SOCIETY OF BROWNFIELD RISK ASSESSMENT

Non-Aqueous Phase Liquid –
Guidance Notes for their Assessment in
Contaminated Land Scenarios in the UK

2. EFFECTIVE SOLUBILITY TOOL

USER GUIDE

PUBLICATION

This series of reports and tools is published by the Society of Brownfield Risk Assessment (SoBRA). It presents work undertaken by a SoBRA sub-group composed of volunteers listed in the acknowledgments below. This publication is part of a series of work packages designed to address various issues in data collection and evaluating risks associated with non-aqueous phase liquid (NAPL).

Calculating the effective solubility of dissolved phase contaminants is an important step in evaluating and risk assessing groundwater concentrations on sites with NAPL sources. This guidance document and the accompanying spreadsheet tool is intended to provide practical guidance and assistance to UK risk assessors to undertake these calculations. As set out in the text, it is imperative that users have read and understand the basis for the derivation of the tool and its limitations as described in the supporting text presented herein.

ACKNOWLEDGMENTS

SoBRA wishes to thank the following individuals for their considerable assistance in the successful delivery of this document:

CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST of APPENDICES

1   INTRODUCTION

The Society of Brownfield Risk Assessment (SoBRA) is a UK-based learned society that aims to:

- improve technical knowledge in risk-based decision-making related to land contamination applications; and

- enhance the professional status and profile of risk assessment practitioners.

The society has a number of working groups (termed "sub-groups") comprising volunteer SoBRA members working on particular aspects to help achieve these aims. This report presents one of several outputs of the non-aqueous phase liquid (NAPL) sub-group.

The technical aims of the sub-group are to:

- support technical excellence in the assessment, estimation and evaluation of risks associated with NAPL; and,

- encourage best practice by delivering practical advice to support decisions regarding the appropriate management of NAPL risks.

It should be noted from the outset it is not the intention of the sub-group or any of its deliverables to replicate existing NAPL guidance. Instead, the overarching aim is to address gaps in current guidance, and to provide practical advice to SoBRA members when undertaking risk assessments at sites where NAPL could be or is present.

1.1   Evolution and Overall Strategy of Sub-Group

The evaluation of contaminated land risk relies on understanding sub-surface processes. NAPL can be difficult to measure, meaning conceptual site models (CSM) may be data deficient. Following several requests from our members, SoBRA created the NAPL sub-group in 2019 with a call out to the SoBRA membership for volunteers to participate.

Once the group of volunteers was assembled, initial sub-group meetings identified and prioritised areas where existing NAPL UK risk assessment guidance was lacking or would benefit from practical advice. As a result of this screening process, a series of seven working groups was formed, each tasked with producing a document or tool to address the identified need.

The overall approach developed by the sub-group to address NAPL risk assessment is summarised in Figure 1. The seven working groups cover all stages of risk assessment, ranging from establishing whether NAPL is likely to be present at a site or

