Development of the partition coefficient (Kd) test method for use in environmental risk assessments

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EXECUTIVE SUMMARY

Recent environmental legislation, such as the Environmental Protection Act 1990, Groundwater Regulations 1998, Pollution Prevention and Control Regulations 2000, the Landfill Regulations 2002 and the Water Framework Directive, includes requirements for environmental risk assessment as part of the permitting process. The Government has issued guidance on environmental risk assessment and management (DETR *et al*., 2000) and the Environment Agency is seeking to ensure that each of its regulatory processes adhere to the tiered approach to environmental risk assessment described therein.

The Environment Agency has published guidance for the waste management and contaminated land sectors on methods to assess pollution risks from their activities to water, and in particular groundwater (Environment Agency, 1999, 2001, 2003). Groundwater risk assessment requires an understanding and evaluation of the fate and transport of substances in the subsurface, and an estimate of the probability and magnitude of the likely impact that would result from any entry of pollutants.

The fate of pollutants in the subsurface is subject to a number of controls, but the velocity with which they migrate relative to water is influenced by retardation processes, including a number of different sorption processes. The Environment Agency previously developed a standard test method to determine ammonium partitioning between landfill leachate and rock, which was published as R&D Technical Report P340 (Environment Agency, 2000). The project reported here sought to develop the partition coefficient (K_d) test method to include a wider range of the substances commonly found on contaminated sites.

Partition coefficients for ammonium are derived using relatively simple batch tests. The aim of this project is to maintain this simplicity, while making the necessary refinements to the ammonium methodology for the other contaminants under study. This should ensure sufficient consistency between different laboratories that might carry out K_d measurements in the future.

The substances considered in this study are:

- Heavy metals (using arsenic, cadmium, lead and zinc as examples);
- Major anions (sulphate);
- Volatile organic compounds – benzene, toluene, xylene, tetrachloroethene (PCE) and trichloroethene (TCE);
- Polycyclic aromatic hydrocarbons (PAHs) – naphthalene and benzo[a]pyrene;
- Pesticides (mecoprop, diazinon, isoproturon and cypermethrin).

This report presents the results of laboratory method development and validation, and recommends modifications to the ammonium K_d test method to make it applicable to a wider range of substances.

Key words: Partition coefficient, K_d, test method, retardation, groundwater pollution

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1. INTRODUCTION

The Environment Agency has previously published a test method to determine partition coefficients (K_d) for ammonium to geological materials, for use in landfill risk assessments. This work was undertaken by the British Geological Survey (BGS) and the method is published, along with its validation, as Environment Agency R&D Technical Report P340 (Environment Agency, 2000). This report was commissioned to meet a specific need within the waste function to assess the migration of ammonium as part of landfill risk assessments, using models such as LandSim (Environment Agency, 2003).

Partition coefficients are being used increasingly in contaminated soil and/or groundwater risk assessments as a result of guidance published by the Environment Agency and others in recent years, such as the Remedial Targets Methodology/P20 (Environment Agency, 1999) and RBCA [risk-based corrective action] (American Society for Testing Materials, 1998). However, little work has been done to validate the test method for contaminants other than ammonium. The objective of this project was to extend the ammonium K_d methodology to a range of other common soil contaminants, to make suitable refinements to the analytical procedures where necessary and to validate those methods through repeat analytical testing.

1.1 Partition Coefficients (K_d)

A partition (or distribution) coefficient, K_d, describes the distribution of a species between a solid and aqueous matrix after equilibration. In groundwater risk assessments, the K_d value describes the degree of sorption of a particular species in the leachate and/or groundwater to the soil or rock that is in contact with that liquid. Partition coefficients are expressed in units of l/kg, or ml/g (volume/mass).

Sorption mechanisms include ion exchange (in particular cation exchange) and surface complexation. For organic contaminants sorption is often affected in a significant way by only two factors: the hydrophobicity of the contaminant and the fraction of organic carbon in the solid phase.

For organic compounds considered to follow a linear sorption model, the relationship in Equation (1) is commonly assumed:

$$K_d = K_{OC}.f_{OC} \tag{1}$$

where: K_{OC} **= organic carbon partition coefficient, ml/g**
                 f_{OC} **= fraction of organic carbon, unitless.**

The measured or calculated partition coefficient, K_d, can subsequently be used to predict the effects of retardation on the velocity and travel times of the contaminants being investigated. Substances subject to sorption processes migrate through an aquifer system more slowly than the water or a conservative (non-reactive) substance. Understanding the likely contaminant velocity allows the assessor to locate monitoring boreholes in the most appropriate locations, predict the imminence of any risks to

receptors and instigate a timely response. The contaminant velocity can be predicted from the relationship in Equation (2):

$$u = \frac{v}{R_f} \tag{2}$$

where R_f is given by Equation (3):

$$R_f = 1 + \left(\frac{K_d \cdot \rho}{n_e} \right) \tag{3}$$

and
$u =$ contaminant velocity, m/s
$v =$ groundwater velocity, m/s
$R_f =$ retardation factor, ml/g
$\rho =$ soil or aquifer bulk density, kg/m^3
$n_e =$ effective porosity, unitless.

1.2 Principle

The K_d values for the different contaminants are derived using batch testing. To a tube is added an amount of crushed rock sample under investigation (typically 1–10 g). Synthetic groundwater is added to the tube (typically 25–40 ml). The tubes are placed on a rotator and rotated through 360° for a period of 72 hours. This is the pre-equilibration stage and it ensures all exchange reactions have taken place before the addition of the contaminant under study. The contaminant is then added to the rock–solution mixture (at the required concentration[1]) and rotated for a further 48 hours. This is the equilibration stage. The equilibration time varies depending on the contaminant and, where possible, it should be determined by conducting tests with different contact times.

The purpose of this study, however, is to produce a method for K_d determination, and therefore individual equilibration times were not investigated. This study has not investigated the kinetics of sorption.

The mass of contaminant added is known and, using the analytical techniques available in the laboratory, the mass remaining in solution after equilibration can be determined. Therefore, the mass of contaminant that has sorbed onto the rock sample can be calculated. The different parameters are put into Equation (4) to derive the individual K_d values for the contaminant under investigation:

$$K_d = \left(\frac{I - F}{F} \right) \times \left(\frac{V}{M} \right) \tag{4}$$

where:
I = initial contaminant concentration, mg/l
F = final contaminant concentration, mg/l
V = volume of liquid, l
M = mass of solid, kg.

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[1] Contaminant concentrations should be representative of the conditions present within the contaminated soil or aquifer under assessment.

1.3 Project Aims

The aims of this project are:

- Complete review of the BGS ammonium methodology (Environment Agency, 2000) for six reference lithologies, to ensure that this method can be replicated in Environment Agency laboratories.
- To validate and refine the ammonium method for sulphate, which was selected as representative of anions present on contaminated sites.
- To validate and refine the ammonium method for arsenic, cadmium, lead and zinc, which were selected as representative of the heavy metals present on contaminated sites.
- Refinement and validation of the ammonium method for a number of organic compounds, namely benzene, toluene, total xylene, trichloroethene (TCE), tetrachloroethene (PCE), naphthalene, benzo[a]pyrene, mecoprop (MCPP), diazinon, isoproturon and cypermethrin.

Partition coefficients were determined for each substance at three different aqueous solute concentrations, to give an estimate of the variability of K_d over the likely pollutant concentration ranges.

2. MATERIALS

2.1 Instrumentation

2.1.1 Orion pH probe

The pH was measured after the pre-equilibration stage to give the 'natural pH'. For the metals and sulphate the pH was also measured after the addition of the contaminant and after the equilibration stage. The pH was not determined further for the organic compounds because of the volatile nature of some of these compounds (i.e., losses to the atmosphere while measuring the pH) and the possibility of other compounds sticking to the probe and affecting the final measurements. The Orion pH probe can measure pH to an accuracy of ±0.05 units.

2.1.2 Polycarbonate tubes (30 ml) and glass screw-cap vials (40 ml)

Polycarbonate tubes (supplied by Fisher Scientific) were used during the sulphate and metals K_d batch tests, and glass tubes (supplied by Varian) were used for the K_d batch tests for organic compounds.

2.1.3 Heraeus sepatech centrifuge

The Heraeus sepatech centrifuge was used to centrifuge the rock–solution mixture after the equilibration stage.

2.1.4 Amicon centriprep cells (30,000 daltons membrane)

Amicon centriprep cells were the centrifugal filtration devices used to remove colloidal material (supplied by Fisher Scientific).

2.1.5 Rugged rotators

The rotators (supplied by Camlab, *Figure 2.1*) were used to pre-equilibrate the crushed rock sample with the synthetic groundwater, and then to equilibrate the contaminant with the rock–solution mixture.

2.2 Reagents

2.2.1 Preparation of rock sample

For the review of the ammonium method, the National Laboratory Service (NLS) obtained samples of the six reference lithologies used by the BGS as part of the development and validation of the ammonium K_d method (Environment Agency, 2000). These materials were received in powder form:

- Mercia Mudstone;
- Lower Oxford Clay;
- Lower Chalk;
- Gault Clay;
- Sherwood Sandstone;
- Lincolnshire Limestone.
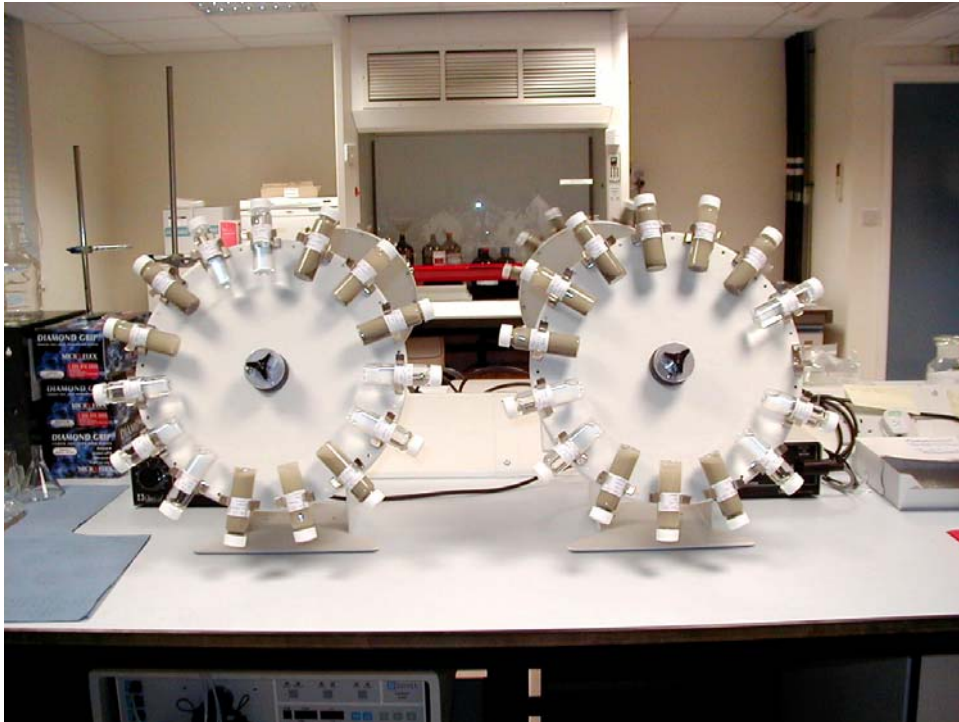
Figure 2.1. Rugged rotators loaded with 40 ml glass vials (volatile organics batch testing).

For the development and application of the ammonium method to other contaminants, a sample of siltstone was collected and prepared. Part of the Tredorn Slate Formation, this lithology is described as a silver–green, finely laminated siltstone, showing post-diagenetic folding and striations. Bedding planes were approximately 20 mm apart, in places flaggy. It was collected from national grid reference SX 053 894, near Tintagel, Cornwall.

About 10 kg of this siltstone was received in a slate form, which was all crushed down to a 3-4 mm particle size using a laboratory jaw crusher. It was then further reduced using a tema mill. The final particle size varied from approximately 1 mm down to <200 μm. Before use for batch testing the ground siltstone was homogenised for 24 hours on a roller.

The moisture content of the siltstone was negligible, and no dry matter adjustment was necessary during the studies. The organic carbon content (f_{oc}) of the siltstone was determined, using an in-house ash test method, to be 1.05 percent.

2.2.2 Preparation of synthetic groundwater

To ensure no other interference, ultra high purity water (UHP) was used to make up the synthetic groundwater. Sodium chloride was added to the UHP to simulate the ionic potential of groundwater – a 0.03M solution was used.

2.2.3 Preparation of contaminant solutions

All the contaminants studied were prepared using certified reference materials and either UHP or pesticide and/or headspace grade solvents (see Appendix 1 for details).

