* has been tested many times in this sediment and both its survival and reproduction have been good (Scott and Redmond, in press). The Ninigret Pond

sediment was a low AVS sand collected from the *Rhepoxynius* collection site. The upper few inches of sediment were collected with a shovel, returned to the laboratory, sieved wet through a 2 mm stainless steel screen, rinsed several times to remove high-organic fine particles, homogenized, and stored at 4°C. The third sediment was a 50/50 (volume) mixture of LI Sound and Ninigret Pond sediments.

Sediments were spiked by adding 1000 mL of wet sediment to 1500 mL of 20°C filtered seawater into which a weighted amount of cadmium chloride had been dissolved. An additional 500 mL of filtered seawater was used to rinse the sediment container. The mixture was stirred with a nylon spatula, capped and placed on a paint shaker for 5 minutes to ensure complete mixing, and held at ambient temperature (~15°C) water bath for 7 days to ensure equilibrium of the cadmium and sediment. A thin layer of cadmium sulfide precipitate that had formed on the surface of the sediment was removed, the test sediments were then homogenized, and 200 mL were transferred to each of three replicate exposure containers. For the experiments with peepers, they were inserted at this time. Exposure containers were placed in the water bath with air and seawater delivery.

E. Toxicity Experiment

The amphipods were sieved from holding containers through a 0.5 mm stainless steel screen and distributed sequentially into 100 mL plastic beakers. After sorting and eliminating dead or outsized animals, the beakers were randomized, air delivery in the exposure system was halted, and one beaker of amphipods was added to the two replicate exposure containers in each treatment. *Rhepoxynius* were added to the Ninigret Pond treatments, and *Ampelisca* to the LI Sound and mixture treatments. The third replicate exposure container in each treatment received no amphipods and was used as a chemical control. Salinity and temperature of the overlying seawater remained relatively constant at 20.7 ± 0.3°C (n = 11) and 30.3 ± 0.5% (n = 11) during the 10 day exposure period.

After termination the contents of each exposure container were sieved through a 0.5 mm screen. For *Ampelisca*, material retained on the sieve was preserved in 5% buffered formalin with

Rose Bengal stain for later sorting. For *Rhepoxynius*, material retained on the sieve was examined immediately after sieving. In both cases, recovered animals were counted, and any missing individuals were counted as mortalities. The peeper interstitial and overlying water cadmium concentrations were determined as was the AVS and solid phase cadmium in the chemical control vessels.

F. Cadmium Determinations and Titrations

The cadmium ion concentration in both the peeper samples and the titrations described below was measured as Cd^{2+} activity using an Orion 94-48 cadmium ion selective electrode and a double junction reference electrode (Orion 90-02). The electrode was standardized with a serial dilution of a 1 g/L cadmium solution that was also used as the titrant. Sediment cadmium was determined using a cold concentrated nitric acid (16M, 5mL) digestion of 10mL wet sediment followed by a peroxide oxidation (10mL 30%) and evaporation to dryness. The residue is reconstitute to 20mL using 0.1M nitric acid and the cadmium measured using an AA.

Cadmium titrations of FeS suspensions (prepared in the same manner as the AVS standards) and sediments were performed using sample sizes of 5 to 10 gm dry wt. added to 50 mL seawater which was constantly stirred. Cadmium chloride was added and dissolved cadmium was monitored using the electrode. Anaerobic conditions were maintained using a nitrogen atmosphere provided by a glove box or by constantly bubbling nitrogen through the covered titration vessel. In the sediment titrations where electrode response was slow, a uniform differential response-time procedure was employed to obtain consistent voltage readings.

EXPERIMENTAL RESULTS AND INTERSTITIAL WATER CORRELATIONS

A. Dry weight normalization

The toxicity of cadmium to *Rhepoxynius hudsoni* in Ninigret Pond sediment; and to *Ampelisca* in Long Island Sound sediment and an equal parts mixture of the two sediments, is shown in Fig.1. The curves are log-logistic concentration response functions with the same slope parameter (Table 1). The LC50s range from 318 μmol/gm to 3200 μmol/gm on a sediment dry weight basis. As shown below these two organisms have virtually the same LC50s in water only exposures: 0.012

mg Cd^{2+}/L (0.23 mg Cd/L) and 0.017 mg Cd $^{2+}$/L (0.34 mg Cd/L) for *Rhepoxynius* and *Ampe-lisca* respectively. The concentrations are for free cadmium, Cd^{2+}, and total dissolved cadmium, Cd, respectively. Hence the differences in the cadmium toxicity are likely to be attributable to varying sediment properties. In addition Swartz et al., (1985) reported the *Rhepoxynius abronius* cadmium LC50 for a Yaquina Bay sediment to be 25 μmol/gm. Thus a factor of ten separates each of the LC50s for these three marine sediments: Long Island Sound (3200 μmol/gm), Ninigret Pond (318 μmol/gm) and Yaquina Bay (25 μmol/gm). An explanation for the over two order of magnitude variation in LC50s would surely be useful.

B. Correlation to Interstitial Water concentration

The correlation between organism toxicity and interstitial water concentration for sediments with different dry weight sediment toxicity has been reported (Adams et al., 1985; Swartz et al., 1985; Kemp and Swartz, 1986). In addition the evidence suggests [Borgmann, 1983] that biological response correlates to chemical activity, in particular to the divalent metal activity, $\{Me^{2+}\}$ [Sunda and Guillard, 1976; Sunda et al., 1978; Zamuda and Sunda, 1982]. The claim is not that the only bioavailable form of the metal is Me^{2+} - for example $MeOH^+$ may also bioavailable - but that the DOC or other ligand complexed fractions are not bioavailable.

These two hypotheses are examined in Fig. 2a, a comparison of the observed mortality to the observed interstitial water cadmium activity, measured with the specific ion electrode, for the three sediments in Fig. 1. The concentration response curves for *Ampelisca* and *Rhepoxynius* in water only exposures are nearly identical. The interstitial water concentration data from the sediment exposures are somewhat scattered. However the grouped data, presented in Fig. 2b as medians (50th percentile) and interquartile ranges (25th to 75th percentiles) parallel the water only expo-sure curve. These results conform to previous observations that the concentration response curves for sediment exposures, which are quite different on a sediment cadmium dry weight basis (Fig. 1), are quite comparable on an interstitial water basis. Table 1 presents the results.

C. Sediment Cadmium vs. Interstitial Water

The prediction of the toxicity of cadmium in sediments requires that the relationship between sediment cadmium concentration and interstitial water concentration be established. A plot of solid phase versus aqueous phase cadmium concentrations - which is regularly used for the analysis of sorption data - is shown in Fig. 3.

The data can be envisioned as a titration in which cadmium is added incrementally to the sediment and the resulting aqueous and solid phase cadmium distribution is measured. Initially the solid phase concentration increases but the aqueous phase concentration remains below the detection limit of the cadmium electrode. Then a critical sediment concentration is reached at which point the aqueous concentration increases sharply - in the region marked "transition" in Fig. 3. Note that the increase is over two orders of magnitude in aqueous concentration while the sediment concentration remains nearly constant. As more cadmium is added, the data then appear to follow a linear trend which is characteristic of a sorption reaction.

It is apparent that the critical part of the relationship between solid and aqueous phase cadmium is the onset of the transition region. There is a sudden increase in interstitial water cadmium activity (mg Cd^{2+}/L) and total dissolved concentration (mg Cd/L) from nonlethal levels below 0.001 mg Cd^{2+}/L (0.02 mg Cd/L), passing the water only LC50: 0.015 mg Cd^{2+}/L (0.30 mg Cd/L) for *Rhepoxynius* and *Ampelisca*, to concentrations in excess of 0.1 mg Cd^{2+}/L (2.0 mg Cd/L). This marks the transition between nontoxic and toxic sediments. The solid phase - aqueous phase relationship at the lower sediment cadmium concentrations is unclear since the aqueous concentrations are below detection. However the data do not appear to conform to a straight line sorption isotherm that would be inferred by extrapolation from the high concentration data since detectable dissolved concentrations would have been present. The more likely possibility is that a precipitation reaction is maintaining the aqueous phase concentration at below detectable values in the region of low sediment concentrations. Since these are marine sediments the possibility of the formation of a cadmium sulfide precipitate is suggested.

METAL SULFIDES AND CADMIUM TITRATIONS

The importance of sulfide in the control of interstitial water metal concentrations of marine sediments is well documented (Boulegue, 1983; Emerson et al., 1983; Davies-Cooley et al.,1985; Morse et al., 1987). Metal sulfides are very insoluble and the equilibrium interstitial water metal concentrations in their presence are small. It is possible that the interstitial water sulfide concentration in the sediment samples used for these toxicity tests was initially high enough that so that as cadmium was added to the sediment, cadmium sulfide was precipitating following the reaction:

$$Cd^{2+} + S^{2-} \rightarrow CdS(s) \tag{1}$$

However direct measurements of the interstitial water sulfide activity, $\{S^{2-}\}$, with a sulfide electrode failed to detect any free sulfide in the unspiked sediments. This was a most puzzling result since it was visually clear that a bright yellow cadmium sulfide precipitate was forming as cadmium was added to the sediment.

The lack of significant quantity of dissolved sulfide in the interstitial water and the evident formation of solid phase cadmium sulfide suggested the following possibility. Most of the sulfide in sediments is in the form of solid phase iron sulfides. Perhaps the source of the sulfide is the *solid phase* sulfide initially present. Then as cadmium is added to the sediment it causes the solid phase iron sulfide to dissolve releasing sulfide which is available for the formation of cadmium sulfide. This possibility is examined below.

A. Solubility Relationships and Displacement Reactions

The majority of sulfide in sediments is in the form of iron monosulfides (mackinawite and greigite) and iron bisulfide (pyrite) of which the former are most reactive [see the review by Morse et al., 1987]. Iron monosulfide, FeS(s), is in equilibrium with aqueous phase sulfide via the reaction:

$$FeS(s) \leftrightarrow Fe^{2+} + S^{2-} \tag{2}$$

If cadmium is added to the aqueous phase, then the result is:

$$Cd^{2+} + FeS(s) \leftrightarrow Cd^{2+} + Fe^{2+} + S^{2-} \tag{3}$$
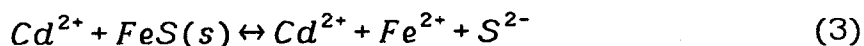
As the cadmium concentration increases, $[Cd^{2+}][S^{2-}]$ will exceed the solubility product of cadmium sulfide and CdS(s) will start to form. Since cadmium sulfide is more insoluble than iron monosulfide, FeS(s) should start to dissolve in response to the lowered sulfide concentration in the interstitial water. The overall reaction is:

$$Cd^{2+} + FeS(s) \rightarrow CdS(s) + Fe^{2+} \tag{4}$$
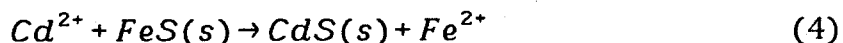
where the iron in FeS(s) is displaced by cadmium to form soluble iron and solid cadmium sulfide, CdS(s). A theoretical analysis of the Cd(II)-Fe(II)-S(II) system, presented in Appendix I, supports this conclusion. The relevant parameter, which can be termed the metal sulfide solubility parameter for any metal, Me, is $\alpha_{Me^{2-}} \cdot K_{MeS}$. It is the product of $\alpha_{Me^{2-}} = [\Sigma Me(aq) / [Me^{2+}]$, the ratio of total dissolved Me to the divalent species concentration; and $K_{MeS} = [Me^{2+}][S^{2-}]$, the metal sulfide solubility product. These are given in Table 2. The sulfide solubility parameters, shown in Fig. 4, determines the behavior of [FeS(s)] and and [MeS(s)] as the metal is added to the sediment. For example since the cadmium sulfide solubility parameter is less than the iron sulfide solubility parameter, cadmium will form a sulfide at the expense of the iron sulfide which will dissolve. Note that all the metals examined in Fig. 4 are predicted to dissolve FeS and MnS.

B. Experimental Results - FeS

The calculations presented above reflect the chemical composition expected at thermodynamic equilibrium. However many solid phase reactions are not at equilibrium with respect to either the aqueous phase of other solid phases because of the slow kinetics involved in the necessary transformations. Therefore a direct test of the extent to which this reaction takes place has been performed.

A quantity of freshly precipitated iron sulfide is titrated by adding dissolved cadmium. The resulting aqueous cadmium activity, measured with the cadmium electrode versus the ratio of cadmium added, $[Cd]_A$, to the amount of FeS initially present, $[FeS(s)]_i$, is shown in Fig. 5. The electrode potentials (left) correspond to a very low cadmium concentration during the initial portion of

the titration. Then a sharp upward inflection occurs near $[Cd]_A \sim [FeS]_i$ indicating that all the iron sulfide has dissolved to form CdS and any additional cadmium added appears as free cadmium. The plot of dissolved cadmium versus cadmium added (right) illustrates the rapid increase in dissolved cadmium that occurs near $[Cd]_A / [FeS]_i = 1$. A similar experiment has been performed for amorphous MnS with comparable results. It is interesting to note that such a replacement reaction was postulated by Pankow (1979) to explain an experimental result using copper and FeS.

These experiments plainly demonstrate that solid phase amorphous iron and manganese sulfide can readily be dissolved by adding cadmium. As a consequence it is a source of available sulfide which must be taken into account in evaluating the relationship between solid phase and aqueous phase cadmium in sediments.

C. Titration results - Sediments

A similar titration procedure has been used to evaluate the behavior of sediment samples taken from four quite different marine environments: Black Rock Harbor; the Long Island Sound and Ninigret Pond sediments used in the toxicity tests; and the Hudson River. The results are shown in Fig. 6. The binding capacity for cadmium is estimated by extrapolating a straight line fit to the dissolved cadmium data. The equation is:

$$[\Sigma Cd(aq)] = \max\{0, m([Cd]_A - [Cd]_B)\} \tag{5}$$

where $[\Sigma Cd(aq)]$ is the total dissolved cadmium, $[Cd]_A$ is the cadmium added, $[Cd]_B$ is the bound cadmium, and m is the slope of the straight line. The sediments exhibit quite different binding capacities for cadmium, listed in Table 3, ranging from approximately 1 μmol/gm to more than 100 μmol/gm. The question is whether this binding capacity is explained by the solid phase acid volatile sulfide present in the samples.

D. Correlation to Sediment AVS

Sulfides in sediments can be partitioned into three broad classes which reflect the techniques used for quantification [Berner, 1971; Goldhaber and Kaplan, 1974; Morse et al., 1987]. The most labile fraction, acid volatile sulfide (AVS), is associated with the more soluble iron and manganese

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monosulfides. The more resistant sulfide mineral phase, iron pyrite, is not soluble in the cold acid extraction used to measure AVS. Neither is the third compartment, organic sulfide associated with the organic matter in sediments [Landers et al., 1983].

The possibility that acid volatile sulfide is a direct measure of the solid phase sulfide that reacts with cadmium is examined in Fig. 7 (left): a plot of the sediment binding capacity for cadmium versus the measured initial AVS for each sediment. The line of perfect agreement is shown. The sediment cadmium binding capacity appears to be somewhat less than the initial AVS for the sediments tested. However a comparison between the initial AVS of the sediments and that remaining after the cadmium titration is completed, Fig. 7 (right), suggests that some AVS is lost during the titration procedure. It is possible that a portion is oxidized even though deoxygenated N_2 gas is passed through the reactor. Or it is possible that some of the AVS is lost as $H_2S(g)$ via stripping into the gas stream. In any case the correlation of sediment binding capacity and final AVS is apparent in Fig. 7. This strongly suggests that AVS is the proper quantification of the solid phase sulfides that can be dissolved by cadmium.

SEDIMENT TOXICITY AND AVS NORMALIZATION

The toxicity experiment illustrated in Fig. 1 was designed to test the utility of AVS as a predictor of the cadmium binding capacity of sediments and therefore a predictor of the concentration of cadmium that would cause sediment toxicity.

A. Experimental Results

Fig. 8 presents the AVS and cadmium concentration data at the start and end of the experiment. The initial concentrations of AVS are averages of multiple measurements from the stock supply. The initial concentrations of cadmium are calculated from the weighted amounts added to the sediments. The final cadmium and AVS concentrations are measured in parallel chemical control vessels.

The AVS results are interesting. A constant amount of AVS, ~2 μmol/gm, is lost from each vessel. Since each sediment is exposed to aerobic overlying water for the same amount of time it is probable that the loss is via oxidation. The final cadmium concentrations are within 70% of the initial values reflecting the loss during initial preparation and via the flowing overlying water.

The toxicity experimental results are shown in Fig. 9. The sediment cadmium is normalized by the AVS for that sediment. The averages of the initial and final values are used for AVS. The relationship in Fig. 8 is used to estimate the final cadmium concentration from the initial concentration if it was not measured. Note that the increase in mortality occurs at the point where the sediment cadmium begins to exceed the sediment AVS on a molar basis. Total mortality occurs at [Cd]/[AVS] > 3. The LC50 that results from a combined fit of the data is 1.97 μmol Cd /μmol AVS.

The critical point is that the sediment AVS can be used to normalize the sediment cadmium concentration in the same way that sediment organic carbon is used to normalize non-ionic organic chemicals. The reason that both methods work is that they properly account for the chemical activity of the chemical in both the aqueous and sediment phases. Below 1 μmol Cd /μmol AVS the cadmium is all precipitated as CdS(s) and the activity of Cd is very low. Above 1 μmol Cd /μmol AVS there exists free cadmium in the interstitial water, sorbed cadmium in the sediment phase, as well as CdS(s). The activity of cadmium in the system is now high enough to cause mortality. This is true for sediments with an appreciable amount of AVS, >1 μmol/gm. The reason is that the additional cadmium added in excess of 1 μmol Cd/gm/ μmol AVS/gm is large enough to exceed the activity of cadmium in the system that causes mortality even in the presence of some sorption phases - see Fig.5.

IMPLICATIONS FOR METAL TOXICITY IN SEDIMENTS

The first order importance of AVS in determining the toxicity of cadmium in sediments has important implications. These are discussed below.

A. Application to Other Metals and Mixtures

The other potentially toxic metals all form metal sulfide precipitates that are more insoluble than iron sulfide. Fig. 4 presents the sulfide solubility parameters for divalent metals. The iron and manganese sulfides have $\log(\alpha K_{sp}) > -25$ whereas the remaining sulfides have $\log(\alpha K_{sp}) < -25$. The implication is that the results found for cadmium are applicable to these other metals as well since, at equilibrium, they can displace iron and manganese sulfide to form a more insoluble sulfide precipitate.

In particular it is likely that the LC50 *for any metal* is at least 1 μmol/μmol AVS. Given the high concentrations of AVS in most sediments, the LC50s of these metals are likely to be large concentrations. For a molecular weight range of Ni ~ 50 to Pb ~ 200 gm/mol, the LC50s for an AVS of 1 (10) μmol AVS/gm would range from 50 (500) to 200 (2000) μg/gm.

A additional conjecture is that the molar AVS normalized toxicity of metals is additive. Since all the divalent metals in Fig. 4 have lower sulfide solubility parameters than FeS, they would all exist as metal sulfides if their molar sum is less than the AVS. For this case no metal toxicity would be expected and:

$$\frac{\sum_i [Me_T]_i}{[AVS]} < 1 \qquad (6)$$

where $[Me_T]_i$ is the total cold acid extractable metal concentration in the sediment. On the other hand if their molar sum is greater than the AVS concentration then a portion of the metals with the lowest sulfide solubility parameters would exist as free metal and presumably exert a toxicity. For this case the following would be true:

$$\frac{\sum_i [Me_T]_i}{[AVS]} > 1 \qquad (7)$$

But these two equations are precisely the formulas that one would employ to determine the extent of metal toxicity in sediments assuming additive behavior and neglecting the effect of partitioning. Whether the normalized sum is less than or greater than one discriminates between non toxic and

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toxic sediments. The additivity does not come from the nature of the mechanism that causes toxicity. Rather it results from their equal ability of the metals to form metal sulfides with the same stoichiometric ratio of Me and S.

This discussion is predicated on the assumption that all the metal sulfides behave similarly to cadmium sulfide. Further it has been assumed that only acid soluble metals are reactive enough to affect the free metal activity. At present no experimental data to support either of these conjectures exists so that this discussion purely speculative.

B. AVS and Sediment Quality Criteria

Since AVS can bind cadmium and presumably metals and thereby reduce their toxicity AVS will obviously play a role in the determination of sediment quality criteria for metals. For sediments with very little or no AVS - fully oxidized sediments for example - an AVS normalization would not be appropriate. Rather the partitioning would be controlled by other sediment phases such as iron and manganese oxides and organic carbon (Jenne et al., 1986). An estimate of when partitioning to other phases can be important can be made using the proposed sediment quality criteria formula [EPA, 1989]:

$$r_{SQC} = K_P c_{WQC} \qquad (8)$$

where r_{SQC} is the sediment quality criteria, K_p is the partition coefficient, and c_{WQC} is the chronic water quality criteria. For the case where there is only one metal competing for the AVS, the molar equivalent of the AVS would not bioavailable. Therefore it should be added to the allowable concentration so that:

$$[r_{SQC}] = [AVS] + K_P[c_{WQC}] \qquad (9)$$

where $[r_{SQC}]$ is the molar sediment quality criteria (μmol/gm), K_p is the partition coefficient (L/gm), and $[c_{WQC}]$ is the molar chronic water quality criteria (μmol/L). The range for freshwater acute (chronic) criteria for the metals in Fig. 4 (hardness = 100 mg/L) is 0.01 to 31. (.0001 to 1.6) μmol/L. The marine criteria are 0.01 to 3.8 (.0001 to 0.88) μmol/L [EPA, 1986]. The

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importance of partitioning can be judged by comparing the product $K_p[c_{w_{QC}}]$ to the AVS concentration. Consider an AVS concentration of 1 µmol/gm. If the partition coefficient is $K_p = 1$ L/gm then a metal with a criteria concentration of 1 µmol/L would have its sediment quality criteria doubled due to the partitioning. For $K_p = 10$ L/gm the criteria concentration at which partitioning doubles the sediment quality criteria drops to 0.1 µmol/L. Hence the effect of partitioning only becomes significant for relatively low AVS concentrations ($\sim$ 1 µmol AVS/gm) and for the metals with larger partition coefficients and criteria concentrations. For all cases with only a single metal involved, the minimum molar sediment quality criterion is [AVS].

C. AVS in Freshwater Sediments

Acid volatile sulfide is commonly found in marine sediments. It is produced by the diagenesis of particulate organic carbon, represented as CH_2O, with sulfate as the electron acceptor [Goldhaber and Kaplan, 1974]:

$$2CH_2O + SO_4^{2-} \rightarrow 2CO_2 + S^{2-} + 2H_2O \tag{10}$$
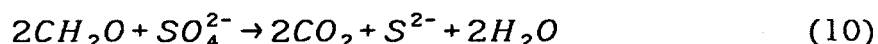
and the precipitation of iron sulfide [Berner, 1971]:

$$Fe^{2+} + S^{2-} \rightarrow FeS(s) \tag{11}$$

It might be expected that AVS is significant only in marine sediments since the concentration of sulfate in seawater is 28 mM = 2700 mg SO_4/L. By contrast average river water sulfate concentration is 0.12 mM = 11.5 mg SO_4/L [Stumm and Morgan, 1981]. However sedimentary organic matter is present in either locale and the sulfate in freshwater may be sufficient to produce a significant quantity of AVS. This is confirmed by the observations reported in Table 4. Surprisingly large values are found for sediments from the Great Lakes, rivers and other freshwater lakes. The magnitudes are nearly 1 µmol/gm to more than 100 µmol/gm. This strongly suggests that the AVS concentration in freshwater sediments must be considered when addressing cadmium and other metal toxicity.

D. Vertical and Temporal AVS Profiles

The normal method for sediment preparation in sediment bioassays is to produce a uniform distribution of chemical and sediment by careful mixing. For these systems the AVS is uniformly distributed and the concentration to be used for normalization is unambiguous.

However the distribution of AVS in intact sediment cores exhibits both vertical and temporal variation over the annual cycle. Table 4 presents a summary of some observations [Aller 1980; Reaves, 1984]. There is a seasonal variation in the surface concentration of AVS at the Long Island Sound NWC station and all stations exhibit a strong vertcal gradient between the surface 1 cm. and the average of the top 10 cm.

This variation in AVS concentration makes it more difficult to decide what AVS concentration should be used in evaluating the potential toxicity of metals in natural sediments. This is in contrast to the distribution of sediment organic carbon which is more spatially uniform and temporally stable. Hence it appears that intact cores should be used for sediment toxicity testing if metal toxicity is suspected. Indigenous predators such as *Nephtys incisa* should be elimated, however, pehaps by asphyxiation [Scott and Redmond, in press].

E. Sediment sampling and interstitial water generation

Ferrous sulfide oxidizes very rapidly in aerobic environments. For suspensions, oxidation is virtually complete within a few hours [Nelson, 1978]. We also have noted a decline in AVS for sediments that are held for a long period or are exposed to air. It is clear, therefore, that care should be taken to keep sediments anaerobic before AVS measurements or toxicity testing.

The use of elutrates as a surrogate for interstitial water is also suspect since oxidation of metal sulfides and release of soluble metals can occur. Procedures for producing large volumes of "pore" water by equilibrating suspensions of sediments must be checked for the extent of AVS oxidation that occurs.

CONCLUSIONS

It has been shown that AVS is the proper normalization parameter for cadmium toxicity in sediments. The observed amphipod mortality versus normalized cadmium concentration, [Cd]/[AVS], is the same for sediments with over an order of magnitude difference in dry weight normalized cadmium LC50s. The correlation between mortality and interstitial water metal activity has also been confirmed. Although the fact that metals can form insoluble sulfides is well known, it apparently has not been recognized that FeS and MnS, quantified as AVS, is a reactive pool of *solid phase* sulfide that is available to bind with metals which have sulfide solubility parameters smaller than FeS.

Titrations of FeS and MnS with cadmium demonstrate that the displacement reaction, Eq. 4. does occur. Further, titrations of sediments with cadmium indicates that an abrupt increase of dissolved cadmium occurs when the added cadmium exceeds the measured AVS. However, these data are not as certain since AVS appears to be lost during the titration and the relationship is only approximate (Fig. 7). Nevertheless, the AVS normalized toxicity data (Fig. 9) does demonstrate that the normalization is quantitative.

Surprisingly, the AVS of freshwater sediments is in the same range as marine sediments. Therefore, AVS should also be the proper normalization for these sediments. The other sorption phases are expected to be important for low AVS sediments and for metals with large partition coefficients and water effect concentrations.

ACKNOWLEDGEMENTS

APPENDIX I

Solubility Relationships for Metal Sulfides

The behavior of iron sulfide during a titration with cadmium can be analyzed using a simplified equilibrium model of the Cd(II)-Fe(II)-S(II) system. The mass action laws for the sulfide solubilities are:

$$\gamma_{Cd^{2+}}[Cd^{2+}]\gamma_{S^{2-}}[S^{2-}] = K_{CdS} \tag{12}$$

$$\gamma_{Fe^{2+}}[Fe^{2+}]\gamma_{S^{2-}}[S^{2-}] = K_{FeS} \tag{13}$$

where $[Cd^{2+}]$, $[Fe^{2+}]$, and $[S^{2-}]$ are the molar concentrations; $\gamma_{Cd^{2+}}$, $\gamma_{Fe^{2+}}$, and $\gamma_{S^{2-}}$ are the activity coefficients; and K_{FeS} and K_{CdS} are the sulfide solubility products. The mass balance equations for total cadmium, iron(II), and sulfide are:

$$\alpha_{Cd^{2+}}[Cd^{2+}] + [CdS(s)] = [Cd]_A \tag{14}$$

$$\alpha_{Fe^{2+}}[Fe^{2+}] + [FeS(s)] = [FeS(s)]_i \tag{15}$$

$$\alpha_{S^{2-}}[S^{2-}] + [CdS(s)] + [FeS(s)] = [FeS(s)]_i \tag{16}$$

where $\alpha_{Cd^{2+}} = [\Sigma Cd(aq)]/[Cd^{2+}]$, $\alpha_{Fe^{2+}} = [\Sigma Fe(aq)]/[Fe^{2+}]$, and $\alpha_{S^{2-}} = [\Sigma S(aq)]/[S^{2-}]$

are the ratios of the total dissolved Cd, Fe(II), and S(II) to the divalent species concentrations, respectively. $[CdS(s)]$ and $[FeS(s)]$ are the concentration of solid phase cadmium and iron sulfide; $[FeS]_i$ is the initial iron sulfide in the sediment, and $[Cd]_A$ is the added cadmium.

The solution of these equations begins with substituting Eqs.(14) and (15) into Eq.(16). Noting that $\alpha_{S^{2-}}[S^{2-}] = [\Sigma S(aq)] \ll [Cd]_A$, which states that the total dissolved sulfide in the interstitial water is much less than the cadmium added, it follows that:

$$\gamma_{S^{2-}}[S^{2-}] \approx \frac{\alpha_{Fe^{2+}} K_{FeS}/\gamma_{Fe^{2+}} + \alpha_{Cd^{2+}} K_{CdS}/\gamma_{Cd^{2+}}}{[Cd]_A} \qquad (17)$$

Then substituting Eqs. (12), (13) and (17) into Eqs.(14) and (15) yields the concentrations of solid phase sulfides:

$$[CdS(s)] \approx [Cd]_A \left(1 - \frac{\alpha_{Cd^{2+}} K_{CdS}}{\alpha_{Cd^{2+}} K_{CdS} + \alpha_{Fe^{2+}} K_{FeS}} \right) \qquad (18)$$

$$[FeS(s)] \approx [FeS]_i - \frac{\alpha_{Fe^{2+}} K_{FeS}}{\alpha_{Cd^{2+}} K_{CdS} + \alpha_{Fe^{2+}} K_{FeS}}[Cd]_A \qquad (19)$$

where it has been assumed that the activity coefficients for Cd^{2+} and Fe^{2+} are equal, $\gamma_{Cd^{2+}} \approx \gamma_{Fe^{2+}}$, since they are both divalent cations. The relative magnitudes of $\alpha_{Fe^{2+}} K_{FeS}$ and $\alpha_{Cd^{2+}} K_{CdS}$ determines the behavior of [FeS(s)] and [CdS(s)] as cadmium is added to the sediment. For this reason they are termed sulfide solubility parameters. Table 2 presents reported values. Since the cadmium solubility parameter is much less than the iron sulfide solubility parameter, i.e., $\alpha_{Cd^{2+}} K_{CdS} \ll \alpha_{Fe^{2+}} K_{FeS}$, Eqs. (18) and (19) become:

$$[CdS(s)] \approx Cd_A \qquad (20)$$

and:

$$[FeS(s)] \approx [FeS]_i - Cd_A \qquad (21)$$

Hence as cadmium is added to this system cadmium sulfide forms at the expense of iron sulfide. The overall reaction is:

$$Cd^{2+} + FeS(s) \rightarrow CdS(s) + Fe^{2+} \qquad (22)$$
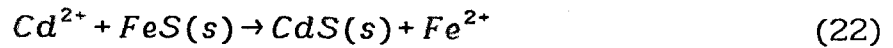
Note that if $\alpha_{Cd^{2+}} K_{CdS} \gg \alpha_{Fe^{2+}} K_{FeS}$ then $[FeS(s)] \approx [FeS]_i$; $[CdS(s)] \approx 0$ and no cadmium sulfide would form.

REFERENCES

Adams, W.J., Kimerle, R.A. and Mosher, R.G. (1985): Aquatic safety assessment of chemicals sorbed to sediments. In: Aquatic Toxicology and Hazard Assessment: Seventh Symposium, pp. 429-453. Editors: R.D. Cardwell, R. Purdy and R.C. Bahner. Am. Soc. for Testing and Materials, Philadelphia, PA.

Aller, R.C. (1980): Diagenetic Processes Near the Sediment-Water Interface of Long Island Sound. I. Decomposition and Nutrient Element Geochemistry (S, N, P). In: Estuarine Physics and Chemistry: Studies in Long Island Sound, pp. 238-350. Editor: B. Saltzman. Academic Press, New York.

Altschuler, Z.S., Schnepfe, M.M., Silber, C.C. and Simon, F.O. (1983): Sulfur Diagenesis in Everglades Peat and Origin of Pyrite in Coal. Science 221: pp. 221-227.

Borgmann, U. (1983): Metal Speciation and Toxicity of Free Metal Ions to Aquatic Biota. In: Aquatic Toxicology, pp. 47-72. Editor: J.O. Nriagu. J. Wiley, New York.

Boulegue, J., Lord III, C.J. and Church, T.M. (1982): Sulfur speciation and associated trace metals (Fe, Cu) in the pore waters of Great Marsh, Delaware. Geochim.. Cosmochim.. Acta. 46: pp. 453-464.

Byrne, R.H., Kump, L.R. and Cantrell, K.J. (1988): The influence of temperature and pH on trace metal speciation in seawater. Marine Chemistry 25: pp. 163-181.

Carignan, R. (1984): Interstitial water sampling by dialysis: Methodological notes. Limnol. Oceanogr. 29(3): pp. 667-670.

Carignan, R., Rapin, F. and Tessier, A. (1985): Sediment porewater sampling for metal analysis: A comparison of techniques. Geochim. Cosmochim. Acta 49: pp. 2493-2497.

Davies-Colley, R.J., Nelson, P.O. and Williamson, K.J. (1985): Sulfide Control of Cadmium and Copper Concentrations in Anaerobic Estuarine Sediments. Marine Chemistry 16: pp. 173-186.