not, through to designing an appropriate remediation strategy. The position of this particular document within this strategy is highlighted.
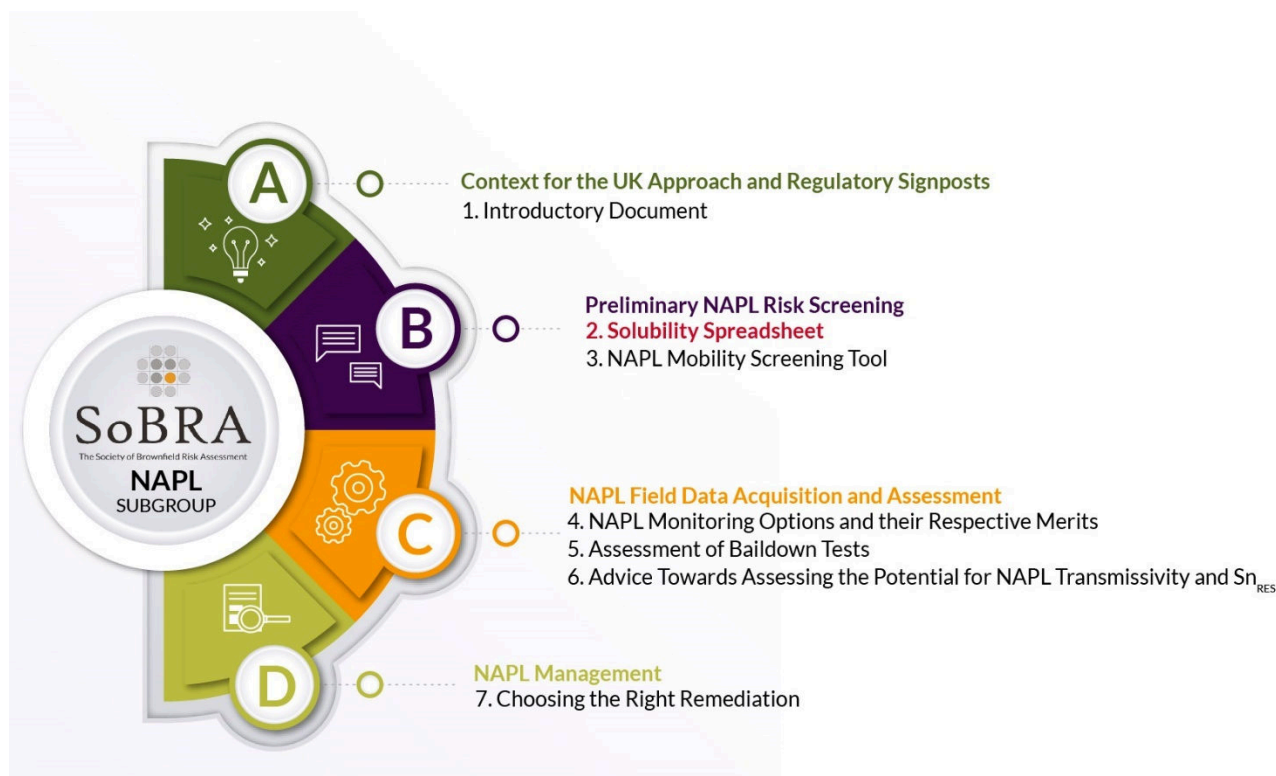
Figure 1 – Publication Strategy for NAPL Sub-Group.

1.2   Background

Non aqueous phase liquids (NAPLs) are described as organic liquids that are only slightly soluble, or immiscible in water (EA 2003, CL:AIRE 2014). NAPLs can be composed of a single component, but it is more common for them to be multicomponent comprising a complex mixture of chemical compounds, for example, petroleum hydrocarbon fuels and oils.

Where multi component NAPLs are present, the dissolved phase solubility of the various chemical components (the 'effective solubility') can be significantly reduced compared to their pure-phase solubility. This has important implications for developing NAPL conceptual site models (NCSM), understanding dissolved phase source terms and assessing contaminant migration risk.

Obtaining representative groundwater samples in proximity to NAPL sources can be problematic and lead to positive sample bias resulting from entrained NAPL or sediment (CL:AIRE 2017, Zemo 2009).

Therefore, calculating the effective solubility limit of the various contaminants of potential concern (CoPC) can help a risk assessor better evaluate the presence of

unrepresentative dissolved phase concentrations, and in most cases, provide a more accurate indication of the likely maximum dissolved phase concentrations that will be present if in equilibrium with the NAPL source. Such a parameter may then be considered for use in contaminant fate and transport modelling.

Additionally, where groundwater samples record CoPC concentrations at or close to calculated effective solubility limits, but where no measurable NAPL is observed, this can also be used as a line of evidence to suggest the presence of potential residual NAPL on site.

1.3   Aims

The aim of this document is to provide a user guide to support a peer reviewed spreadsheet tool that may be used by a competent person to calculate and assess dissolved phase effective solubility limits for a range of hydrocarbon contaminants where these derive from NAPL sources.

The tool has been produced based on equations published in a variety of recognised technical guidance and has been subject to a rigorous programme of 'road testing' and quality control with the sub-group.