3. METHODS

3.1 Ammonium review experimental procedure

Two contaminant concentrations were studied: 10 mg/l and 40 mg/l.

Twelve polycarbonate tubes (30 ml) with screw caps were weighed and recorded.

The rock (10 g) under study was added to eight of the tubes each. The weight of solid added was recorded. This was followed by the addition of 24 ml of synthetic groundwater to each of the eight tubes, the weight of which was recorded. The four remaining tubes served as positive controls, to which only the synthetic groundwater was added and no solid (rock sample). All twelve tubes were placed on the rotator at 36 revolutions per minute (rpm) for a period of 72 hours. This was the *pre-equilibration process*.

All tubes were then removed and allowed to settle, and the pH of the supernatant was measured and recorded.

To each of three tubes (containing solid) was added a 1 ml aliquot of ammonium (250 mg/l), which is equivalent to 10 mg/l after dilution in 25 ml of groundwater. To a further three tubes (containing solid) was added a 1 ml aliquot of ammonium (1000 mg/l), which is equivalent to 40 mg/l after dilution in 25 ml groundwater. To the two remaining tubes (containing solid) a 1 ml portion of groundwater was added – these were blanks. The weight of all the 1 ml portions added were recorded. The pH of the supernatant in each tube was recorded.

Two of the remaining tubes (containing no solid) were spiked with a 1 ml aliquot of 250 mg/l ammonium. The other two (containing no solid) were spiked with a 1 ml aliquot of 1000 mg/l ammonium.

All twelve tubes were placed on the rotator for 48 hours. This was the *equilibration process*.

The tubes were then removed and centrifuged for 5 minutes at 2500 rpm. The supernatant from each tube was transferred to clean tubes and the pH was measured and recorded for each (this transfer to clean tubes is only to allow the following acidification stage, and is not necessary for the other contaminants under study). *The glass tubes used for the organic contaminants under study were centrifuged at 1900 rpm, because of possible breakage at higher speeds.*

The supernatant was acidified with one drop of 8M HCl (this prevents the loss of ammonium as ammonia gas). The pH was re-measured and recorded. *The acidification stage is unique to the ammonium method and is not necessary for the other contaminants under study.*

Finally, the supernatant from each of the tubes was poured into separate Amicon centriprep cells. The cells were then centrifuged at 2700 rpm for 15 minutes. The filtrates from each cell were added to clean polycarbonate tubes.

The ammonium concentration in each tube was measured using an Aqua 800 according to the in-house method of analysis AQUA 001, details of which are available on request (see Appendix 2 for data).

The above was undertaken for each of the six lithologies.

Also, a chemical wash was performed on each lithology to assess the chemical content of the groundwater after pre-equilibration. A chemical wash was also carried out for the siltstone (see Appendix 2 for data).

3.2 K_d determination for arsenic, cadmium, lead and zinc: experimental procedure

Three contaminant concentrations were studied: 10 mg/l, 50 mg/l and 100 mg/l.

Scoping tests were performed for each contaminant, so as to ascertain the most suitable solid–solution ratio to use in the batch testing. Where possible, a solid–solution ratio was chosen that resulted in between 25 percent and 75 percent sorption from the aqueous to solid phases. This increases the accuracy of the K_d measurement. For a given contaminant the ratio of the mass of solid material to liquid may be different depending on the concentration being studied.

During batch testing no adjustment to the above ammonium methodology was necessary.

The cadmium, lead and zinc samples were analysed according to the in-house method PE0002, using an inductively coupled plasma optical-emission spectrometer, for which details are available on request (see Appendix 2 for data).

The arsenic samples were analysed according to the in-house method PE4001, using flow injection hydride analysis and atomic absorption spectrometry, for which details are available on request (see Appendix 2 for data).

3.3 K_d determination for sulphate – experimental procedure

Three contaminant concentrations were studied: 125 mg/l, 250 mg/l and 500 mg/l.

Scoping tests were performed before batch testing. No adjustment to the ammonium methodology was necessary.

The sulphate samples were analysed according to the in-house method SKA003, using continuous flow analysis, details of which are available on request (see Appendix 2 for data).

3.4 K_d determination for mecoprop (MCPP), diazinon and isoproturon – experimental procedure

Three contaminant concentrations were studied: 10 μg/l, 50 μg/l and 100 μg/l.

Scoping tests were performed first. Instead of polycarbonate tubes, glass screw-cap 40 ml tubes were used. This was to minimise interactions between the contaminant and the tube itself. Instead of adding 1 ml portions of the contaminant to each tube as above, 10 μl was added because the spiking solution has to be made up in acetone and not UHP (this facilitates dissolving the organic contaminants in the groundwater). The 10 μl solvent spiking volume is negligible when added to 25 ml of groundwater.

The pH was measured after the pre-equilibration stage only.

After the filtration of the samples using the centriprep cells, they were set-up for analysis using the in-house methodology. A volume was taken from each tube and added to separate 1 l aliquots of UHP in glass pyrex bottles. The volume added depends on the initial concentration of the contaminant under study, and on the calibration range of the in-house method used to analyse the final contaminant concentration. Typically for mecoprop, spiked initially at 100 μg/l, 2ml of the final supernatant was added to 998ml of UHP. It was then ready for quantitative analysis.

The above are the only deviations from the ammonium method.

The mecoprop samples were analysed according to the in-house method SX020, using Gas Chromatography Mass Spectrometry (GCMS), for which details are available on request (see Appendix 2 for data).

The diazinon samples were analysed according to in-house method SX007, using GCMS, for which details are available on request (see Appendix 2 for data).

The isoproturon samples were analysed according to in-house method SX009, using Liquid Chromatography Mass Spectrometry (LCMS), for which details are available on request (see Appendix 2 for data).

3.5 K_d determination for cypermethrin and benzo[a]pyrene – experimental procedure

The same experimental procedure was adopted for cypermethrin and benzo[a]pyrene, as for the above organic substances. However, insufficient quantities were left in solution after the centriprep stage to detect by analysis, because of the very hydrophobic nature of these two compounds. It is therefore assumed that they are not mobile and would normally be strongly retarded by the soil and/or rock. Through the positive controls (no rock present) it was also determined that these compounds partition strongly to the glass of the tubes and, in particular, to the centriprep cells and/or membranes. Therefore, a K_d experimental procedure based on the simple ammonium method used here is not recommended for cypermethrin or benzo[a]pyrene.

3.6 K_d determination for benzene, toluene, total xylene, trichloroethene, tetrachloroethene and naphthalene–experimental procedure

Three contaminant concentrations were studied: 0.1 mg/l, 1.0 mg/l and 10 mg/l.

Scoping tests were performed first, for which 40 ml screw-cap glass tubes were used. After the addition of the rock sample, it is imperative that there is no headspace volume, so enough groundwater has to be added to minimise the headspace volume sufficiently (typically, with 10 g of rock, 38 ml of groundwater is required). Owing to the volatile nature of these compounds there could be significant losses from the aqueous and/or solid phases to air if the relative headspace volume is significant.

The pH is not measured, to avoid volatilisation of the substances during the measurement procedure. The 'natural' pH could be obtained, if required, by pre-equilibrating a separate tube solely for this purpose, decanting off the supernatant and then measuring the pH.

The spiking volume of the different contaminants is 10.86 μl, which is negligible compared to the 38 ml into which they are spiked.

The centriprep stage is performed immediately after the equilibration process to minimise any losses caused by volatilisation, if for example, the samples were left to stand overnight. During the centriprep stage the samples are exposed to the atmosphere, which results in losses of each contaminant through volatilisation. To correct for this, positive controls are run in duplicate at each concentration level, but are not put through the centriprep stage. These are compared with positive controls (run in duplicate at each concentration level) that *are* put through the centriprep stage, and a factor can then be applied.

It is important after the centriprep stage to promptly set-up the samples for analysis with minimal headspace volume. Typically for the 1 mg/l concentration, 1.4 ml of the filtrate is added to 40.6 ml of UHP in another 40 ml glass tube (this occupies the neck space volume of the tube, and keeps any headspace to an absolute minimum). This should be done immediately after the centriprepping process. This dilution also ensures that quantification is within the calibration range of the in-house methodology used to finally analyse the samples

The above are the only deviations from the ammonium method.

The samples are now ready for analysis according to the in-house method SX022 using GCMS with a purge and trap sampling system, for which details are available on request (see Appendix 2 for data).

4. RESULTS

All the data from each of the batch tests is presented In Appendix 2 and the calculated K_d values are summarised in Tables 4.1 and 4.2. The variability of K_d with solute concentrations are shown graphically in Figure 4.1. These results demonstrate the applicability of the method to contaminants other than ammonium.

These results are not intended to be used as a database of acceptable values for any specific risk assessment. Values obtained from detailed site specific or laboratory investigation will always be preferred for use in groundwater risk assessments.

Table 4.1 Comparison of K_d values for ammonium reported by the BGS and Environment Agency NLS for reference lithologies

	Average K_d (ml/g) BGS		Average K_d (ml/g) NLS	
Ammonium concentration	*~10 mg/l*	*~40 mg/l*	*~10 mg/l*	*~40 mg/l*
Gault Clay	6.91	6.28	5.55	5.40
Sherwood Sandstone	1.79	1.72	2.23	1.68
Mercia Mudstone	7.78	5.49	6.59	5.41
Lincolnshire Limestone	0.77	0.66	0.33	0.29
Lower Chalk	1.63	1.20	1.67	1.36
Lower Oxford Clay	1.48	2.27	1.02	2.40

Table 4.2 Summary of average K_d values determined for selected contaminants across experimental concentration ranges (Cornish siltstone sample)

Initial solute concentration	*10 μg/l*	*50 μg/l*	*0.1 mg/l*	*1 mg/l*	*10 mg/l*	*50 mg/l*	*100 mg/l*	*125 mg/l*	*250 mg/l*	*500 mg/l*
Arsenic					17.33	5.89	2.90			
Cadmium					13.60	7.26	5.48			
Lead					317.51	76.43	37.45			
Zinc					44.63	14.23	8.01			
Sulphate								0.048	0.43	0.23
Diazinon	8.79	2.62	2.16							
Isoproturon	ND	ND	0.038							
Mecoprop	ND	ND	ND							
Benzene			10.93	6.53	3.53					
Naphthalene			ND	0.45	0.47					
Xylene (total)			12.98	6.50	2.25					
Toluene			16.20	16.34	4.90					
TCE			10.90	2.57	4.53					
PCE			3.36	3.31	2.33					

ND, not determined since sorption too low to allow calculation of K_d.
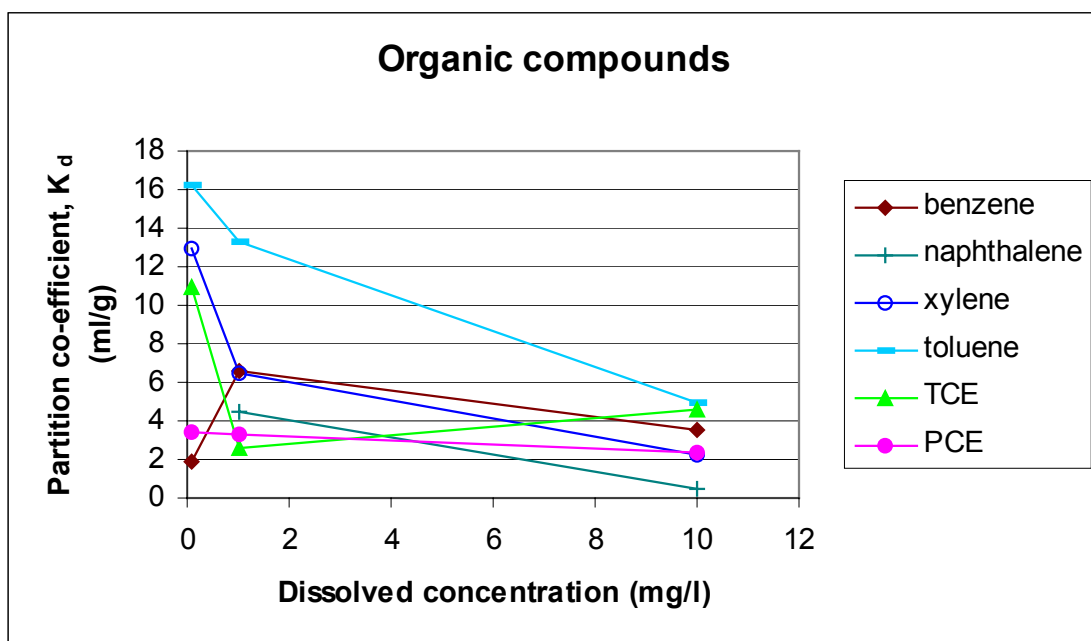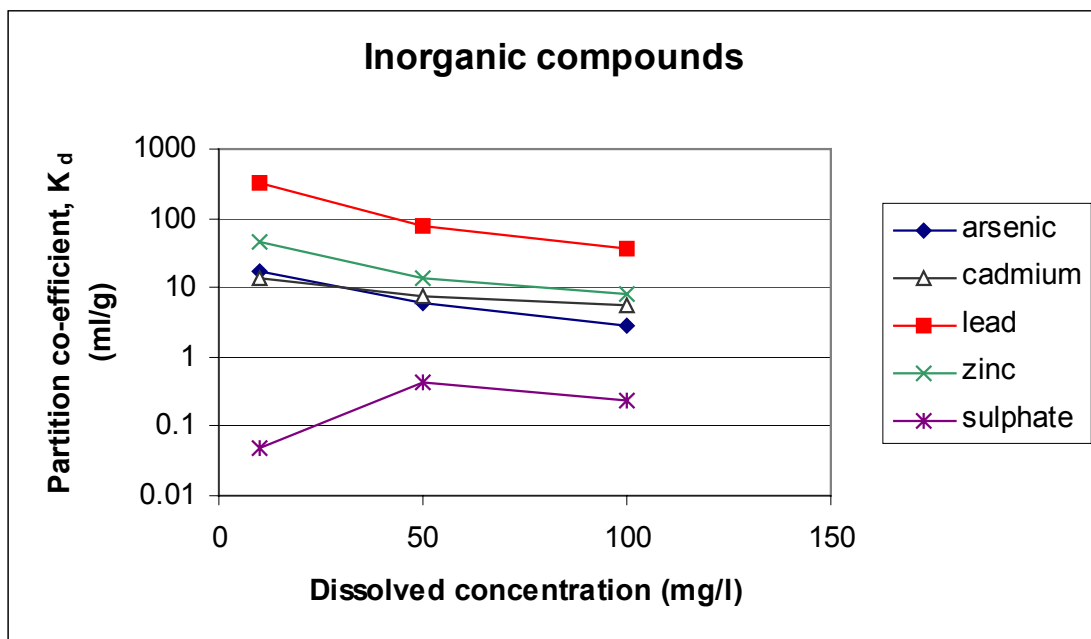
Figure 4.1. Variability of K_d with solute concentration for the Cornish siltstone. The upper graph shows inorganic substances, the lower graph shows the organic compounds.