Emerson, S., Jacobs, L. and Tebo, B. (1983): The behavior of trace metals in marine anoxic waters: Solubilities at the oxygen- hydrogen sulfide interface. In: Trace Metals in Sea Water, pp. 579-608. Editors: C.S. Wong, E. Boyle, K.W. Bruland and J.D. Burton. Plenum Press, New York.

EPA (1986): Quality Criteria for Water, 1986. EPA 440/5-86-001. EPA Office of Water, Wash. DC 20460.

EPA (1989): Briefing Report to the EPA Science Advisory Board on the Equilibrium Partitioning Approach to Generating Sediment Quality Criteria. EPA 440/5-89-002. US EPA, Criteria and Standards Division, Washington, DC.

Gardner, L.R. (1974): Organic versus inorganic trace metal complexes in sulfidic marine waters - some speculative calculations based on available stability constants. Geochim. Cosmochim. Acta. 38: p. 1297.

Goldhaber, M.B. and Kaplan, I.R. (1974): The Sulfur Cycle. In: The Sea. Volume 5. Marine Chemistry, pp. 569-655. Editor: E.D. Goldberg. J. Wiley & Sons, New York.

Hesslein, R.H. (1976): An in situ sampler for close interval pore water studies. Limnol. Oceanogr. 21: pp. 912-914.

Kemp, P.F. and Swartz, R.C. (1986): Acute Toxicity of Interstitial and Particle-Bound Cadmium to a Marine Infaunal Amphipod. Submitted to J. Exp. Marine Biol. Ecol. :.

Matisoff, G., Fisher, J.B. and McCall, P.L. (1981): Kinetics of nutrient and metal release from decomposing lake sediments. Geochim. Cosmochim. Acta 45: pp. 2333-2347.

Morse, J.W., Millero, F.J., Cornwell, J.C. and Rickard, D. (1987): The Chemistry of the Hydrogen Sulfide and Iron Sulfide Systems in Natural Waters. Earth Science Reviews 24: pp. 1-42.

Nelson, M.B. (1978): Kinetics and Mechanisms of the Oxidation of Ferrous Sulfide. Ph.D. Thesis. Stanford University, Palo Alto, Calif. pp. 1-288.

Nriagu, J.O. (1968): Sulfur Metabolism and Sedimentary Environment: Lake Mendota, Wisconsin. Limnol. Oceanogr. 13(2): pp. 430-439.

Nriagu, J.O. and Coker, R.D. (1976): Emission of sulfur from Lake Ontario sediments. Limnol. Oceanogr. 21(4): pp. 485-489.

Oakley, S.M., Delphey, C.E., Williamson, K.J. and Nelson, P.O. (1980): Kinetics of trace metal partitioning in model anoxic marine sediments. Water Research 14: pp. 1067-1072.

Pankow, J.F. (1979): The dissolution rates and mechanisms of tetragonal ferrous sulfide (Mackinawite) in anoxic aqueous systems. Ph.D thesis. California Inst. of Technology, Pasadena, Calif. pp. 1-146.

Presley, B.J., Kolodny, R., Nissenbaum, A. and Kaplan, I.R. (1972): Early diagenesis in a reducing fjord, Saanich Inlet, B.C. - II. Trace element distribution in interstitial water and sediment. Geochim. Cosmochim. Acta. 36: p. 1073.

Reaves, C. (1984): The Migration of Iron and Sulfur During the Early Diagenesis of Marine Sediments. Ph.D Thesis. Yale University, New Haven, Conn. pp. 1-413.

Schoonen, M.A.A. and Barnes, H.L. (1988): An approximation of the second dissociation constant for H_2S. Geochim. Cosmochim. Acta 52: pp. 649-654.

Scott, K.J. and Redmond, M.S. (In press): The effects of a contaminated dredged material on laboratory populations of the tubicolous amphipod, *Ampelisca abdita*. Aquatic Toxicology and Hazard Assessment: Twelfth Symposium. American Society for Testing and Materials, Philadelphia, PA.

Sunda, W. and Guillard, R.R.L. (1976): The relationship between cupric ion activity and the toxicity of copper to phytoplankton. J. Mar. Res. 34: pp. 511-529.

Sunda, W.G., Engel, D.W. and Thuotte, R.M. (1978): Effect of chemical speciation of toxicity of cadmium to Grass Shrimp, *Palaemonetes pugio*: Importance of free cadmium ion. Environ. Sci. Tech. 12: pp. 409-413.

Sunda, W.G. and Lewis, J.M. (1978): Effect of complexation by natural organic ligands on the toxicity of copper to a unicellular alga, *Monochrysis lutheri*. Limnol. Oceanogr. 23(5): pp. 870-876.

Swartz, R.C., Ditsworth, G.R., Schults, D.W. and Lamberson, J.O. (1985): Sediment toxicity to a marine infaunal amphipod: Cadmium and its interaction with sewage sludge. Marine Environ. Res. 18: pp. 133-153.

Swartz, R.C., Schults, D.W., DeWitt, T.H., Ditsworth, G.R. and Lamberson, J.O. (1987): Toxicity of Fluoranthene in Sediment to Marine Amphipods: A Test of the Equilibrium Partitioning Approach to Sediment Quality Criteria. Presented at the 8th Annual Meeting, Society for Environmental Toxicology and Chemistry., Pensacola, Fl.

TABLE 1

Log-Logistic Parameters[a]

Experiment	R_0 (%)	β	LC50	Units	Fig. No.
LI Sound[b]	3.32	4.50	3200.	µg Cd/gm	(1)
Mixture[b]	"	"	1130.	"	"
Ninigret Pd[b]	"	"	318.	"	"
Yaquina Bay	0.0	3.34	25.5		
Water Only[c]					
A. abdita	0.0	2.34	0.34	mg Cd/L[d]	(2)
R. hudsoni	0.0	2.33	0.24	"	"
Joint[f]	0.0	2.12	0.29	"	"
All Sediments AVS Normalized	5.88	4.48	1.97	µmol Cd/ µmol AVS	(9)

(a) Concentration - response formula:

$$R = R_o + \frac{100 - R_o}{1 + (LC50/c)^\beta}$$

R = mortality (%) at concentration c

R_0 = control mortality (%)

LC50 = concentration for 50% mortality

β = population sensitivity parameter

(b) The three sediments are fit assuming one value of R_0 and β.

(c) Water only exposures - no sediment present in the exposure vessels. Exposure for 96 hrs.

(d) Divide by 20 to obtain mg Cd^{2+}/L.

(e) Data from Swartz et al., (1985) is fit to the log-logistic function.

(f) Joint fit of the *Ampelisca abdita* and *Rhepoxynius hudsoni* water only exposure data.

TABLE 2

Metal Sulfide Solubility and

Ratio of Total Dissolved to Free Cation Metal Concentration

Metal Sulfide	$\log K_{sp,2}$	$\log K_{sp}$	$\log \alpha$		$\log(\alpha K_{sp})$
			pH = 7.6	pH = 8.2	Average
HgS	-38.50	-57.25	15.10	15.10	-42.15
CuS	-22.19	-40.94	0.50	0.92	-40.23
PbS	-14.67	-33.42	1.12	1.32	-32.20
CdS	-14.10	-32.85	1.50	1.50	-31.35
ZnS	-9.64	-28.39	0.12	0.14	-28.26
NiS	-9.23	-27.98	0.11	0.17	-27.84
FeS	-3.64	-22.39	0.10	0.12	-22.28
FeS(am)	-3.05	-21.80	0.10	0.12	-21.69
MnS	-0.40	-19.15	0.13	0.13	-19.02

Solubility products, $K_{sp,2}$, for the reaction: $Me^{2+} \, HS^- \leftrightarrow MeS(s) + H^+$ for CdS (Greenockite), FeS(amorphous) and Mackinawite, MnS (Alabandite), and NiS (Millerite), from Emerson et al., (1983). Solubility products for CuS (Covellite), HgS (Metacinnabar), PbS (Galena), and ZnS (Wurtzite), and $pK_2 = 18.57$ for the reaction $HS^- \leftrightarrow H^+ + S^{2-}$, from Schoonen and Barnes, (1988). K_{sp} is for the reaction: $Me^{2+} \, S^{2-} \leftrightarrow MeS(s)$ is computed from $\log K_{sp,2}$ and pK_2. Ratios of total to free metal concentrations: $\alpha = [\Sigma Me(aq)]/[Me^{2+}]$, from Byrne et al., (1988) at $T = 5 °C$. $\log(\alpha K_{sp}) = \log \alpha + \log K_{sp}$. All logs are $\log_{10}$.

TABLE 3

Cadmium Binding Capacity and AVS of Sediments

Sediment	Initial AVS (μmol/g)[a]	Final AVS (μmol/g)[b]	Cd Binding Capacity (μmol/g)
Black Rock Harbor	175.	-	114.
Hudson River	12.6	-	8.58
LI Sound	15.9	13.9	4.57
Mixture	5.45	3.23	-
Ninigret Pond	2.34	0.28	1.12

[a] Average AVS of repeated measurements of the stock

[b] AVS after the sediment toxicity experiment

TABLE 4

AVS in Freshwater and Marine Sediments

Location	T°C[a] Depth Interval	AVS (μmol/gm)		Reference
		(0 - 1 cm)	(0 - 10 cm)	
Fresh Water Sediments				
Everglades peat basin	-	-	0.31 - 1.3	Altschuler et al., 1983
Lake Mendota	-	-	8.7 - 112.	Nriagu, 1968
Lake Ontario	-	11.6	27.1	Nriagu et al., 1976
Lake Erie	(W)	15.0	7.5	Matisoff et al., 1981
Marine Sediments				
Long Island Sound				Aller, 1980
NWC	3.0	0.0	8.35	
NWC	13.2	0.60	10.5	
NWC	19.0	0.097	10.3	
DEEP-1	18.5	0.62	17.4	
FOAM-1	20.0	7.50	13.3	
Sapelo Island				Reaves, 1984
Mud Flat	(W)	1.88	14.6	
Mud Flat	(S)	3.44	43.2	
Tidal Ck.	(W)	9.69	28.4	
Tidal Ck.	(S)	5.94	31.9	

[a] (W) = Winter; (S) = Summer

FIGURE CAPTIONS

Figure 1. Toxicity test results for sediments from Ninigret Pond (*Ampelisca*) Long Island Sound and the mixture (*Rhepoxynius*). Cadmium concentrations on a sediment dry weight basis.

Figure 2. Mortality versus interstitial water cadmium activity. Water only exposure data for *Ampelisca* and *Rhepoxynius*. The line is a joint fit to both data sets (Table 1). Toxicity test results for the sediments in Fig. 1. Top panel - individual data. Bottom panel - statistical summary of all the sediment interstitial water data

Figure 3. Sediment cadmium versus interstitial water cadmium activity for LI Sound sediment.

Figure 4. Metal sulfide solubility parameters for seawater: $\alpha_{M^{2+}} \cdot K_{MeS}$ for the metals as indicated. pH = 7.2 to 8.2; T = 20°C (Table 2).

Figure 5. Cadmium titrations of amorphous FeS. Abscissa is cadmium added normalized by FeS initially present. Ordinate is cadmium electrode response (left panel) and total dissolved cadmium (right panel).

Figure 6. Cadmium titration of sediments: Black Rock Harbor, Long Island Sound, Hudson River, Ninigret Pond. Cadmium added per unit dry weight of sediment versus total dissolved cadmium.

Figure 7. Sediment binding capacity - from the x axis intercepts of the data in Fig. 6. versus sediment AVS concentration at the start of the titration (left). Initial AVS versus final AVS at the end of the cadmium titration.

Figure 8. AVS and cadmium concentrations for the sediments used in the toxicity test (Fig. 1). Initial and final AVS (left); initial and final cadmium (right).

Figure 9. Mortality versus AVS normalized sediment cadmium for Lond Island Sound, Ninigret Pond, and a 50/50 volume mixture.
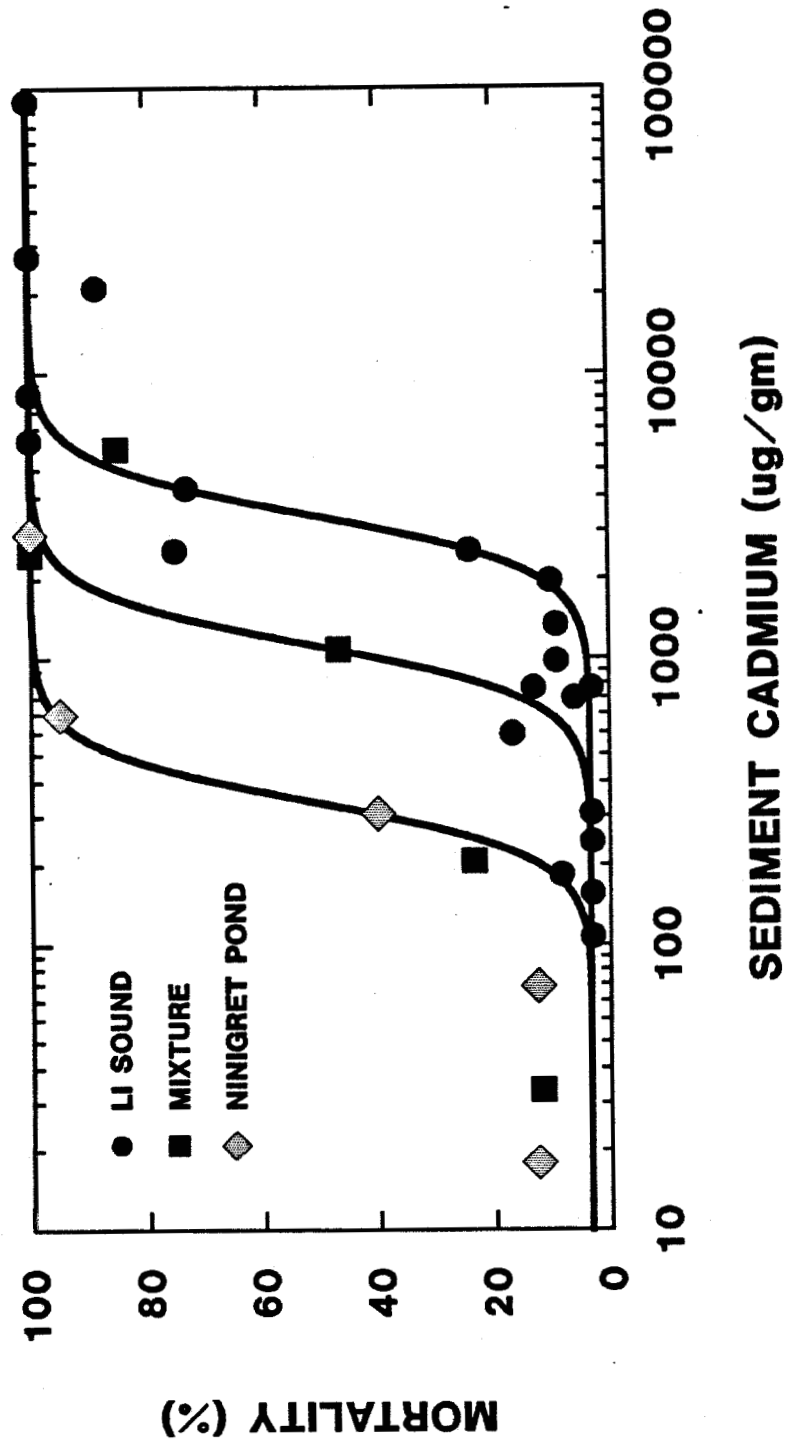
Figure 1. Toxicity test results for sediments from Ninigret Pond (*Ampelisca*) Long Island Sound and the mixture (*Rhepoxynius*). Cadmium concentrations on a sediment dry weight basis.

MORTALITY vs INTERSTITIAL WATER CADMIUM
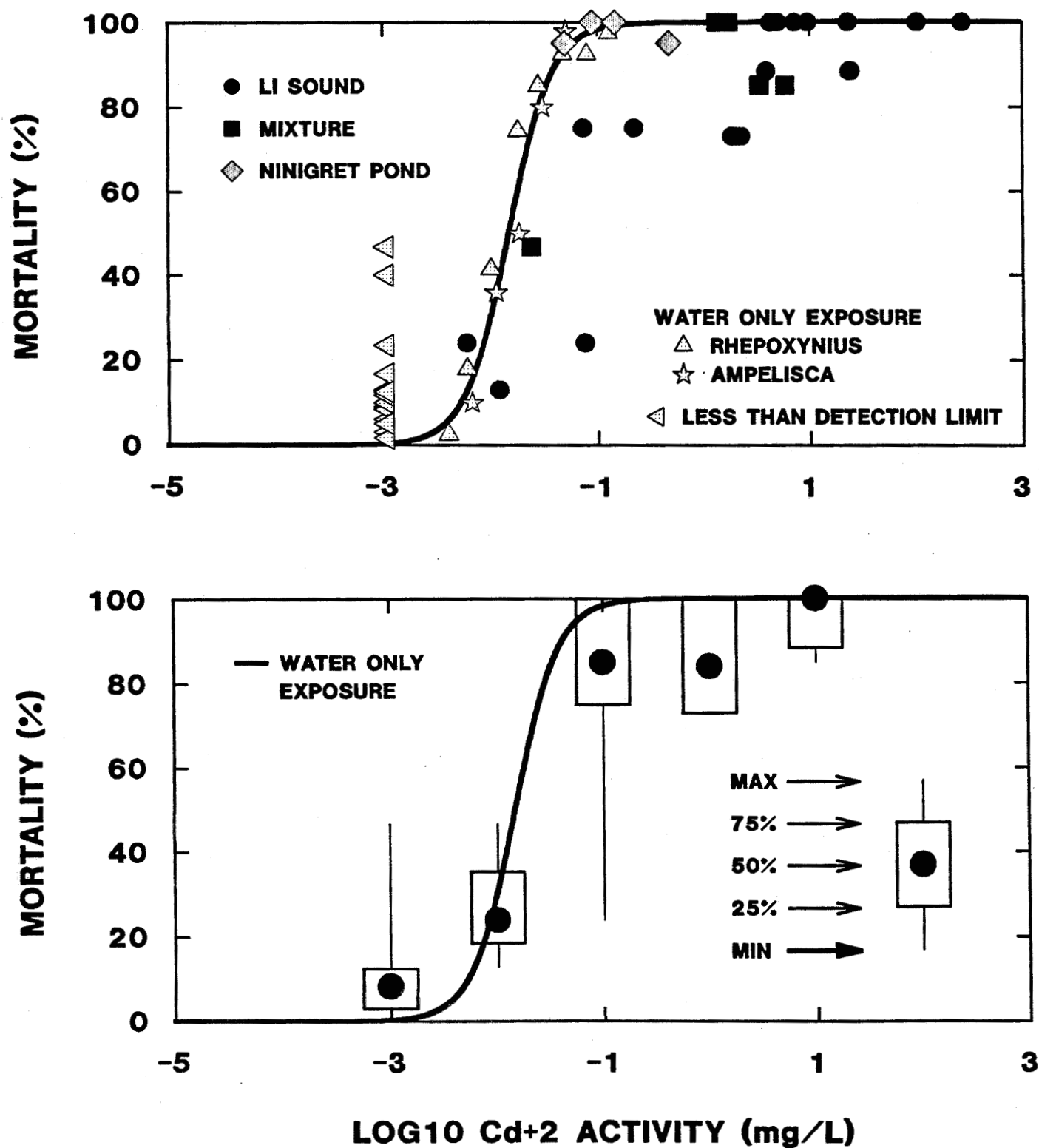
Figure 2. Mortality versus interstitial water cadmium activity. Water only exposure data for *Ampelisca* and *Rhepoxynius*. The line is a joint fit to both data sets (Table 1). Toxicity test results for the sediments in Fig. 1. Top panel - individual data. Bottom panel - statistical summary of all the sediment interstitial water data

SEDIMENT vs INTERSTITIAL WATER CADMIUM
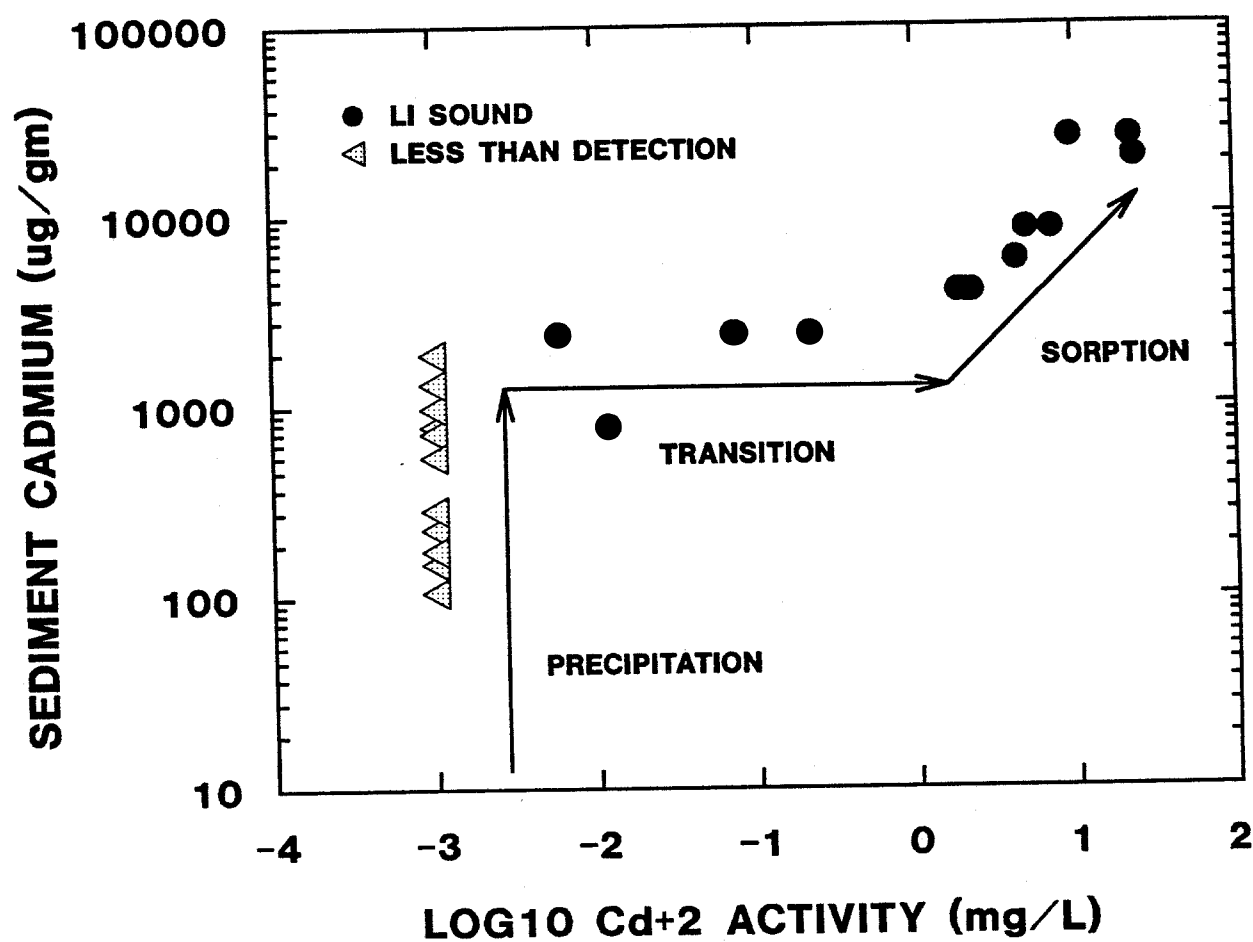
Figure 3. Sediment cadmium versus interstitial water cadmium activity for LI Sound sediment.
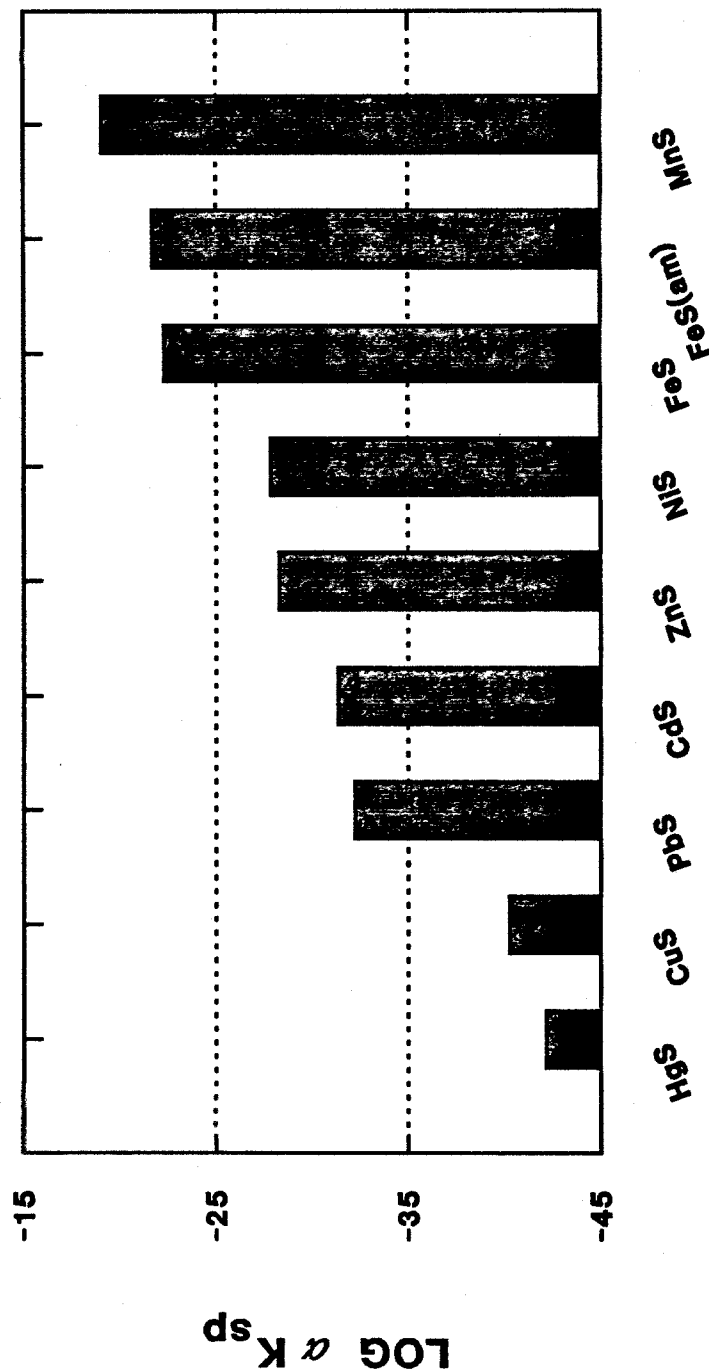
Figure 4. Metal sulfide solubility parameters for seawater: $\alpha_{Me^{2+}} \cdot K_{MeS}$ for the metals as indicated.

pH = 7.2 to 8.2; T = 20°C (Table 2).

CADMIUM TITRATION OF IRON SULFIDE
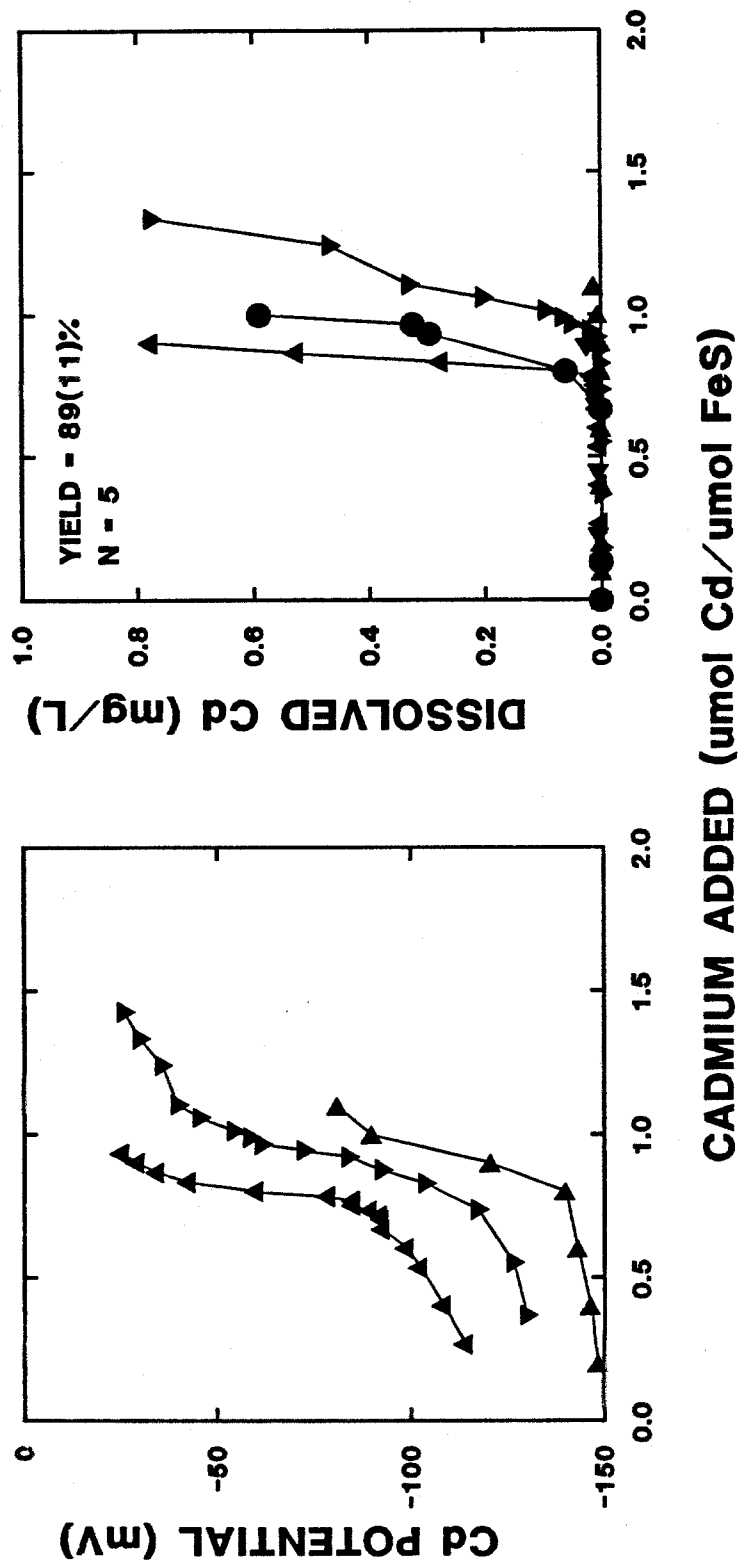
Figure 5. Cadmium titrations of amorphous FeS. Abscissa is cadmium added normalized by FeS initially present. Ordinate is cadmium electrode response (left panel) and total dissolved cadmium (right panel).
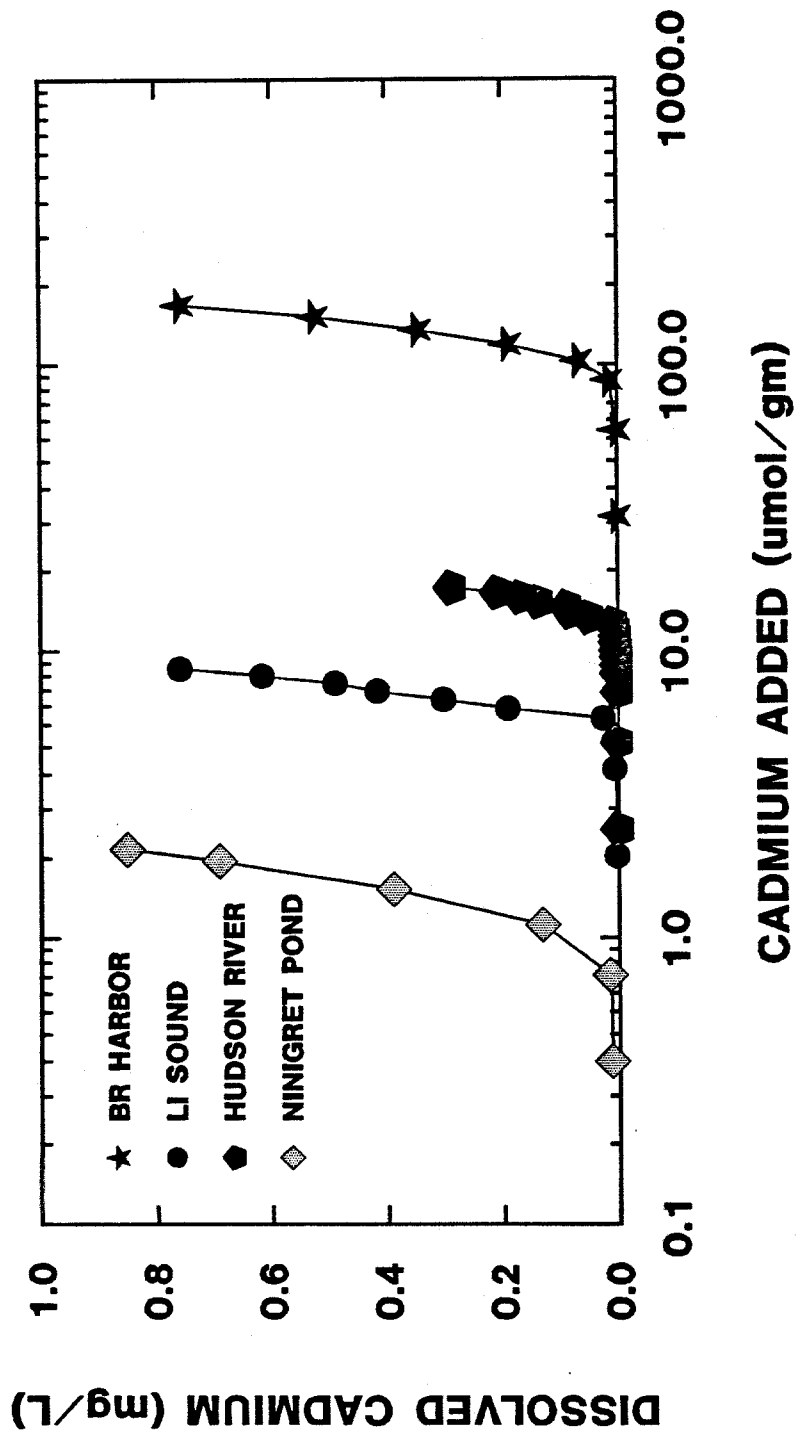
Figure 6. Cadmium titration of sediments: Black Rock Harbor, Long Island Sound, Hudson River, Ninigret Pond. Cadmium added per unit dry weight of sediment versus total dissolved cadmium.