As part of this document the following have been set out:

- the limitations of the tools use;

- a list of information to be obtained prior to its use; and,

- the methodologies and information sources used in the production of the tool.

It includes worked examples of calculations for a range of NAPL types to demonstrate its application in real-world settings.

Ultimately, our aim is that this spreadsheet tool may be used as part of the standard suite of tools that a competent assessor will employ to carry out risk assessment on sites with NAPL sources, in accordance with the principles set out under the Land Contamination Risk Management (LCRM) framework (EA 2020).

2 KEY PRINCIPLES

2.1 NAPL Dissolution & Raoult's Law

NAPL dissolution is described for light non aqueous phase liquids (LNAPLs) in CL:AIRE (2014, 2017) and for dense non aqueous phase liquids (DNAPLs) in EA (2003), and is briefly summarised below.

Following a release of NAPL to the subsurface, the NAPL body will expand until it becomes trapped by capillary forces, or as a mobile pool above a capillary barrier or the groundwater table, where it acts as a long-term source for groundwater contamination.

As groundwater flows through this NAPL source zone (be it LNAPL or DNAPL) soluble components dissolve from the NAPL body and partition into the passing groundwater (Figure 1).
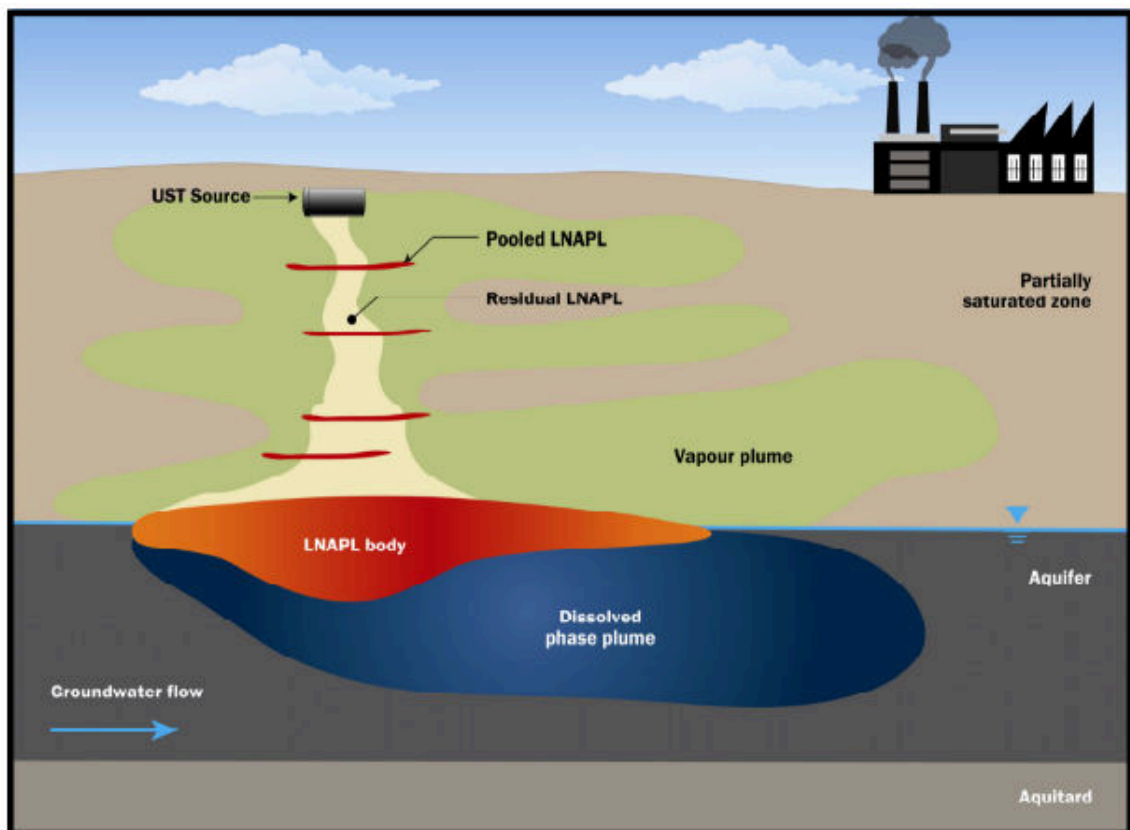
Figure 2. A Schematic conceptual model of an LNAPL release (Image from CL:AIRE 2014).