5. CONCLUSIONS

The required amendments are summarised in *Table 5.1*.

When performing batch tests it is important to use the correct type of tube and/or vial. For all inorganic contaminants 30 ml screw-cap polycarbonate tubes were found to be the most suitable. For the organic contaminants 40 ml screw-cap glass vials were preferred. The reason for the different tubes is to minimise interactions between the contaminant and the tube itself.

Before batch testing for each contaminant can begin, it is necessary to carry out scoping tests. These tests are used to establish the correct solid-to-solution ratio so that, where possible, between 25 percent and 75 percent sorption of the contaminant occurs onto the rock (this increases the accuracy of the K_d measurement). For substances with a high K_d value (e.g. lead) a small solid-to-solution ratio is required, such as 1 g of rock and 25 ml of groundwater. This ensures measurable concentrations are left in solution. For the smaller K_d values a large solid-to-solution ratio is best, such as 10 g of rock and 25 ml of groundwater.

For the inorganic contaminants and the non-volatile organics the batch tests operate as a three-phase system (i.e., solid, liquid and air). For the volatile organics it is imperative that the headspace (air) is kept to an absolute minimum (ideally zero), otherwise significant losses of the contaminant into the vapour phase can occur.

Three contaminant concentrations were studied, so as to ascertain any variability of sorption with solute concentration. For the four metal compounds studied there was little linearity between the different concentrations. For sulphate there was no sorption, because sulphate is an anionic species, and anion exchange is often not important with clay materials. Sorption of anions may be important when considering strata with iron oxyhydroxide minerals present. Also there were levels of sulphate in the groundwater after the pre-equilibration stage which made blank subtraction necessary.

The organic substances mecoprop and isoproturon displayed no measurable sorption onto the siltstone. For diazinon there was some linearity of sorption. For cypermethrin and benzo[a]pyrene this experimental method was not able to produce a K_d value as a result of the highly hydrophobic nature of these compounds. Both compounds stick to the glass tube as well as the centriprep cell. With the exception of naphthalene, the volatile organics all showed moderate levels of sorption, with little indication of any linearity.

Table 5.1 Summary of required amendments to published K_d test method (R&D Technical Report P340) for groups of substances considered in this study

Substance	Comment on K_d batch test method
Heavy metals	K_d test method published in R&D TR P340 can be used without modification (other than that acidification to prevent NH_3 production is unnecessary)
Anions	K_d test method published in R&D TR P340 can be used without modification (other than that acidification to prevent NH_3 production is unnecessary)
VOCs (BTEX)	Necessary modifications to P340 method: • use glass vials to prevent sorption to plastic test apparatus • ensure no headspace in batch test to prevent volatilisation
VOCs (chlorinated solvents)	Necessary modifications to P340 method: • use glass vials to prevent sorption to plastic test apparatus • ensure no headspace in batch test to prevent volatilisation
SVOCs (e.g. naphthalene)	Necessary modifications to P340 method: • use glass vials to prevent sorption to plastic test apparatus • ensure no headspace in batch test to prevent volatilisation
Pesticides (i.e. mecoprop, isoproturon and diazinon)	Necessary modifications to P340 method: • use glass vials to prevent sorption to plastic test apparatus
Highly hydrophobic organics (e.g. B[a]P, cypermethrin)	The K_d batch test method is not recommended for these substances. The substances are so hydrophobic that sorption to test apparatus (e.g. membranes and glass vials) renders the analytical results questionable.

B[a]P, benzo[a]pyrene; BTEX, benzene, toluene, ethylbenzene and xylene; SVOC, semi-volatile organic compounds; VOC, volatile organic compounds.

Each concentration level was studied in triplicate. For some of the compounds (namely some of the volatile organic compounds) the relative standard deviation (RSD) was rather high (for a given concentration level). This can be attributed to analytical variability and the low number of replicate analyses. Also, for the organic substances the RSDs are generally higher than for the inorganic determinands, because of the more complex nature of organic analysis.

For the organic compounds, partition coefficient RSDs are perhaps not particularly useful numbers, because the concentration values themselves are mostly within the RSD targets set for the method of analysis, which in this instance was 15 percent. Further, this target does not take into account the additional work involved in the production of a K_d measurement and that we are only evaluating a population of three K_d values. The nature of analysis for metals and inorganic compounds results in much smaller RSD values.

K_d determinations for very high solute concentrations (e.g., volatile organics at levels in the region of 100 mg/l, which might be present in the source area of a pollutant plume where non-aqueous phase liquids (NAPL) is present) would be difficult. This arises from solubility problems when making up what would need to be very concentrated standards used to spike the groundwater.

The batch tests attempt to simulate the interaction of contaminated leachate or groundwater with the soil or rock through which it is migrating. In reality, the field situation is far more complex than the laboratory environment and a number of other, often competing, chemical interactions will be occurring. The laboratory set-up also involves the use of ground rock with its significantly increased surface area for sorption. However, the laboratory K_d measurements do give an indication of the level of sorption that can take place. This can then be used along with a number of other parameters as part of the risk assessment process.

Future enhancements of the above methodology should include using synthetic or authentic leachate, and studying mixtures of contaminants instead of compounds in isolation. Also, the rock sample used could be ground up to different particle sizes, and a comparison made between a coarse sample (2-4 mm) and a fine sample (<200 μm).

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APPENDIX 1: SOLUTIONS USED

Ammonium solutions – for review experiments

1. 0.03M NaCl solution (synthetic groundwater)

To 1 l of UHP add 1.76 g of NaCl.

2. 0.1M ammonium chloride solution

To 1 l of UHP add 5.349 g of ammonium chloride.

3. 250 mg/l ammonium solution

To a 25 ml volumetric add 3.465 ml of 0.1M ammonium chloride. Make up to the mark with 0.03M NaCl solution.

4. 1000 mg/l ammonium solution

To a 25 ml volumetric add 13.859 ml of 0.1M ammonium chloride. Make up to the mark with 0.03M NaCl solution.

1 ml of solutions 3 and 4 added to 24 ml of groundwater gives ammonium concentrations of 10 mg/l and 40 mg/l, respectively.

Arsenic, Cadmium, Lead and Zinc solutions

1. 2500 mg/l arsenic solution

To 200 ml of UHP water add 2.0823 g of sodium arsenate ($Na_2HAsO_4.7H_2O$).

2. 1250 mg/l arsenic solution

To a 20 ml volumetric add 10 ml of solution 1. Make up to the mark with UHP.

3. 250 mg/l arsenic solution

To a 20 ml volumetric add 2 ml of solution 1. Make up to the mark with UHP.

4. 2500 mg/l cadmium solution

To 200 ml of UHP water add 0.8154 g of cadmium chloride ($CdCl_2$).

5. 1250 mg/l cadmium solution

To a 20 ml volumetric add 10 ml of solution 4. Make up to the mark with UHP.

6. 250 mg/l cadmium solution

To a 20 ml volumetric add 2 ml of solution 4. Make up to the mark with UHP.

7. *2500 mg/l lead solution*

To 200 ml of UHP add 0.7993 g of lead II nitrate $(Pb(NO_3)_2)$.

8. *1250 mg/l lead solution*

To a 20 ml volumetric add 10 ml of solution 7. Make up to the mark with UHP.

9. *250m g/l lead solution*

To a 20 ml volumetric add 2 ml of solution 7. Make up to the mark with UHP.

10. *2500 mg/l zinc solution*

To 200 ml of UHP water add 2.1990 g of zinc sulphate $(ZnSO_4.7H_2O)$.

11. *1250 mg/l zinc solution*

To a 20 ml volumetric add 10 ml of solution 10. Make up to the mark with UHP.

12. *250 mg/l zinc solution*

To a 20 ml volumetric add 2 ml of solution 10. Make up to the mark with UHP.

1 ml of the 2500 mg/l solution added to 24 ml of groundwater gives a concentration of 100 mg/l.
1 ml of the 1250 mg/l solution added to 24 ml of groundwater gives a concentration of 50 mg/l.
1 ml of the 250 mg/l solution added to 24 ml of groundwater gives a concentration of 10 mg/l.

Sulphate solutions

1. *12,500 mg/l sulphate solution*

To 1 l of UHP add 22.6757 g of potassium sulphate (K_2SO_4).

2. *6250 mg/l sulphate solution*

To a 20 ml volumetric add 10 ml of solution 1. Make up to the mark with UHP.

3. *3125 mg/l sulphate solution*

To a 20 ml volumetric add 5 ml of solution 1. Make up to the mark with UHP.

1 ml of the 12,500 mg/l solution added to 24 ml of groundwater gives a concentration of 500 mg/l.

1 ml of the 6250 mg/l solution added to 24 ml of groundwater gives a concentration of 250 mg/l.
1 ml of the 3125 mg/l solution added to 24 ml of groundwater gives a concentration of 125 mg/l.

Mecoprop, diazinon, cypermethrin, isoproturon and benzo[a]pyrene solutions

1. 10,000 mg/l mecoprop (MCPP) solution

To 10 ml of acetone add 100 mg of Mecoprop.

2. 250 mg/l mecoprop solution

To a 20 ml volumetric add 500 μl of solution 1. Make up to the mark with acetone.

3. 125 mg/l mecoprop solution

To a 20 ml volumetric add 250 μl of solution 1. Make up to the mark with acetone.

4. 25 mg/l mecoprop solution

To a 20 ml volumetric add 50 μl of solution 1. Make up to the mark with acetone.

For compounds diazinon, cypermethrin, isoproturon and benzo[a]pyrene the exact same format as that for mecoprop is used. Certified reference materials were used.

10 μl of the 250 mg/l solution added to 25 ml of groundwater gives a concentration of 100 μg/l.
10 μl of the 125 mg/l solution added to 25 ml of groundwater gives a concentration of 50 μg/l.
10 μl of the 25 mg/l solution added to 25 ml of groundwater gives a concentration of 10 μg/l.

Volatile organic compound solutions

1. 35,000 mg/l benzene solution

To a 10 ml volumetric add 397.73 μl of benzene. Make up to the mark with methanol.

2. 3500 mg/l benzene solution

To a 10 ml volumetric add 39.77 μl of benzene. Make up to the mark with methanol.

3. 350 mg/l benzene solution

To a 100 ml volumetric add 39.77 μl of benzene. Make up to the mark with methanol.

For the compounds toluene, total xylene, TCE and PCE the exact same format as that for benzene is used. However, the different densities need to be taken into account.

Naphthalene was made up from solid material at the following levels: 17,500 mg/l (in acetone because of solubility issues), and 3500 mg/l and 350 mg/l, both in methanol.