SEDIMENT CADMIUM BINDING CAPACITY
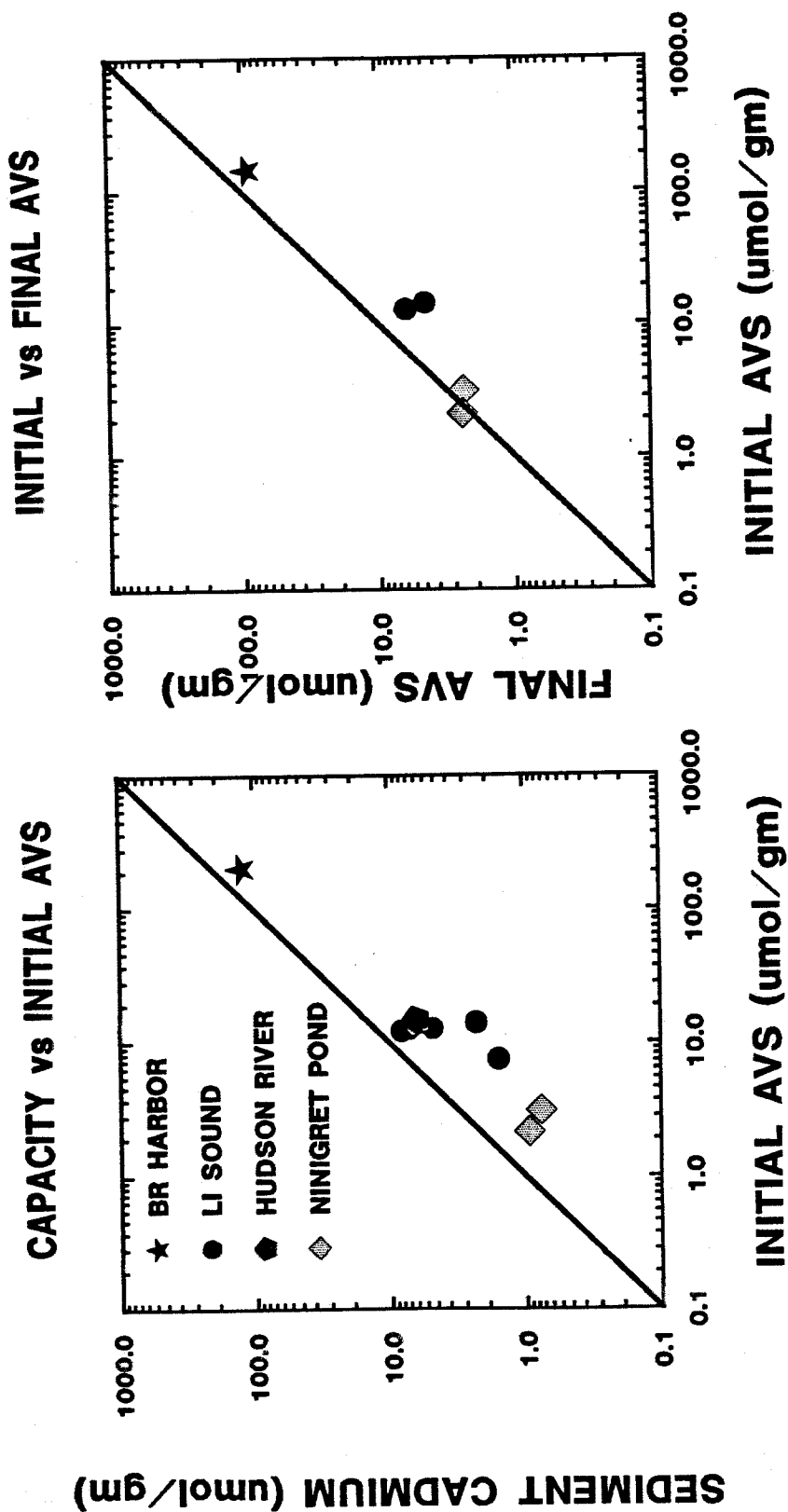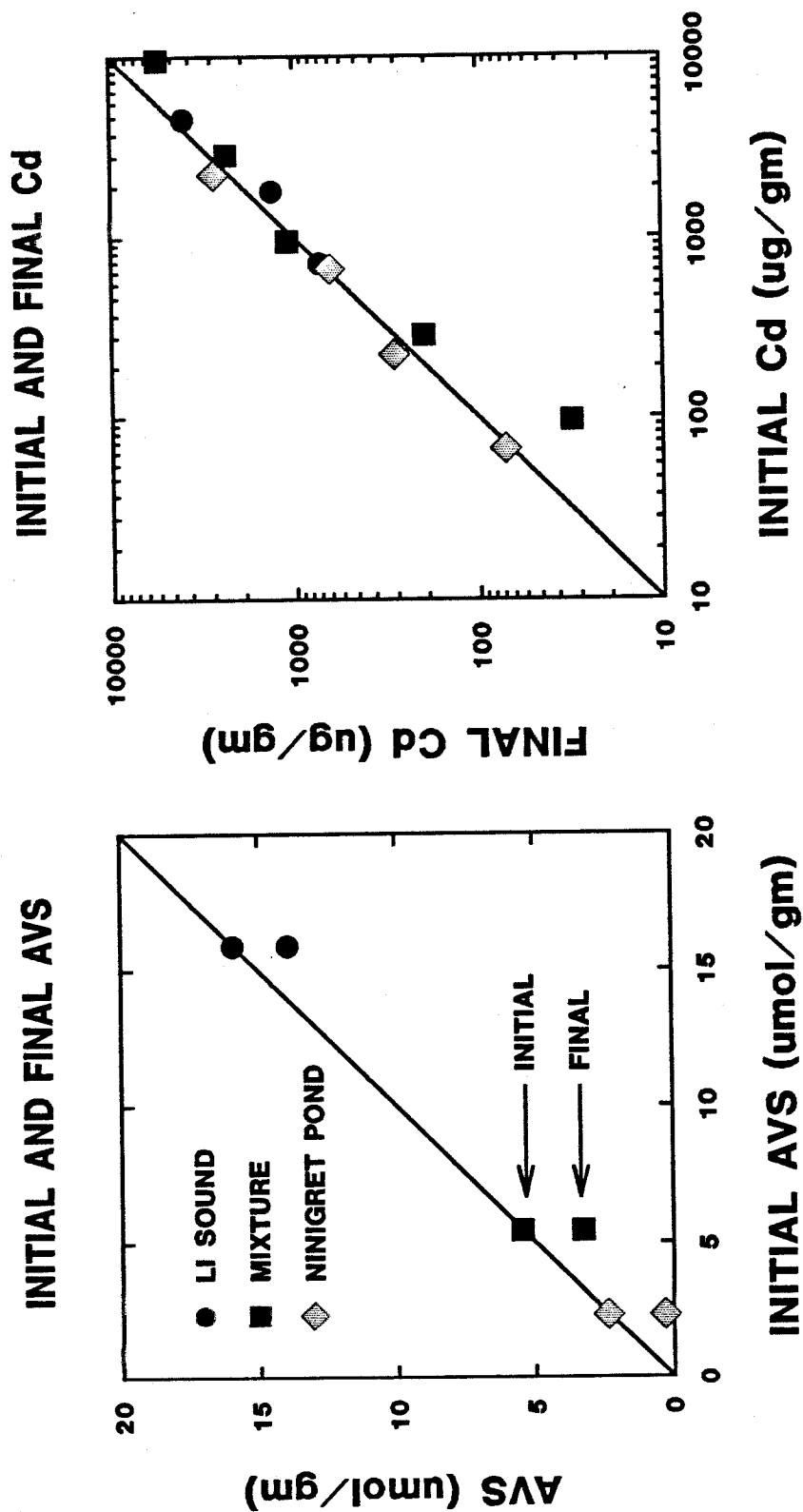
CAPACITY vs INITIAL AVS

INITIAL vs FINAL AVS

Figure 7. Sediment binding capacity - from the x axis intercepts of the data in Fig. 6. versus sediment AVS concentration at the start of the titration (left). Initial AVS versus final AVS at the end of the cadmium titration.

AVS AND CADMIUM CONCENTRATIONS

INITIAL AND FINAL Cd

INITIAL AND FINAL AVS

Figure 8. AVS and cadmium concentrations for the sediments used in the toxicity test (Fig. 1). Initial and final AVS (left); initial and final cadmium (right).
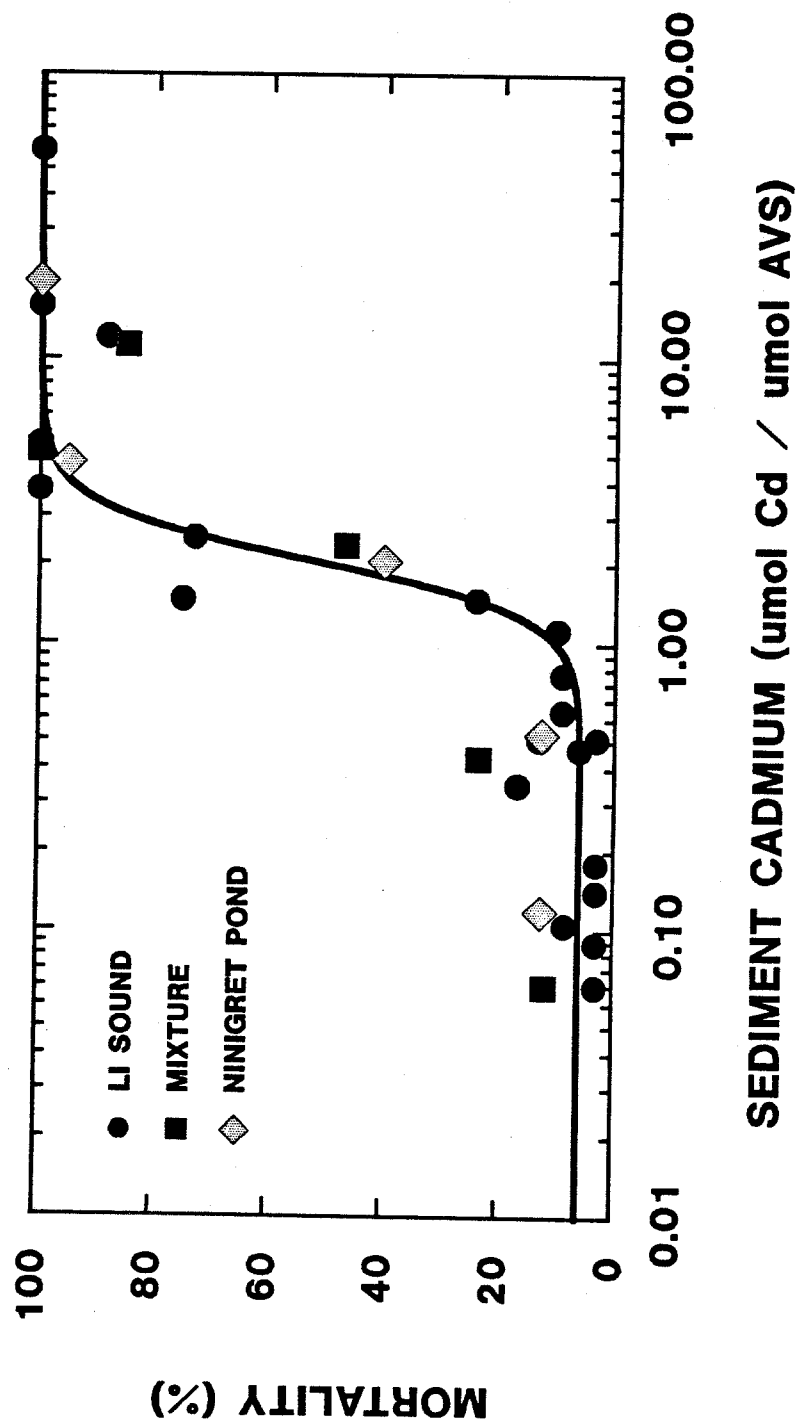
Figure 9. Mortality versus AVS normalized sediment cadmium for Lond Island Sound, Ninigret Pond, and a 50/50 volume mixture.

APPENDIX II

DATA TABLES

Table 1

Final Data for Toxicity Experiments

Expt.#	Sediment	r (ug/g)	[Cd]/[AVS] (mol/mol)	Dissolved Cd[a] (mg Cd^{2+}/L) 1 cm	4 cm	centrf.[b]	Mortality (%)
1.000	LI Sound	0.0	0.0	0.001	0.001	.	3.000
1.000	"	106.748	0.064	0.001	0.001	.	3.000
1.000	"	150.995	0.090	0.001	0.001	.	3.000
1.000	"	229.153	0.137	0.001	0.001	.	3.000
1.000	"	288.237	0.172	0.001	0.001	.	3.000
1.000	"	789.775	0.472	0.001	0.001	.	3.000
2.000	"	0.0	0.0	0.001	0.001	.	3.000
2.000	"	789.775	0.472	0.012	0.001	.	13.000
2.000	"	2396.442	1.431	0.222	0.074	.	75.000
2.000	"	8423.713	5.030	7.210	5.030	.	100.000
2.000	"	25560.363	15.262	22.890	9.580	.	100.000
2.000	"	89846.995	53.648	268.260	101.380	.	100.000
3.000	"	0.0	0.0	0.001	0.001	.	6.000
3.000	"	726.606	0.434	0.001	0.001	.	6.000
3.000	"	980.801	0.586	0.001	0.001	.	9.000
3.000	"	1315.596	0.786	0.001	0.001	.	9.000
3.000	"	2396.442	1.431	0.006	0.076	.	24.000
3.000	"	3961.468	2.365	1.880	2.280	.	73.000
4.000	"	0.0	0.0	0.001	.	0.001	1.65
4.000	"	175.533	0.105	0.001	.	0.001	8.350
4.000	"	544.771	0.325	0.001	.	0.001	16.700
4.000	"	1872.224	1.118	0.001	.	0.001	10.000
4.000	"	5810.512	3.469	4.330	.	1.420	100.000
4.000	"	19969.073	11.924	24.200	.	3.940	88.400
4.000	Mixture	0.000	0.000	0.001	.	0.001	16.700
4.000	"	31.078	0.064	0.001	.	0.001	11.700
4.000	"	196.491	0.403	0.001	.	0.001	23.400
4.000	"	1082.707	2.219	0.001	.	0.024	46.700
4.000	"	2325.815	4.768	1.740	.	1.350	100.000
4.000	"	5443.609	11.159	5.900	.	3.400	85.000
4.000	Ninigret	0.000	0.000	0.000	.	0.000	5.000
4.000	"	17.195	0.117	0.001	.	0.001	12.500
4.000	"	71.788	0.488	0.001	.	0.001	12.500
4.000	"	287.150	1.950	0.001	.	0.001	40.000
4.000	"	638.191	4.334	0.475	.	0.050	95.000
4.000	"	2727.925	18.527	0.146	.	0.090	100.000

[a] Detection limit = 0.001 mg Cd^{+2}/L
[b] Centrifugate from the sediment of the chemical control sediment

Table 2

Toxicity Tests - Water Only Exposure

Organism	Dissolved Cd ($mg\ Cd^{2+}/L$)	Mortality (%)
Ampelisca	0.000	2.000
"	0.007	10.000
"	0.011	36.000
"	0.018	50.000
"	0.031	80.000
"	0.051	98.000
Rhepoxynius	0.000	0.000
"	0.010	2.500
"	0.015	17.900
"	0.025	41.500
"	0.045	74.400
"	0.070	85.000
"	0.120	92.500
"	0.200	92.500
"	0.320	97.500

Table 2
Toxicity Tests - Water Only Exposure

Organism	Dissolved Cd (mg Cd^{2+}/L)	Mortality (%)
Ampelisca	0.000	2.000
"	0.007	10.000
"	0.011	36.000
"	0.018	50.000
"	0.031	80.000
"	0.051	98.000
Rhepoxynius	0.000	0.000
"	0.004	2.500
"	0.006	17.900
"	0.010	41.500
"	0.018	74.400
"	0.028	85.000
"	0.048	92.500
"	0.080	92.500
"	0.128	97.500

TABLE 3

Chemistry and Toxicity Data for Sediment Toxicity Tests

Variable Identification and Units for Data Table

EXPT	Experiment number
SED$	Sediment ID
DEPTH	Depth of peeper sampling. Depth = 0 corresponds to water only exposures.
CDCL2	Concentration of $CdCl_2$ in the sediment mixture (g $CdCl_2$/L) based on the initial weighed sample.
CDCL2H2O	Concentration of $CdCl2 \cdot 2.5H_2O$ in the sediment mixture (g $CdCl_2 \cdot 2.5H_2O$/L) based on the initial weighed sample.
CT	Concentration of Cd in the sediment mixture (g Cd/L) based on the initial weighed sample.
CT_OBS	Observed concentration of Cd in the sediment mixture (g Cd/L)
CT_FNL	Final concentration of Cd in the sediment mixture (g Cd/L). CT_FNL = CT_OBS if it was measured. If not then $CT\_FNL = 10^{\wedge}(-0.1568 + 1.028 \log 10(CT))$ which is the regression of log CT_OBS versus log CT.
M	Concentration of sediment solids in the sediment mixture (g/L).
R	Cd concentration on the solids based on CT (μg/gm). R = CT/M
R_OBS	Cd concentration on the solids based on CT_OBS (μg/gm). R = CT_OBS/M
R_FNL	Cd concentration on the solids based on CT_FNL (μg/gm). R = CT_FNL/M
RM	Molar Cd concentration on the solids based on CT_FNL (μmol/gm). R = CT_FNL/M/112.4
CD	Dissolved cadmium activity (mg Cd^{2+}/L) for the water only experiments (EXPT = 0).
CD_PEEP	Dissolved cadmium activity (mg Cd^{2+}/L) for the peeper cavities within the sediment. All cavities in the overlying water were below detection.

CD_CENTR   Dissolved cadmium activity (mg Cd^{2+}/L) for the centrifugate separated from the sediment in the chemical controls at the end of the experiment.

LCD_PEEP Log_{10}(CD_PEEP)

LCD_CENT Log_{10}(CD_CEMTR)

AVS1   Final AVS at the end of the experiment (μmol/gm)

AVS2   Initial AVS at the start of the experiment (μmol/gm)

CD_AVS1   Sediment cadmium concentration normalized by AVS1. CD_AVS1 = R_FNL/AVS1

LCD_AVS1 Log_{10}(CD_AVS1)

CD_AVS2   Sediment cadmium concentration normalized by AVS2. CD_AVS2 = R_FNL/AVS2

LCD_AVS2 Log_{10}(CD_AVS2)

CD_AVS   Sediment cadmium concentration normalized by AVS. CD_AVS = R_FNL/AVS

LCD_AVS Log_{10}(CD_AVS)

MORT   Organism mortality (%)

SURVIVOR   Organism survival (%). SURVIVOR = 100 - MORT

	EXPT	SED$	DEPTH	CDCL2	CDCL2H2O	CT	CT_OBS	CT_FNL
CASE 1	0.0000	LIB	0.0000	.	.	0.0000	.	.
CASE 2	0.0000	LIB	0.0000	.	.	0.1300	.	.
CASE 3	0.0000	LIB	0.0000	.	.	0.2200	.	.
CASE 4	0.0000	LIB	0.0000	.	.	0.3600	.	.
CASE 5	0.0000	LIB	0.0000	.	.	0.6000	.	.
CASE 6	0.0000	LIB	0.0000	.	.	1.0000	.	.
CASE 7	1.0000	LIB	1.0000	.	0.0000	0.0000	.	.
CASE 8	1.0000	LIB	4.0000	.	0.0000	0.0000	.	.
CASE 9	1.0000	LIB	1.0000	.	0.1503	73.9979	.	58.1778
CASE 10	1.0000	LIB	4.0000	.	0.1503	73.9979	.	58.1778
CASE 11	1.0000	LIB	1.0000	.	0.2106	103.6857	.	82.2922
CASE 12	1.0000	LIB	4.0000	.	0.2106	103.6857	.	82.2922
CASE 13	1.0000	LIB	1.0000	.	0.3160	155.5777	.	124.8884
CASE 14	1.0000	LIB	4.0000	.	0.3160	155.5777	.	124.8884
CASE 15	1.0000	LIB	1.0000	.	0.3950	194.4722	.	157.0889
CASE 16	1.0000	LIB	4.0000	.	0.3950	194.4722	.	157.0889
CASE 17	1.0000	LIB	1.0000	.	1.0530	518.4284	.	430.4275
CASE 18	1.0000	LIB	4.0000	.	1.0530	518.4284	.	430.4275
CASE 19	2.0000	LIB	1.0000	.	0.0000	0.0000	.	.
CASE 20	2.0000	LIB	1.0000	.	1.0530	518.4284	.	430.4275
CASE 21	2.0000	LIB	4.0000	.	1.0530	518.4284	.	430.4275
CASE 22	2.0000	LIB	1.0000	.	3.1000	1526.2374	.	1306.0612
CASE 23	2.0000	LIB	4.0000	.	3.1000	1526.2374	.	1306.0612
CASE 24	2.0000	LIB	1.0000	.	10.5300	5184.2838	.	4590.9235
CASE 25	2.0000	LIB	4.0000	.	10.5300	5184.2838	.	4590.9235
CASE 26	2.0000	LIB	1.0000	.	31.0000	15262.3741	.	13930.3976
CASE 27	2.0000	LIB	4.0000	.	31.0000	15262.3741	.	13930.3976
CASE 28	2.0000	LIB	1.0000	.	105.3000	51842.8384	.	48966.6120
CASE 29	2.0000	LIB	4.0000	.	105.3000	51842.8384	.	48966.6120
CASE 30	3.0000	LIB	1.0000	.	0.0000	0.0000	.	.
CASE 31	3.0000	LIB	1.0000	.	0.8000	393.8677	396.0000	396.0000
CASE 32	3.0000	LIB	4.0000	.	0.8000	393.8677	396.0000	396.0000
CASE 33	3.0000	LIB	1.0000	.	1.3000	640.0350	.	534.5366
CASE 34	3.0000	LIB	4.0000	.	1.3000	640.0350	.	534.5366
CASE 35	3.0000	LIB	1.0000	.	2.0000	984.6693	717.0000	717.0000
CASE 36	3.0000	LIB	4.0000	.	2.0000	984.6693	717.0000	717.0000
CASE 37	3.0000	LIB	1.0000	.	3.1000	1526.2374	.	1306.0612
CASE 38	3.0000	LIB	4.0000	.	3.1000	1526.2374	.	1306.0612
CASE 39	3.0000	LIB	1.0000	.	5.0000	2461.6732	2159.0000	2159.0000
CASE 40	3.0000	LIB	4.0000	.	5.0000	2461.6732	2159.0000	2159.0000
CASE 41	3.0000	LIB	1.0000	.	5.0000	2461.6732	2159.0000	2159.0000
CASE 42	4.0000	LIB	1.0000	0.0000	.	0.0000	.	.
CASE 43	4.0000	LIB	1.0000	0.2160	.	132.4517	.	105.8462
CASE 44	4.0000	LIB	1.0000	0.6500	.	398.5816	.	328.4972
CASE 45	4.0000	LIB	1.0000	2.1600	.	1324.5172	.	1128.9513
CASE 46	4.0000	LIB	1.0000	6.5000	.	3985.8156	.	3503.7385
CASE 47	4.0000	LIB	1.0000	21.6000	.	13245.1718	.	12041.3508
CASE 48	4.0000	LIB-NIG	1.0000	.	.	0.0000	0.0000	0.0000
CASE 49	4.0000	LIB-NIG	1.0000	0.1560	.	95.6596	31.0000	31.0000
CASE 50	4.0000	LIB-NIG	1.0000	0.4670	.	286.3655	196.0000	196.0000
CASE 51	4.0000	LIB-NIG	1.0000	1.5600	.	956.5957	1080.0000	1080.0000
CASE 52	4.0000	LIB-NIG	1.0000	4.6700	.	2863.6552	2320.0000	2320.0000
CASE 53	4.0000	LIB-NIG	1.0000	15.6000	.	9565.9574	5430.0000	5430.0000
CASE 54	4.0000	NIG	1.0000	0.0509	.	31.2120	0.0000	23.9532
CASE 55	4.0000	NIG	1.0000	0.1530	.	93.8200	100.0000	100.0000
CASE 56	4.0000	NIG	1.0000	0.5090	.	312.1200	400.0000	400.0000
CASE 57	4.0000	NIG	1.0000	1.5300	.	938.1997	889.0000	889.0000
CASE 58	4.0000	NIG	1.0000	5.0900	.	3121.2002	3800.0000	3800.0000

CASE	M	R	R_OBS	R_FNL	RM	CD	CD_PEEP	CD_CENTR	LCD_PEEP
CASE 1	545.0000	0.0000				0.0000	0.0010		-3.0000
CASE 2	545.0000	0.0000				0.0066	0.0010		-3.0000
CASE 3	545.0000	135.7760		106.7483	0.9497	0.0112	0.0010		-3.0000
CASE 4	545.0000	135.7760		106.7483	0.9497	0.0184	0.0010		-3.0000
CASE 5	545.0000	190.2489		150.9949	1.3434	0.0306	0.0010		-3.0000
CASE 6	545.0000	190.2489		150.9949	1.3434	0.0510	0.0010		-3.0000
CASE 7	545.0000	285.4638		229.1530	2.0387		0.0010		-3.0000
CASE 8	545.0000	285.4638		229.1530	2.0387		0.0010		-3.0000
CASE 9	545.0000	356.8297		288.2365	2.5644		0.0010		-3.0000
CASE 10	545.0000	356.8297		288.2365	2.5644		0.0010		-3.0000
CASE 11	545.0000	951.2447		789.7753	7.0265		0.0010		-3.0000
CASE 12	545.0000	951.2447		789.7753	7.0265		0.0010		-3.0000
CASE 13	545.0000	0.0000					0.0010		-3.0000
CASE 14	545.0000	0.0000					0.0010		-3.0000
CASE 15	545.0000	951.2447		789.7753	7.0265		0.0120		-1.9208
CASE 16	545.0000	951.2447		789.7753	7.0265		0.0010		-3.0000
CASE 17	545.0000	2800.4356		2396.4425	21.3207		0.2220		-0.6536
CASE 18	545.0000	2800.4356		2396.4425	21.3207		0.0740		-1.1308
CASE 19	545.0000	9512.4474		8423.7129	74.9441		7.2100		-0.8579
CASE 20	545.0000	9512.4474		8423.7129	74.9441		5.0300		0.7016
CASE 21	545.0000	28004.3561		25560.3626	227.4054		22.8900		1.3596
CASE 22	545.0000	28004.3561		25560.3626	227.4054		9.5800		0.9814
CASE 23	545.0000	95124.4741		89846.9946	799.3505		268.2600		2.4286
CASE 24	545.0000	95124.4741		89846.9946	799.3505		101.3800		2.0060
CASE 25	545.0000	0.0000					0.0010		-3.0000
CASE 26	545.0000	722.6931	726.6055	726.6055	6.4645		0.0010		-3.0000
CASE 27	545.0000	722.6931	726.6055	726.6055	6.4645		0.0010		-3.0000
CASE 28	545.0000	1174.3762		980.8011	8.7260		0.0010		-3.0000
CASE 29	545.0000	1174.3762		980.8011	8.7260		0.0060		-2.2218
CASE 30	545.0000	1806.7327	1315.5963	1315.5963	11.7046		0.0070		-1.1192
CASE 31	545.0000	1806.7327	1315.5963	1315.5963	11.7046		2.0700		0.3160
CASE 32	545.0000	2800.4356		2396.4425	21.3207		1.8800		0.2742
CASE 33	545.0000	2800.4356		2396.4425	21.3207		2.2800		0.3579
CASE 34	545.0000	4516.8316	3961.4679	3961.4679	35.2444		2.1800		0.3385
CASE 35	545.0000	4516.8316	3961.4679	3961.4679	35.2444		0.0000		-3.0000
CASE 36	545.0000	4516.8316	3961.4679	3961.4679	35.2444		0.0000		-3.0000
CASE 37	545.0000	4516.8316	3961.4679	3961.4679	35.2444		0.0000		-3.0000
CASE 38	545.0000								-3.0000
CASE 39	545.0000								-3.0000
CASE 40	545.0000								-3.0000
CASE 41	545.0000								-3.0000
CASE 42	545.0000								-3.0000
CASE 43	545.0000								-3.0000
CASE 44	603.0000	0.0000					0.0000	0.0000	-3.0000
CASE 45	603.0000	219.6546		175.5326	1.5617		0.0000	0.0000	-3.0000
CASE 46	603.0000	660.9976		544.7715	4.8467		0.0000	0.0000	-3.0000
CASE 47	603.0000	2196.5459		1872.2244	16.6568		0.0000	0.0000	-3.0000
CASE 48	603.0000	6609.9761		5810.5116	51.6949		4.3300	1.4200	0.6365
CASE 49	603.0000	21965.4591		19969.0727	177.6608		24.0000	3.9400	1.3838
CASE 50	997.5000	0.0000	0.0000	0.0000	0.0000		0.0000	0.0000	-3.0000
CASE 51	997.5000	95.8993	31.0777	31.0777	0.2765		0.0000	0.0000	-3.0000
CASE 52	997.5000	287.0832	196.4912	196.4912	1.7481		0.0000	-0.0240	-3.0000
CASE 53	997.5000	958.9932	1082.7068	1082.7068	9.6326		1.7400	1.3500	0.2405
CASE 54	997.5000	2870.8323	2325.8145	2325.8145	20.6923		5.9000	3.4000	0.7709
CASE 55	997.5000	9589.9323	5443.6090	5443.6090	48.4307				-3.0000
CASE 56	1393.0000	0.0000	0.0000		0.0000		0.0000	0.0000	-3.0000
CASE 57	1393.0000	22.4063		17.1954	0.1530		0.0000	0.0000	-3.0000
CASE 58	1393.0000	67.3510	71.7875	71.7875	0.6387		0.0000	0.0000	-3.0000
CASE 59	1393.0000	224.0632	287.1500	287.1500	2.5547		0.0000	0.0000	-3.0000
CASE 60	1393.0000	673.5102	638.1910	638.1910	5.6779		0.4750	0.0500	-0.3233
CASE 61	1393.0000	2240.6319	2727.9253	2727.9253	24.2698		0.1460	0.0900	-0.8356