10.86 µl of the 35,000 mg/l solution added to 38 ml of groundwater gives a concentration of 10 mg/l.

10.86 µl of the 3500 mg/l solution added to 38 ml of groundwater gives a concentration of 1 mg/l.

10.86 µl of the 350 mg/l solution added to 38 ml of groundwater gives a concentration of 0.1 mg/l.

APPENDIX 2: ANALYTICAL RESULTS

Table A2.1 Chemical composition of 0.03M NaCl in UHP after contact with geological material for 72 hours

	pH	NH$_4$ mg/l	NO$_3$ mg/l	NO$_2$ mg/l	Ca mg/l	Mg mg/l	Na mg/l	K mg/l	HCO$_3$ mg/l	Cl mg/l	SO$_4$ mg/l	Si mg/l	Mn mg/l	Fe mg/l	Al mg/l	Cd µg/l	As µg/l	Pb mg/l
Mercia Mudstone	8.03	<0.04	**<0.9**	<0.03	**91.8**	30.5	**550.3**	8.57	**68.0**	1080.0	**24.7**	13.2	**<0.01**	<0.03	**0.01**	<0.1	**3.85**	<0.002
Lower Oxford Clay	7.38	3.01	**<0.9**	<0.03	**635.6**	132.1	**844.6**	116.4	**130.0**	1110.0	**2468.0**	15.8	**0.079**	<0.03	**0.018**	0.57	**<1.0**	<0.002
Lower Chalk	8.09	<0.04	**<0.9**	0.05	**90.6**	16.9	**636.9**	16.8	**51.0**	1100.0	**180.5**	17.0	**<0.01**	<0.03	**0.036**	<0.1	**<1.0**	<0.002
Gault Clay	7.80	0.19	**2.39**	0.03	**180.8**	41.9	**507.0**	51.6	**64.0**	1120.0	**236.2**	11.1	**0.013**	<0.03	**<0.01**	<0.1	**1.09**	<0.002
Sherwood Sandstone	8.55	0.04	**<0.9**	<0.03	**34.4**	17.6	**622.4**	38.2	**75.0**	1120.0	**16.8**	13.6	**<0.01**	<0.03	**0.053**	<0.1	**6.25**	<0.002
Lincolnshire Limestone	7.69	0.18	**<0.9**	<0.03	**718.0**	23.0	**664.0**	16.2	**78.0**	1100.0	**1797.0**	9.14	**0.012**	<0.03	**0.037**	<0.1	**<1.0**	<0.002
Cornish Siltstone (Tredorn Slate Formation)	6.35	1.03	**0.43**	<0.004	**4.41**	15.88	**689.0**	29.2	**<10.0**	1156.3	**13.0**	15.96	**0.01**	<0.03	**0.011**	0.34	**2.1**	<0.002

Table A2.2 Comparison of the K_d values for ammonium between the BGS and the NLS in various lithologies

	Average K_d (ml/g) BGS		Average K_d (ml/g) NLS (this study)	
	Low spike (~10 mg/l)	High spike (~40 mg/l)	Low spike (~10 mg/l)	High spike (~40 mg/l)
Gault Clay	6.91	6.25	5.55	5.40
Sherwood Sandstone	1.79	1.72	2.23	1.68
Mercia Mudstone	7.78	5.49	6.59	5.41
Lincolnshire Limestone	0.77	0.66	0.33	0.29
Lower Chalk	1.63	1.20	1.67	1.36
Lower Oxford Clay	1.48	2.27	1.02	2.40

The tables on the following pages include the raw data used to calculate the K_d values with the equation below:

$$K_d = \left(\frac{I - F}{F} \right) \times \left(\frac{V}{M} \right)$$

where:
- I = initial contaminant concentration, mg/l
- F = final contaminant concentration, mg/l
- V = volume of liquid, l
- M = mass of solid, kg.

For some experiments with isoproturon (Table A2.15), mecoprop (Table A2.16), and naphthalene (Table A2.18), the final contaminant concentration was equal to or greater than the initial contaminant concentration ($F/I \geq 1$). This is due to little or no sorption and so it is not possible to calculate a K_d value.

Table A2.3 NLS batch test data for ammonium in Gault Clay (powder form)

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibrium	Wt NH₄ added (g)	Total wt tube + liquid (g)	pH after addition of NH₄	pH ratio after addition of NH₄	Total wt liquid (g) (V)
1 +ve control 10 mg/l (no solid)										
2 +ve control 10 mg/l (no solid)										
3 +ve control 40mg/l (no solid)										
4 +ve control 40 mg/l. (no solid)										
5 Low spike 10 mg/l	12.68	10.00	24.84	47.52	7.90	0.99	48.51	7.86	0.99	25.83
6 Low spike 10 mg/l	12.65	10.02	24.85	47.52	7.88	0.99	48.51	7.86	1.00	25.84
7 Low spike 10 mg/l	12.67	10.00	24.83	47.50	7.91	0.99	48.49	7.86	0.99	25.82
8 High spike 40 mg/l	12.68	10.04	24.91	47.63	7.89	0.99	48.62	7.80	0.99	25.90
9 High spike 40 mg/l	12.71	10.02	24.86	47.59	7.88	0.99	48.58	7.80	0.99	25.85
10 High spike 40 mg/l	12.66	10.01	24.86	47.53	7.82	0.98	48.51	7.80	1.00	25.84
11 Blank	12.67	10.01	24.85	47.53	7.88	0.99	48.52	7.90	1.00	25.84
12 Blank	12.65	10.02	24.85	47.52	7.88	0.99	48.51	7.90	1.00	25.84

Table A2.3 (cont.) NLS batch test data for ammonium in Gault Clay (powder form)

Tube No.	Calc. NH$_4$ conc. (mg/l)	Actual NH$_4$ conc. (mg/l)	NH$_4$ conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	NH$_4$ ratio finish/start (F/I)	pH after adding HCl	Final NH$_4$ conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk average (mg/l)	Standard deviation	Relative SD
1 +ve control			9.60				9.48					
2 +ve control			9.60				9.49					
3 +ve control			38.44				37.91					
4 +ve control			38.44				39.97					
5 Low spike	250	**249.72**	9.60	**7.80**	0.32	**2.09**	3.04	5.57				
6 Low spike	250	**249.72**	9.60	**7.82**	0.32	**2.05**	3.05	5.54				
7 Low spike	250	**249.72**	9.60	**7.83**	0.32	**2.00**	3.05	5.54	5.55		0.017	0.312
8 High spike	1000	**999.37**	38.44	**7.82**	0.32	**2.21**	12.41	5.41				
9 High spike	1000	**999.37**	38.44	**7.83**	0.32	**2.07**	12.48	5.37				
10 High spike	1000	**999.37**	38.44	**7.80**	0.32	**2.03**	12.40	5.42	5.40		0.026	0.489
11 Blank				**7.80**		**2.07**	0.32					
12 Blank				**7.80**		**2.01**	0.27			0.29		

Table A2.4 NLS batch test data for ammonium in Lincolnshire Limestone (powder form)

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt NH₄ added (g)	Total wt tube & liquid (g)	pH after addition of NH₄	pH ratio after addition of NH₄	Total wt liquid (g) (V)
1 +ve control 10 mg/l (**no solid**)										
2 +ve control 10 mg/l (**no solid**)										
3 +ve control 40 mg/l (**no solid**)										
4 +ve control 40 mg/l. (**no solid**)										
5 Low spike 10 mg/l	12.67	**10.08**	25.06	**47.81**	7.58	**1.00**	48.81	**7.58**	1.00	**26.06**
6 Low spike 10 mg/l	12.63	**10.09**	25.05	**47.77**	7.55	**0.99**	48.76	**7.55**	1.00	**26.04**
7 Low spike 10 mg/l	12.67	**9.96**	25.02	**47.65**	7.58	**1.00**	48.65	**7.58**	1.00	**26.02**
8 High spike 40 mg/l	12.61	**10.08**	25.02	**47.71**	7.55	**1.00**	48.71	**7.55**	1.00	**26.02**
9 High spike 40 mg/l	12.64	**10.08**	25.02	**47.74**	7.55	**1.00**	48.74	**7.55**	1.00	**26.02**
10 High spike 40 mg/l	12.65	**10.03**	25.00	**47.68**	7.52	**1.00**	48.68	**7.52**	1.00	**26.00**
11 Blank	12.66	**10.07**	25.02	**47.75**	7.52	**1.00**	48.75	**7.59**	1.01	**26.02**
12 Blank	12.66	**10.06**	25.05	**47.77**	7.52	**1.00**	48.77	**7.59**	1.01	**26.05**

Table A2.4 (cont.) NLS Batch test data for ammonium in Lincolnshire Limestone (powder form)

Tube No.	Calc. NH$_4$ conc. (mg/l)	Actual NH$_4$ conc. mg/l	NH$_4$ conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	NH$_4$ ratio finish/start (F/I)	pH after adding HCl	Final NH$_4$ conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk average (mg/l)	Standard deviation	Relative SD
1 +ve control			9.58				9.67					
2 +ve control			9.58				9.72					
3 +ve control			38.70				38.28					
4 +ve control			38.70				38.31					
5 Low spike	250	248.97	9.58	7.48	0.87	2.29	8.33	0.34				
6 Low spike	250	248.97	9.58	7.48	0.88	2.39	8.47	0.34				
7 Low spike	250	248.97	9.58	7.46	0.89	2.42	8.57	0.31	0.33		0.017	5.15
8 High spike	1000	1006.16	38.70	7.50	0.90	2.39	34.72	0.30				
9 High spike	1000	1006.16	38.70	7.46	0.90	2.29	34.73	0.30				
10 High spike	1000	1006.16	38.70	7.46	0.98	2.52	37.94	0.28	0.29		0.012	4.14
11 Blank				7.46		2.42	0.42					
12 Blank				7.46		2.54	0.55			0.49		

Table A2.5 NLS batch test data for ammonium in Lower Chalk (powder form)

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt NH_4 added (g)	Total wt tube + liquid (g)	pH after addition of NH_4	pH ratio after addition of NH_4	Total wt liquid (g) (V)
1 +ve control 10 mg/l (**no solid)**										
2 +ve control 10 mg/l (**no solid)**										
3 +ve control 40 mg/l (**no solid)**										
4 +ve control 40 mg/l. (**no solid)**										
5 Low spike 10 mg/l	12.67	**10.00**	24.06	**46.73**	8.14	**1.00**	47.73	**8.19**	1.01	**25.06**
6 Low spike 10 mg/l	12.68	**10.00**	24.06	**46.74**	8.19	**1.00**	47.74	**8.19**	1.00	**25.06**
7 Low spike 10 (mg/l)	12.64	**10.08**	24.03	**46.75**	8.21	**1.00**	47.75	**8.24**	1.00	**25.03**
8 High spike 40 mg/l	12.78	**10.07**	24.02	**46.87**	8.20	**0.99**	47.86	**8.11**	0.99	**25.01**
9 High spike 40 mg/l	12.62	**10.01**	24.00	**46.63**	8.21	**0.99**	47.62	**8.12**	0.99	**24.99**
10 High spike 40 mg/l	12.72	**10.05**	23.98	**46.75**	8.21	**0.99**	47.74	**8.12**	0.99	**24.97**
11 Blank	12.71	**10.04**	23.93	**46.68**	8.22	**0.99**	47.67	**8.21**	1.00	**24.92**
12 Blank	12.64	**10.02**	23.94	**46.60**	8.23	**0.99**	47.59	**8.22**	1.00	**24.93**

Table A2.5 (cont.) NLS batch test data for ammonium in Lower Chalk (powder form)

Tube No.	Calc. NH$_4$ conc. (mg/l)	Actual NH$_4$ conc. (mg/l)	NH$_4$ conc. after dilution in 25 ml mg/l (I)	pH after equilibration	NH$_4$ ratio finish/start (F/I)	pH after adding HCl	Final NH$_4$ conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk average (mg/l)	Standard deviation	Relative SD
1 +ve control			9.98				9.98					
2 +ve control			9.98				9.99					
3 +ve control			39.82				40.35					
4 +ve control			39.82				40.34					
5 Low spike	250	**249.38**	9.98	**8.11**	0.62	**2.26**	6.21	1.52				
6 Low spike	250	**249.38**	9.98	**8.15**	0.59	**2.28**	5.88	1.75				
7 Low spike	250	**249.38**	9.98	**8.17**	0.59	**2.22**	5.88	1.73	1.67		0.13	7.78
8 High spike	1000	**995.40**	39.82	**8.14**	0.65	**2.13**	25.79	1.35				
9 High spike	1000	**995.40**	39.82	**8.15**	0.64	**2.47**	25.53	1.40				
10 High spike	1000	**995.40**	39.82	**8.14**	0.65	**2.21**	25.89	1.34	1.36		0.032	2.35
11 Blank				**8.17**		**2.35**	0.15					
12 Blank				**8.18**		**2.54**						

Table A2.6 NLS batch test data for ammonium in Lower Oxford Clay (powder form)

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt NH$_4$ added (g)	Total wt tube + liquid (g)	pH after addition of NH$_4$	pH ratio after addition of NH$_4$	Total wt liquid (g) (V)
1 +ve control 10 mg/l (**no solid)**										
2 +ve control 10 mg/l (**no solid)**										
3 +ve control 40 mg/l (**no solid)**										
4 +ve control 40 mg/l. (**no solid)**										
5 Low spike 10 mg/l	12.65	**10.04**	24.05	**46.74**	7.60	**1.00**	47.74	**7.51**	0.99	**25.05**
6 Low spike 10 mg/l	12.74	**10.00**	24.08	**46.82**	7.61	**1.00**	47.82	**7.52**	0.99	25.08
7 Low spike 10 mg/l	12.66	**10.08**	24.06	**46.80**	7.59	**1.00**	47.80	**7.50**	0.99	25.06
8 High spike 40 mg/l	12.67	**10.06**	24.08	**46.81**	7.56	**1.00**	47.81	**7.23**	0.96	25.08
9 High spike 40 mg/l	12.67	**10.00**	24.06	**46.73**	7.58	**1.00**	47.73	**7.25**	0.96	25.06
10 High spike 40 mg/l	12.66	**10.08**	24.05	**46.79**	7.55	**0.99**	47.78	**7.24**	0.96	25.04
11 Blank	12.71	**10.06**	24.04	**46.81**	7.55	**1.00**	47.81	**7.54**	1.00	**25.04**
12 Blank	12.71	**10.05**	23.97	**46.73**	7.55	**1.00**	47.73	**7.55**	1.00	**24.97**

Table A2.6 (cont.) NLS Batch test data for ammonium in Lower Oxford Clay (powder form)

Tube No.	Calc. NH$_4$ conc. (mg/l)	Actual NH$_4$ conc. (mg/l)	NH$_4$ conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	NH$_4$ ratio finish/start (F/I)	pH after adding HCl	Final NH$_4$ conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk average (mg/l)	Standard deviation	Relative SD
1 +ve control			9.98				9.98					
2 +ve control			9.98				9.99					
3 +ve control			39.82				40.35					
4 +ve control			39.82				40.34					
5 Low spike	250	**249.38**	9.98	**7.30**	0.77	**2.44**	7.73	0.73				
6 Low spike	250	**249.38**	9.98	**7.26**	0.69	**2.54**	6.86	1.14				
7 Low spike	250	**249.38**	9.98	**7.25**	0.68	**2.42**	6.77	1.18	1.02		0.25	24.5
8 High spike	1000	**995.40**	39.82	**7.26**	0.50	**2.40**	20.02	2.47				
9 High spike	1000	**995.40**	39.82	**7.23**	0.50	**2.52**	20.09	2.46				
10 High spike	1000	**995.40**	39.82	**7.25**	0.52	**2.49**	20.78	2.28	2.40		0.11	4.58
11 Blank				**7.26**		**2.50**	2.86					
12 Blank				**7.27**		**2.46**	2.67					

Table A2.7 NLS batch test data for ammonium in Mercia Mudstone (powder form)

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt NH$_4$ added (g)	Total wt tube + liquid (g)	pH after addition of NH$_4$	pH ratio after addition of NH$_4$	Total wt liquid (g) (V)
1 +ve control 10 mg/l (no solid)										
2 +ve control 10 mg/l (no solid)										
3 +ve control 40 mg/l (no solid)										
4 +ve control 40 mg/l. (no solid)										
5 Low spike 10 mg/l	12.65	10.01	25.02	47.68	7.96	1.00	48.68	7.86	0.99	26.02
6 Low spike 10 mg/l	12.59	9.97	25.03	47.59	7.96	1.00	48.59	7.86	0.99	26.03
7 Low spike 10 mg/l	12.67	10.07	24.98	47.72	7.98	1.00	48.72	7.88	0.99	25.98
8 High spike 40 mg/l	12.66	10.06	25.01	47.73	7.94	1.00	48.73	7.69	0.97	26.01
9 High spike 40 mg/l	12.67	10.07	24.94	47.68	7.96	1.00	48.68	7.71	0.97	25.94
10 High spike 40 mg/l	12.69	10.03	25.01	47.73	7.98	1.00	48.73	7.73	0.97	26.01
11 Blank	12.68	9.99	24.96	47.63	7.96	1.00	48.63	8.01	1.01	25.96
12 Blank	12.76	10.05	24.96	47.77	7.96	1.00	48.77	8.01	1.01	25.96

Table A2.7 (cont.) NLS batch test data for ammonium in Mercia Mudstone (powder form)

Tube No.	Calc. NH$_4$ conc. (mg/l)	Actual NH$_4$ conc. (mg/l)	NH$_4$ conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	NH$_4$ ratio finish/start (F/I)	pH after adding HCl	Final NH$_4$ conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk average (mg/l)	Standard deviation	Relative SD
1 +ve control			9.58				9.67					
2 +ve control			9.58				9.72					
3 +ve control			38.70				38.28					
4 +ve control			38.70				38.31					
5 Low spike	250	248.97	9.58	7.85	0.30	2.21	2.83	6.20				
6 Low spike	250	248.97	9.58	7.88	0.28	2.17	2.65	6.83				
7 Low spike	250	248.97	9.58	7.89	0.28	2.35	2.65	6.75	6.59		0.34	5.16
8 High spike	1000	1006.16	38.70	7.85	0.32	2.40	12.43	5.46				
9 High spike	1000	1006.16	38.70	7.85	0.32	2.62	12.54	5.37				
10 High spike	1000	1006.16	38.70	7.86	0.32	2.61	12.56	5.40	5.41		0.046	0.85
11 Blank				7.93		2.75	0.70					
12 Blank				7.93		2.90	0.10			0.4		

Table A2.8 NLS Batch test data for Ammonium in Sherwood Sandstone (powder form)

Tube No.	Wt. tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt NH₄ added (g)	Total wt tube + liquid (g)	pH after addition of NH₄	pH ratio after addition of NH₄	Total wt liquid (g) (V)
1 +ve control 10 mg/l (**no solid**)										
2 +ve control 10 mg/l (**no solid**)										
3 +ve control 40 mg/l (**no solid**)										
4 +ve control 40 mg/l. (**no solid**)										
5 Low spike 10 mg/l	12.67	**10.03**	24.89	**47.59**	8.70	**1.00**	48.59	**8.46**	0.97	**25.89**
6 Low spike 10 mg/l	12.66	**9.99**	24.89	**47.54**	8.71	**0.99**	48.53	**8.46**	0.96	**25.88**
7 Low spike 10 mg/l	12.65	**10.00**	24.89	**47.54**	8.68	**0.99**	48.53	**8.46**	0.97	**25.88**
8 High spike 40 mg/l	12.68	**10.00**	24.90	**47.58**	8.68	**0.99**	48.57	**8.06**	0.93	**25.89**
9 High spike 40 mg/l	12.69	**10.03**	24.87	**47.59**	8.70	**0.99**	48.58	**8.06**	0.93	**25.86**
10 High spike 40 mg/l	12.65	**10.06**	24.89	**47.60**	8.70	**0.99**	48.59	**8.06**	0.92	**25.88**
11 Blank	12.68	**10.02**	24.84	**47.54**	8.71	**0.99**	48.53	**8.68**	1.00	**25.83**
12 Blank	12.65	**10.04**	24.92	**47.61**	8.71	**0.99**	48.60	**8.68**	1.00	**25.91**

Table A2.8 (cont.) NLS batch test data for ammonium in Sherwood Sandstone (powder form)

Tube No.	Calc. NH$_4$ conc. (mg/l)	Actual NH$_4$ conc. (mg/l)	NH$_4$ conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	NH$_4$ ratio finish/start (F/I)	pH after adding HCl	Final NH$_4$ conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk average (mg/l)	Standard deviation	Relative SD
1 +ve control			9.60				9.48					
2 +ve control			9.60				9.49					
3 +ve control			38.44				37.91					
4 +ve control			38.44				37.97					
5 Low spike	250	**249.72**	9.60	**8.56**	0.55	**2.15**	5.26	2.12				
6 Low spike	250	**249.72**	9.60	**8.56**	0.53	**2.10**	5.09	2.30				
7 Low spike	250	**249.72**	9.60	**8.56**	0.53	**2.09**	5.11	2.27	2.23		0.096	4.32
8 High spike	1000	**999.37**	38.44	**8.52**	0.61	**2.09**	23.32	1.68				
9 High spike	1000	**999.37**	38.44	**8.52**	0.60	**2.10**	23.22	1.69				
10 High spike	1000	**999.37**	38.44	**8.52**	0.61	**2.19**	23.39	1.66	1.68		0.015	0.91
11 Blank				**8.59**		**2.13**	0.21					
12 Blank				**8.59**		**2.12**	0.17			0.19		

Table A2.9 NLS batch test data for arsenic in siltstone – sorption equilibration time 48 hours

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt As added (g)	Total wt tube + liquid (g)	pH after addition of As	pH ratio after addition of As	Total wt liquid (g) (V)
1 100 mg/l (no solid)										
2 100 mg/l (no solid)										
3 10 mg/l spike	12.65	**2.55**	24.01	**39.21**	6.74	**0.99**	40.20	**7.71**	1.14	**25.00**
4 10 mg/l spike	12.72	**2.51**	24.04	**39.27**	6.73	**0.99**	40.26	**7.72**	1.15	**25.03**
5 10 mg/l spike	12.70	**2.50**	24.03	**39.23**	6.73	**0.99**	40.22	**7.72**	1.15	**25.02**
6 50 mg/l spike	12.60	**7.52**	24.11	**44.23**	6.71	**0.99**	45.22	**7.98**	1.19	**25.10**
7 50 mg/l spike	12.71	**7.48**	24.11	**44.30**	6.73	**0.99**	45.29	**8.00**	1.19	**25.10**
8 50 mg/l spike	12.60	**7.54**	24.05	**44.19**	6.72	**0.99**	45.18	**7.99**	1.19	**25.04**
9 100 mg/l spike	12.71	**10.01**	24.03	**46.75**	6.69	**1.00**	47.75	**8.19**	1.22	**25.03**
10 100 mg/l spike	12.62	**10.03**	24.08	**46.73**	6.71	**1.01**	47.74	**8.17**	1.22	**25.09**
11 100 mg/l spike	12.61	**9.97**	24.06	**46.64**	6.71	**1.01**	47.65	**8.19**	1.22	**25.07**
12 Blank	12.70	**10.02**	24.03	**46.75**	6.71	**0.99**	47.74	**6.83**	1.02	**25.02**
13 Blank	12.59	**10.03**	24.01	**46.63**	6.74	**0.99**	47.62	**6.83**	1.01	**25.00**

Table A2.9 (cont.) NLS batch test form for Arsenic in siltstone – sorption equilibration time 48 hours

Tube No.	Calc. As conc. (mg/l)	Actual As conc. (mg/l)	As conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	As ratio finish/start (F/I)	Final As conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Average bulk (mg/l)	Standard deviation	Relative SD
1 100 mg/l (no solid)			100.23			94.51					
2 100 mg/l (no solid)			100.23			94.07					
3 10 mg/l spike	250	247.86	9.91	7.18	0.36	3.60	17.18				
4 10 mg/l spike	250	247.86	9.91	7.19	0.37	3.64	17.18				
5 10 mg/l spike	250	247.86	9.91	7.19	0.36	3.59	17.62	17.33		0.25	1.44
6 50 mg/l spike	1250	1251.89	50.08	7.30	0.35	17.52	6.20				
7 50 mg/l spike	1250	1251.89	50.08	7.32	0.37	18.68	5.64				
8 50 mg/l spike	1250	1251.89	50.08	7.31	0.36	18.20	5.82	5.89		0.29	4.92
9 100 mg/l spike	2500	2505.69	100.23	7.40	0.46	46.21	2.92				
10 100 mg/l spike	2500	2505.69	100.23	7.38	0.47	46.76	2.86				
11 100 mg/l spike	2500	2505.69	100.23	7.40	0.46	46.43	2.91	2.90		0.03	1.03
12 Blank				6.84		0.0042					
13 Blank				6.84		0.0028			0.0035		

Table A2.10 NLS batch test data for Cadmium in siltstone – sorption equilibration time 48 hours