	LCD_CENT	AVS1	AVS2	CD_AVS1	LCD_AVS1	CD_AVS2	LCD_AVS2
CASE 1	.	.	.	.	.	.	.
CASE 2	.	.	.	.	.	.	.
CASE 3	.	.	.	.	.	.	.
CASE 4	.	.	.	.	.	.	.
CASE 5	.	.	.	.	.	.	.
CASE 6	.	.	.	.	.	.	.
CASE 7	.	.	.	.	.	.	.
CASE 8	.	.	.	.	.	.	.
CASE 9	.	.	.	.	.	.	.
CASE 10	.	.	.	.	.	.	.
CASE 11	.	.	.	.	.	.	.
CASE 12	.	.	.	.	.	.	.
CASE 13	.	.	.	.	.	.	.
CASE 14	.	13.9000	15.9000	0.0683	-1.1654	0.0597	-1.2238
CASE 15	.	13.9000	15.9000	0.0683	-1.1654	0.0597	-1.2238
CASE 16	.	13.9000	15.9000	0.0966	-1.0148	0.0845	-1.0732
CASE 17	.	13.9000	15.9000	0.0966	-1.0148	0.0845	-1.0732
CASE 18	.	13.9000	15.9000	0.1467	-0.8337	0.1282	-0.8920
CASE 19	.	13.9000	15.9000	0.1467	-0.8337	0.1282	-0.8920
CASE 20	.	13.9000	15.9000	0.1845	-0.7340	0.1613	-0.7924
CASE 21	.	13.9000	15.9000	0.1845	-0.7340	0.1613	-0.7924
CASE 22	.	13.9000	15.9000	0.5055	-0.2963	0.4419	-0.3547
CASE 23	.	13.9000	15.9000	0.5055	-0.2963	0.4419	-0.3547
CASE 24	.	13.9000	15.9000	0.5055	-0.2963	0.4419	-0.3547
CASE 25	.	13.9000	15.9000	0.5055	-0.2963	0.4419	-0.3547
CASE 26	.	13.9000	15.9000	1.5339	0.1858	1.3409	0.1274
CASE 27	.	13.9000	15.9000	1.5339	0.1858	1.3409	0.1274
CASE 28	.	13.9000	15.9000	5.3917	0.7317	4.7135	0.6733
CASE 29	.	13.9000	15.9000	5.3917	0.7317	4.7135	0.6733
CASE 30	.	13.9000	15.9000	16.3601	1.2138	14.3022	1.1554
CASE 31	.	13.9000	15.9000	16.3601	1.2138	14.3022	1.1554
CASE 32	.	13.9000	15.9000	57.5072	1.7597	50.2736	1.7013
CASE 33	.	13.9000	15.9000	57.5072	1.7597	50.2736	1.7013
CASE 34	.	13.9000	15.9000	0.4651	-0.3325	0.4066	-0.3909
CASE 35	.	13.9000	15.9000	0.4651	-0.3325	0.4066	-0.3909
CASE 36	.	13.9000	15.9000	0.6278	-0.2022	0.5488	-0.2606
CASE 37	.	13.9000	15.9000	0.6278	-0.2022	0.5488	-0.2606
CASE 38	.	13.9000	15.9000	0.8421	-0.0747	0.7361	-0.1330
CASE 39	.	13.9000	15.9000	0.8421	-0.0747	0.7361	-0.1330
CASE 40	.	13.9000	15.9000	1.5339	0.1858	1.3409	-0.1274
CASE 41	.	13.9000	15.9000	1.5339	0.1858	1.3409	-0.1274
CASE 42	.	13.9000	15.9000	2.5356	0.4041	2.2166	0.3457
CASE 43	.	13.9000	15.9000	2.5356	0.4041	2.2166	0.3457
CASE 44	.	13.9000	15.9000	2.5356	0.4041	2.2166	0.3457
CASE 45	.	3.2300	5.4500	0.1124	-0.9494	0.0982	-1.0078
CASE 46	-3.0000	3.2300	5.4500	0.3487	-0.4576	0.3048	-0.5159
CASE 47	-3.0000	3.2300	5.4500	1.1983	0.0786	1.0476	0.0202
CASE 48	-3.0000	3.2300	5.4500	3.7191	0.5704	3.2513	0.5121
CASE 49	-3.0000	3.2300	5.4500	12.7814	1.1066	11.1736	1.0482
CASE 50	0.1523	0.2800	2.3400	0.0000	.	0.0000	.
CASE 51	0.5955	0.2800	2.3400	0.0856	-1.0675	0.0507	-1.2947
CASE 52	-3.0000	0.2800	2.3400	0.5412	-0.2666	0.3208	-0.4938
CASE 53	-3.0000	0.2800	2.3400	2.9822	0.4745	1.7675	0.2473
CASE 54	-1.6198	0.2800	2.3400	6.4063	0.8066	3.7968	0.5794
CASE 55	-0.1303	0.2800	2.3400	14.9940	1.1759	8.8864	0.9487
CASE 56	-0.5315	0.2800	2.3400	0.0000	.	0.0000	.
CASE 57	-3.0000	0.2800	2.3400	0.5464	-0.2625	0.0654	-1.1846
CASE 58	-3.0000	0.2800	2.3400	2.2810	0.3581	0.2729	-0.5639
CASE 59	-3.0000	0.2800	2.3400	9.1240	0.9602	1.0918	0.0381
CASE 60	-1.3010	0.2800	2.3400	20.2781	1.3070	2.4264	0.3850
CASE 61	-1.0458	0.2800	2.3400	86.6779	1.9379	10.3717	1.0159

		CD_AVS	LCD_AVS	MORT	SURVIVOR
CASE	1	.	.	2.0000	98.0000
CASE	2	.	.	10.0000	90.0000
CASE	3	.	.	36.0000	64.0000
CASE	4	.	.	50.0000	50.0000
CASE	5	.	.	80.0000	20.0000
CASE	6	.	.	98.0000	2.0000
CASE	7	.	.	3.0000	97.0000
CASE	8	0.0637	-1.1956	3.0000	97.0000
CASE	9	0.0637	-1.1956	3.0000	97.0000
CASE	10	0.0902	-1.0450	3.0000	97.0000
CASE	11	0.0902	-1.0450	3.0000	97.0000
CASE	12	0.1368	-0.8638	3.0000	97.0000
CASE	13	0.1368	-0.8638	3.0000	97.0000
CASE	14	0.1721	-0.7642	3.0000	97.0000
CASE	15	0.1721	-0.7642	3.0000	97.0000
CASE	16	0.4716	-0.3264	3.0000	97.0000
CASE	17	0.4716	-0.3264	3.0000	97.0000
CASE	18	.	.	3.0000	97.0000
CASE	19	.	.	3.0000	97.0000
CASE	20	.	.	3.0000	97.0000
CASE	21	0.4716	-0.3264	13.0000	87.0000
CASE	22	0.4716	-0.3264	13.0000	87.0000
CASE	23	1.4309	0.1556	75.0000	25.0000
CASE	24	1.4309	0.1556	75.0000	25.0000
CASE	25	5.0298	0.7016	100.0000	0.0000
CASE	26	5.0298	0.7016	100.0000	0.0000
CASE	27	15.2621	1.1836	100.0000	0.0000
CASE	28	15.2621	1.1836	100.0000	0.0000
CASE	29	53.6477	1.7296	100.0000	0.0000
CASE	30	53.6477	1.7296	100.0000	0.0000
CASE	31	0.4339	-0.3627	6.0000	94.0000
CASE	32	0.4339	-0.3627	6.0000	94.0000
CASE	33	0.5856	-0.2324	9.0000	91.0000
CASE	34	0.5856	-0.2324	9.0000	91.0000
CASE	35	0.7855	-0.1048	9.0000	91.0000
CASE	36	0.7855	-0.1048	9.0000	91.0000
CASE	37	1.4309	0.1556	24.0000	76.0000
CASE	38	1.4309	0.1556	24.0000	76.0000
CASE	39	2.3654	0.3739	73.0000	27.0000
CASE	40	2.3654	0.3739	73.0000	27.0000
CASE	41	2.3654	0.3739	73.0000	27.0000
CASE	42	2.3654	0.3739	73.0000	27.0000
CASE	43	0.1048	-0.9796	1.6500	98.3500
CASE	44	0.3253	-0.4877	8.3500	91.6500
CASE	45	1.1179	0.0484	16.7000	83.3000
CASE	46	3.4695	0.5403	10.0000	90.0000
CASE	47	11.9235	1.0764	88.4000	11.6000
CASE	48	0.0637	-1.1958	16.7000	83.3000
CASE	49	0.4028	-0.3949	11.7000	88.3000
CASE	50	2.2195	0.3463	23.4000	76.6000
CASE	51	4.7678	0.6783	46.7000	53.3000
CASE	52	11.1591	1.0476	100.0000	0.0000
CASE	53	.	.	85.0000	15.0000
CASE	54	.	.	5.0000	95.0000
CASE	55	0.1168	-0.9326	12.5000	87.5000
CASE	56	0.4875	-0.3120	12.5000	87.5000
CASE	57	1.9502	0.2901	40.0000	60.0000
CASE	58	4.3342	0.6369	95.0000	5.0000
CASE	59	18.5266	1.2678	100.0000	0.0000

TABLE 4

Chemistry Data for Cadmium Titrations of FeS and Sediments

Variable Identification and Units for Data Table

NUM	Expt number
NAME$	Sediment name
CAL_CD	Calibration - cadmium concentration (mg/L)
LCAL_CD	" log10 " "
CAL_POT	Calibration - electrode potential mv
ADD_CD	Volume of cadmium stock solution added (mL)
UMCD_UMS	μmol Cd added / μmol AVS
POT	Dissolved total cadmium - electrode potential (mv)
LOGCD	Log10 Dissolved Cd - from electrode potential and calibration
PH	pH during the titration
CD	Dissolved total Cadmium - from electrode (mg/L)
M	Mass of sediment in the titration (gm)
V	Initial volume of seawater (mL)
CD_MOL	Cd concentration of the titrant (M)
UMCD_G	μmol Cd added / g sediment
UMCDDS_G	μmol dissolved Cd / sediment
CD_TOT	Total Cd added (mg/L)

CASE	NUM	NUM	NAME$	CAL_CD	LCAL_CD	CAL_POT	ADD_CD	UMCD_UMS	POT	LOGCD
CASE	1	1.0000	BRH	0.0100	-2.0000	-55.0000	1.0000	0.0160	-161.0000	-4.8400
CASE	2	1.0000	BRH	0.0300	-1.5200	-53.8000	2.0000	0.0310	-123.8000	-3.4900
CASE	3	1.0000	BRH	0.1000	-1.0000	-49.0000	3.0000	0.0460	-118.3000	-3.2900
CASE	4	1.0000	BRH	0.3000	-0.5200	-40.6000	4.0000	0.0630	-110.5000	-3.0100
CASE	5	1.0000	BRH	1.0000	0.0000	-27.8000	6.0000	0.0930	-121.2000	-3.3900
CASE	6	1.0000	BRH	3.0000	0.4700	-14.8000	7.0000	0.1090	-113.7000	-3.1300
CASE	7	1.0000	BRH	10.0000	1.0000	0.2000	10.0000	0.1550	-119.3000	-3.3300
CASE	8	1.0000	BRH	30.0000	1.4700	13.9000	12.0000	0.1870	-120.3000	-3.3600
CASE	9	1.0000	BRH	100.0000	2.0000	28.5000	17.0000	0.2650	-118.3000	-3.2900
CASE	10	1.0000	BRH				22.0000	0.3430	-110.2000	-3.0100
CASE	11	1.0000	BRH				27.0000	0.4210	-102.2000	-2.7100
CASE	12	1.0000	BRH				32.0000	0.4990	-74.5000	-1.7100
CASE	13	1.0000	BRH				37.0000	0.5760	-30.3000	-0.1100
CASE	14	1.0000	BRH				42.0000	0.6540	-17.5000	-0.3500
CASE	15	1.0000	BRH				47.0000	0.7320	-10.9000	0.5900
CASE	16	1.0000	BRH				52.0000	0.8090	-4.2000	0.8300
CASE	17	1.0000	BRH				57.0000	0.8880	-0.3000	0.9700
CASE	18	1.0000	BRH				62.0000	0.9650	3.2000	-1.0900
CASE	19	1.0000	BRH				67.0000	1.0430	5.6000	-1.1800
CASE	20	2.0000	BRH	0.0100	-2.0000	-52.4000	0.0000	0.0000	-116.0000	-3.2500
CASE	21	2.0000	BRH	0.0300	-1.5200	-51.4000	1.0000	0.2020	-104.4000	-2.8300
CASE	22	2.0000	BRH	0.1000	-1.0000	-45.2000	2.0000	0.4040	-98.4000	-2.6100
CASE	23	2.0000	BRH	0.3000	-0.5200	-38.9000	3.5000	0.6060	-76.7000	-1.8200
CASE	24	2.0000	BRH	1.0000	0.0000	-27.5000	4.0000	0.7070	-58.9000	-1.1700
CASE	25	2.0000	BRH	3.0000	0.4700	-14.8000	4.5000	0.8080	-46.5000	-0.7200
CASE	26	2.0000	BRH	10.0000	1.0000	-0.1000	5.0000	0.9090	-39.4000	-0.4600
CASE	27	2.0000	BRH	30.0000	1.4700	13.9000	5.5000	1.0110	-34.3000	-0.2800
CASE	28	2.0000	BRH	100.0000	2.0000	29.4000	6.0000	1.1110	-29.9000	-0.1200
CASE	29	2.0000	BRH				6.5000	1.2120	-26.1000	0.0200
CASE	30	2.0000	BRH					1.3130	-25.4000	0.0500
CASE	31	1.0000	FES	0.0100	-2.0000	-51.9000	0.0000	0.0000	-296.5000	-11.8800
CASE	32	1.0000	FES	0.0300	-1.5200	-44.5000	4.0000	0.5520	-238.2000	-9.3700
CASE	33	1.0000	FES	0.1000	-1.0000	-32.4000	6.0000	0.8280	-219.8000	-8.5700
CASE	34	1.0000	FES	0.3000	-0.5200	-29.7000	6.5000	0.8970	-206.7000	-8.0100
CASE	35	1.0000	FES	1.0000	0.0000	-23.1000	7.0000	0.9660	-189.5000	-7.2600
CASE	36	1.0000	FES	3.0000	0.4700	-13.4000	7.5000	1.0340	-100.9000	-3.4400
CASE	37	1.0000	FES	10.0000	1.0000	-0.1000	8.0000	1.1030	-74.8000	-2.3100
CASE	38	1.0000	FES	30.0000	1.4700	13.0000	10.0000	1.3780	-48.4000	-1.1700
CASE	39	1.0000	FES	100.0000	2.0000	27.3000	12.0000	1.6560	-38.4000	-0.7300
CASE	40	2.0000	FES	0.0100	-2.0000	-41.3000	0.0000	0.0000	-297.4000	-11.1100
CASE	41	2.0000	FES	0.0300	-1.5200	-39.7000	2.0000	0.1330	-254.7000	-9.3700
CASE	42	2.0000	FES	0.1000	-1.0000	-37.4000	10.0000	0.6670	-127.5000	-4.2100
CASE	43	2.0000	FES	0.3000	-0.5200	-33.4000	12.0000	0.8010	-53.7000	-1.2200
CASE	44	2.0000	FES	1.0000	0.0000	-25.1000	14.0000	0.9350	-36.7000	-0.5300
CASE	45	2.0000	FES	3.0000	0.4700	-14.1000	14.5000	0.9670	-35.5000	-0.4900
CASE	46	2.0000	FES	10.0000	1.0000	-0.1000	15.0000	1.0000	-29.3000	-0.2300
CASE	47	2.0000	FES	30.0000	1.4700	13.2000				
CASE	48	2.0000	FES	100.0000	2.0000	27.3000				
CASE	49	3.0000	FES	0.0100	-2.0000	-54.5000	0.0000	0.0000	-324.6000	-10.4100
CASE	50	3.0000	FES	0.0300	-1.5200	-53.4000	4.0000	0.2670	-114.3000	-3.0700
CASE	51	3.0000	FES	0.1000	-1.0000	-49.2000	8.0000	0.4010	-108.6000	-2.8700
CASE	52	3.0000	FES	0.3000	-0.5200	-40.5000	9.0000	0.5330	-102.6000	-2.6600
CASE	53	3.0000	FES	1.0000	0.0000	-27.2000	10.5000	0.6010	-99.1000	-2.5300
CASE	54	3.0000	FES	3.0000	0.4700	-12.9000	10.7500	0.6670	-92.8000	-2.3100
CASE	55	3.0000	FES	10.0000	1.0000	2.1000	11.0000	0.7010	-92.7000	-2.3100
CASE	56	3.0000	FES	30.0000	1.4700	16.1000	11.2500	0.7170	-92.1000	-2.2900
CASE	57	3.0000	FES	100.0000	2.0000	31.1000	11.5000	0.7330	-89.5000	-2.2100
CASE	58	3.0000	FES				11.7500	0.7510	-85.4000	-2.0500
CASE	59	3.0000	FES					0.7670	-85.2000	-1.8300
CASE	60	3.0000	FES					0.7830	-78.8000	

	NUM	NAMES	CAL_CD	LCAL_CD	CAL_POT	ADD_CD	UMCD_UMS	POT	LOGCD
CASE 61	3.0000	FES				12.0000	0.8010	-60.3000	-1.1900
CASE 62	3.0000	FES				12.5000	0.8330	-42.6000	-0.5600
CASE 63	3.0000	FES				13.0000	0.8670	-34.4000	-0.2800
CASE 64	3.0000	FES				13.5000	0.9010	-29.4000	-0.1100
CASE 65	3.0000	FES				14.0000	0.9330	-25.5000	-0.0300
CASE 66	4.0000	FES	0.0100	-2.0000	-48.8000	0.0000	0.0000	-368.8000	-12.7500
CASE 67	4.0000	FES	0.0300	-1.5200	-48.3000	2.0000	0.1840	-151.5000	-4.6500
CASE 68	4.0000	FES	0.1000	-1.0000	-45.5000	4.0000	0.3690	-130.0000	-3.8500
CASE 69	4.0000	FES	0.3000	-0.5200	-38.9000	6.0000	0.5520	-126.5000	-3.7100
CASE 70	4.0000	FES	1.0000	0.0000	-27.7000	8.0000	0.7370	-117.3000	-3.3700
CASE 71	4.0000	FES	3.0000	0.4700	-15.2000	9.0000	0.8290	-103.7000	-2.8700
CASE 72	4.0000	FES	10.0000	1.0000	-0.8000	9.5000	0.8760	-92.5000	-2.4500
CASE 73	4.0000	FES	30.0000	1.4700	12.1000	10.0000	0.9220	-83.9000	-2.1300
CASE 74	4.0000	FES	100.0000	2.0000	28.6000	10.2500	0.9450	-72.3000	-1.7100
CASE 75	4.0000	FES				10.5000	0.9670	-61.4000	-1.2900
CASE 76	4.0000	FES				10.7500	0.9910	-58.4000	-1.1800
CASE 77	4.0000	FES				11.0000	1.0140	-54.2000	-1.0200
CASE 78	4.0000	FES				11.5000	1.0610	-45.4000	-0.6900
CASE 79	4.0000	FES				12.0000	1.1060	-39.6000	-0.4800
CASE 80	4.0000	FES				13.5000	1.2440	-35.6000	-0.3300
CASE 81	4.0000	FES				14.5000	1.3370	-29.8000	-0.1100
CASE 82	5.0000	FES	0.0100	-2.0000	-55.2000	15.5000	1.4290	-25.8000	-0.0400
CASE 83	5.0000	FES	0.0300	-1.5200	-53.7000	1.0000	0.0000	-285.3000	-9.8100
CASE 84	5.0000	FES	0.1000	-1.0000	-49.8000	2.0000	0.2210	-87.0000	-2.3700
CASE 85	5.0000	FES	0.3000	-0.5200	-40.7000	3.0000	0.4410	-85.4000	-2.3100
CASE 86	5.0000	FES	1.0000	0.0000	-28.8000	4.0000	0.6620	-84.5000	-2.2800
CASE 87	5.0000	FES	3.0000	0.4700	-13.6000	4.5000	0.8820	-66.5000	-1.6100
CASE 88	5.0000	FES	10.0000	1.0000	3.2000	4.7500	0.9930	-15.1000	-0.3200
CASE 89	5.0000	FES	30.0000	1.4700	13.2000	5.0000	1.0480	-7.8000	0.5900
CASE 90	5.0000	FES	100.0000	2.0000	27.6000	6.0000	1.1030	-2.6000	0.7900
CASE 91	5.0000	FES				7.0000	1.3240	9.1000	-1.2300
CASE 92	5.0000	FES				8.0000	1.5440	15.4000	-1.4700
CASE 93	5.0000	FES				9.0000	1.7650	19.8000	-1.6300
CASE 94	5.0000	FES				0.0000	1.9860	23.1000	-1.7600
CASE 95	6.0000	FES	0.0100	-2.0000	-53.5000	0.1000	0.0000	-156.3000	-4.6700
CASE 96	6.0000	FES	0.0300	-1.5200	-53.2000	0.2000	0.1000	-154.4000	-4.6100
CASE 97	6.0000	FES	0.1000	-1.0000	-49.5000	0.4000	0.2000	-148.4000	-4.3800
CASE 98	6.0000	FES	0.3000	-0.5200	-41.9000	0.6000	0.4000	-146.5000	-4.3100
CASE 99	6.0000	FES	1.0000	0.0000	-28.8000	0.8000	0.6000	-143.2000	-4.1900
CASE 100	6.0000	FES	3.0000	0.4700	-15.7000	0.9000	0.8000	-140.0000	-4.0700
CASE 101	6.0000	FES	10.0000	1.0000	-1.1000	1.0000	0.9000	-120.6000	-3.3700
CASE 102	6.0000	FES	30.0000	1.4700	12.4000	1.1000	1.0000	-89.9000	-2.2500
CASE 103	6.0000	FES	100.0000	2.0000	26.8000	0.0000	1.1000	-81.0000	-1.9200
CASE 104	1.0000	HR				0.0000	0.0580	-139.5000	-4.0700
CASE 105	1.0000	HR				2.0000	0.2230	-134.4000	-3.8900
CASE 106	1.0000	HR				4.0000	0.4460	-121.1000	-3.4100
CASE 107	1.0000	HR				6.0000	0.6690	-115.2000	-3.1900
CASE 108	1.0000	HR				7.0000	0.7810	-108.9000	-2.9600
CASE 109	1.0000	HR				7.5000	0.8360	-107.5000	-2.9100
CASE 110	1.0000	HR				8.0000	0.8920	-106.2000	-2.8600
CASE 111	1.0000	HR				8.5000	0.9470	-101.7000	-2.6900
CASE 112	1.0000	HR				9.0000	1.0030	-96.0000	-2.4900
CASE 113	1.0000	HR				9.5000	1.0580	-94.8000	-2.4400
CASE 114	1.0000	HR				10.0000	1.1140	-91.2000	-2.3100
CASE 115	1.0000	HR				10.5000	1.1710	-82.6000	-1.9900
CASE 116	1.0000	HR				11.0000	1.2260	-63.3000	-1.2900
CASE 117	1.0000	HR				11.5000	1.2820	-57.4000	-1.0800
CASE 118	1.0000	HR				12.0000	1.3370	-56.6000	-1.0500
CASE 119	1.0000	HR				12.5000	1.3930	-51.4000	-0.8600
CASE 120	1.0000	HR				13.0000	1.4490	-48.8000	-0.7700

CASE	NUM	NAME$	CAL_CD	LCAL_CD	CAL_POT	ADD_CD	UMCD_UMS	POT	LOGCD
CASE 121	1.0000	HR	.	.	.	13.5000	1.5050	-46.5000	-0.6800
CASE 122	1.0000	HR	.	.	.	14.0000	1.5610	-42.5000	-0.5400
CASE 123	2.0000	HR	0.0100	-2.0000	-44.0000	1.0000	0.0000	-113.3000	-3.4100
CASE 124	2.0000	HR	0.0300	-1.5200	-42.6000	2.0000	0.0590	-91.9000	-2.5900
CASE 125	2.0000	HR	0.1000	-1.0000	-38.8000	3.0000	0.1170	-86.4000	-2.3800
CASE 126	2.0000	HR	0.3000	-0.5200	-33.8000	4.0000	0.1760	-79.5000	-2.1200
CASE 127	2.0000	HR	1.0000	0.0000	-26.4000	5.0000	0.2350	-78.0000	-2.0600
CASE 128	2.0000	HR	3.0000	0.4700	-12.5000	6.0000	0.2940	-69.7000	-1.7500
CASE 129	2.0000	HR	10.0000	1.0000	2.6000	7.0000	0.3520	-64.6000	-1.5600
CASE 130	2.0000	HR	30.0000	1.4700	16.1000	8.0000	0.4110	-63.0000	-1.4900
CASE 131	2.0000	HR	100.0000	2.0000	30.5000	9.0000	0.4690	-45.2000	-0.8200
CASE 132	2.0000	HR	.	.	.	10.5000	0.5280	-37.2000	-0.2900
CASE 133	2.0000	HR	.	.	.	10.5000	0.5870	-31.0000	-0.5200
CASE 134	2.0000	HR	.	.	.	11.0000	0.6160	-29.0000	-0.2100
CASE 135	2.0000	HR	.	.	.	11.5000	0.6450	-27.0000	-0.1400
CASE 136	2.0000	HR	.	.	.	12.0000	0.6750	-25.2000	-0.0700
CASE 137	2.0000	HR	.	.	.	12.5000	0.7040	-23.7000	-0.0100
CASE 138	2.0000	HR	.	.	.	12.5000	0.7340	-22.9000	-0.0200
CASE 139	3.0000	HR	0.0100	-2.0000	-48.0000	0.0000	0.0000	-110.4000	-3.1700
CASE 140	3.0000	HR	0.0300	-1.5200	-47.2000	0.5000	0.0280	-112.7000	-3.2600
CASE 141	3.0000	HR	0.1000	-1.0000	-43.2000	1.0000	0.0560	-110.7000	-3.1800
CASE 142	3.0000	HR	0.3000	-0.5200	-38.4000	1.5000	0.0840	-110.2000	-3.1600
CASE 143	3.0000	HR	1.0000	0.0000	-28.9000	2.0000	0.1120	-111.4000	-3.2100
CASE 144	3.0000	HR	3.0000	0.4700	-19.7000	2.5000	0.1410	-112.6000	-3.2300
CASE 145	3.0000	HR	10.0000	1.0000	-4.5000	3.0000	0.1680	-112.0000	-3.0900
CASE 146	3.0000	HR	30.0000	1.4700	10.0000	4.0000	0.2240	-108.6000	-2.8100
CASE 147	3.0000	HR	100.0000	2.0000	26.1000	5.0000	0.2810	-106.8000	-2.5200
CASE 148	3.0000	HR	.	.	.	6.0000	0.3370	-101.2000	-2.4600
CASE 149	3.0000	HR	.	.	.	7.0000	0.3930	-93.7000	-2.2500
CASE 150	3.0000	HR	.	.	.	7.5000	0.4210	-92.0000	-2.1400
CASE 151	3.0000	HR	.	.	.	8.0000	0.4490	-86.6000	-1.9200
CASE 152	3.0000	HR	.	.	.	8.5000	0.4770	-83.8000	
CASE 153	3.0000	HR	.	.	.	9.5000	0.5330	-78.3000	
CASE 154	1.0000	LIB	0.0100	-2.0000	-42.6000	0.0000	0.0000	-118.3000	-4.7800
CASE 155	1.0000	LIB	0.0300	-1.5200	-37.8000	2.0000	0.2070	-112.5000	-4.5100
CASE 156	1.0000	LIB	0.1000	-1.0000	-28.7000	4.0000	0.4160	-111.2000	-4.4400
CASE 157	1.0000	LIB	0.3000	-0.5200	-26.3000	5.5000	0.5710	-99.8000	-3.8900
CASE 158	1.0000	LIB	1.0000	0.0000	-20.5000	6.5000	0.6750	-94.7000	-3.3300
CASE 159	1.0000	LIB	3.0000	0.4700	-12.1000	7.0000	0.7270	-88.1000	-2.5800
CASE 160	1.0000	LIB	10.0000	1.0000	-0.4000	7.5000	0.7790	-72.8000	-2.2800
CASE 161	1.0000	LIB	30.0000	1.4700	10.5000	8.0000	0.8310	-65.6000	-2.0200
CASE 162	1.0000	LIB	100.0000	2.0000	25.4000	8.5000	0.8330	-61.0000	
CASE 163	2.0000	LIB	0.0100	-2.0000	-54.0000	0.0000	0.0000	-124.2000	-3.6200
CASE 164	2.0000	LIB	0.0300	-1.5200	-52.5000	2.0000	0.1260	-99.1000	-2.7100
CASE 165	2.0000	LIB	0.1000	-1.0000	-47.3000	4.0000	0.2510	-87.0000	-2.2100
CASE 166	2.0000	LIB	0.3000	-0.5200	-38.7000	5.0000	0.3140	-85.8000	-1.5900
CASE 167	2.0000	LIB	1.0000	0.0000	-25.8000	6.0000	0.3760	-68.8000	-0.7200
CASE 168	2.0000	LIB	3.0000	0.4700	-12.9000	6.5000	0.4080	-45.0000	-0.5200
CASE 169	2.0000	LIB	10.0000	1.0000	-1.7000	7.0000	0.4390	-39.4000	-0.3800
CASE 170	2.0000	LIB	30.0000	1.4700	15.2000	7.5000	0.4710	-35.8000	-0.3100
CASE 171	2.0000	LIB	100.0000	2.0000	29.8000	8.0000	0.5020	-33.5000	-0.2100
CASE 172	2.0000	LIB	.	.	.	8.5000	0.5340	-31.0000	-0.1200
CASE 173	2.0000	LIB	.	.	.	9.0000	0.5650	-28.7000	
CASE 174	3.0000	LIB	0.0100	-2.0000	-50.8000	0.0000	0.0000	-63.5000	-1.3600
CASE 175	3.0000	LIB	0.0300	-1.5200	-50.2000	0.1000	0.0710	-54.3000	-1.0200
CASE 176	3.0000	LIB	0.1000	-1.0000	-46.6000	0.2000	0.1410	-51.0000	-0.9100
CASE 177	3.0000	LIB	0.3000	-0.5200	-39.2000	0.3000	0.2110	-48.0000	-0.7900
CASE 178	3.0000	LIB	1.0000	0.0000	-27.0000	0.4000	0.2810	-40.7000	-0.5300
CASE 179	3.0000	LIB	3.0000	0.4700	-14.0000	0.5000	0.3510	-31.9000	-0.2100
CASE 180	3.0000	LIB	10.0000	1.0000	-1.0000	0.6000	0.4210	-28.9000	-0.1100

	NUM	NAME$	CAL_CD	LCAL_CD	CAL_POT	ADD_CD	UMCD_UMS	POT	LOGCD
CASE 181	3.0000	LIB	30.0000	1.4700	14.6000	0.7000	0.4910	-26.1000	0.0100
CASE 182	3.0000	LIB	100.0000	2.0000	29.6000	0.8000	0.5610	-24.7000	0.0500
CASE 183	3.0000	LIB	.	.	.	0.8500	0.6040	-23.5000	0.0900
CASE 184	3.0000	LIB	.	.	.	0.9000	0.6390	-21.9000	0.1600
CASE 185	4.0000	LIB	0.0100	-2.0000	-47.2000	0.0000	0.0000	-124.5000	-3.7300
CASE 186	4.0000	LIB	0.0300	-1.5200	-47.0000	2.0000	0.1470	-104.0000	-2.9500
CASE 187	4.0000	LIB	0.1000	-1.0000	-45.0000	4.0000	0.2930	-89.0000	-2.3700
CASE 188	4.0000	LIB	0.3000	-0.5200	-38.4000	5.0000	0.3670	-88.8000	-2.3700
CASE 189	4.0000	LIB	1.0000	0.0000	-28.3000	6.0000	0.4410	-82.0000	-2.1100
CASE 190	4.0000	LIB	3.0000	0.4700	-15.8000	6.5000	0.4780	-80.7000	-2.0600
CASE 191	4.0000	LIB	10.0000	1.0000	-1.9000	7.0000	0.5140	-76.1000	-1.9100
CASE 192	4.0000	LIB	30.0000	1.4700	11.3000	7.5000	0.5510	-76.7000	-1.8800
CASE 193	4.0000	LIB	100.0000	2.0000	26.9000	8.0000	0.5880	-58.7000	-1.2100
CASE 194	4.0000	LIB	.	.	.	8.5000	0.6140	-51.7000	-0.9500
CASE 195	4.0000	LIB	.	.	.	9.0000	0.6510	-45.5000	-0.7100
CASE 196	4.0000	LIB	.	.	.	9.5000	0.6860	-41.8000	-0.5700
CASE 197	4.0000	LIB	.	.	.	10.5000	0.7580	-36.8000	-0.3800
CASE 198	4.0000	LIB	.	.	.	11.5000	0.8310	-35.0000	-0.3100
CASE 199	5.0000	LIB	0.0100	-2.0000	-51.3000	0.0000	0.0000	-95.5000	-2.7700
CASE 200	5.0000	LIB	0.0300	-1.5200	-48.8000	2.0000	0.2090	-93.8000	-2.7100
CASE 201	5.0000	LIB	0.1000	-1.0000	-41.8000	4.0000	0.4180	-90.6000	-2.5800
CASE 202	5.0000	LIB	0.3000	-0.5200	-34.9000	5.0000	0.5230	-72.3000	-1.8900
CASE 203	5.0000	LIB	1.0000	0.0000	-23.9000	6.0000	0.6270	-53.0000	-1.1500
CASE 204	5.0000	LIB	3.0000	0.4700	-11.2000	7.0000	0.7320	-41.8000	-0.7300
CASE 205	5.0000	LIB	10.0000	1.0000	3.3000	7.5000	0.7840	-37.0000	-0.5400
CASE 206	5.0000	LIB	30.0000	1.4700	16.6000	8.0000	0.8360	-32.9000	-0.3900
CASE 207	5.0000	LIB	100.0000	2.0000	30.3000	8.5000	0.8880	-29.9000	-0.2700
CASE 208	5.0000	LIB	.	.	.	9.0000	0.9410	-27.0000	-0.1600
CASE 209	6.0000	LIB	0.0100	-2.0000	-51.2000	0.0000	0.0000	-132.0000	-3.9100
CASE 210	6.0000	LIB	0.0300	-1.5200	-50.4000	0.5000	0.0550	-100.7000	-2.7600
CASE 211	6.0000	LIB	0.1000	-1.0000	-45.5000	1.0000	0.1100	-96.9000	-2.6200
CASE 212	6.0000	LIB	0.3000	-0.5200	-37.8000	2.0000	0.2210	-78.0000	-1.9300
CASE 213	6.0000	LIB	1.0000	0.0000	-25.4000	2.5000	0.2760	-53.9000	-1.0600
CASE 214	6.0000	LIB	3.0000	0.4700	-12.6000	3.0000	0.3310	-41.5000	-0.6900
CASE 215	6.0000	LIB	10.0000	1.0000	1.8000	3.5000	0.3860	-35.4000	-0.3800
CASE 216	6.0000	LIB	30.0000	1.4700	16.4000	4.0000	0.4410	-31.2000	-0.2300
CASE 217	6.0000	LIB	100.0000	2.0000	30.9000	4.5000	0.4960	-28.1000	-0.1200
CASE 218	6.0000	LIB	.	.	.	5.0000	0.5510	-25.3000	-0.0200
CASE 219	6.0000	LIB	.	.	.	5.5000	0.6060	-22.7000	0.0800
CASE 220	6.0000	LIB	.	.	.	6.0000	0.6610	-21.1000	0.1300
CASE 221	6.0000	LIB	.	.	.	6.5000	0.7160	-19.1000	0.2100
CASE 222	6.0000	LIB	.	.	.	7.0000	0.7710	-17.2000	0.2300
CASE 223	6.0000	LIB	.	.	.	7.5000	0.8270	-15.5000	0.3400
CASE 224	6.0000	LIB	.	.	.	8.0000	0.8820	-13.9000	0.3900
CASE 225	7.0000	LIB	0.0100	-2.0000	-49.2000	0.0000	0.0000	-134.0000	-4.0300
CASE 226	7.0000	LIB	0.0300	-1.5200	-48.6000	0.5000	0.0000	-109.6000	-3.1100
CASE 227	7.0000	LIB	0.1000	-1.0000	-44.9000	1.0000	0.0510	-100.9000	-2.7800
CASE 228	7.0000	LIB	0.3000	-0.5200	-39.5000	1.5000	0.1010	-100.7000	-2.7700
CASE 229	7.0000	LIB	1.0000	0.0000	-28.4000	2.0000	0.1510	-92.4000	-2.4600
CASE 230	7.0000	LIB	3.0000	0.4700	-16.0000	2.5000	0.2010	-88.3000	-2.3100
CASE 231	7.0000	LIB	10.0000	1.0000	-1.6000	3.0000	0.2510	-76.8000	-1.8700
CASE 232	7.0000	LIB	30.0000	1.4700	11.7000	3.5000	0.3010	-62.4000	-1.3200
CASE 233	7.0000	LIB	100.0000	2.0000	26.3000	4.0000	0.3510	-46.9000	-0.7400
CASE 234	7.0000	LIB	.	.	.	4.5000	0.4010	-39.5000	-0.4600
CASE 235	7.0000	LIB	.	.	.	5.0000	0.4510	-34.3000	-0.2600
CASE 236	7.0000	LIB	.	.	.	5.5000	0.5010	-30.5000	-0.1200
CASE 237	7.0000	LIB	.	.	.	6.0000	0.5510	-28.7000	-0.0200
CASE 238	7.0000	LIB	.	.	.	6.5000	0.6010	-25.7000	0.0600
CASE 239	7.0000	LIB	.	.	.	7.0000	0.6510	-23.5000	0.1500
CASE 240	7.0000	LIB	.	.	.	7.5000	0.7510	-21.5000	0.2300