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt Cd added (g)	Total wt tube + liquid (g)	pH after addition of Cd	pH ratio after addition of Cd	Total wt liquid (g) (V)
1 100 mg/l (no solid)										
2 100 mg/l (no solid)										
3 10 mg/l spike	12.66	**5.04**	23.98	**41.68**	6.57	**0.99**	42.67	**6.59**	1.00	**24.97**
4 10 mg/l spike	12.68	**5.06**	24.00	**41.74**	6.53	**0.99**	42.73	**6.55**	1.00	**24.99**
5 10 mg/l spike	12.67	**5.05**	23.97	**41.69**	6.53	**0.99**	42.68	**6.55**	1.00	**24.96**
6 50 mg/l spike	12.72	**5.04**	23.98	**41.74**	6.53	**0.99**	42.73	**6.56**	1.00	**24.97**
7 50 mg/l spike	12.69	**5.01**	23.98	**41.68**	6.53	**0.99**	42.67	**6.56**	1.00	**24.97**
8 50 mg/l spike	12.66	**5.00**	23.98	**41.64**	6.53	**0.99**	42.63	**6.56**	1.00	**24.97**
9 100 mg/l spike	12.60	**5.03**	23.98	**41.61**	6.52	**1.00**	42.61	**6.53**	1.00	**24.98**
10 100 mg/l spike	12.60	**5.00**	23.96	**41.56**	6.52	**1.00**	42.56	**6.53**	1.00	**24.96**
11 100 mg/l spike	12.66	**5.03**	23.94	**41.63**	6.53	**1.00**	42.63	**6.54**	1.00	**24.94**
12 Blank	12.64	**5.03**	23.95	**41.62**	6.53	**0.99**	42.61	**6.75**	1.03	**24.94**
13 Blank	12.67	**5.03**	23.96	**41.66**	6.53	**0.99**	42.65	**6.75**	1.03	**24.95**

Table A2.10 (cont.) NLS batch test data for cadmium in siltstone – sorption equilibration time 48 hours

Tube No.	Calc. Cd conc. (mg/l)	Actual Cd conc. (mg/l)	Cd conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	Cd ratio finish/start (F/I)	Final Cd conc. (mg/l) (F)	K_d (ml/g)m	Average K_d (ml/g)m	Average bulk (mg/l)	Standard deviation	Relative SD
1 100 mg/l (no solid)			**99.56**			95.77					
2 100 mg/l (no solid)			**99.56**			93.07					
3 10 mg/l spike	**250**	246.59	**9.86**	6.59	**0.27**	2.67	13.34				
4 10 mg/l spike	**250**	246.59	**9.86**	6.55	**0.26**	2.59	13.86				
5 10 mg/l spike	**250**	246.59	**9.86**	6.55	**0.27**	2.63	13.59	13.60		0.26	1.91
6 50 mg/l spike	**1250**	1243.71	**49.75**	6.48	**0.41**	20.15	7.28				
7 50 mg/l spike	**1250**	1243.71	**49.75**	6.48	**0.41**	20.23	7.27				
8 50 mg/l spike	**1250**	1243.71	**49.75**	6.48	**0.41**	20.33	7.23	7.26		0.026	0.36
9 100 mg/l spike	**2500**	2488.9	**99.56**	6.41	**0.48**	47.93	5.35				
10 100 mg/l spike	**2500**	2488.9	**99.56**	6.41	**0.49**	48.87	5.18				
11 100 mg/l spike	**2500**	2488.9	**99.56**	6.42	**0.46**	45.43	5.91	5.48		0.38	6.93
12 Blank				6.62		0.007					
13 Blank				6.62		0.02			0.014		

Table A2.11 NLS batch test data for lead in siltstone – sorption equilibration time 48 hours

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt Pb added (g)	Total wt tube + liquid (g)	pH after addition of Pb	pH ratio after addition of Pb	Total wt liquid (g) (V)
1 100 mg/l (no solid)										
2 100 mg/l (no solid)										
3 10 mg/l spike	12.70	**0.106**	23.98	**36.79**	6.32	**0.99**	37.78	**5.86**	0.93	**24.97**
4 10 mg/l spike	12.66	**0.104**	24.01	**36.77**	6.27	**0.99**	37.76	**5.81**	0.93	**25.00**
5 10 mg/l spike	12.66	**0.099**	23.95	**36.71**	6.27	**0.99**	37.70	**5.81**	0.93	**24.94**
6 50 mg/l spike	12.70	**1.04**	23.95	**37.69**	6.41	**0.99**	38.68	**6.09**	0.95	**24.94**
7 50 mg/l spike	12.72	**1.02**	23.94	**37.68**	6.41	**0.99**	38.67	**6.09**	0.95	**24.93**
8 50 mg/l spike	12.74	**1.03**	23.92	**37.69**	6.41	**0.99**	38.68	**6.09**	0.95	**24.91**
9 100 mg/l spike	12.66	**1.00**	24.02	**37.68**	6.54	**0.99**	38.67	**5.94**	0.91	**25.01**
10 100 mg/l spike	12.65	**1.02**	23.95	**37.62**	6.44	**0.99**	38.61	**5.84**	0.91	**24.94**
11 100 mg/l spike	12.69	**1.00**	23.93	**37.62**	6.44	**0.99**	38.61	**5.84**	0.91	**24.92**
12 Blank	12.65	**1.00**	23.97	**37.62**	6.46	**1.00**	38.62	**6.96**	1.08	**24.97**
13 Blank	12.65	**1.00**	23.92	**37.57**	6.46	**0.99**	38.56	**6.96**	1.08	**24.91**

Table A2.11 (cont.) NLS batch test data for lead in siltstone – sorption equilibration time 48 hours

Tube No.	Calc. Pb conc. (mg/l)	Actual Pb conc. (mg/l)	Pb conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	Pb ratio finish/start (F/I)	Final Pb conc. (mg/l) (F)	K_d (ml/g)m	Average K_d (ml/g)m	Average bulk (mg/l)	Standard deviation	Relative SD
1 100 mg/l (no solid)			**99.96**			92.92					
2 100 mg/l (no solid)			**99.96**			92.13					
3 10 mg/l spike	**250**	246.87	**9.87**	5.74	**0.43**	4.28	307.54				
4 10 mg/l spike	**250**	246.87	**9.87**	5.69	**0.44**	4.33	307.69				
5 10 mg/l spike	**250**	246.87	**9.87**	5.69	**0.43**	4.22	337.29	317.51		17.13	5.40
6 50 mg/l spike	**1250**	1256.50	**50.26**	5.68	**0.24**	11.83	77.90				
7 50 mg/l spike	**1250**	1256.50	**50.26**	5.68	**0.25**	12.35	75.03				
8 50 mg/l spike	**1250**	1256.50	**50.26**	5.68	**0.24**	12.09	76.35	76.43		1.44	1.88
9 100 mg/l spike	**2500**	2499.03	**99.96**	5.54	**0.39**	39.17	38.81				
10 100 mg/l spike	**2500**	2499.03	**99.96**	5.44	**0.39**	39.24	37.84				
11 100 mg/l spike	**2500**	2499.03	**99.96**	5.44	**0.41**	41.09	35.70	37.45		1.59	4.25
12 Blank				6.56		0.019					
13 Blank				6.56		0.004			0.012		

Table A2.12 NLS batch test data for zinc in siltstone – sorption equilibration time 48 hours

Tube No.	Wt tube + lid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt Zn added (g)	Total wt tube + liquid (g)	pH after addition of Zn	pH ratio after addition of Zn	Total wt liquid (g) (V)
1 100 mg/l (no solid)										
2 100 mg/l (no solid)										
3 10 mg/l spike	12.60	**0.759**	23.98	**37.34**	6.57	**0.99**	38.33	**6.36**	0.97	**24.97**
4 10 mg/l spike	12.64	**0.758**	23.97	**37.37**	6.66	**0.99**	38.36	**6.45**	0.97	**24.96**
5 10 mg/l spike	12.62	**0.751**	24.00	**37.37**	6.83	**0.99**	38.36	**6.62**	0.97	**24.99**
6 50 mg/l spike	12.64	**5.01**	24.02	**41.67**	6.55	**1.00**	42.67	**6.44**	0.98	**25.02**
7 50 mg/l spike	12.71	**5.05**	24.01	**41.77**	6.55	**0.99**	42.76	**6.44**	0.98	**25.00**
8 50 mg/l spike	12.70	**5.04**	24.04	**41.78**	6.55	**0.99**	42.77	**6.44**	0.98	**25.03**
9 100 mg/l spike	12.67	**5.03**	24.02	**41.72**	6.55	**1.00**	42.72	**6.42**	0.98	**25.02**
10 100 mg/l spike	12.66	**5.03**	24.04	**41.73**	6.55	**1.00**	42.73	**6.42**	0.98	**25.04**
11 100 mg/l spike	12.68	**5.02**	24.02	**41.72**	6.55	**1.00**	42.72	**6.42**	0.98	**25.02**
12 Blank	12.66	**5.05**	24.02	**41.73**	6.55	**0.99**	42.72	**6.98**	1.07	**25.01**
13 Blank	12.67	**5.08**	24.00	**41.75**	6.55	**0.99**	42.74	**6.98**	1.07	**24.99**

Table A2.12 (cont.) NLS batch test data for zinc in siltstone – sorption equilibration time 48 hours

Tube No.	Calc. Zn conc. (mg/l)	Actual Zn conc. (mg/l)	Zn conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	Zn ratio finish/start (F/I)	Final Zn conc. (mg/l) (F)	K_d (ml/g)m	Average K_d (ml/g)	Average bulk (mg/l)	Standard deviation	Relative SD
1 100 mg/l (no solid)			**100.44**			97.47					
2 100 mg/l (no solid)			**100.44**			97.44					
3 10 mg/l spike	**250**	248.01	**9.92**	6.19	**0.43**	4.35	42.13				
4 10 mg/l spike	**250**	248.01	**9.92**	6.28	**0.43**	4.25	43.93				
5 10 mg/l spike	**250**	248.01	**9.92**	6.53	**0.41**	4.07	47.83	44.63		2.91	6.52
6 50 mg/l spike	**1250**	1256.90	**50.28**	6.01	**0.26**	13.10	14.17				
7 50 mg/l spike	**1250**	1256.90	**50.28**	6.01	**0.26**	12.93	14.30				
8 50 mg/l spike	**1250**	1256.90	**50.28**	6.01	**0.26**	13.02	14.21	14.23		0.067	0.47
9 100 mg/l spike	**2500**	2511.12	**100.44**	5.86	**0.39**	38.71	7.93				
10 100 mg/l spike	**2500**	2511.12	**100.44**	5.86	**0.38**	38.47	8.02				
11 100 mg/l spike	**2500**	2511.12	**100.44**	5.86	**0.38**	38.35	8.07	8.01		0.071	0.89
12 Blank				6.52		0.03					
13 Blank				6.52		0.013			0.022		

Table A2.13 NLS batch test data for sulphate in siltstone – sorption equilibration time 48 hours (final SO$_4$ conc. bulk corrected)

Tube No.	Wt tube + lid	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt after adding NaCl (g)	pH after pre-equilibration	Wt SO$_4$ added (g)	Total wt tube + liquid (g)	pH after addition of SO$_4$	pH ratio after addition of SO$_4$	Total wt liquid (g) (V)
1 QC 500 mg/l (no solid)										
2 QC 500 mg/l (no solid)										
3 125 mg/l spike	12.68	10.03	23.98	46.69	6.32	1.00	47.69	6.42	1.02	24.98
4 125 mg/l spike	12.67	10.02	23.97	46.66	6.35	0.99	47.65	6.45	1.02	24.96
5 125 mg/l spike	12.66	9.99	23.98	46.63	6.34	1.00	47.63	6.44	1.02	24.98
6 250 mg/l spike	12.73	10.05	24.01	46.79	6.34	1.00	47.79	6.41	1.01	25.01
7 250 mg/l spike	12.71	10.03	23.96	46.70	6.32	1.00	47.70	6.39	1.01	24.96
8 250 mg/l spike	12.71	10.05	23.96	46.72	6.34	1.00	47.72	6.41	1.01	24.96
9 500 mg/l spike	12.70	10.01	23.98	46.69	6.34	1.02	47.71	6.38	1.01	25.00
10 500 mg/l spike	12.63	10.04	23.93	46.60	6.32	1.01	47.61	6.36	1.01	24.94
11 500 mg/l spike	12.67	10.01	23.95	46.63	6.39	1.01	47.64	6.43	1.01	24.96
12 Blank	12.66	10.04	23.94	46.64	6.42	0.99	47.63	6.42	1.00	24.93
13 Blank	12.73	9.98	23.89	46.60	6.42	0.99	47.59	6.42	1.00	24.88

Table A2.13 (cont.) NLS batch test data for sulphate in siltstone – sorption equilibration time 48 hours (final SO$_4$ conc. bulk corrected)

Tube No.	Calc. SO$_4$ conc. (mg/l)	Actual SO$_4$ conc. (mg/l)	SO$_4$ conc. after dilution in 25 ml (mg/l) (I)	pH after equilibration	SO$_4$ ratio start/finish (F/I)	Final SO$_4$ conc. (mg/l) (F)	K_d (ml/g)m	Average K_d (ml/g)m	Bulk average (mg/l)	Standard deviation	Relative SD
1 QC 500 mg/l (no solid)			499.92			**499**					
2 QC 500 mg/l (no solid)			499.92			**499**					
3 125 mg/l spike	3125.0	**3093.95**	123.76	**6.46**	0.98	**122**	0.061				
4 125 mg/l spike	3125.0	**3093.95**	123.76	**6.44**	0.98	**123**	0.041				
5 125 mg/l spike	3125.0	**3093.95**	123.76	**6.44**	0.98	**123**	0.041	0.048			
6 250 mg/l spike	6250.0	**6259.33**	250.37	**6.38**	0.90	**224**	0.29				
8 250 mg/l spike	6250.0	**6259.33**	250.37	**6.41**	0.91	**227**	0.25				
9 250 mg/l spike	6250.0	**6259.33**	250.37	**6.38**	0.77	**192**	0.75	0.43			
10 500 mg/l spike	12500.0	**12498.03**	499.92	**6.32**	0.96	**480**	0.10				
11 500 mg/l spike	12500.0	**12498.03**	499.92	**6.32**	0.86	**430**	0.40				
12 500 mg/l spike	12500.0	**12498.03**	499.92	**6.33**	0.93	**464**	0.19	0.23			
13 Blank				**6.50**		**13**					
14 Blank				**6.50**		**11**			12.0		

RSDs have not been calculated because of the small amount of sorption.