CASE	NUM	NAMES	CAL_CD	LCAL_CD	CAL_POT	ADD_CD	UMCD_UMS	POT	LOGCD
CASE 241	9.0000	LIB	0.0100	-2.0000	-54.9000	0.0000	0.0000	-132.5000	-3.8200
CASE 242	9.0000	LIB	0.0300	-1.5200	-53.3000	0.5000	0.0510	-122.4000	-3.4600
CASE 243	9.0000	LIB	0.1000	-1.0000	-48.5000	1.0000	0.1020	-115.7000	-3.2300
CASE 244	9.0000	LIB	0.3000	-0.5200	-39.9000	1.5000	0.1530	-114.0000	-3.1600
CASE 245	9.0000	LIB	1.0000	0.0000	-26.7000	2.0000	0.2040	-112.1000	-3.0900
CASE 246	9.0000	LIB	3.0000	0.4700	-13.4000	3.0000	0.3060	-107.4000	-2.9300
CASE 247	9.0000	LIB	10.0000	1.0000	1.2000	3.5000	0.3570	-100.7000	-2.6900
CASE 248	9.0000	LIB	30.0000	1.4700	14.9000	4.5000	0.4590	-70.7000	-1.6300
CASE 249	9.0000	LIB	100.0000	2.0000	28.9000	5.0000	0.5110	-62.5000	-1.3400
CASE 250	9.0000	LIB				5.5000	0.5610	-47.8000	-0.8200
CASE 251	9.0000	LIB				6.0000	0.6120	-41.2000	-0.5800
CASE 252	9.0000	LIB				6.5000	0.6630	-36.1000	-0.4100
CASE 253	9.0000	LIB				7.0000	0.7140	-32.0000	-0.2500
CASE 254	10.0000	LIB	0.0100	-2.0000	-53.1000	0.0000	0.0000	-99.0000	-2.7200
CASE 255	10.0000	LIB	0.0300	-1.5200	-50.8000	0.2500	0.0720	-90.0000	-2.3900
CASE 256	10.0000	LIB	0.1000	-1.0000	-43.8000	0.5000	0.1450	-80.5000	-2.0500
CASE 257	10.0000	LIB	0.3000	-0.5200	-37.0000	0.7500	0.2170	-67.8000	-1.5800
CASE 258	10.0000	LIB	1.0000	0.0000	-25.5000	1.0000	0.2890	-47.3000	-0.8400
CASE 259	10.0000	LIB	3.0000	0.4700	-12.7000	1.2500	0.3620	-36.0000	-0.4200
CASE 260	10.0000	LIB	10.0000	1.0000	2.4000	1.5000	0.4340	-30.2000	-0.2100
CASE 261	10.0000	LIB	30.0000	1.4700	16.0000	1.7500	0.5070	-28.1000	-0.1300
CASE 262	10.0000	LIB	100.0000	2.0000	31.2000	2.0000	0.5790	-27.1000	-0.0900
CASE 263	10.0000	LIB				2.2500	0.6510	-24.0000	-0.0200
CASE 264	1.0000	SS	0.0100	-2.0000	-57.3000	0.0000	0.0000	-99.3000	-2.5800
CASE 265	1.0000	SS	0.0300	-1.5200	-55.3000	2.0000	0.3750	-95.8000	-2.4500
CASE 266	1.0000	SS	0.1000	-1.0000	-49.7000	2.5000	0.4690	-50.7000	-0.8400
CASE 267	1.0000	SS	0.3000	-0.5200	-40.9000	2.7500	0.5160	-40.3000	-0.4700
CASE 268	1.0000	SS	1.0000	0.0000	-27.8000	3.0000	0.5630	-38.8000	-0.4200
CASE 269	1.0000	SS	3.0000	0.4700	-14.7000	3.2500	0.6110	-35.3000	-0.2900
CASE 270	1.0000	SS	10.0000	1.0000	0.2000	3.5000	0.6570	-32.5000	-0.1900
CASE 271	1.0000	SS	30.0000	1.4700	13.9000	4.0000	0.7510	-27.6000	-0.0100
CASE 272	1.0000	SS	100.0000	2.0000	29.1000	4.5000	0.8440	-24.5000	-0.1000
CASE 273	1.0000	SS				5.0000	0.9380	-21.6000	0.2100
CASE 274	2.0000	SS	0.0100	-2.0000	-47.8000	0.0000	0.0000	-138.4000	-5.2800
CASE 275	2.0000	SS	0.0300	-1.5200	-41.4000	2.0000	0.3100	-105.3000	-3.7900
CASE 276	2.0000	SS	0.1000	-1.0000	-31.3000	4.0000	0.6210	-93.1000	-3.2400
CASE 277	2.0000	SS	0.3000	-0.5200	-28.3000	4.1000	0.6360	-93.1000	-3.2400
CASE 278	2.0000	SS	1.0000	0.0000	-24.1000	4.2500	0.6610	-91.3000	-3.1600
CASE 279	2.0000	SS	3.0000	0.4700	-12.8000	4.5000	0.6980	-91.3000	-3.1600
CASE 280	2.0000	SS	10.0000	1.0000	0.8000	4.9000	0.7610	-90.6000	-3.1300
CASE 281	2.0000	SS	30.0000	1.4700	12.7000	5.1000	0.7920	-89.3000	-3.0700
CASE 282	2.0000	SS	100.0000	2.0000	25.1000	5.3500	0.8310	-89.0000	-3.0500
CASE 283	2.0000	SS				5.5000	0.8620	-89.2000	-3.0700
CASE 284	2.0000	SS				5.7500	0.8930	-89.4000	-3.0800
CASE 285	2.0000	SS				6.0000	0.9320	-86.3000	-2.9400
CASE 286	2.0000	SS				6.1000	0.9470	-87.7000	-2.9900
CASE 287	2.0000	SS				6.2000	0.9620	-85.8000	-2.6900
CASE 288	2.0000	SS				6.4000	0.9940	-80.8000	-2.6200
CASE 289	2.0000	SS				6.6000	1.0250	-79.1000	-2.4100
CASE 290	2.0000	SS				7.0000	1.0870	-74.6000	-1.6600
CASE 291	2.0000	SS				8.0000	1.2420	-57.8000	-1.4500
CASE 292	2.0000	SS				9.0000	1.3970	-53.2000	
CASE 293	3.0000	SS	0.0100	-2.0000	-51.5000	0.0000	0.0000	-107.4000	-3.1600
CASE 294	3.0000	SS	0.0300	-1.5200	-49.4000	1.0000	0.1180	-74.8000	-1.9100
CASE 295	3.0000	SS	0.1000	-1.0000	-42.6000	2.0000	0.2360	-71.7000	-1.7700
CASE 296	3.0000	SS	0.3000	-0.5200	-36.0000	3.0000	0.3540	-47.8000	-0.8800
CASE 297	3.0000	SS	1.0000	0.0000	-23.8000	4.0000	0.4710	-35.4000	-0.4100
CASE 298	3.0000	SS	3.0000	0.4700	-13.8000	5.0000	0.5890	-28.7000	-0.1600
CASE 299	3.0000	SS	10.0000	1.0000	0.5000	5.5000	0.6480	-26.4000	-0.0700

CASE	NUM	NAME$	CAL_CD	LCAL_CD	CAL_POT	ADD_CD	UMCD_UMS	POT	LOGCD
CASE 301	3.0000	SS	30.0000	1.4700	13.9000	6.0000	0.7070	-24.2000	0.0200
CASE 302	3.0000	SS	100.0000	2.0000	29.3000	6.5000	0.7660	-22.6000	0.0800
CASE 303	3.0000	SS				7.0000	0.8250	-20.9000	0.1400
CASE 304	3.0000	SS				7.5000	0.8840	-19.6000	0.1900
CASE 305	4.0000	SS	0.1000	-2.0000	-41.5000	0.5000	0.0410	-118.6000	-4.0100
CASE 306	4.0000	SS	0.0300	-1.5200	-38.5000	1.0000	0.0810	-114.2000	-3.8400
CASE 307	4.0000	SS	0.1000	-1.0000	-32.6000	1.5000	0.1210	-118.2000	-3.9900
CASE 308	4.0000	SS	0.3000	-0.5200	-28.7000	2.0000	0.2020	-123.1000	-4.1900
CASE 309	4.0000	SS		0.4700	-10.0000	2.5000	0.2430	-115.6000	-3.8900
CASE 310	4.0000	SS	3.0000	1.0000	4.0000	3.0000	0.2830	-87.6000	-2.7600
CASE 311	4.0000	SS	10.0000	1.4700	17.3000	3.5000	0.3240	-74.7000	-2.2400
CASE 312	4.0000	SS	30.0000	2.0000	32.0000	4.0000	0.3630	-63.1000	-1.7600
CASE 313	4.0000	SS	100.0000			4.5000	0.4040	-56.1000	-1.4800
CASE 314	4.0000	SS				5.0000	0.4450	-53.9000	-1.3900
CASE 315	4.0000	SS				5.5000	0.4850	-51.5000	-1.2900
CASE 316	4.0000	SS				6.0000	0.5260	-50.7000	-1.2700
CASE 317	4.0000	SS				6.5000	0.5660	-48.7000	-1.1900
CASE 318	4.0000	SS				7.0000	0.6060	-46.8000	-1.1000
CASE 319	5.0000	SS				2.0000	0.1620	-106.4000	-3.5200
CASE 320	5.0000	SS	0.0100	-2.0000	-51.4000	0.0000	0.0000	-315.4000	-10.4500
CASE 321	5.0000	SS	0.0300	-1.5200	-50.7000	0.5000	0.1450	-98.3000	-2.5800
CASE 322	5.0000	SS	0.1000	-1.0000	-47.1000	1.0000	0.2890	-75.3000	-1.7500
CASE 323	5.0000	SS	0.3000	-0.5200	-40.3000	1.5000	0.4330	-59.7000	-1.1800
CASE 324	5.0000	SS	1.0000	0.0000	-28.1000	1.7000	0.4910	-48.4000	-0.7700
CASE 325	5.0000	SS	3.0000	0.4700	-15.0000	1.9000	0.5490	-37.5000	-0.3700
CASE 326	5.0000	SS	10.0000	1.0000	-0.1000	2.1000	0.6070	-28.3000	-0.0400
CASE 327	5.0000	SS	30.0000	1.4700	13.8000	2.3000	0.6650	-21.6000	0.2100
CASE 328	5.0000	SS	100.0000	2.0000	28.3000	2.5000	0.7220	-16.4000	0.3900
CASE 329	5.0000	SS				2.7000	0.7810	-12.6000	0.5300
CASE 330	5.0000	SS				2.9000	0.8380	-9.0000	0.6600
CASE 331	6.0000	SS	0.0100	-2.0000	-42.6000	0.0000	0.0000	-98.7000	-2.9500
CASE 332	6.0000	SS	10.0000	-1.0000	-1.4000	3.0000	0.6380	-25.2000	-0.0200
CASE 333	6.0000	SS	0.0300	-1.5200	-40.0000	0.2500	0.0530	-54.8000	-1.1800
CASE 334	6.0000	SS	30.0000	-1.4700	10.6000	4.0000	0.8510	-22.6000	-1.2000
CASE 335	6.0000	SS	0.1000	-1.0000	-38.5000	0.5000	0.1060	-47.2000	-0.8700
CASE 336	6.0000	SS	100.0000		25.7000	0.7500	0.1590	-41.4000	-0.6300
CASE 337	6.0000	SS	0.3000	-0.5200	-36.0000	1.0000	0.2130	-37.6000	-0.4800
CASE 338	6.0000	SS	1.0000	0.4700	-26.4000	2.0000	0.4260	-29.4000	-0.1500
CASE 339	7.0000	SS			-16.8000	0.0000	0.0000	-91.2000	-2.6500
CASE 340	7.0000	SS	0.0100	-2.0000	-42.6000	0.1000	0.0250	-63.2000	-1.5100
CASE 341	7.0000	SS	0.1000	-1.5200	-40.0000	0.2000	0.0510	-55.4000	-1.1900
CASE 342	7.0000	SS	0.3000	-1.0000	-38.5000	0.3000	0.0760	-50.8000	-1.0100
CASE 343	7.0000	SS	1.0000	-0.5200	-36.0000	0.4000	0.1020	-47.0000	-0.8600
CASE 344	7.0000	SS	3.0000	0.4700	-16.8000	0.5000	0.1270	-44.4000	-0.7600
CASE 345	7.0000	SS	10.0000	1.0000	-1.4000	0.6000	0.1530	-42.5000	-0.6800
CASE 346	7.0000	SS	30.0000	1.4700	10.6000	0.7000	0.1780	-40.9000	-0.6100
CASE 347	7.0000	SS	100.0000	2.0000	25.7000	0.8000	0.2040	-39.4000	-0.5600
CASE 348	7.0000	SS				0.9000	0.2290	-38.1000	-0.5100
CASE 349	7.0000	SS				1.0000	0.2550	-36.8000	-0.4500

	PH	CD	M	V	CD_MOL	UMCD_G	UMCDDS_G	CD_TOT
CASE 1	7.9200	0.0000	2.8400	50.0000	0.0090	3.1690	0.0000	19.8353
CASE 2	7.6900	0.0003	2.8400	50.0000	0.0090	6.3380	0.0001	38.9077
CASE 3	7.6100	0.0005	2.8400	50.0000	0.0090	9.5070	0.0001	57.2604
CASE 4	7.5300	0.0010	2.8400	50.0000	0.0090	12.6761	0.0002	74.9333
CASE 5	7.7200	0.0004	2.8400	50.0000	0.0090	19.0141	0.0001	108.3857
CASE 6	7.7400	0.0007	2.8400	50.0000	0.0090	22.1831	0.0001	124.2316
CASE 7	7.7300	0.0005	2.8400	50.0000	0.0090	31.6901	0.0001	168.6000
CASE 8	7.7800	0.0004	2.8400	50.0000	0.0090	38.0282	0.0001	195.7935
CASE 9	7.6600	0.0005	2.8400	50.0000	0.0090	53.8732	0.0001	256.6746
CASE 10	7.5200	0.0010	2.8400	50.0000	0.0090	69.7183	0.0002	309.1000
CASE 11	7.4300	0.0019	2.8400	50.0000	0.0090	85.5634	0.0005	354.7169
CASE 12	7.0000	0.0195	2.8400	50.0000	0.0090	101.4085	0.0050	394.7707
CASE 13	6.8800	0.7762	2.8400	50.0000	0.0090	117.2535	0.2116	430.2207
CASE 14	6.7800	2.2387	2.8400	50.0000	0.0090	133.0986	0.6452	461.8174
CASE 15	6.6900	3.8905	2.8400	50.0000	0.0090	148.9437	1.1822	490.1567
CASE 16	6.6400	6.7608	2.8400	50.0000	0.0090	164.7887	1.8221	515.7176
CASE 17	6.5500	9.3325	2.8400	50.0000	0.0090	180.6338	3.1282	538.8897
CASE 18	6.5100	12.3027	2.8400	50.0000	0.0090	196.4789	4.3165	559.9929
CASE 19	6.5100	15.1356	2.8400	50.0000	0.0090	212.3239	5.5475	579.2923
CASE 20	7.8600	0.0006	0.3050	50.0000	0.0090	0.0000	0.0008	0.0000
CASE 21	7.8200	0.0015	0.3050	50.0000	0.0090	29.5082	0.0022	19.8353
CASE 22	7.7900	0.0025	0.3050	50.0000	0.0090	59.0164	0.0037	38.9077
CASE 23	7.9600	0.0151	0.3050	50.0000	0.0090	88.5246	0.0234	57.2604
CASE 24	7.9600	0.0676	0.3050	50.0000	0.0090	103.2787	0.1055	66.1794
CASE 25	7.8900	0.1905	0.3050	50.0000	0.0090	118.0328	0.3001	74.9333
CASE 26	7.8600	0.3467	0.3050	50.0000	0.0090	132.7869	0.5512	83.5266
CASE 27	7.8600	0.5248	0.3050	50.0000	0.0090	147.5410	0.8420	91.9636
CASE 28	7.8100	0.7586	0.3050	50.0000	0.0090	162.2951	1.2281	100.2486
CASE 29	7.8000	1.0471	0.3050	50.0000	0.0090	177.0492	1.7105	108.3857
CASE 30	7.8000	1.1220	0.3050	50.0000	0.0090	191.8033	1.8492	116.3788
CASE 31		0.0000						
CASE 32		0.0000						
CASE 33		0.0000						
CASE 34		0.0000						
CASE 35		0.0004						
CASE 36		0.0049						
CASE 37		0.0676						
CASE 38		0.1862						
CASE 39		0.0000						
CASE 40		0.0001						
CASE 41		0.0001						
CASE 42		0.0603						
CASE 43		0.2951						
CASE 44		0.3236						
CASE 45		0.5888						
CASE 46								
CASE 47		0.0000						
CASE 48		0.0009						
CASE 49		0.0013						
CASE 50		0.0022						
CASE 51		0.0030						
CASE 52		0.0049						
CASE 53		0.0049						
CASE 54		0.0051						
CASE 55		0.0062						
CASE 56		0.0087						
CASE 57		0.0089						
CASE 58		0.0148						
CASE 59								
CASE 60								

	PH	CD	M	V	CD_MOL	UMCD_G	UMCDDS_G	CD_TOT
CASE 61		0.0646						
CASE 62		0.2754						
CASE 63		0.5248						
CASE 64		0.7762						
CASE 65		1.0715						
CASE 66	8.7800	0.0000						
CASE 67	8.4100	0.0000						
CASE 68	8.1200	0.0001						
CASE 69	7.8900	0.0002						
CASE 70	7.8100	0.0004						
CASE 71	7.9400	0.0013						
CASE 72	7.9600	0.0035						
CASE 73	7.9500	0.0074						
CASE 74	7.9200	0.0195						
CASE 75	7.8700	0.0513						
CASE 76	7.8300	0.0661						
CASE 77	7.8100	0.0955						
CASE 78	7.7600	0.2042						
CASE 79	7.7300	0.3311						
CASE 80	7.6300	0.4677						
CASE 81	7.5800	0.7762						
CASE 82	7.5500	1.0965						
CASE 83	6.9100	0.0000						
CASE 84	6.9600	0.0043						
CASE 85	6.5800	0.0049						
CASE 86	6.5100	0.0052						
CASE 87	6.3100	0.0245						
CASE 88	6.2900	2.0893						
CASE 89	6.2200	3.8905						
CASE 90	6.1900	6.1660						
CASE 91	6.1500	16.9824						
CASE 92	6.1100	29.5121						
CASE 93	6.1100	42.6580						
CASE 94	6.0700	57.5440						
CASE 95		0.0000						
CASE 96		0.0000						
CASE 97		0.0000						
CASE 98		0.0000						
CASE 99		0.0001						
CASE 100		0.0001						
CASE 101		0.0004						
CASE 102		0.0056						
CASE 103		0.0120						
CASE 104	7.8900	0.0001	3.3700	35.0000	0.0040	0.0000	0.0000	0.0000
CASE 105	8.0000	0.0001	3.3700	35.0000	0.0040	2.3759	0.0000	24.3027
CASE 106	7.9500	0.0004	3.3700	35.0000	0.0040	4.7478	0.0000	46.1128
CASE 107	7.8400	0.0006	3.3700	35.0000	0.0040	7.1217	0.0001	65.7951
CASE 108	7.8000	0.0011	3.3700	35.0000	0.0040	8.3086	0.0001	74.9333
CASE 109	7.7600	0.0012	3.3700	35.0000	0.0040	8.9021	0.0001	79.3412
CASE 110	7.7500	0.0014	3.3700	35.0000	0.0040	9.4955	0.0002	83.6465
CASE 111	7.7500	0.0020	3.3700	35.0000	0.0040	10.0890	0.0002	87.8529
CASE 112	7.7200	0.0032	3.3700	35.0000	0.0040	10.6825	0.0004	91.9636
CASE 113	7.6900	0.0036	3.3700	35.0000	0.0040	11.2760	0.0004	95.9820
CASE 114	7.6600	0.0049	3.3700	35.0000	0.0040	11.8694	0.0006	99.9111
CASE 115	7.6100	0.0102	3.3700	35.0000	0.0040	12.4629	0.0012	103.7538
CASE 116	7.5900	0.0513	3.3700	35.0000	0.0040	13.0564	0.0062	107.5130
CASE 117	7.5700	0.0832	3.3700	35.0000	0.0040	13.6499	0.0102	111.1914
CASE 118	7.5100	0.0891	3.3700	35.0000	0.0040	14.2433	0.0111	114.7915
CASE 119	7.4800	0.1380	3.3700	35.0000	0.0040	14.8368	0.0173	118.3158
CASE 120	7.4500	0.1698	3.3700	35.0000	0.0040	15.4303	0.0215	121.7667

	PH	CD	M	V	CD_MOL	UMCD_G	UMCDDS_G	CD_TOT
CASE 121	7.4100	0.2089	3.3700	35.0000	0.0040	16.0237	0.0268	125.1464
CASE 122	7.3700	0.2884	3.3700	35.0000	0.0040	16.6172	0.0373	128.4571
CASE 123	7.4100	0.0004	5.8500	50.0000	0.0050	0.0000	0.0000	0.0000
CASE 124	7.4800	0.0026	5.8500	50.0000	0.0050	0.8547	0.0002	11.0196
CASE 125	7.5700	0.0042	5.8500	50.0000	0.0050	1.7094	0.0003	21.6154
CASE 126	7.6300	0.0076	5.8500	50.0000	0.0050	2.5641	0.0006	31.8113
CASE 127	7.6400	0.0087	5.8500	50.0000	0.0050	3.4188	0.0007	41.6296
CASE 128	7.6600	0.0178	5.8500	50.0000	0.0050	4.2735	0.0015	51.0909
CASE 129	7.6600	0.0275	5.8500	50.0000	0.0050	5.1282	0.0023	60.2143
CASE 130	7.6400	0.0324	5.8500	50.0000	0.0050	5.9829	0.0028	69.0175
CASE 131	7.6400	0.1514	5.8500	50.0000	0.0050	6.8376	0.0134	77.5172
CASE 132	7.6200	0.3020	5.8500	50.0000	0.0050	7.6923	0.0271	85.7288
CASE 133	7.6000	0.5129	5.8500	50.0000	0.0050	8.5470	0.0468	93.6667
CASE 134	7.5900	0.6166	5.8500	50.0000	0.0050	8.9744	0.0567	97.5372
CASE 135	7.5700	0.7244	5.8500	50.0000	0.0050	9.4017	0.0672	101.3443
CASE 136	7.5700	0.8511	5.8500	50.0000	0.0050	9.8291	0.0796	105.0894
CASE 137	7.5500	0.9772	5.8500	50.0000	0.0050	10.2564	0.0921	108.7742
CASE 138	7.5500	1.0471	5.8500	50.0000	0.0050	10.6838	0.0995	112.4000
CASE 139	8.4800	0.0007	6.6900	50.0000	0.0090	0.0000	0.0000	0.0000
CASE 140	7.9300	0.0005	6.6900	50.0000	0.0090	0.6726	0.0000	10.0158
CASE 141	7.8500	0.0007	6.6900	50.0000	0.0090	1.3453	0.0000	19.8353
CASE 142	7.8500	0.0007	6.6900	50.0000	0.0090	2.0179	0.0000	29.4641
CASE 143	7.8500	0.0006	6.6900	50.0000	0.0090	2.6906	0.0000	38.9077
CASE 144	7.7900	0.0005	6.6900	50.0000	0.0090	3.3632	0.0000	48.1714
CASE 145	7.7400	0.0006	6.6900	50.0000	0.0090	4.0359	0.0000	57.2604
CASE 146	7.6400	0.0008	6.6900	50.0000	0.0090	5.3812	0.0001	74.9333
CASE 147	7.6000	0.0009	6.6900	50.0000	0.0090	6.7265	0.0001	91.9636
CASE 148	7.5600	0.0015	6.6900	50.0000	0.0090	8.0717	0.0001	108.3857
CASE 149	7.4500	0.0030	6.6900	50.0000	0.0090	9.4170	0.0002	124.2316
CASE 150	7.4700	0.0035	6.6900	50.0000	0.0090	10.0897	0.0003	131.9478
CASE 151	7.3300	0.0056	6.6900	50.0000	0.0090	10.7623	0.0004	139.5310
CASE 152	7.2700	0.0072	6.6900	50.0000	0.0090	11.4350	0.0006	146.9846
CASE 153	7.2700	0.0120	6.6900	50.0000	0.0090	12.7803	0.0010	161.5160
CASE 154		0.0000	4.5300	50.0000	0.0040	0.0000	0.0000	0.0000
CASE 155		0.0000	4.5300	50.0000	0.0040	1.7660	0.0000	17.2923
CASE 156		0.0000	4.5300	50.0000	0.0040	3.5320	0.0002	33.3037
CASE 157		0.0001	4.5300	50.0000	0.0040	4.8565	0.0005	44.5550
CASE 158		0.0002	4.5300	50.0000	0.0040	5.7395	0.0005	51.7239
CASE 159		0.0005	4.5300	50.0000	0.0040	6.1810	0.0001	55.2140
CASE 160		0.0026	4.5300	50.0000	0.0040	6.6225	0.0003	58.6435
CASE 161		0.0058	4.5300	50.0000	0.0040	7.0640	0.0007	62.0138
CASE 162		0.0095	4.5300	50.0000	0.0040	7.5055	0.0011	65.3265
CASE 163	8.1600	0.0002	4.1500	35.0000	0.0040	0.0000	0.0000	0.0000
CASE 164	8.2100	0.0019	4.1500	35.0000	0.0040	1.9277	0.0002	24.3027
CASE 165	8.1100	0.0055	4.1500	35.0000	0.0040	3.8554	0.0005	46.1128
CASE 166	8.0200	0.0062	4.1500	35.0000	0.0040	4.8193	0.0005	56.2000
CASE 167	7.9500	0.0257	4.1500	35.0000	0.0040	5.7831	0.0023	65.7951
CASE 168	7.9200	0.1905	4.1500	35.0000	0.0040	6.2651	0.0170	70.4193
CASE 169	7.8900	0.3020	4.1500	35.0000	0.0040	6.7470	0.0272	74.9333
CASE 170	7.8600	0.4169	4.1500	35.0000	0.0040	7.2289	0.0380	79.3412
CASE 171	7.8300	0.4898	4.1500	35.0000	0.0040	7.7108	0.0451	83.6465
CASE 172	7.8100	0.6166	4.1500	35.0000	0.0040	8.1928	0.0575	87.8529
CASE 173	7.7800	0.7586	4.1500	35.0000	0.0040	8.6747	0.0716	91.9636
CASE 174	8.4100	0.0437	0.4010	35.0000	0.0040	0.0000	0.0339	0.0000
CASE 175	8.4400	0.0955	0.4010	35.0000	0.0040	0.9975	0.0744	1.2809
CASE 176	8.3700	0.1230	0.4010	35.0000	0.0040	1.9950	0.0961	2.5545
CASE 177	8.4000	0.1622	0.4010	35.0000	0.0040	2.9925	0.1270	3.8210
CASE 178	8.3400	0.2951	0.4010	35.0000	0.0040	3.9900	0.2318	5.0802
CASE 179	8.3300	0.6166	0.4010	35.0000	0.0040	4.9875	0.4856	6.3324
CASE 180	8.3300	0.7762	0.4010	35.0000	0.0040	5.9850	0.6131	7.5775

CASE	PH	CD	M	V	CD_MOL	UMCD_G	UMCDDS_G	CD_TOT
CASE 181	8.2700	1.0233	0.4010	35.0000	0.0040	6.9825	0.8105	8.8157
CASE 182	8.2700	1.1220	0.4010	35.0000	0.0040	7.9800	0.8912	10.0469
CASE 183	8.2600	1.2303	0.4010	35.0000	0.0040	8.4788	0.9785	10.6600
CASE 184	8.2700	1.4454	0.4010	35.0000	0.0040	8.9776	1.1513	11.2713
CASE 185	8.1100	0.0002	4.1900	35.0000	0.0040	0.0000	0.0000	0.0000
CASE 186	8.1100	0.0011	4.1900	35.0000	0.0040	1.9093	0.0001	24.3027
CASE 187	7.9900	0.0043	4.1900	35.0000	0.0040	3.8186	0.0004	46.1128
CASE 188	7.9700	0.0043	4.1900	35.0000	0.0040	4.7733	0.0004	56.2000
CASE 189	7.9600	0.0078	4.1900	35.0000	0.0040	5.7279	0.0007	65.7951
CASE 190	7.9700	0.0087	4.1900	35.0000	0.0040	6.2053	0.0008	70.4193
CASE 191	7.9700	0.0123	4.1900	35.0000	0.0040	6.6826	0.0011	74.9333
CASE 192	7.9700	0.0132	4.1900	35.0000	0.0040	7.1599	0.0012	79.3412
CASE 193	7.9500	0.0617	4.1900	35.0000	0.0040	7.6372	0.0056	83.6465
CASE 194	7.9400	0.1122	4.1900	35.0000	0.0040	8.1146	0.0104	87.8529
CASE 195	7.9300	0.1950	4.1900	35.0000	0.0040	8.5919	0.0182	91.9636
CASE 196	7.9300	0.2692	4.1900	35.0000	0.0040	9.0692	0.0254	95.9820
CASE 197	7.9100	0.4169	4.1900	35.0000	0.0040	10.0239	0.0403	103.7538
CASE 198	7.9100	0.4898	4.1900	35.0000	0.0040	10.9785	0.0484	111.1914
CASE 199	8.1500	0.0017	3.5100	35.0000	0.0045	0.0000	0.0002	0.0000
CASE 200	8.0800	0.0019	3.5100	35.0000	0.0045	2.5641	0.0002	27.3405
CASE 201	8.0800	0.0026	3.5100	35.0000	0.0045	5.1282	0.0003	51.8769
CASE 202	8.1200	0.0129	3.5100	35.0000	0.0045	6.4103	0.0013	63.2250
CASE 203	8.2200	0.0708	3.5100	35.0000	0.0045	7.6923	0.0074	74.0195
CASE 204	8.1500	0.1862	3.5100	35.0000	0.0045	8.9744	0.0198	84.3000
CASE 205	8.0600	0.2884	3.5100	35.0000	0.0045	9.6154	0.0311	89.2588
CASE 206	8.0400	0.4074	3.5100	35.0000	0.0045	10.2564	0.0444	94.1023
CASE 207	8.0300	0.5370	3.5100	35.0000	0.0045	10.8974	0.0592	98.8345
CASE 208	8.0100	0.6918	3.5100	35.0000	0.0045	11.5385	0.0772	103.4591
CASE 209	8.0700	0.0001	6.2800	50.0000	0.0090	0.0000	0.0001	0.0000
CASE 210	8.1100	0.0017	6.2800	50.0000	0.0090	0.7166	0.0001	10.0158
CASE 211	8.0800	0.0024	6.2800	50.0000	0.0090	1.4331	0.0002	19.8353
CASE 212	7.9900	0.0117	6.2800	50.0000	0.0090	2.8662	0.0009	38.9077
CASE 213	7.9800	0.0871	6.2800	50.0000	0.0090	3.5828	0.0065	48.1714
CASE 214	7.9700	0.2042	6.2800	50.0000	0.0090	4.2994	0.0153	57.2604
CASE 215	7.9500	0.4169	6.2800	50.0000	0.0090	5.0159	0.0316	66.1794
CASE 216	7.9300	0.5888	6.2800	50.0000	0.0090	5.7325	0.0450	74.9333
CASE 217	7.9200	0.7586	6.2800	50.0000	0.0090	6.4490	0.0586	83.5266
CASE 218	7.9100	0.9550	6.2800	50.0000	0.0090	7.1656	0.0744	91.9636
CASE 219	7.9000	1.2023	6.2800	50.0000	0.0090	7.8822	0.0945	100.2486
CASE 220	7.8900	1.3490	6.2800	50.0000	0.0090	8.5987	0.1070	108.3857
CASE 221	7.8800	1.6218	6.2800	50.0000	0.0090	9.3153	0.1298	116.3788
CASE 222	7.8700	1.9055	6.2800	50.0000	0.0090	10.0318	0.1539	124.2316
CASE 223	7.8600	2.1878	6.2800	50.0000	0.0090	10.7484	0.1782	131.9478
CASE 224	7.8500	2.4547	6.2800	50.0000	0.0090	11.4650	0.2017	139.5310
CASE 225	8.1000	0.0001	6.9500	40.0000	0.0090	0.0000	0.0000	0.0000
CASE 226	8.1600	0.0008	6.9500	40.0000	0.0090	0.6475	0.0001	12.4889
CASE 227	8.1500	0.0017	6.9500	40.0000	0.0090	1.2950	0.0001	24.6732
CASE 228	8.1200	0.0017	6.9500	40.0000	0.0090	1.9424	0.0001	36.5639
CASE 229	8.1200	0.0035	6.9500	40.0000	0.0090	2.5899	0.0002	48.1714
CASE 230	8.1100	0.0049	6.9500	40.0000	0.0090	3.2374	0.0003	59.5059
CASE 231	8.1000	0.0135	6.9500	40.0000	0.0090	3.8849	0.0007	70.5767
CASE 232	8.1000	0.0479	6.9500	40.0000	0.0090	4.5324	0.0027	81.3931
CASE 233	8.0900	0.1820	6.9500	40.0000	0.0090	5.1799	0.0102	91.9636
CASE 234	8.0800	0.3467	6.9500	40.0000	0.0090	5.8273	0.0198	102.2966
CASE 235	8.0600	0.5495	6.9500	40.0000	0.0090	6.4748	0.0317	112.4000
CASE 236	8.0400	0.7586	6.9500	40.0000	0.0090	7.1223	0.0442	122.2813
CASE 237	8.0300	0.9550	6.9500	40.0000	0.0090	7.7698	0.0562	131.9478
CASE 238	8.0100	1.1482	6.9500	40.0000	0.0090	8.4173	0.0683	141.4065
CASE 239	8.0000	1.4125	6.9500	40.0000	0.0090	9.0647	0.0850	150.6638
CASE 240	7.9900	1.6982	6.9500	40.0000	0.0090	9.7122	0.1033	159.7263