Table A2.14 NLS batch test data for diazinon in siltstone – 87 hours sorption equilibration time

Tube No.	Wt tube + Liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	pH after pre-equilibration	Total wt liquid (g) (V)	Diazinon conc. (mg/l).	Diazinon conc. after dilution in 25 ml (µg/l) (I)
1. QC 100 µg/l (no solid)							100
2. QC 100 µg/l (no solid)							100
3. 10 µg/l spike	27.44	**0.99**	25.10	**6.96**	25.10	**25**	10
4. 10 µg/l spike	27.37	**1.02**	25.11	**6.96**	25.11	**25**	10
5. 10 µg/l spike	27.26	**1.07**	25.08	**6.96**	25.08	**25**	10
6. 50 µg/l spike	27.38	**4.97**	25.07	**6.84**	25.07	**125**	50
7. 50 µg/l spike	27.38	**4.98**	25.08	**6.84**	25.08	**125**	50
8. 50 µg/l spike	27.13	**5.04**	25.02	**6.84**	25.02	**125**	50
9. 100 µg/l spike	27.40	**4.97**	25.01	**6.84**	25.01	**250**	100
10. 100 µg/l spike	27.30	**5.00**	25.09	**6.84**	25.09	**250**	100
11. 100 µg/l spike	27.63	**5.06**	25.07	**6.84**	25.07	**250**	100
12. Blank	27.15	**5.07**	25.02	**6.84**	25.02		
13. Blank	27.41	**5.00**	25.00	**6.84**	25.00		

Table A2.14 (cont.) NLS batch test data for diazinon in siltstone – 87 hours sorption equilibration time

Tube No.	Diazinon ratio finish/start (F/I)	Final diazinon conc. (µg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk (µg/l)	Standard deviation	Relative SD
1. QC 100 µg/l (no solid)		**88.72**					
2. QC 100 µg/l (no solid)		**91.70**					
3. 10 µg/l spike	0.72	**7.19**	9.91				
4. 10 µg/l spike	0.74	**7.38**	8.74				
5. 10 µg/l spike	0.75	**7.52**	7.73	8.79		1.09	12.40
6. 50 µg/l spike	0.69	**34.40**	2.29				
7. 50 µg/l spike	0.66	**32.99**	2.60				
8. 50 µg/l spike	0.63	**31.32**	2.96	2.62		0.34	13.00
9. 100 µg/l spike	0.69	**69.46**	2.21				
10. 100 µg/l spike	0.70	**69.62**	2.19				
11. 100 µg/l spike	0.71	**70.58**	2.07	2.16		0.08	3.70
12. Blank		**ND**					
13. Blank		**ND**			ND		

ND, not detected.

Table A2.15 NLS batch test data for Isoproturon in siltstone – 87 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	pH after pre-equilibration	Total wt liquid (g) (V)	Isoproturon conc. (mg/l)	Isoproturon conc. after dilution in 25 ml (μg/l) (I)
1. QC 100 μg/l (no solid)							100
2. QC 100 μg/l (no solid)							100
3. 10 μg/l spike	27.44	**30.10**	25.02	**6.50**	25.02	**25**	10
4. 10 μg/l spike	27.30	**29.99**	25.00	**6.50**	25.00	**25**	10
5. 10 μg/l spike	27.43	**30.13**	24.96	**6.50**	24.96	**25**	10
6. 50 μg/l spike	27.23	**29.98**	25.11	**6.50**	25.11	**125**	50
7. 50 μg/l spike	27.48	**29.95**	25.04	**6.50**	25.04	**125**	50
8. 50 μg/l spike	27.44	**30.02**	25.03	**6.50**	25.03	**125**	50
9. 100 μg/l spike	27.26	**30.12**	25.00	**6.50**	25.00	**250**	100
10. 100 μg/l spike	27.55	**30.04**	24.97	**6.50**	24.97	**250**	100
11. 100 μg/l spike	27.49	**30.03**	24.96	**6.50**	24.96	**250**	100
12. Blank	26.94	**10.07**	24.91	**6.73**	24.91		
13. Blank	27.41	**10.03**	24.86	**6.73**	24.86		

Table A2.15 (cont.) NLS batch test data for isoproturon in siltstone – 87 hours sorption equilibration time

Tube No.	Isoproturon ratio finish/start (F/I)	Final isoproturon conc. (µg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Bulk (µg/l)	Standard deviation	Relative SD
1. QC 100 µg/l (no solid)		**109.30**					
2. QC 100 µg/l (no solid)		**105.65**					
3. 10 µg/l spike	1.17	**11.73**	<				
4. 10 µg/l spike	1.13	**11.27**	<				
5. 10 µg/l spike	1.08	**10.76**	<				
6. 50 µg/l spike	1.07	**53.72**	<				
7. 50 µg/l spike	1.02	**50.98**	<				
8. 50 µg/l spike	1.03	**51.69**	<				
9. 100 µg/l spike	0.96	**96.43**	0.031				
10. 100 µg/l spike	0.96	**95.84**	0.036				
11. 100 µg/l spike	0.95	**94.68**	0.047				
12. Blank		**ND**					
13. Blank		**ND**					

ND, not detected; < K_d not calculated since sorption too low.

Table A2.16 NLS batch test data for mecoprop in siltstone – 87 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	pH after pre-equilibration	Total wt liquid (g) (V)	Mecoprop conc. (mg/l).	Mecoprop conc. after dilution in 25 ml (µg/l) (I)
1. QC 100 µg/l (no solid)							100
2. QC 100 µg/l (no solid)							100
3. 10 µg/l spike	27.43	**10.00**	25.04	**6.73**	25.04	**25**	10
4. 10 µg/l spike	27.09	**10.06**	25.01	**6.73**	25.01	**25**	10
5. 10 µg/l spike	27.34	**10.06**	25.00	**6.73**	25.00	**25**	10
6. 50 µg/l spike	27.22	**20.07**	24.98	**6.67**	24.98	**125**	50
7. 50 µg/l spike	27.38	**20.01**	24.94	**6.67**	24.94	**125**	50
8. 50 µg/l spike	27.40	**20.07**	24.94	**6.67**	24.94	**125**	50
9. 100 µg/l spike	27.49	**19.97**	24.90	**6.67**	24.90	**250**	100
10. 100 µg/l spike	27.16	**20.03**	24.97	**6.67**	24.97	**250**	100
11. 100 µg/l spike	27.16	**20.04**	24.93	**6.67**	24.93	**250**	100
12. Blank	27.27	**10.04**	24.94	**6.73**	24.94		
13. Blank	27.26	**10.07**	24.90	**6.73**	24.90		

Table A2.16 (cont.) NLS batch test data for mecoprop in siltstone – 87 hours sorption equilibration time

Tube No.	Mecoprop ratio finish/start (F/I)	Final mecoprop conc. (µg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Average bulk (µg/l)	Standard Deviation	Relative SD
1. QC 100 µg/l (no solid)		**111.28**					
2. QC 100 µg/l (no solid)		**129.40**					
3. 10 µg/l spike	1.10	**11.04**	<				
4. 10 µg/l spike	1.27	**12.68**	<				
5. 10 µg/l spike	1.10	**11.00**	<				
6. 50 µg/l spike	0.92	**45.83**	0.11				
7. 50 µg/l spike	1.25	**62.59**	<				
8. 50 µg/l spike	1.00	**49.87**	0.003				
9. 100 µg/l spike	1.04	**104.09**	<				
10. 100 µg/l spike	1.07	**106.82**	<				
11. 100 µg/l spike	1.27	**127.11**	<				
12. Blank		**ND**					
13. Blank		**ND**					

ND, not detected; < K_d not calculated since sorption too low.

Table A2.17 NLS batch test data for benzene in siltstone – 48 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt liquid (g) (V)	Benzene conc. (mg/l)	Benzene conc. after dilution in 38 ml (mg/l) (I)
1. QC 1.0 mg/l (no solid)					**3500**	1.0
2. QC 1.0 mg/l (no solid)					**3500**	1.0
3. 0.1 mg/l spike	27.56	**10.07**	37.83	37.83	**350**	0.1
4. 0.1 mg/l spike	27.61	**10.01**	37.83	37.83	**350**	0.1
5. 0.1 mg/l spike	27.65	**10.03**	37.81	37.81	**350**	0.1
6. 1.0 mg/l spike	27.49	**10.04**	37.82	37.82	**3500**	1.0
7. 1.0 mg/l spike	27.21	**10.06**	37.78	37.78	**3500**	1.0
8. 1.0 mg/l spike	27.53	**10.07**	37.79	37.79	**3500**	1.0
9. 10 mg/l spike	27.58	**9.99**	37.81	37.81	**35000**	10.0
10. 10 mg/l spike	27.52	**10.00**	37.83	37.83	**35000**	10.0
11. 10 mg/l spike	27.54	**10.01**	37.85	37.85	**35000**	10.0
12. Blank	27.70	**9.97**	38.00	38.00		
13. Blank	27.57	**10.02**	37.86	37.86		

Table A2.17 (cont.) NLS batch test data for benzene in siltstone – 48 hours sorption equilibration time

Tube No.	Benzene ratio finish/start (F/I)	Final benzene conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Average K_{oc} (ml/g OC)	Average bulk (mg/l)	Standard deviation	Relative SD
1. QC 1.0 mg/l (no solid)		**0.92**						
2. QC 1.0 mg/l (no solid)		**0.92**						
3. 0.1 mg/l spike	0.25	**0.025**	11.27					
4. 0.1 mg/l spike	0.25	**0.025**	11.34					
5. 0.1 mg/l spike	0.27	**0.027**	10.19	10.93	**1040.95**		0.64	5.90
6. 1.0 mg/l spike	0.35	**0.35**	7.00					
7. 1.0 mg/l spike	0.43	**0.43**	4.98					
8. 1.0 mg/l spike	0.33	**0.33**	7.62	6.53	**621.90**		1.38	21.14
9. 10 mg/l spike	0.51	**5.06**	3.70					
10. 10 mg/l spike	0.53	**5.31**	3.34					
11. 10 mg/l spike	0.52	**5.16**	3.55	3.53	**336.19**		0.18	5.12
12. Blank		**ND**						
13. Blank		**ND**				ND		

ND, not detected.