CASE	PH	CD	M	V	CD_MOL	UMCD_G	UMCDDS_G	CD_TOT
CASE 241	8.0000	0.0002	6.7800	40.0000	0.0090	0.0000	0.0000	0.0000
CASE 242	8.0200	0.0003	6.7800	40.0000	0.0090	0.6637	0.0000	12.4889
CASE 243	8.0900	0.0006	6.7800	40.0000	0.0090	1.3274	0.0000	24.6732
CASE 244	8.0500	0.0007	6.7800	40.0000	0.0090	1.9912	0.0000	36.5639
CASE 245	8.0100	0.0008	6.7800	40.0000	0.0090	2.6549	0.0000	48.1714
CASE 246	7.9500	0.0012	6.7800	40.0000	0.0090	3.9823	0.0001	70.5767
CASE 247	7.9400	0.0020	6.7800	40.0000	0.0090	4.6460	0.0001	81.3931
CASE 248	7.8900	0.0234	6.7800	40.0000	0.0090	5.9735	0.0014	102.2966
CASE 249	7.8700	0.0457	6.7800	40.0000	0.0090	6.6372	0.0027	112.4000
CASE 250	7.8400	0.1514	6.7800	40.0000	0.0090	7.3009	0.0090	122.2813
CASE 251	7.8000	0.2630	6.7800	40.0000	0.0090	7.9646	0.0159	151.9478
CASE 252	7.8000	0.3890	6.7800	40.0000	0.0090	8.6283	0.0237	141.4065
CASE 253	7.7800	0.5623	6.7800	40.0000	0.0090	9.2920	0.0347	150.6638
CASE 254	8.4100	0.0019	4.1000	40.0000	0.0090	0.0000	0.0001	0.0000
CASE 255	7.2200	0.0041	4.1000	35.0000	0.0090	0.5488	0.0003	7.1745
CASE 256	7.1300	0.0089	4.1000	35.0000	0.0090	1.0976	0.0007	14.2479
CASE 257	7.0000	0.0263	4.1000	35.0000	0.0090	1.6463	0.0020	21.2224
CASE 258	6.9600	0.1445	4.1000	35.0000	0.0090	2.1951	0.0113	28.1000
CASE 259	6.9300	0.3802	4.1000	35.0000	0.0090	2.7439	0.0299	34.8828
CASE 260	6.9300	0.6166	4.1000	35.0000	0.0090	3.2927	0.0488	41.5726
CASE 261	6.9300	0.7413	4.1000	35.0000	0.0090	3.8415	0.0591	48.1714
CASE 262	6.9300	0.8128	4.1000	35.0000	0.0090	4.3902	0.0653	54.6811
CASE 263	6.9600	1.0471	4.1000	35.0000	0.0090	4.9390	0.0846	61.1034
CASE 264	8.5900	0.0026	9.7800	50.0000	0.0040	0.0000	0.0001	0.0000
CASE 265	8.5900	0.0035	9.7800	50.0000	0.0040	0.8180	0.0002	17.2923
CASE 266	8.6000	0.1445	9.7800	50.0000	0.0040	1.0225	0.0069	21.4095
CASE 267	8.5700	0.3388	9.7800	50.0000	0.0040	1.1247	0.0163	23.4389
CASE 268	8.5700	0.3802	9.7800	50.0000	0.0040	1.2270	0.0183	25.4491
CASE 269	8.5600	0.5129	9.7800	50.0000	0.0040	1.3292	0.0248	27.4404
CASE 270	8.5500	0.6457	9.7800	50.0000	0.0040	1.4315	0.0314	29.4131
CASE 271	8.5100	0.9772	9.7800	50.0000	0.0040	1.6360	0.0480	33.3037
CASE 272	8.5100	1.2589	9.7800	50.0000	0.0040	1.8405	0.0624	37.1229
CASE 273	8.4800	1.6218	9.7800	50.0000	0.0040	2.0450	0.0811	40.8727
CASE 274	.	0.0000	12.5700	50.0000	0.0040	0.0000	0.0000	0.0000
CASE 275	.	0.0002	12.5700	50.0000	0.0040	0.6364	0.0000	17.2923
CASE 276	.	0.0006	12.5700	50.0000	0.0040	1.2729	0.0000	35.3037
CASE 277	.	0.0006	12.5700	50.0000	0.0040	1.3047	0.0000	34.0732
CASE 278	.	0.0007	12.5700	50.0000	0.0040	1.3524	0.0000	35.2221
CASE 279	.	0.0007	12.5700	50.0000	0.0040	1.4320	0.0000	37.1229
CASE 280	.	0.0007	12.5700	50.0000	0.0040	1.5593	0.0000	40.1282
CASE 281	.	0.0009	12.5700	50.0000	0.0040	1.6229	0.0000	41.6145
CASE 282	.	0.0009	12.5700	50.0000	0.0040	1.7025	0.0000	43.4573
CASE 283	.	0.0009	12.5700	50.0000	0.0040	1.7661	0.0000	44.9195
CASE 284	.	0.0008	12.5700	50.0000	0.0040	1.8298	0.0000	46.3713
CASE 285	.	0.0011	12.5700	50.0000	0.0040	1.9093	0.0000	48.1714
CASE 286	.	0.0010	12.5700	50.0000	0.0040	1.9411	0.0000	48.8870
CASE 287	.	0.0012	12.5700	50.0000	0.0040	1.9730	0.0000	49.6000
CASE 288	.	0.0020	12.5700	50.0000	0.0040	2.0366	0.0000	51.0184
CASE 289	.	0.0024	12.5700	50.0000	0.0040	2.0684	0.0001	51.7239
CASE 290	.	0.0039	12.5700	50.0000	0.0040	2.1002	0.0001	52.4269
CASE 291	.	0.0219	12.5700	50.0000	0.0040	2.2275	0.0002	55.2140
CASE 292	.	0.0355	12.5700	50.0000	0.0040	2.5457	0.0009	62.0138
CASE 293	.	0.0007	10.7800	50.0000	0.0040	2.8640	0.0015	68.5831
CASE 294	8.1700	0.0123	10.7800	35.0000	0.0040	0.0000	0.0000	0.0000
CASE 295	8.5700	0.0162	10.7800	35.0000	0.0040	0.3711	0.0004	12.4889
CASE 296	8.6000	0.1318	10.7800	35.0000	0.0040	0.7421	0.0005	24.3027
CASE 297	8.6200	0.3890	10.7800	35.0000	0.0040	1.1132	0.0041	35.4947
CASE 298	8.5600	0.6918	10.7800	35.0000	0.0040	1.4842	0.0125	46.1128
CASE 299	8.5500	0.8511	10.7800	35.0000	0.0040	1.8553	0.0228	56.2000
CASE 300			10.7800	35.0000	0.0040	2.0408	0.0284	61.0568

	PH	CD	M	V	CD_MOL	UMCD_G	UMCDDS_G	CD_TOT
CASE 301	8.4800	1.0471	10.7800	35.0000	0.0040	2.2263	0.0354	65.7951
CASE 302	.	1.2023	10.7800	35.0000	0.0040	2.4119	0.0412	70.4193
CASE 303	.	1.3804	10.7800	35.0000	0.0040	2.5974	0.0478	74.9333
CASE 304		1.5488	10.7800	35.0000	0.0040	2.7829	0.0543	79.3412
CASE 305	8.5000	0.0001	17.6700	35.0000	0.0045	0.0000	0.0000	0.0000
CASE 306	8.6600	0.0001	17.6700	35.0000	0.0045	0.1273	0.0000	7.1239
CASE 307	8.7200	0.0001	17.6700	35.0000	0.0045	0.2547	0.0000	14.0500
CASE 308	8.7200	0.0001	17.6700	35.0000	0.0045	0.3820	0.0000	20.7863
CASE 309	8.8000	0.0001	17.6700	35.0000	0.0045	0.6367	0.0000	33.7200
CASE 310	8.8200	0.0017	17.6700	35.0000	0.0045	0.7640	0.0000	39.9316
CASE 311	8.0000	0.0058	17.6700	35.0000	0.0045	0.8913	0.0001	45.9818
CASE 312	8.6500	0.0174	17.6700	35.0000	0.0045	1.0187	0.0003	51.8769
CASE 313	8.5900	0.0331	17.6700	35.0000	0.0045	1.1460	0.0007	57.6228
CASE 314	8.5900	0.0407	17.6700	35.0000	0.0045	1.2733	0.0008	63.2250
CASE 315	8.5900	0.0513	17.6700	35.0000	0.0045	1.4007	0.0010	68.6889
CASE 316	8.5900	0.0537	17.6700	35.0000	0.0045	1.5280	0.0011	74.0195
CASE 317	8.5600	0.0646	17.6700	35.0000	0.0045	1.6553	0.0013	79.2217
CASE 318	8.7600	0.0776	17.6700	35.0000	0.0045	1.7827	0.0016	84.3000
CASE 319	9.0000	0.0003	17.6700	35.0000	0.0045	0.5093	0.0000	27.3405
CASE 320	8.8000	0.0000	14.7600	40.0000	0.0090	0.0000	0.0000	0.0000
CASE 321	8.8000	0.0026	14.7600	40.0000	0.0090	0.3049	0.0001	12.4889
CASE 322	8.5100	0.0178	14.7600	40.0000	0.0090	0.6098	0.0004	24.6732
CASE 323	8.4500	0.0661	14.7600	40.0000	0.0090	0.9146	0.0017	36.5639
CASE 324	8.5700	0.1698	14.7600	40.0000	0.0090	1.0366	0.0043	41.2403
CASE 325	8.5000	0.4266	14.7600	40.0000	0.0090	1.1585	0.0108	45.8721
CASE 326	8.5200	0.9120	14.7600	40.0000	0.0090	1.2805	0.0231	50.4599
CASE 327	8.4600	1.6218	14.7600	40.0000	0.0090	1.4024	0.0414	55.0043
CASE 328	8.4100	2.4547	14.7600	40.0000	0.0090	1.5244	0.0629	59.5059
CASE 329	8.3400	3.3884	14.7600	40.0000	0.0090	1.6463	0.0872	63.9653
CASE 330	8.2900	4.5709	14.7600	40.0000	0.0090	1.7683	0.1182	68.3832
CASE 331	7.8800	0.0011	17.2200	50.0000	0.0090	0.0000	0.0000	0.0000
CASE 332	8.0600	1.0471	17.2200	50.0000	0.0090	1.5679	0.0287	57.2604
CASE 333	8.0900	0.0661	17.2200	50.0000	0.0090	0.1307	0.0017	5.0328
CASE 334	8.0600	1.3183	17.2200	50.0000	0.0090	2.0906	0.0368	74.9333
CASE 335	8.0400	0.1349	17.2200	50.0000	0.0090	0.2613	0.0035	10.0158
CASE 336								
CASE 337	8.0300	0.2344	17.2200	50.0000	0.0090	0.3920	0.0061	14.9498
CASE 338	8.0300	0.3311	17.2200	50.0000	0.0090	0.5226	0.0087	19.8353
CASE 339	8.0500	0.7079	17.2200	50.0000	0.0090	1.0453	0.0190	38.9077
CASE 340	7.8500	0.0022	13.5500	50.0000	0.0090	0.0000	0.0001	0.0000
CASE 341	7.8800	0.0309	13.5500	50.0000	0.0090	0.0665	0.0010	2.0192
CASE 342	7.8800	0.0646	13.5500	50.0000	0.0090	0.1330	0.0021	4.0303
CASE 343	7.8800	0.0977	13.5500	50.0000	0.0090	0.1996	0.0032	6.0334
CASE 344	7.8800	0.1380	13.5500	50.0000	0.0090	0.2661	0.0046	8.0286
CASE 345	7.8800	0.1738	13.5500	50.0000	0.0090	0.3326	0.0058	10.0158
CASE 346	7.8800	0.2089	13.5500	50.0000	0.0090	0.3991	0.0070	11.9953
CASE 347	7.9700	0.2655	13.5500	50.0000	0.0090	0.4656	0.0082	13.9669
CASE 348	7.9500	0.2754	13.5500	50.0000	0.0090	0.5322	0.0092	15.9307
CASE 349	7.9600	0.3090	13.5500	50.0000	0.0090	0.5987	0.0103	17.8868
CASE 350	7.9400	0.3548	13.5500	50.0000	0.0090	0.6652	0.0119	19.8353

TABLE 5

AVS Determinations

Variable Identification and Units for Data Table

NAME$ Sediment identifier

DATE$ Date of the experiment

DRYWT   Dry weight of sediment extracted

AG2S   Weight of Ag_2S in sulfide trap

UMS_G $\mu mol/gm$ AVS

UMS_G1 $\mu mol/gm$ AVS - These were extractions after a cadmium titration was
               completed.

RATIO   Ratio of UMS_G1 to UMS_G

		NAME$	DATE$	DRYWT	AG2S	UMS_G	UMS_G1	RATIO
CASE	1	BRH	8/5/88	3.9554	0.1998	203.8500	.	.
CASE	2	BRH	9/22/88	2.1800	0.0789	146.0600	92.4600	0.6330
CASE	3	HR	7/11/88	11.8200	0.0312	10.6500	.	.
CASE	4	HR	7/22/88	5.8500	0.0211	14.5600	.	.
CASE	5	HR1	10/11/88A	10.5300	0.0350	27.9100	.	.
CASE	6	HR1	10/13/88A	7.1300	0.0426	24.1100	.	.
CASE	7	HR1	9/27/88	13.0700	0.0340	23.9900	.	.
CASE	8	HR1	9/27/88B	11.4800	0.0387	24.8800	.	.
CASE	9	LIB	7/11/88	8.9100	0.0339	15.3500	.	.
CASE	10	LIB	7/11/88	8.9200	0.0336	15.2100	.	.
CASE	11	LIB	7/13/88	6.7100	0.0237	14.2500	.	.
CASE	12	LIB	7/13/88	15.9300	0.0503	12.7500	.	.
CASE	13	LIB	7/13/88	15.8000	0.0467	11.9300	.	.
CASE	14	LIB	7/14/88	17.9200	0.0545	12.2700	.	.
CASE	15	LIB	7/15/88	7.9200	0.0279	14.2200	.	.
CASE	16	LIB	7/15/88	6.0500	0.0243	16.2100	.	.
CASE	17	LIB	7/18/88	13.0800	0.0431	12.6000	.	.
CASE	18	LIB	7/19/88	15.8000	0.0408	10.4200	.	.
CASE	19	LIB	7/7/88	11.5200	0.0400	13.9700	.	.
CASE	20	LIB	7/8/88	11.0100	0.0419	15.3500	.	.
CASE	21	LIB	8/1/88	.	.	14.4000	4.5000	0.3125
CASE	22	LIB1	7/24/88	16.2500	0.0581	14.4300	.	.
CASE	23	LIB1	8/2/88	7.1170	0.0228	12.9300	6.2100	0.4803
CASE	24	LIB1	9/20/88	12.6600	0.0238	7.5900	.	.
CASE	25	LIB1	9/23/88	10.7800	0.0305	11.4100	.	.
CASE	26	SS	7/18/88	40.0500	0.0313	3.1500	.	.
CASE	27	SS	7/19/88	41.1600	0.0302	2.9600	.	.
CASE	28	SS	7/8/88	18.7000	0.0101	2.1800	.	.
CASE	29	SS	8/3/88	11.5200	0.0090	3.1500	2.3700	0.7524
CASE	30	SS	8/4/88	15.1000	0.0079	2.1100	2.4400	1.1564
CASE	31	SS	9/23/88	25.2100	0.0199	3.1900	.	.
CASE	32	SS1	9/27/88	15.9400	0.0103	2.6100	.	.

TABLE 6

Comparison of Initial AVS and Cadmium Binding

Variable Identification and Units for Data Table

NAME$	Sediment identifier
NUM	Expt number
DATE$	Date of the experiment
AVS	Initial AVS at the start of the titration (μmol/gm)
CD_G	Binding capacity of the sediment (μmol Cd/g sediment

		NAME$	NUM	DATE$	AVS	CD_G
CASE	1	BRH	1.0000	8/5/88	203.8500	122.9768
CASE	2	BRH	2.0000	9/22/88	.	105.8089
CASE	3	HR	1.0000	7/12/88	.	12.4965
CASE	4	HR	2.0000	7/22/88	14.5600	6.3564
CASE	5	HR	3.0000	10/03/88	.	7.9552
CASE	6	LIB	1.0000	7/5/88	.	6.1573
CASE	7	LIB	2.0000	7/8/88	.	5.5622
CASE	8	LIB	3.0000	7/13/88	14.2500	2.2627
CASE	9	LIB	4.0000	7/13/88	12.7500	7.1214
CASE	10	LIB	5.0000	7/14/88	12.2700	8.1084
CASE	11	LIB	6.0000	8/1/88	.	3.8762
CASE	12	LIB	7.0000	8/2/88	12.9000	4.7734
CASE	13	LIB	9.0000	8/3/88	.	6.4904
CASE	14	LIB	10.0000	9/19/88	7.5900	1.5547
CASE	15	SS	1.0000	7/8/88	2.1800	0.9381
CASE	16	SS	2.0000	7/1/88	.	2.0620
CASE	17	SS	3.0000	7/14/88	.	1.0127
CASE	18	SS	4.0000	7/18/88	3.1500	0.7589
CASE	19	SS	5.0000	8/4/88	.	1.1768

TABLE 7

AVS in Long Island Sound Sediments[#]

Variable Identification and Units for Data Table

ID$	Sediment identifier
TABLE$	Table number in the reference from which the data were taken
T	Temperature °C
DEPTH1	Starting depth of the core slice (cm)
DEPTH2	Ending depth of the core slice (cm)
DEPTH	Average depth of the core slice (cm)
FES	Measured AVS in the slice (μmol/g)

[#][Aller, 1980]

	IDS	TABLES	T	DEPTH1	DEPTH2	DEPTH	FES
CASE 1	FOAM1	B1	20.0000	0.0000	1.0000	0.5000	7.5000
CASE 2	FOAM1	B1	20.0000	1.0000	2.0000	1.5000	11.0000
CASE 3	FOAM1	B1	20.0000	2.0000	3.0000	2.5000	8.1000
CASE 4	FOAM1	B1	20.0000	3.0000	4.0000	3.5000	12.0000
CASE 5	FOAM1	B1	20.0000	4.0000	5.0000	4.5000	23.0000
CASE 6	FOAM1	B1	20.0000	5.0000	6.0000	5.5000	20.0000
CASE 7	FOAM1	B1	20.0000	6.0000	7.0000	6.5000	18.0000
CASE 8	FOAM1	B1	20.0000	7.0000	8.0000	7.5000	13.0000
CASE 9	FOAM1	B1	20.0000	8.0000	9.0000	8.5000	11.0000
CASE 10	FOAM1	B1	20.0000	9.0000	10.0000	9.5000	12.0000
CASE 11	FOAM1	B1	20.0000	10.0000	11.0000	10.5000	11.0000
CASE 12	FOAM1	B1	20.0000	11.0000	12.0000	11.5000	7.2000
CASE 13	FOAM1	B1	20.0000	12.0000	13.0000	12.5000	8.4000
CASE 14	FOAM1	B1	20.0000	13.0000	14.0000	13.5000	6.6000
CASE 15	FOAM1	B1	20.0000	14.0000	15.0000	14.5000	7.2000
CASE 16	FOAM1	B1	20.0000	15.0000	16.0000	15.5000	10.0000
CASE 17	FOAM1	B1	20.0000	16.0000	17.0000	16.5000	10.0000
CASE 18	FOAM1	B1	20.0000	17.0000	18.0000	17.5000	10.0000
CASE 19	FOAM1	B1	20.0000	18.0000	24.0000	21.0000	7.5000
CASE 20	NWC-2	B7	13.2000	0.0000	1.0000	0.5000	0.6000
CASE 21	NWC-2	B7	13.2000	1.0000	2.0000	1.5000	9.0400
CASE 22	NWC-2	B7	13.2000	2.0000	3.0000	2.5000	13.7000
CASE 23	NWC-2	B7	13.2000	3.0000	4.0000	3.5000	16.5000
CASE 24	NWC-2	B7	13.2000	4.0000	5.0000	4.5000	14.0000
CASE 25	NWC-2	B7	13.2000	5.0000	6.0000	5.5000	9.3600
CASE 26	NWC-2	B7	13.2000	6.0000	7.0000	6.5000	10.6000
CASE 27	NWC-2	B7	13.2000	7.0000	8.0000	7.5000	0.0000
CASE 28	NWC-3	B8	3.0000	0.0000	1.0000	0.5000	0.0000
CASE 29	NWC-3	B8	3.0000	1.0000	2.0000	1.5000	2.1000
CASE 30	NWC-3	B8	3.0000	2.0000	3.0000	2.5000	19.0000
CASE 31	NWC-3	B8	3.0000	3.0000	4.0000	3.5000	23.3000
CASE 32	NWC-3	B8	3.0000	4.0000	5.0000	4.5000	15.2000
CASE 33	NWC-3	B8	3.0000	5.0000	6.0000	5.5000	8.4500
CASE 34	NWC-3	B8	3.0000	6.0000	7.0000	6.5000	5.7100
CASE 35	NWC-3	B8	3.0000	7.0000	8.0000	7.5000	4.8800
CASE 36	NWC-3	B8	3.0000	8.0000	9.0000	8.5000	3.1800
CASE 37	NWC-3	B8	3.0000	9.0000	10.0000	9.5000	1.7000
CASE 38	NWC-4	B9	19.0000	0.0000	1.0000	0.5000	0.0970
CASE 39	NWC-4	B9	19.0000	1.0000	2.0000	1.5000	7.3600
CASE 40	NWC-4	B9	19.0000	2.0000	3.0000	2.5000	16.9000
CASE 41	NWC-4	B9	19.0000	3.0000	4.0000	3.5000	18.6000
CASE 42	NWC-4	B9	19.0000	4.0000	5.0000	4.5000	12.0000
CASE 43	NWC-4	B9	19.0000	5.0000	6.0000	5.5000	10.1000
CASE 44	NWC-4	B9	19.0000	6.0000	7.0000	6.5000	6.8600
CASE 45	NWC-4	B9	19.0000	7.0000	8.0000	7.5000	
CASE 46	DEEP-1	B12	18.5000	0.0000	1.0000	0.5000	0.6200
CASE 47	DEEP-1	B12	18.5000	1.0000	2.0000	1.5000	4.4300
CASE 48	DEEP-1	B12	18.5000	2.0000	3.0000	2.5000	9.9200
CASE 49	DEEP-1	B12	18.5000	3.0000	4.0000	3.5000	11.0000
CASE 50	DEEP-1	B12	18.5000	4.0000	5.0000	4.5000	22.7000
CASE 51	DEEP-1	B12	18.5000	5.0000	6.0000	5.5000	30.7000
CASE 52	DEEP-1	B12	18.5000	6.0000	7.0000	6.5000	30.8000
CASE 53	DEEP-1	B12	18.5000	7.0000	8.0000	7.5000	23.3000
CASE 54	DEEP-1	B12	18.5000	8.0000	10.0000	9.0000	24.6000
CASE 55	DEEP-1	B12	18.5000	10.0000	12.0000	11.0000	16.0000
CASE 56	DEEP-1	B12	18.5000	12.0000	14.0000	13.0000	13.9000

TABLE 8

AVS in Sapelo Island Sediments[#]

Variable Identification and Units for Data Table

STA$	Sediment identifier
SEASON$	Table number in the reference from which the data were taken
DEPTH1	Starting depth of the core slice (cm)
DEPTH2	Ending depth of the core slice (cm)
FES_W	Measured AVS in the slice (weight %)
FES	Measured AVS in the slice (μmol/g)

[#][Reaves, 1984]

		STA$	SEASON$	DEPTH1	DEPTH2	FES_W	FES
CASE	1	MUD	W	0.000	1.000	0.006	1.875
CASE	2	MUD	W	1.000	2.000	0.005	1.563
CASE	3	MUD	W	2.000	3.000	0.012	3.750
CASE	4	MUD	W	3.000	4.000	0.066	20.625
CASE	5	MUD	W	4.000	5.000	0.079	24.688
CASE	6	MUD	W	5.000	6.000	0.058	18.125
CASE	7	MUD	W	6.000	7.000	0.061	19.063
CASE	8	MUD	W	7.000	8.000	0.051	15.938
CASE	9	MUD	W	8.000	9.000	0.047	14.688
CASE	10	MUD	W	9.000	10.000	0.060	18.750
CASE	11	MUD	W	10.000	11.000	0.069	21.563
CASE	12	MUD	W	11.000	12.000	0.035	10.938
CASE	13	MUD	W	12.000	13.000	0.039	12.188
CASE	14	MUD	W	13.000	14.000	0.046	14.375
CASE	15	MUD	W	14.000	15.000	0.036	11.250
CASE	16	MUD	S	0.000	1.000	0.075	23.438
CASE	17	MUD	S	1.000	2.000	0.058	18.125
CASE	18	MUD	S	2.000	3.000	0.090	28.125
CASE	19	MUD	S	3.000	4.000	0.097	30.313
CASE	20	MUD	S	4.000	5.000	0.120	37.500
CASE	21	MUD	S	5.000	6.000	0.229	71.563
CASE	22	MUD	S	6.000	7.000	0.165	51.563
CASE	23	MUD	S	7.000	8.000	0.153	47.813
CASE	24	MUD	S	8.000	9.000	0.164	51.250
CASE	25	MUD	S	9.000	10.000	0.193	60.313
CASE	26	MUD	S	10.000	11.000	0.176	55.000
CASE	27	MUD	S	11.000	12.000	0.222	69.375
CASE	28	MUD	S	12.000	13.000	0.201	62.813
CASE	29	MUD	S	13.000	14.000	0.222	69.375
CASE	30	MUD	S	14.000	15.000	0.220	68.750
CASE	31	CK	W	0.000	1.000	0.031	9.688
CASE	32	CK	W	1.000	2.000	0.088	27.500
CASE	33	CK	W	2.000	3.000	0.077	24.063
CASE	34	CK	W	3.000	4.000	0.073	22.813
CASE	35	CK	W	4.000	5.000	0.103	32.188
CASE	36	CK	W	5.000	6.000	0.113	35.313
CASE	37	CK	W	6.000	7.000	0.087	27.188
CASE	38	CK	W	7.000	8.000	0.053	16.563
CASE	39	CK	W	8.000	9.000	0.116	36.250
CASE	40	CK	W	9.000	10.000	0.133	41.563
CASE	41	CK	W	10.000	11.000	0.124	38.750
CASE	42	CK	W	11.000	12.000	0.124	38.750
CASE	43	CK	W	12.000	13.000	0.070	21.875
CASE	44	CK	W	13.000	14.000	0.090	28.125
CASE	45	CK	W	14.000	15.000	0.099	30.938
CASE	46	CK	S	0.000	1.000	0.019	5.938
CASE	47	CK	S	1.000	2.000	0.018	5.625
CASE	48	CK	S	2.000	3.000	0.039	12.188
CASE	49	CK	S	3.000	4.000	0.075	23.438
CASE	50	CK	S	4.000	5.000	0.115	35.938
CASE	51	CK	S	5.000	6.000	0.196	61.250
CASE	52	CK	S	6.000	7.000	0.155	48.438
CASE	53	CK	S	7.000	8.000	0.144	45.000
CASE	54	CK	S	8.000	9.000	0.135	42.188
CASE	55	CK	S	9.000	10.000	0.125	39.063
CASE	56	CK	S	10.000	11.000	0.103	32.188
CASE	57	CK	S	11.000	12.000	0.102	31.875
CASE	58	CK	S	12.000	13.000	0.088	27.500
CASE	59	CK	S	13.000	14.000	0.102	31.875
CASE	60	CK	S	14.000	15.000	0.103	32.188

DEVELOPMENT OF EXPERIMENTAL METHODOLOGY

A. Measuring Cadmium Activity

The most direct method to measure activity of a metal is to use an ion specific electrode (Orion Model 94-48). Ion selective electrodes measure the activity of the target species only - in this case Cd^{2+}). The determination of a reliable standard curve is the first step in the establishment of an analytical method. For the ion selective electrode this involves the measurement of relative potential in conjunction with a double function reference electrode as a function of activity, of the analyte (Cd^{2+}).

Because Cd^{2+} forms several stable complexes with Cl^-, the standardization cannot be done in seawater. A noncomplexing matrix of the same ionic strength as seawater, 0.7 M $NaNO_3$, was used. The results are shown in Fig. 1. The linear behavior of the potential versus cadmium activity to 0.1 mg/L with a slope of 28.2 is consistent with the Nernst equation. When a hydrogen carbonate buffer is added to mimic seawater conditions no significant change occurs in the standard curve (Fig. 2). If the 0.7 M $NaNO_3$ Cd^{2+} potentials are compared with those obtained for the same total cadmium in seawater, the Cd^{2+} fraction is about 5%, which is consistent with values calculated from simultaneous equilibrium models of cadmium speciation in seawater.

To further investigate the performance of the cadmium electrode, several titrations were performed using ions that are known to complex with Cd^{2+} and for which the formation constants are known. The results of a hydroxide titration are shown in Fig. 3. The value of $pK_1 = 9.75$ is consistent with literature values. The results of a chloride titration are shown in Fig. 4. The initial total cadmium concentrations are 10 and 1 mg/L. The value of 26.4 which is obtained for the formation constant of $CdCl^+$ is consistent with reported values.

B. Water Only Exposure - Bioassay Results

The above experiments demonstrated that the cadmium electrode was indeed measuring the cadmium activity in the systems of interest. During this period water-only bioassays were being performed at the Narraganset EPA Environmental Research Lab (ERL) to determine the total

cadmium (Cd_T) LC_{50} for the organism, <u>Ampelisca</u> <u>abdita</u>, that was to be used in the sediment exposure studies. The results are shown in Fig. 5 for both the definitive and range finding experiments.

Following this preliminary work, total cadmium samples bracketing the LC_{50} values of 0.32 - 0.55 mg/L were prepared in seawater. The Cd^{2+} concentration was determined by the electrode, while total cadmium was measured by anodic stripping voltametry and graphite furnace atomic absorption spectrometry using an ammonium phosphate matrix modification procedure. The results are shown in Fig. 6. The data from the two methods are combined in Fig. 7 and the ratio of cadmium activity to total cadmium concentration is found to be $Cd^{2+}/Cd_T = 0.051$. This result is used to convert the total cadmium concentrations in the water only exposure experiment to the cadmium activity.

C. Interstitial Water Diffusion Sampler

The final task that had to be completed before sediment Bioassay studies could be undertaken was the design and construction of a suitable sampling device. The final design of the peeper is shown in Fig. 8. The device is constructed of acrylic material. The body is 1.5 in. thick with three 0.5 in. holes bored at six different levels 0.75 in. apart. A solid 0.25 in. base plate is fused to the back. The front contains a nucleopore membrane, on top of which is a 20 mil polyethylene gasket and a 0.5 in. cover plate. The entire assembly is held together with six 0.25 in. PVC nuts and bolts. The volume of each cell is 5.0 mL, which provides the necessary minimum sample volume of 15 mL required for the electrode measurement, at each sampling level. This sample volume size was determined by experiment to be adequate for reliable measurement.

The interstitial water sampling device depends upon diffusion across the membrane to measure the interstitial water concentrations. In order to establish the equilibration time for transfer across the membrane the cells of the assembled peeper were filled with distilled water. The device was then immersed in seawater. The cells were sampled periodically and the conductivity of the sample was measured. The results are shown in Fig. 9. As can be seen the 12 micron membrane

equilibrated quite rapidly. However even the 1 micron membrane reached equilibrium within 24 hours. Since this equilibration time is well within the time scale of the toxicity experiments, it was decided to use this porosity membrane in subsequent experiments.

D. Initial Toxicity Experiments

When sediment exposure experiments are performed it is necessary to be able to predict the interstitial cadmium concentration that will be obtained from initially combining a quantity of a cadmium salt with measured amount of reference sediment and seawater. To provide this information solutions were prepared with total cadmium concentrations of 200 to 6000 ppm. Each of these contained 1000 mL of control sediment (55% water). The peepers were then placed in the settled sediment-water systems. After two days the cadmium concentration was measured as a function of depth. The results are shown in Fig. 10. Initially it was believed that the interstitial cadmium concentration was being controlled by simple partitioning between a sediment bound component and the aqueous component. The amount of cadmium used in preparing the systems for the interstitial water Bioassay experiments was determined from these results. The attempt was made to bracket the cadmium LC_{50} obtained in the water only exposure. However, in all of the systems the final interstitial cadmium concentration was not sufficient to produce mortality.

The first bioassay results indicated that an additional process was operating in the cadmium-sediment water system. The observation of a yellow precipitate (probably CdS) when preparing the more concentrated systems suggested that sediment generated sulfide was depressing the aqueous cadmium concentration during the actual exposure.

E. Development of Acid Volatile Sulfide Extraction Method

The most labile sulfide component of sediments is the acid volatile sulfide (AVS). It is the solid phase sulfide in the sediment that is soluble in cold acid. The measurement technique is to convert the sulfides to $H_2S(aq)$, purge it with a gas, and trap it [see Morse et al., 1987 for a review]. A 500 mL Erlenmeyer flask reaction vessel fitted with a three-hole stopper is followed by three sequentially connected 250 mL Erlenmeyer flask trapping vessels. The first is a chloride trap

with 200 mL of pH 4 buffer (0.05M potassium hydrogen phthlate) to prevent chloride carry over. The second and third traps contain 200 mL of a 0.1M silver nitrate solution for trapping H_2S. The four flasks are connected with airtight appropriately shaped glass and Tygon tubing.

A nitrogen gas flow allows continuous purging of the system. In order to prevent oxidation the gas flows through an oxygen-scrubbing system consisting of a vanadous chloride solution in the first scrubbing tower and the matrix of the analyte (seawater) in the second tower. Vanadous chloride is prepared using four grams of ammonium metavanadate boiled with 50 mL of concentrated hydrochloric acid and diluted to 500 mL. Amalgamated zinc, prepared by taking about 15 grams of zinc, covering it with deionized water and adding 3 drops of concentrated hydrochloric acid before adding a small amount of mercury to complete the amalgamation, is then added to the vanadous chloride solution.

The sediment sample (10-15 grams of wet sediment) or standard to be analyzed is placed in the reaction vessel after the entire system has been purged with nitrogen for about an hour. The system is again purged for 5-10 minutes, and deaerated 6M hydrochloric acid is added from a thistle tube to achieve a final concentration in the vessel of 0.5M. The system is run at room temperature for one hour which has been found to be sufficient to complete the extraction. Fig. 11 present the results of an experiment in which the time course of AVS extraction from a sediment (Long Island Sediment) is followed. It is clear that one hour is sufficiently long for the extraction to be completed.

F. Figure Captions

Figure. 1 Cadmium electrode calibration curve in 0.7M $NaNO_3$, pH = 8 corresponding to the ionic strength of seawater. Slope = 28.2. Sensitivity of the electrode is 0.1 mg/L

Figure. 2 Cadmium electrode calibration curve in 0.7M $NaNO_3$, 0.002M $NaHCO_3$, pH = 8, corresponding to the ionic strength and bicarbonate concentration of seawater. Slope = 28.2. Sensitivity of the electrode is 0.1 mg/L.

Figure 3. Hydroxide titration to determine pK_1 for the reaction: $Cd^{2+} + OH^- <-> CdOH^+$.

Figure 4. Chloride titrations to determine K_1 for the reaction: $Cd^{2+} + Cl^- <-> CdCl^+$.

Figure 5. Ampelisca Toxicity Test: Water Only Exposure. LC50 = 0.32 mg Cd/L (top) and 0.55 mg Cd/L

Figure 6. Cadmium concentrations in the toxicity test samples (mg Cd/L) determined using a polaragraphic method (top) and using an AA graphite furnace method (bottom) versus electrode concentration (mg Cd^{2+}/L).

Figure 7. Cadmium concentrations in the toxicity test samples (mg Cd/L) determined using both a polaragraphic and AA graphite furnace method versus electrode concentration (mg Cd^{2+}/L). Regression line is Cd^{2+} = 0.051 Cd, which implies a K_1 of the chloride reaction of K_1 = 26.4 M_{-1}.

Figure 8. Design of diffusion sampler "peeper"

Figure 9. Time to equilibrium for membrane transfer.

Figure 10. Initial interstitial water sampling results. Static exposure.

Figure 11. Time course experiment for AVS extraction of Long Island Sound sediment.

Figure. 1 Cadmium electrode calibration curve in 0.7M NaNO3, pH = 8 corresponding to the

ionic strength of seawater. Slope = 28.2. Sensitivity of the electrode is 0.1 mg/L

Figure. 2 Cadmium electrode calibration curve in 0.7M NaNO₃, 0.002M NaHCO₃, pH = 8, corresponding to the ionic strength and bicarbonate concentration of seawater. Slope = 28.2. Sensitivity of the electrode is 0.1 mg/L.

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PEEPER DESIGN
DIMENSIONS (CM)
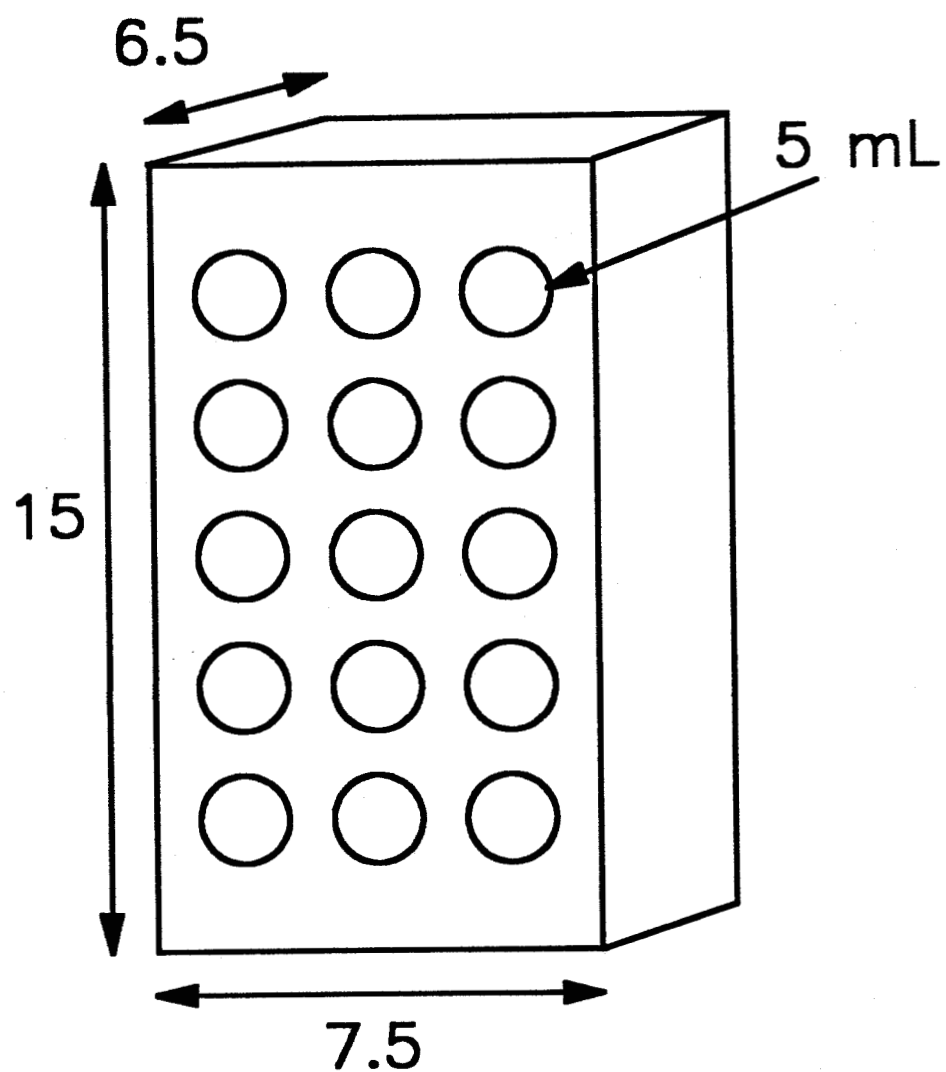
Figure 8. Design of diffusion sampler "peeper"
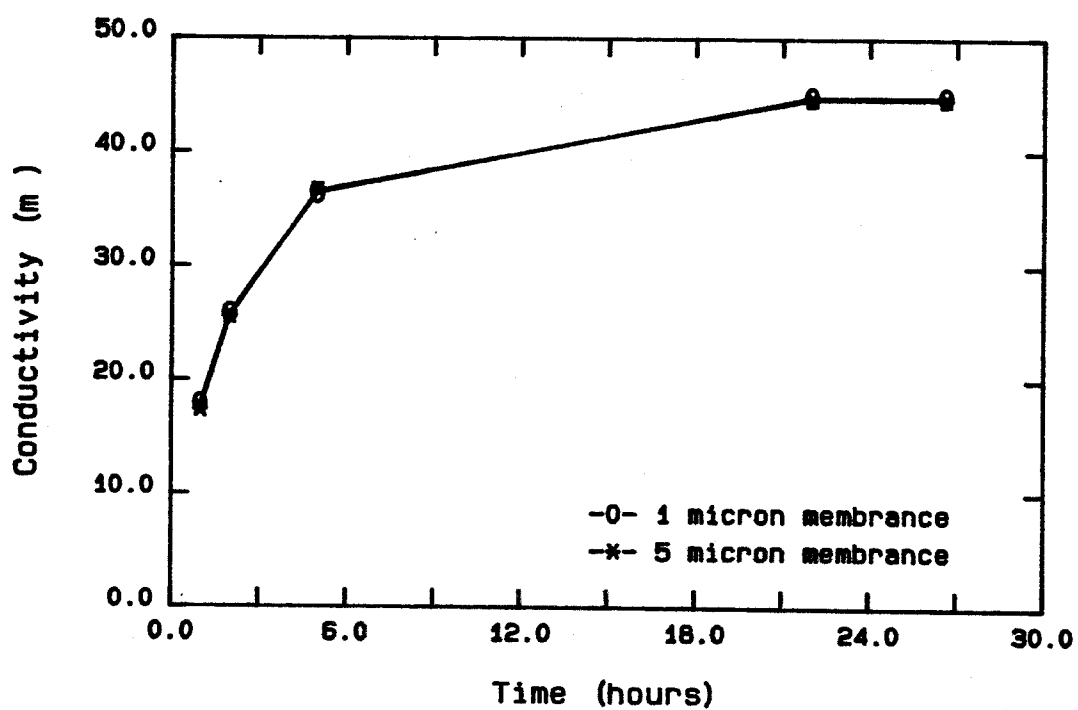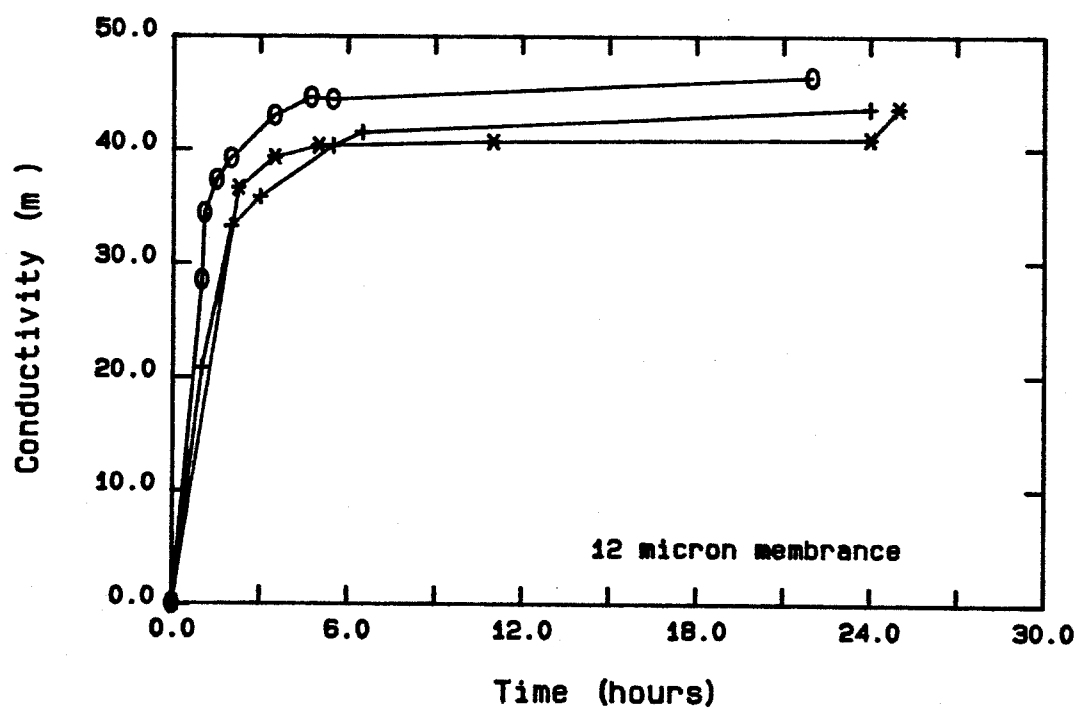
Figure 9. Time to equilibrium for membrane transfer.
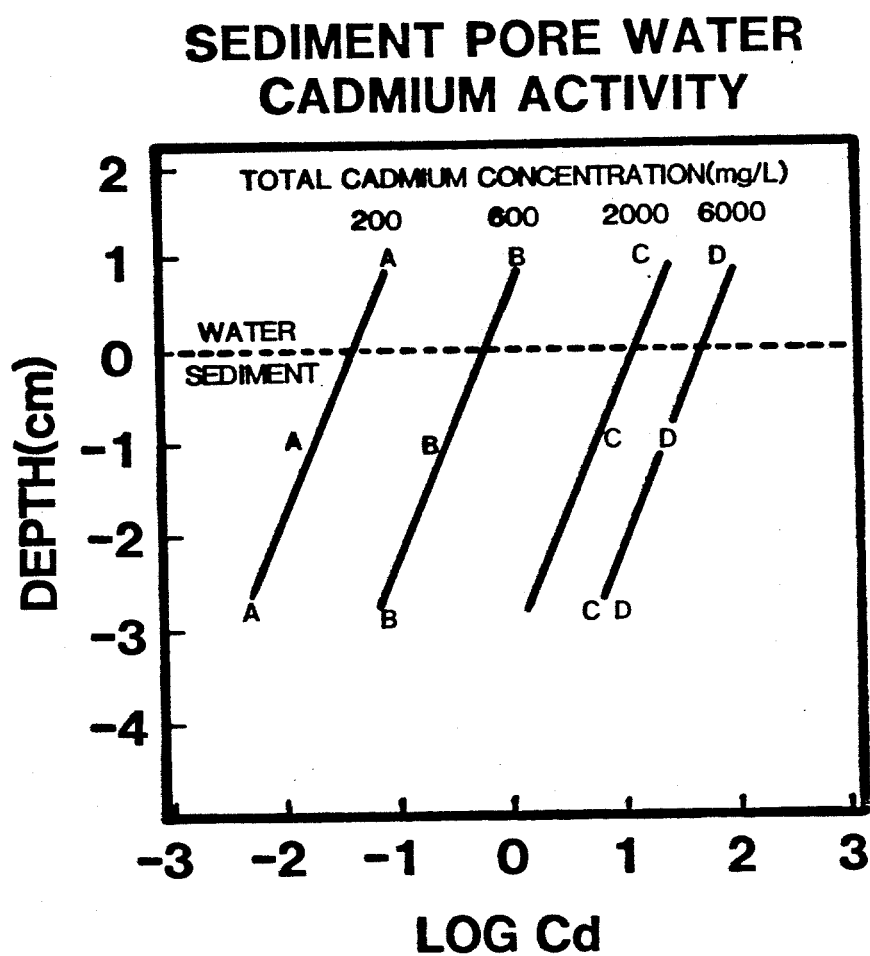
Figure 10. Initial interstitial water sampling results. Static exposure.
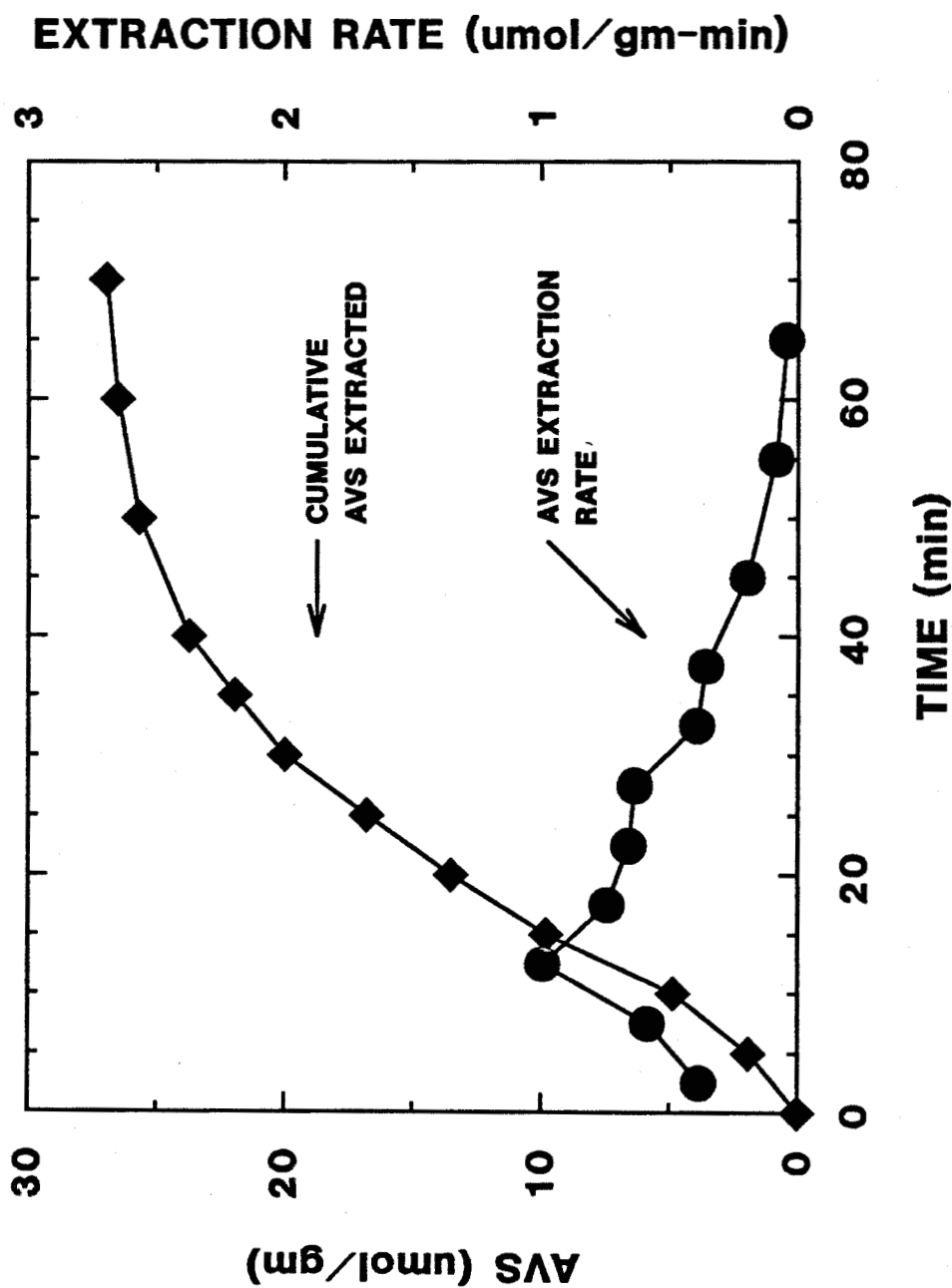
Figure 11. Time course experiment for AVS extraction of Long Island Sound sediment.

DEVELOPMENT AND VERIFICATION OF A KINETIC

MODEL OF POLLUTANT DESORPTION

FROM DREDGE SEDIMENT AND SEWAGE SLUDGE

I. Introduction

The purpose of this project is to develop a kinetic model of heavy metal desorption from sludges and sediments. This reaction significantly influences the fate of these chemicals during the ocean disposal of sludge and dredged sediments since the rapidity with which metals desorb determines, to a large extent, their ultimate fate. If desorption is rapid then the chemical is primarily in the aqueous phase and water column transport determines its fate. However if the metal remains in particulate form then settling and sedimentation will occur. Thus the rate and degree of desorption greatly influence the fate of these chemicals.

Significant progress has been made in the development of the models for this reaction. An equilibrium desorption model for reversibly bound heavy metals and organic chemicals was developed in a previous project (Di Toro and Mahony, 1986). The model describes the initial desorption of heavy metals from sewage sludge and Black Rock Harbor sediment upon mixing with seawater at various particle concentrations. Only a small fraction of the total particulate metal initially desorbes. Consecutive desorptions confirmed that only a small fraction was available during short term (1 hour) desorptions. However, it was noted that although desorption of the reversibly bound (or labile) metal fraction was rapid there was a distinct and slower reaction which also released particle bound metal into the aqueous phase. The time scales of this reaction is days rather than hours. This slow release phenomena, which had been observed experimentally by Rohatgi and Chen (1975) for digested sewage sludge, was confirmed by us for Black Rock Harbor sediment. Rohatgi and Chen speculated that the release might be due to an oxidation reaction which liberated heavy metals that either were bound to organic carbon or which were present as metal sulfides.

These observations, and our own experimental experience, lead us to propose a three component model of heavy metal desorption. Particulate metal was assumed to exist as either reversibly sorbed metal, for which the reversible partition coefficient follows the particle interaction model which we had developed in the previous project, and two other com-

ponents. A resistant component which initially is not desorbed but is gradually released over a period of five to ten days; and a refractory fraction which resists release for the duration of the experiment. This model was fit to Rohatgi and Chen's data and it provides a reasonable fit to the observations. An example is shown in fig. 1.

However, Rohatgi and Chen's experiments could not be used to distinguish between a number of other possible models that could easily fit the data as well. For example it is possible that the increase in dissolved concentration of metals during the experiment is due to slow, reversible, desorption kinetics. That is, it is possible that the desorption reaction for these particles takes a number of days before it reaches equilibrium so that the slow release is just due to the slowness of the desorption reaction. Desorption kinetics which are initially rapid but are followed by a slow phase have been observed for hydrophobic organic chemicals (Karickhoff, 1980).

Alternately it may be that the partition coefficient is decreasing during the experiment due to a change in particle properties. If the particle surface properties are being altered by exposure to oxygenated seawater during the experiment then the desorption reaction might still be rapid but it is adjusting to the slowly changing surface properties of the particles. The oxidation of particlulate reactive organic carbon would influence the partitioning in this way.

The purpose of this research project is to experimentally distinguish between these possibilities and to determine, to the extent possible, the mechanism responsible for the slow release of metals and to incorporate any necessary changes into the desorption model. The experiments conducted to date, using Black Rock Harbor sediment and two digested sewage sludges from the Bergen County and Ridgewood sewage treatment plants, appear to confirm the three component model as originally formulated. It appears that the slow release of metals are from the fraction of the metal which is initially present as particulate metal sulfides. These are released as the particulate sulfides is oxidized to sulfate in the reactor. An initial experiment in sulfate free seawater exhibited an increase in sulfate over time confirming the oxidation of sulfide to sulfate. Additionally, an anaerobic reactor, for

2

which nitrogen gas bubbling was substituted for oxygen containing air bubbling, exhibited no increase in dissolved metal over time. Parallel experiments with radiotagged metal appear to confirm this interpretation although some short term (less than one day) effects are still to be explained.

Hence the data appears to confirm the three component desorption kinetic model. It remains to actually fit these data to the model equations in order to obtain the model parameters. The final version would then be applicable to the evaluation of the fate of heavy metals during the ocean disposal of sludges and dredged sediments.

II. Experimental Design and Results to Date

The experiments are all conducted in small (350 mL) reaction vessels. Metal free seawater and sludge or sediment particles are initially added. The reactors are kept aerobic by bubbling filtered air and are mixed using magnetic stirring. Duplicate reactors at two particle concentrations, 300 and 3000 mg/L, are used. A particle free control reactor which receives the same air, stirring, and sampling, is monitored to detect possible contamination. At various times during the experiment samples are taken and analyzed for total and dissolved metal (the separation is by centrifugation). The duration of the experiment is twenty to thirty days.

Fig. 2 presents the results obtained for copper from Black Rock Harbor sediment and Bergen County sewage sludge for two particle concentrations (300 and 3000 mg/l). The log scales for the concentration are increased by a factor of ten for the 3000 mg/L reactor so that the results for both reactors can be directly compared. The increase in dissolved copper concentration is approximately one order of magnitude for both particle types with the larger dissolved concentrations associated with the smaller particle concentration. This is a result of the decreased fraction of the metal that reversibly partitions to the particles at lower particle concentrations. Fig. 3 presents the results for zinc and cadmium for Black Rock Harbor sediment. Again the release increases by approximately an order of magnitude. However, the chromium

results in fig. 4 show no significant increase for either Black Rock
Harbor sediment or Bergen County sludge. The significance of this fact
is discussed below.

Changes in pH and total organic carbon (TOC) are shown in fig. 5.
For Black Rock Harbor sediment the pH and TOC are essentially constant.
For Bergen County sludge the pH increases slightly during the first day
and stayed approximately constant thereafter. Although this may have
affected the reversible partition coefficient during this time (it would
increase with increasing pH) the release continues during the period of
constant pH. The TOC decreased from 400 (40) mgC/L to 200 (20) mgC/L in
the 3000 (300) mg/L reactor during the experiment. However the release
patterns of metals is similar for Black Rock Harbor sediment and Bergen
County sludge. Since no change in TOC or pH was observed for Black Rock
Harbor sediment, it is unlikely that the pH and TOC changes were respon-
sible for the metal release.

The results of an anaerobic reactor experiment are shown in fig. 6.
The arrangement is the same as the aerobic reactor, the only difference
is that nitrogen gas is substituted for the air that is bubbled through
the reactors. As can be seen the dissolved copper concentration stayed
constant for Black Rock Harbor sediment and the two sludges. The TOC
also remained constant as expected since the experiment did not last
long enough to initiate significant anaerobic breakdown of the sludges.
Thus the presence of oxygen is clearly necessary for the slow metal
release to occur.

The fact that copper, cadmium, and zinc are slowly released while
chromium concentrations are constant is consistent with the hypothesis
that the slow release of metals is due to the oxidation of particulate
metal sulfides. The solubility of these metal-sulfides is very low as
indicated below (Lindsay, 1979):

Solubility of MeS	Log Ksp
CuS (covellite)	−36.10
CdS (greennokite)	−27.07
ZnS (wurtzite)	−22.5

However no Cr(III) sulfide solid phase is reported in tabulations of sulfide mineral solubilities (Naumov et al., 1974).

A possible approach to a direct verification that particulate sulfide is being oxidized is to monitor the oxidation end product, sulfate, and observe its concentration in time. An increase in sulfate would indicate that reduced sulfur, presumably sulfide, was being oxidized in the reactor. The experiment is conducted in sulfate-free artificial seawater so that the large naturally occurring sulfate background does not obscure the increase. The results are shown in fig. 7. The upper panel presents the actual observations. The initial sulfate concentration is due to the sulfate in the supernatant of the Black Rock Harbor sediment stock which was added at the start of the experiment. Future experiments will separate the particles from the supernatant. The bottom panel presents the excess sulfate, defined as the difference between that initially present and that observed at the indicated time. It is interesting to note that the pattern of sulfate release is similar to that observed for the metal release.

In addition to measurements of the total and dissolved metal concentrations over time additional parallel experiments were conducted with radiotagged metals. The purpose of these experiments was to examine the question of the time scale of adsorption and the possible variation of the partition coefficient over time. The kinetic experiment used the same reactor setup. After the particles were added the reactor was tagged with radioactive metal. The total and dissolved radiotagged metal was monitored in time. Changes in the distribution between total and dissolved metal could be due to either slow adsorption kinetics or changes in the adsorption partition coefficient. But the absence of change would eliminate both mechanisms as significantly contributing to the release phenomena.

The results from these kinetic experiments are shown in fig. 8 for zinc. The Bergen County sludge results indicate that very little change occurred in the dissolved concentration suggesting that the variation of TOC did not significantly change the partitioning. However the Black Rock Harbor sediment results indicated a substantial increase in dissolved concentration and a decrease in total concentration that is

attributed to the accumulation of sediment particles on the walls of the reactor. However the changing total concentration casts some doubt on the validity of the experiment so we plan to repeat it.

The results for cadmium are shown in fig. 9. With the exception of the data for less than one day, the dissolved cadmium concentration remained constant for the duration of the experiment for both Black Rock Harbor sediment and Bergen County sludge.

These experiments do not yield a completely consistent interpretation. However they do eliminate one possible model - that the adsorption and desorption kinetics are slow and reversible. If sorption is slow but ultimately reversible then for an adsorption experiment the dissolved concentration should initially be large, since adsorption has not yet had an opportunity to occur, and it should decrease with time. For the experiments where changes were observed the reverse pattern was observed so that slow reversible sorption kinetics appear to be ruled out.

In order to discriminate between adsorption kinetics and partition coefficient changes, an additional set of parallel experiments were performed in order to examine if the partition coefficient is varying in time. A parallel reactor was used which was not initially tagged with radioactive metal. Rather, at various times during the experiment a small sample was taken. This sample was then spiked with a small amount of radioactive metal. The sample was agitated for one hour after which the total and dissolved radioactive metal concentration was determined. Following the adsorption step, a desorption step was performed in order to examine the behavior of the reversibly sorbed metal. If the distribution of total and dissolved metal was changing with time, that would indicate that the partition coefficients were changing with time.

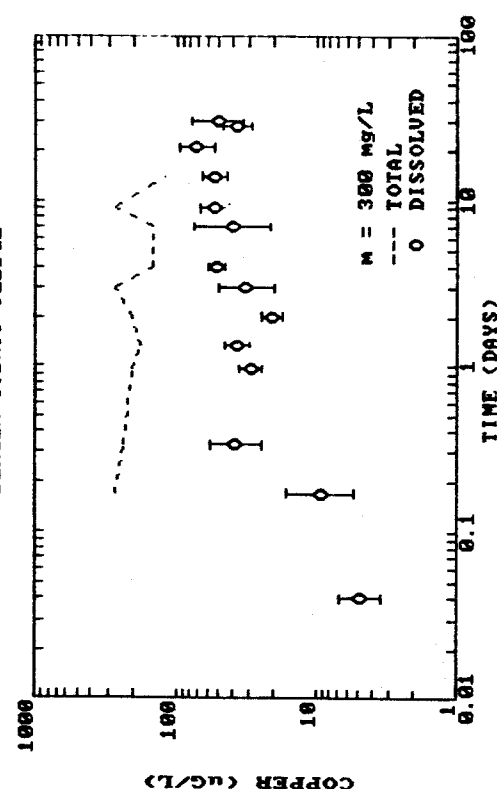The results from these spiking experiments are shown in fig. 10 for zinc. With the exception of the changing adsorption partition coefficient for Black Rock Harbor sediment, the other partition coefficients are constant. It is interesting that the desorption partition coefficient is constant for both Black Rock Harbor sediment and Bergen County sludge.

The results of the spiking experiments for cadmium are shown in fig. 11. Once again the partition coefficients appear to be quite constant for times greater than one day. But both the adsorption and desorption partition coefficients are changing initially.

The results of the kinetic and spiking experiments are not consistent with a single explanation. On the one hand, the Bergen County sludge zinc kinetic and the spike adsorption-desorption data, the Black Rock Harbor sediment spike desorption data, and both the kinetic and spike adsorption-desorption Black Rock Harbor sediment and Bergen County sludge cadmium data for time greater than one day suggest that no partition coefficient changes are occurring since the dissolved concentrations are essentially constant. However, the Black Rock Harbor sediment zinc kinetic and spike adsorption data, and all the less than one day cadmium data, suggest that something was changing during these time periods. Additional experiments are planned to investigate the cause of these unexpected and as yet unexplained results.

III. Future Directions

The major focus of this portion of the research will be to complete the development of the kinetic model for metal desorption from sediments and sludges. The reactor data will be fit to the model equations to estimate the parameters. Additional radiotag experiments will be performed in an attempt to understand the somewhat anomalous results described above. However the focus of the work will be to complete the development with a minimum of experimental effort so that the Sediment Criteria work can begin. A project report will be written that includes all the experimental data as well as the modeling results. A journal article will also be prepared.