Table A2.18 NLS batch test data for naphthalene in siltstone – 48 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt liquid (g) (V)	Naphthalene conc. (mg/l).	Naphthalene conc. after dilution in 38 ml (mg/l) (I)
1. QC 1.0 mg/l (no solid)					**3500**	1.0
2. QC 1.0 mg/l (no solid)					**3500**	1.0
3. 0.1 mg/l spike	**27.28**	5.04	**39.77**	39.77	**350**	0.1
4. 0.1 mg/l spike	**27.47**	5.04	**39.81**	39.81	**350**	0.1
5. 0.1 mg/l spike	**27.73**	5.03	**39.75**	39.75	**350**	0.1
6. 1.0 mg/l spike	**27.32**	7.48	**37.89**	37.89	**3500**	1.0
7. 1.0 mg/l spike	**27.27**	7.51	**37.83**	37.83	**3500**	1.0
8. 1.0 mg/l spike	**27.43**	7.48	**37.78**	37.78	**3500**	1.0
9. 10 mg/l spike	**27.44**	10.08	**37.77**	37.77	**17500**	10.0
10. 10 mg/l spike	**27.40**	10.01	**37.72**	37.72	**17500**	10.0
11. 10 mg/l spike	**27.49**	10.06	**37.73**	37.73	**17500**	10.0
12. Blank	**27.53**	5.04	**39.65**	39.65		
13. Blank	**27.44**	5.03	**39.72**	39.72		

Table A2.18 (cont.) NLS batch test data for naphthalene in siltstone – 48 hours sorption equilibration time

Tube No.	Naphthalene ratio finish/start (F/I)	Final naphthalene conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Average K_{oc} (ml/g OC)	Average bulk (mg/l)	Standard deviation	Relative SD
1. QC 1.0 mg/l (no solid)		**0.93**						
2. QC 1.0 mg/l (no solid)		**0.95**						
3. 0.1 mg/l spike	1.00	**0.10**	<					
4. 0.1 mg/l spike	1.00	**0.10**	<					
5. 0.1 mg/l spike	1.00	**0.10**	<					
6. 1.0 mg/l spike	0.93	**0.93**	0.38					
7. 1.0 mg/l spike	0.96	**0.96**	0.21					
8. 1.0 mg/l spike	0.87	**0.87**	0.75	0.45	**42.86**			
9. 10 mg/l spike	0.90	**9.02**	0.41					
10. 10 mg/l spike	0.88	**8.84**	0.49					
11. 10 mg/l spike	0.88	**8.78**	0.52	0.47	**44.76**			
12. Blank		**ND**						
13. Blank		**ND**						

ND, not detected; < K_d not calculated since sorption too low. RSDs have not been calculated because of the small amount of sorption.

Table A2.19 NLS batch test data for total xylene in siltstone – 48 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt liquid (g) (V)	Total xylene conc. (mg/l).	Total xylene conc. after dilution in 38 ml (mg/l) (I)
1. QC 1.0 mg/l (no solid)					**3500**	1.0
2. QC 1.0 mg/l (no solid)					**3500**	1.0
3. 0.1 mg/l spike	**27.23**	10.01	**37.80**	37.80	**350**	0.1
4. 0.1 mg/l spike	**27.48**	10.00	**37.77**	37.77	**350**	0.1
5. 0.1 mg/l spike	**27.23**	9.99	**37.76**	37.76	**350**	0.1
6. 1.0 mg/l spike	**27.14**	9.98	**37.75**	37.75	**3500**	1.0
7. 1.0 mg/l spike	**27.39**	10.01	**37.80**	37.80	**3500**	1.0
8. 1.0 mg/l spike	**27.27**	9.99	**37.81**	37.81	**3500**	1.0
9. 10 mg/l spike	**27.54**	10.07	**37.77**	37.77	**35000**	10.0
10. 10 mg/l spike	**27.51**	10.04	**37.78**	37.78	**35000**	10.0
11. 10 mg/l spike	**27.20**	10.04	**37.77**	37.77	**35000**	10.0
12. Blank	**27.50**	10.03	**37.75**	37.75		
13. Blank	**27.55**	10.02	**37.72**	37.72		

Table A2.19 (cont.) NLS batch test data for total xylene in siltstone – 48 hours sorption equilibration time

Tube No.	Total xylene ratio finish/start (F/I)	Final total xylene conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Average K_{oc} (ml/g OC)	Average bulk (mg/l)	Standard deviation	Relative SD
1. QC 1.0 mg/l (no solid)		**0.99**						
2. QC 1.0 mg/l (no solid)		**0.89**						
3. 0.1 mg/l spike	0.22	**0.022**	13.39					
4. 0.1 mg/l spike	0.25	**0.025**	11.33					
5. 0.1 mg/l spike	0.21	**0.021**	14.22	12.98	**1236.19**		1.49	11.46
6. 1.0 mg/l spike	0.35	**0.35**	7.02					
7. 1.0 mg/l spike	0.44	**0.44**	4.81					
8. 1.0 mg/l spike	0.33	**0.33**	7.68	6.50	**619.05**		1.50	23.13
9. 10 mg/l spike	0.64	**6.35**	2.16					
10. 10 mg/l spike	0.44	**4.44***						
11. 10 mg/l spike	0.62	**6.17**	2.34	2.25	**214.29**		0.13	5.66
12. Blank		**ND**						
13. Blank		**ND**						

ND, not detected; *, Faulty centriprep cell (not used for average K_d measurement).

Table A2.20 NLS batch test data for toluene in siltstone – 48 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt liquid (g) (V)	Toluene conc. (mg/l)	Toluene conc. after dilution in 38 ml (mg/l) (I)
1. QC 1.0 mg/l (no solid)					**3500**	1.0
2. QC 1.0 mg/l (no solid)					**3500**	1.0
3. 0.1 mg/l spike	27.40	**10.04**	37.83	37.83	**350**	0.1
4. 0.1 mg/l spike	27.40	**10.05**	37.78	37.78	**350**	0.1
5. 0.1 mg/l spike	27.46	**10.01**	37.91	37.91	**350**	0.1
6. 1.0 mg/l spike	27.39	**9.98**	37.89	37.89	**3500**	1.0
7. 1.0 mg/l spike	27.35	**10.03**	37.86	37.86	**3500**	1.0
8. 1.0 mg/l spike	27.42	**9.98**	37.83	37.83	**3500**	1.0
9. 10 mg/l spike	27.19	**10.03**	37.86	37.86	**35000**	10.0
10. 10 mg/l spike	27.35	**9.99**	37.82	37.82	**35000**	10.0
11. 10 mg/l spike	27.40	**10.05**	37.81	37.81	**35000**	10.0
12. Blank	27.65	**10.05**	37.75	37.75		
13. Blank	27.55	**9.99**	37.74	37.74		

Table A2.20 (cont.) NLS batch test data for toluene in siltstone – 48 hours sorption equilibration time

Tube No.	Toluene ratio finish/start (F/I)	Final Toluene conc. (mg/l) (F)	K_d (ml/g)m	Average K_d (ml/g)m	Average K_{oc} (ml/g OC)	Average bulk (mg/l)	Standard Deviation	Relative SD
1. QC 1.0 mg/l (no solid)		**0.96**						
2. QC 1.0 mg/l (no solid)		**0.94**						
3. 0.1 mg/l spike	0.17	**0.017**	18.40					
4. 0.1 mg/l spike	0.20	**0.020**	15.04					
5. 0.1 mg/l spike	0.20	**0.020**	15.15	16.20	**1542.86**		1.91	11.78
6. 1.0 mg/l spike	0.17	**0.17**	18.54					
7. 1.0 mg/l spike	0.24	**0.24**	11.96					
8. 1.0 mg/l spike	0.17	**0.17**	18.51	16.34	**1556.19**		3.79	23.20
9. 10 mg/l spike	0.53	**5.29**	3.36					
10. 10 mg/l spike	0.34	**3.43**	7.25					
11. 10 mg/l spike	0.48	**4.80**	4.08	4.90	**466.67**		2.07	42.24
12. Blank		**ND**						
13. Blank		**ND**				ND		

ND, not detected.

Table A2.21 NLS batch test data for trichloroethene in siltstone – 48 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt liquid (g) (V)	Trichloroethene conc. (mg/l).	Trichloroethene conc. after dilution in 38 ml (mg/l) (I)
1. QC 1.0 mg/l (no solid)					**3500**	1.0
2. QC 1.0 mg/l (no solid)					**3500**	1.0
3. 0.1 mg/l spike	**27.22**	9.99	**37.67**	37.67	**350**	0.1
4. 0.1 mg/l spike	**27.59**	9.99	**37.66**	37.66	**350**	0.1
5. 0.1 mg/l spike	**27.59**	10.05	**37.67**	37.67	**350**	0.1
6. 1.0 mg/l spike	**27.47**	10.02	**37.74**	37.74	**3500**	1.0
7. 1.0 mg/l spike	**27.63**	10.03	**37.64**	37.64	**3500**	1.0
8. 1.0 mg/l spike	**27.66**	10.02	**37.65**	37.65	**3500**	1.0
9. 10 mg/l spike	**27.60**	9.99	**37.65**	37.65	**35000**	10.0
10. 10 mg/l spike	**27.20**	10.05	**37.64**	37.64	**35000**	10.0
11. 10 mg/l spike	**27.59**	10.05	**37.68**	37.68	**35000**	10.0
12. Blank	**27.69**	9.99	**37.68**	37.68		
13. Blank	**27.36**	10.03	**37.68**	37.68		

Table A2.21 (cont.) NLS batch test data for trichloroethene in siltstone – 48 hours sorption equilibration time

Tube No.	Trichloroethene ratio finish/start (F/I)	Final trichloroethene conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Average K_{oc} (ml/g OC)	Average bulk (mg/l)	Standard deviation	Relative SD
1. QC 1.0 mg/l (no solid)		**0.93**						
2. QC 1.0 mg/l (no solid)		**0.93**						
3. 0.1 mg/l spike	0.26	**0.026**	10.73					
4. 0.1 mg/l spike	0.26	**0.026**	10.73					
5. 0.1 mg/l spike	0.25	**0.025**	11.24	10.90	**1038.10**		0.29	2.70
6. 1.0 mg/l spike	0.52	**0.52**	3.48					
7. 1.0 mg/l spike	0.62	**0.62**	2.30					
8. 1.0 mg/l spike	0.66	**0.66**	1.94	2.57	**244.76**		0.81	31.34
9. 10 mg/l spike	0.54	**5.42**	3.18					
10. 10 mg/l spike	0.38	**3.82**	6.06					
11. 10 mg/l spike	0.46	**4.63**	4.35	4.53	**431.43**		1.45	32.00
12. Blank		**ND**						
13. Blank		**ND**						

ND, Not detected.

Table A2.22 NLS batch test data for tetrachloroethene in siltstone – 48 hours sorption equilibration time

Tube No.	Wt tube + liquid (g)	Wt solid added (g) (M)	Wt NaCl added (g)	Total wt liquid (g) (V)	Tetrachloroethene conc. (mg/l)	Tetrachloroethene conc. after dilution in 38 ml (mg/l) (I)
1. QC 1.0 mg/l (no solid)					**3500**	1.0
2. QC 1.0 mg/l (no solid)					**3500**	1.0
3. 0.1 mg/l spike	**27.51**	5.01	**39.82**	39.82	**350**	0.1
4. 0.1 mg/l spike	**27.35**	5.06	**39.78**	39.78	**350**	0.1
5. 0.1 mg/l spike	**27.46**	5.07	**39.78**	39.78	**350**	0.1
6. 1.0 mg/l spike	**27.15**	10.01	**37.84**	37.84	**3500**	1.0
7. 1.0 mg/l spike	**27.40**	10.05	**37.80**	37.80	**3500**	1.0
8. 1.0 mg/l spike	**27.27**	10.01	**37.82**	37.82	**3500**	1.0
9. 10 mg/l spike	**27.41**	9.98	**37.76**	37.76	**35000**	10.0
10. 10 mg/l spike	**27.35**	9.99	**37.76**	37.76	**35000**	10.0
11. 10 mg/l spike	**27.32**	10.07	**37.72**	37.72	**35000**	10.0
12. Blank	**27.29**	5.03	**39.71**	39.71		
13. Blank	**27.32**	4.98	**39.69**	39.69		

Table A2.22 (cont.) NLS batch test data for tetrachloroethene in siltstone – 48 hours sorption equilibration time

Tube No.	Tetrachloroethene ratio finish/start (F/I)	Final tetrachloroethene conc. (mg/l) (F)	K_d (ml/g)	Average K_d (ml/g)	Average K_{oc} (ml/g OC)	Average bulk (mg/l)	Standard deviation	Relative SD
1. QC 1.0 mg/l (no solid)		**0.83**						
2. QC 1.0 mg/l (no solid)		**0.80**						
3. 0.1 mg/l spike	0.80	**0.080**	1.99					
4. 0.1 mg/l spike	0.66	**0.066**	4.05					
5. 0.1 mg/l spike	0.66	**0.066**	4.04	3.36	**320.00**		1.19	35.31
6. 1.0 mg/l spike	0.60	**0.60**	2.52					
7. 1.0 mg/l spike	0.49	**0.49**	3.91					
8. 1.0 mg/l spike	0.52	**0.52**	3.49	3.31	**315.24**		0.71	21.53
9. 10 mg/l spike	0.61	**6.12**	2.40					
10. 10 mg/l spike	0.73	**7.34**	1.37					
11. 10 mg/l spike	0.54	**5.38**	3.22	2.33	**221.90**		0.93	39.78
12. Blank		**ND**						
13. Blank		**ND**						

ND, not detected.