References

[1] Di Toro, D.M. and Mahony, J.D. (1986): An Experimental and
     Modeling Study of the Adsorption and Desorption of Heavy
     Metals and Organic Chemicals with Applications to Sewage
     Sludge and Dredged Sediments in the Marine Environment.
     Final Report. Environmental Engineering and Chemistry Dept.
     Manhattan College, Bronx, NY.

[2] Karickhoff, S.W. (1980): Sorption Kinetics of Hydrophobic
     Pollutants in Natural Sediments. In: Contaminants and
     Sediments, pp. 193-205. Editor: R.A. Baker. Ann Arbor
     Sci., Ann Arbor, Mich.

[3] Lindsay, W.L. (1979): Chemical Equilibria in Soils. J.
     Wiley & Sons, New York,N.Y.

[4] Naumov, G.B., Ryzhenko, B.N. and Khodakovsky, I.L. (1974):
     Handbook of Thermodynamic Data PB-226-722. US Geological
     Survey, Water Res., Menlo Park, CA 94025.

[5] Rohatgi, N. and Chen, K.Y. (1975): Transport of trace
     metals by suspended particulates on mixing with seawater.
     J. Water Pollut. Control Fed. 47: pp. 2298-2316.

FIGURE CAPTIONS

1. Experimental data (Rohatgi and Chen, 1975) and the three component model fit for cadmium and chromium.

2. Total and dissolved copper concentrations versus time for Black Rock Harbor sediment and Bergen County sludge at 3000 mg/L (left side) and 300 mg/L (right side). Control reactor concentrations (C) are also shown.
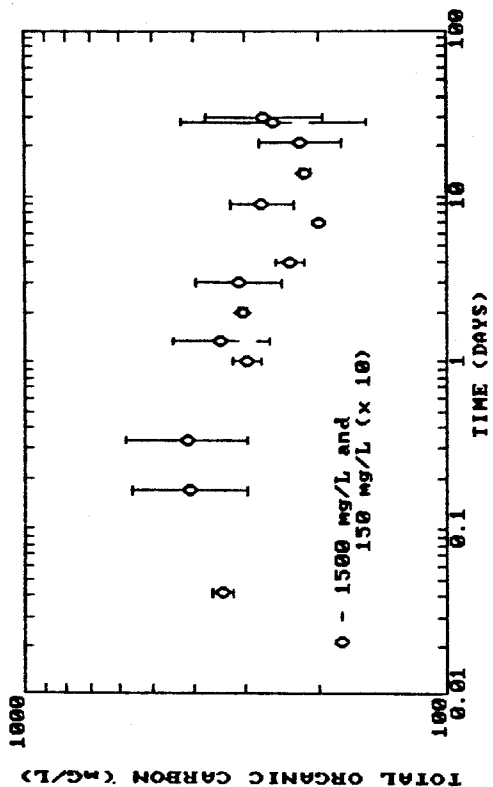
3. Total and dissolved zinc (top) and cadmium (bottom) concentrations versus time for Black Rock Harbor sediment and Bergen County sludge at 3000 mg/L (left side) and 300 mg/L (right side).

4. Total and dissolved chromium concentrations versus time for Black Rock Harbor sediment and Bergen County sludge at 3000 mg/L (left side) and 300 mg/L (right side).

5. pH (top) and Total Organic Carbon (bottom) versus time for Black Rock Harbor sediment (left) and Bergen County sludge (right) reactors.
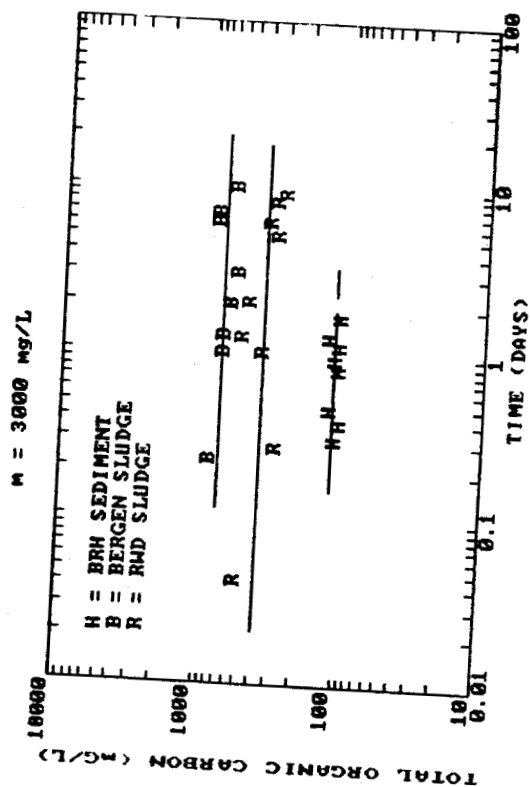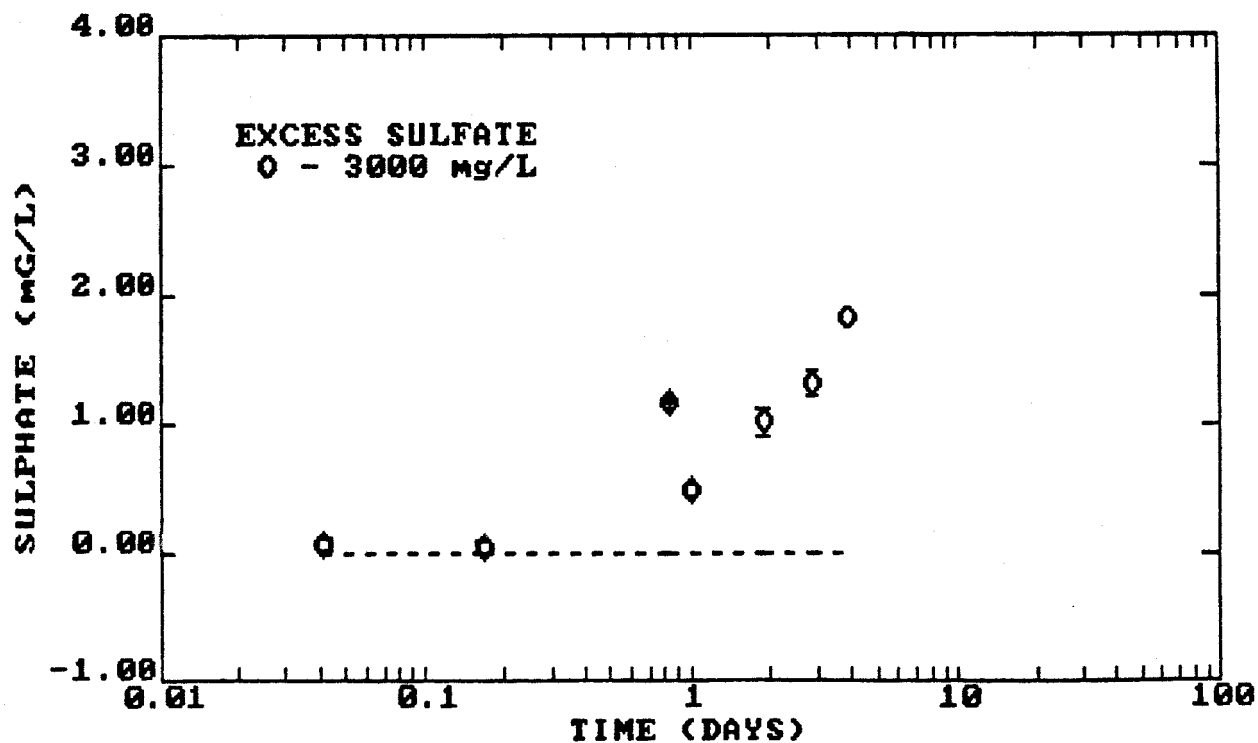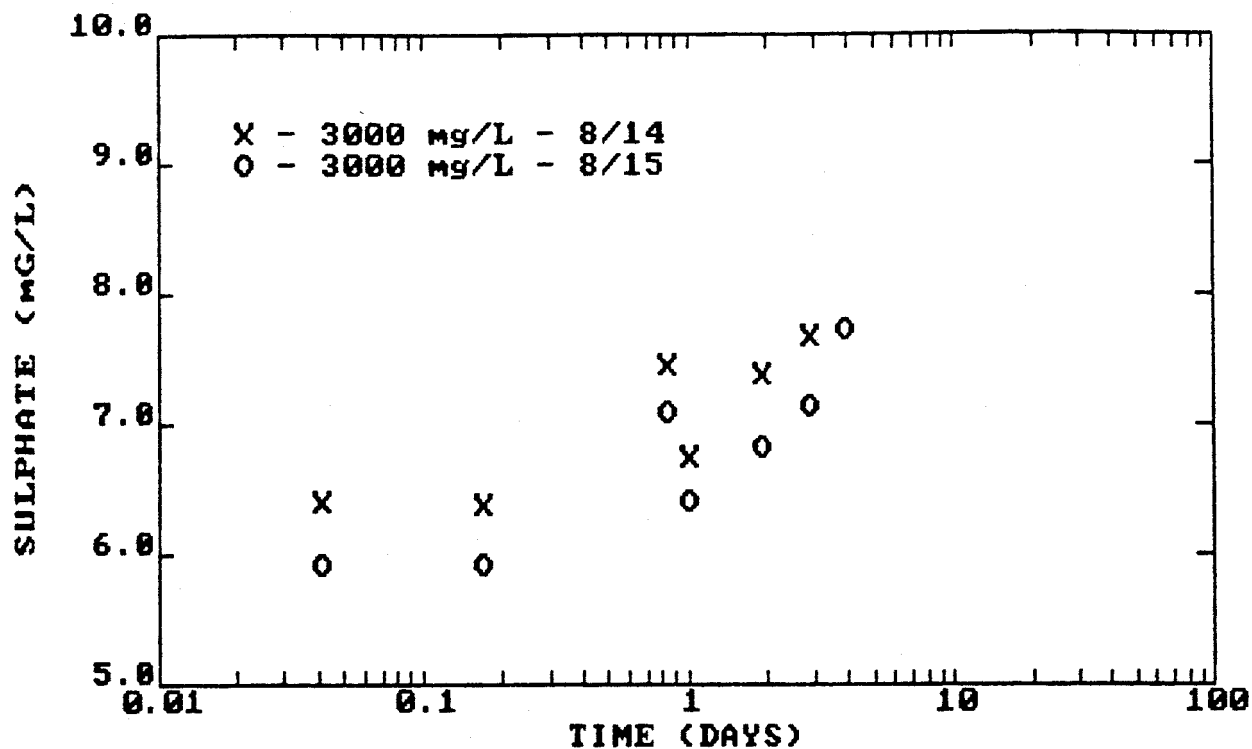
6. Anaerobic Reactor dissolved copper concentrations versus time for Black Rock Harbor (top left), Ridgewood (bottom left) and Bergen County (top right). Total organic carbon concentrations versus time for the three reactors are also shown (bottom right).
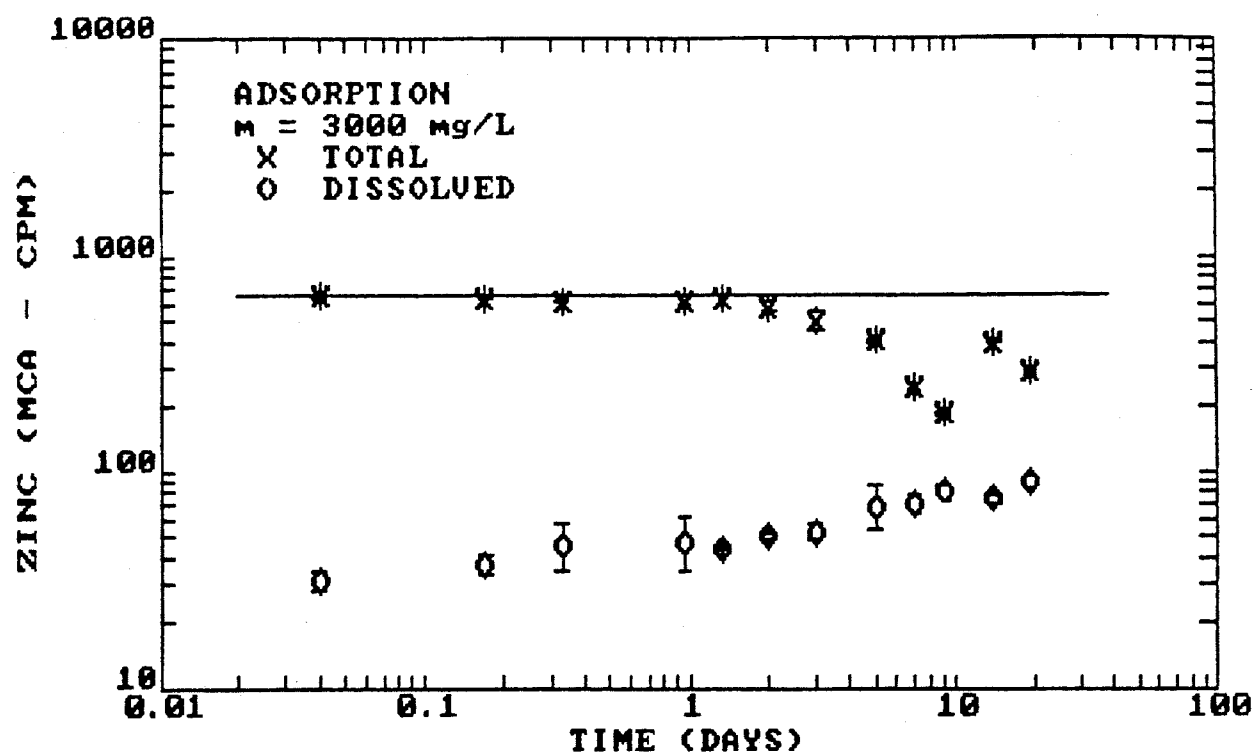
7. Sulfate (top) and excess sulfate (bottom) concentration versus time for Black Rock Harbor sediment.

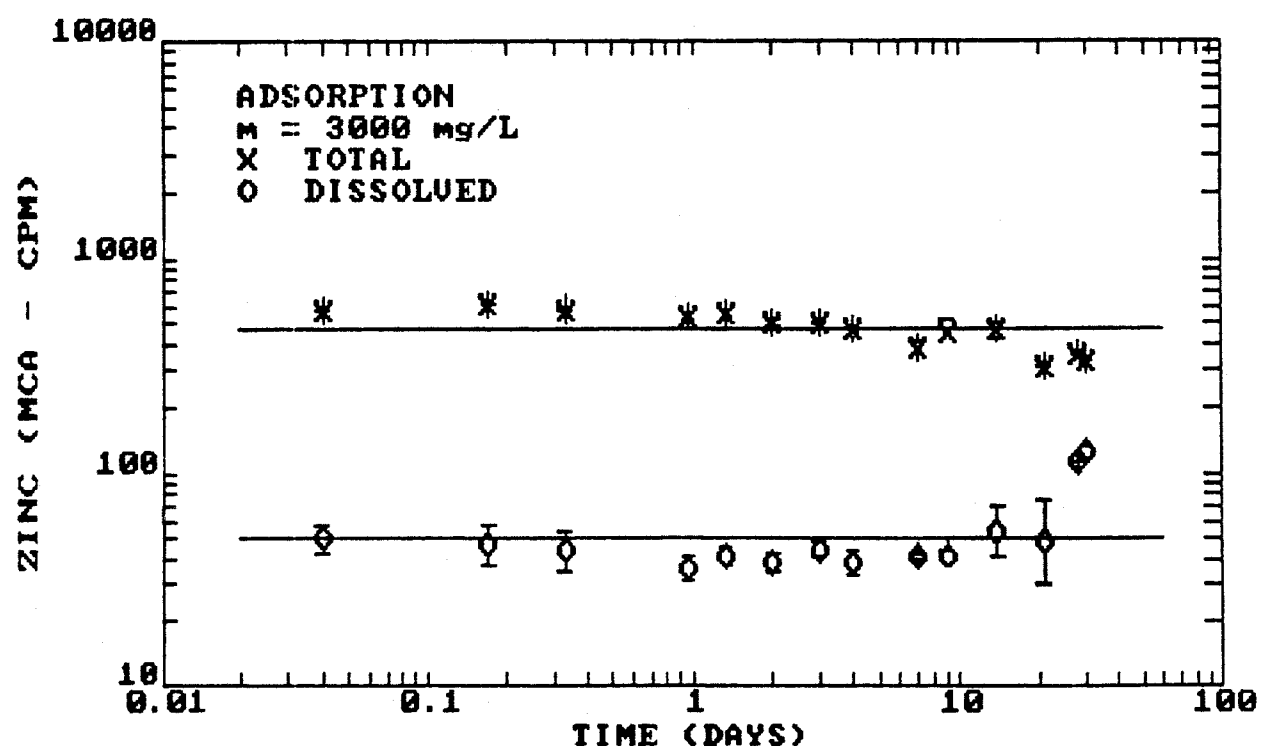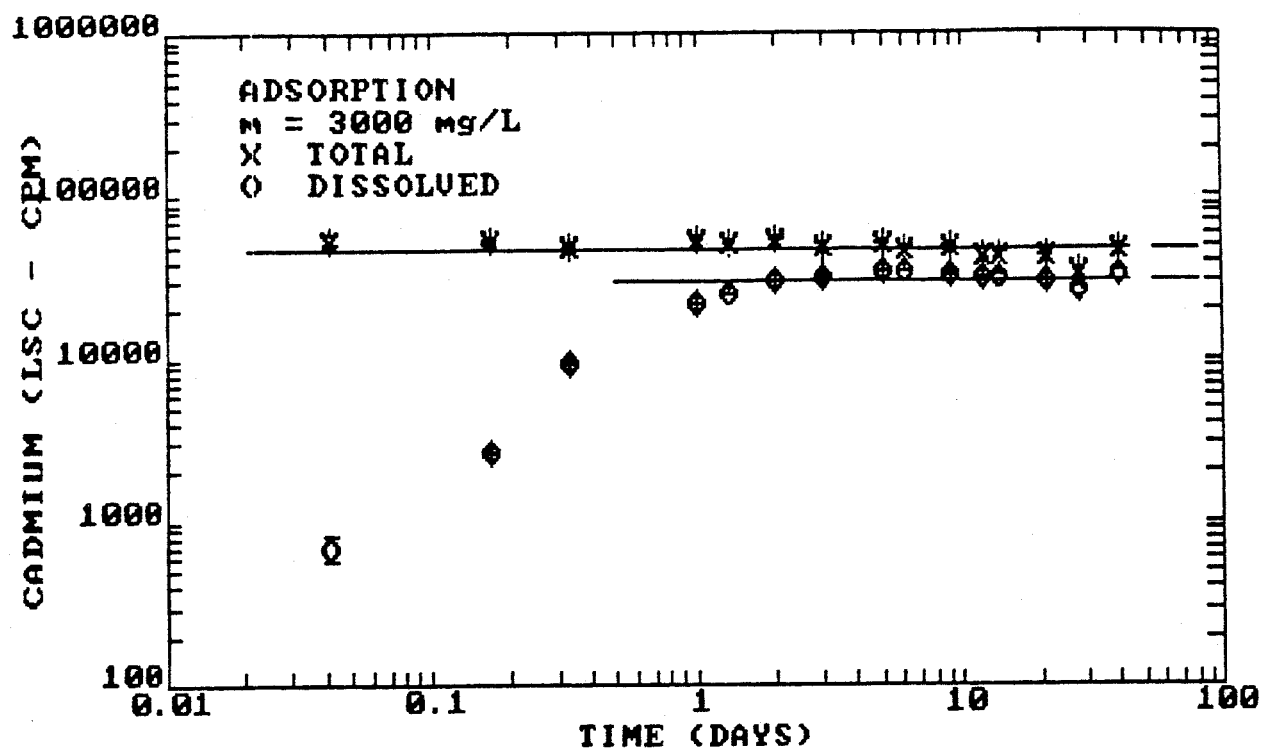8. Concentration of total and dissolved radioactive zinc versus time. Radioactive zinc is added at the start (t=0) of the experiment.

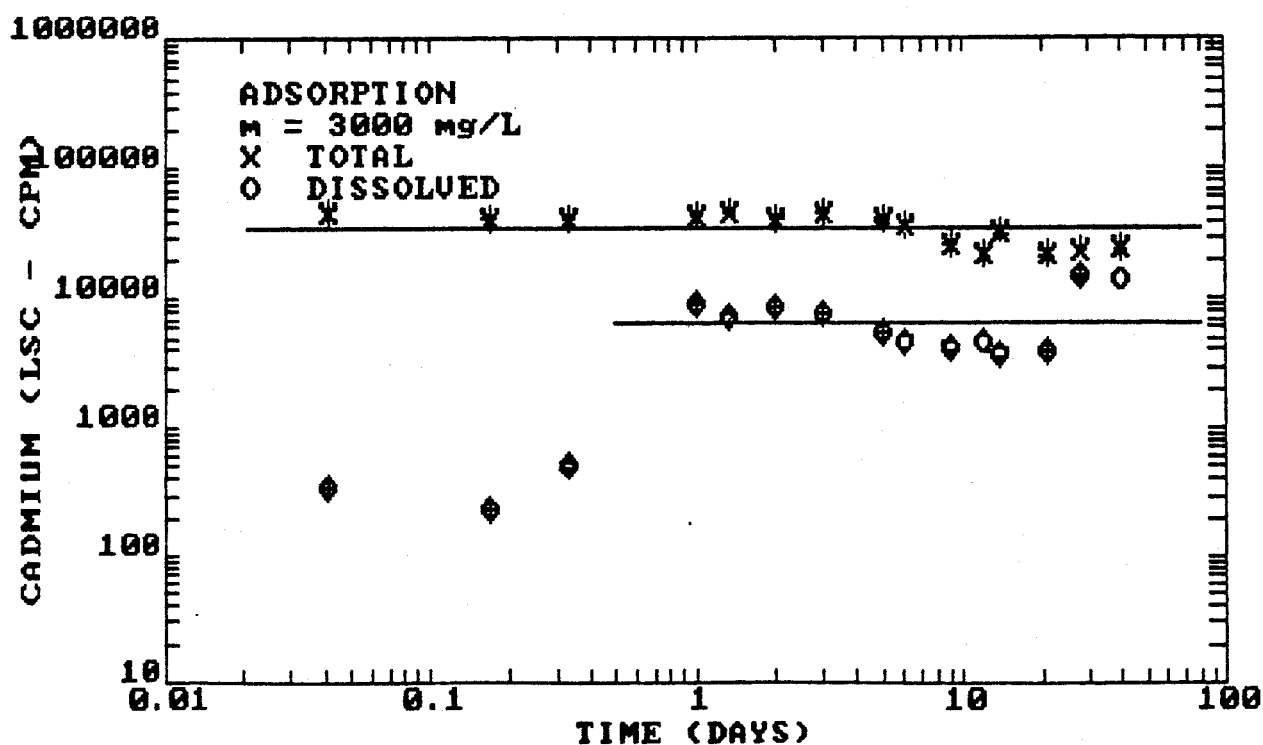9. Concentration of total and dissolved radioactive cadmium versus time. Radioactive cadmium is added at the start (t=0) of the experiment.

10. Concentration of total and dissolved radioactive zinc at various times. Radioactive zinc is added to a subsample taken at the indicated time and a one hour – one hour adsorption-desorption measurement is made. The total and dissolved zinc at adsorption (top) and desorption (bottom) is shown for Black Rock Harbor (left) and Bergen County (right).

11. Concentration of total and dissolved radioactive cadmium at various times. Radioactive cadmium is added to a subsample taken at the indicated time and a one hour – one hour adsorption-desorption measurement is made. The total and dissolved cadmium at adsorption (top) and desorption (bottom) is shown for Black Rock Harbor (left) and Bergen County (right).

CHROMIUM

DILUTION 1:50

DILUTION 1:100

DILUTION 1:200

Time (days)

CADMIUM

DILUTION 1:50

DILUTION 1:100

DILUTION 1:200

Time (days)

1. Experimental data (Rohatgi and Chen, 1975) and the three component
    model fit for cadmium and chromium.

2. Total and dissolved copper concentrations versus time for Black Rock Harbor sediment and Bergen County sludge at 3000 mg/L (left side) and 300 mg/L (right side). Control reactor concentrations (C) are also shown.

3. Total and dissolved zinc (top) and cadmium (bottom) concentrations versus time for Black Rock Harbor sediment and Bergen County sludge at 3000 mg/L (left side) and 300 mg/L (right side).

4. Total and dissolved chromium concentrations versus time for Black Rock Harbor sediment and Bergen County sludge at 3000 mg/L (left side) and 300 mg/L (right side).

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5. pH (top) and Total Organic Carbon (bottom) versus time for Black Rock Harbor sediment (left) and Bergen County sludge (right) reactors.

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6. Anaerobic Reactor dissolved copper concentrations versus time for Black Rock Harbor (top left), Ridgewood (bottom left) and Bergen County (top right). Total organic carbon concentrations versus time for the three reactors are also shown (bottom right).

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BLACK ROCK HARBOR SEDIMENT

7. Sulfate (top) and excess sulfate (bottom) concentration versus time for Black Rock Harbor sediment.

BLACK ROCK HARBOR SEDIMENT - #2

PARTITION COEFFICIENT KINETICS

BERGEN COUNTY SLUDGE - #2

PARTITION COEFFICIENT KINETICS

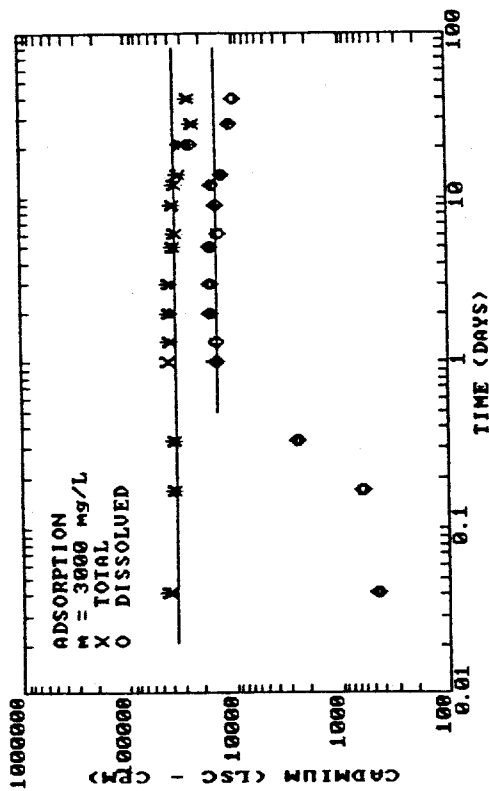8. Concentration of total and dissolved radioactive zinc versus time. Radioactive zinc is added at the start (t=0) of the experiment.

BLACK ROCK HARBOR SEDIMENT - #6

PARTITION COEFFICIENT KINETICS

BERGEN COUNTY SLUDGE - #7

PARTITION COEFFICIENT KINETICS

9. Concentration of total and dissolved radioactive cadmium versus time. Radioactive cadmium is added at the start (t=0) of the experiment.

10. Concentration of total and dissolved radioactive zinc at various times. Radioactive zinc is added to a subsample taken at the indicated time and a one hour – one hour adsorption-desorption measurement is made. The total and dissolved zinc at adsorption (top) and desorption (bottom) is shown for Black Rock Harbor (left) and Bergen County (right).

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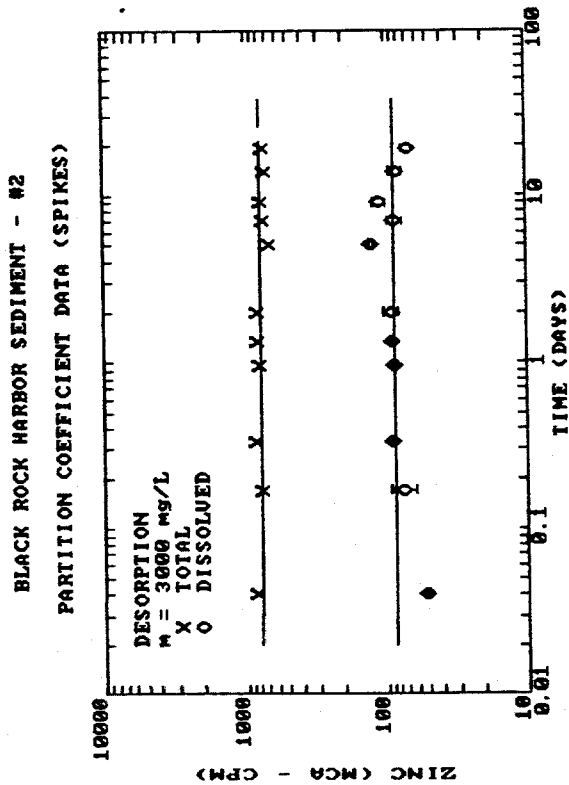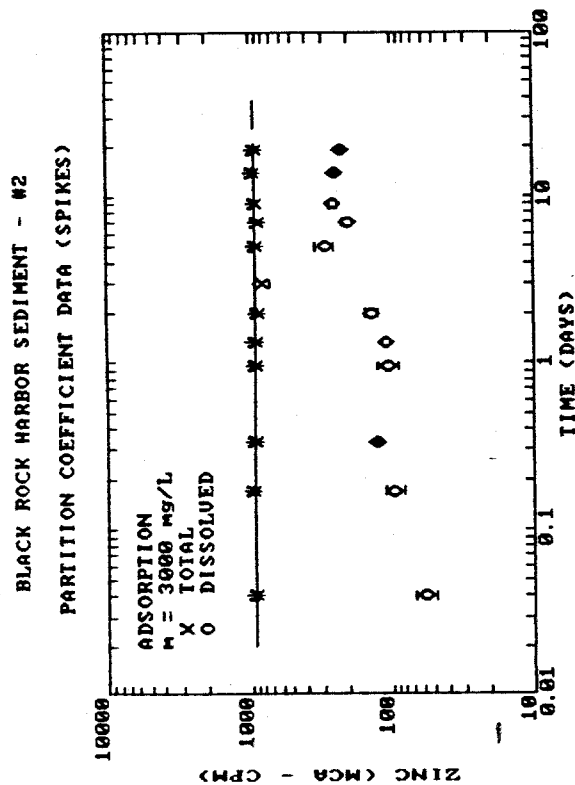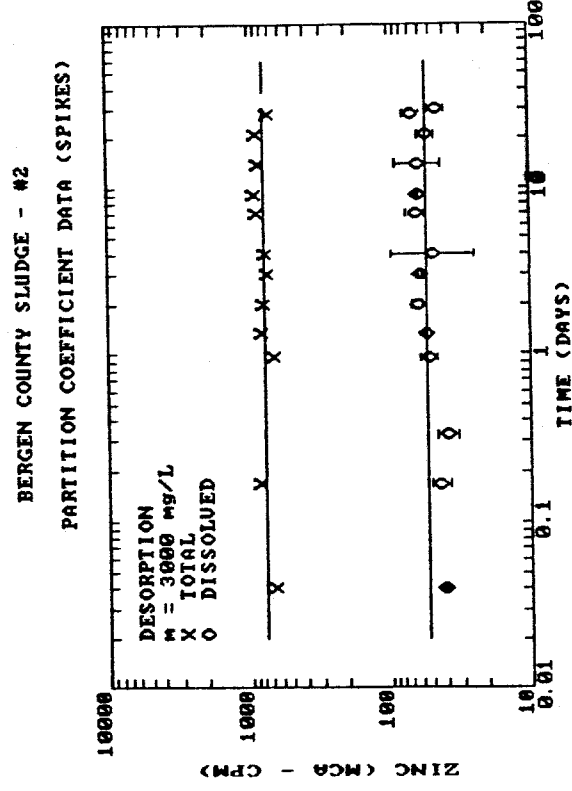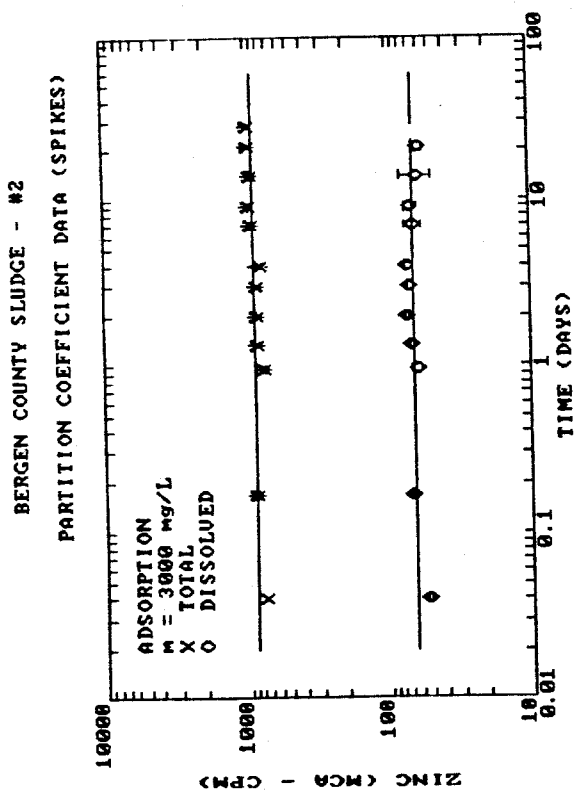
11. Concentration of total and dissolved radioactive cadmium at various times. Radioactive cadmium is added to a subsample taken at the indicated time and a one hour adsorption-desorption measurement is made. The total and dissolved cadmium at adsorption (top) and desorption (bottom) is shown for Black Rock Harbor (left) and Bergen County (right).