For multi component NAPLs, the various components do not dissolve into groundwater at their single component, pure phase, textbook solubility limit, as the various components each effect the solubility of the other components. Therefore, the equilibrium dissolved-phase concentration of each individual component within this

mixture is generally much lower than its pure phase solubility, and is described as its "effective" solubility.

This effective solubility can be estimated using an analogy to Raoult's Law[1].

2.2 Calculating Effective Solubility using Raoult's Law

The approach of using Raoult's Law to calculate effective solubility has been taken from the methodology set out in CL:AIRE (2017), this is summarised in Box 1.

Box 1: Raoult's Law

$$C_i = x_i C_i^o$$

Where:

C_i = effective solubility of a compound *i* (in the mixture) at equilibrium (mg.L^{-1})

x_i = mole fraction of *i* in the mixture

C_i^o = aqueous solubility concentration of the pure phase compound (usually reported at 25 ^{0}C) (mg.L^{-1})

The mole fraction, x_i, is defined as:

$$x_i = MF_i \times \left({MW_o}/{MW_i} \right)$$

Where:

MF_i = mass fraction of compound *i* in hydrocarbon mixture (g.g^{-1})

MW_i = molecular weight of the compound *i* (g.mole^{-1})

MW_o = approximated molecular weight of the whole hydrocarbon mixture (g.mole^{-1})

---

[1] Existing guidance (CL:AIRE 2014, 2017) indicates that for larger, higher molecular mass compounds (such as polycyclic aromatic hydrocarbons (PAHs) in coal tar as a typical example), which in their pure state are solids at normal environmental temperatures, these can have a higher effective solubility than predicted by Raoult's Law. In most cases these larger compounds are rarely dissolved phase risk drivers due to their low pure phase solubilities and large partition coefficients, and therefore are not considered further within this document. See CL:AIRE (2017) for the proposed approach to address this should a more accurate estimate be required.

2.3   Deriving the Mole Fraction

The mole fraction (x_i) of an individual compound is calculated using the equation described in Box 1.

This calculation requires an evaluation of the **mass fraction** of the compound within the hydrocarbon mixture in units of g.g^{-1} (this provides a unitless fraction for this value), the **molecular weight of the compound** in g.mole^{-1} and the **molecular weight of the whole NAPL** hydrocarbon mixture in units of g.mole^{-1}.

2.3.1   Determining Mass Fraction

Mass fraction (MF_i) is usually determined by submitting a sample of NAPL for laboratory analysis by gas chromatography flame ionisation detector (GC-FID) or gas chromatography mass spectrometry (GC-MS) for the range of suspected substances present. This could range from an analysis of speciated petroleum hydrocarbons according to the Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG) method and a volatile organic compound (VOC) suite (for example for a standard petrol or diesel fuel), to a variety of analytical suites such as United States Environmental Protection Agency (US EPA) VOC and semi-volatile organic compounds SVOCs, speciated PAHs or polychlorinated biphenyls (PCBs) (for example for an unidentified NAPL from an industrial site). Example analyses reports are included in Appendix 1.

Box 2: Mass Fraction Unit Conversions

Depending on the laboratory and the analytical suite carried out to determine the NAPL composition, this analysis can be reported as a % composition of each carbon band (common for TPHCWG analysis), or in units of mg.kg^{-1}. Either way, these results will need to be converted to those reported in Box 1 (g.g), to provide a result presented as a unitless fraction.

For example:

- a NAPL composition reported as % distribution will need to be divided by 100 to derive the mass fraction value.

- a NAPL analysis reported in mg.kg^{-1} will need to be divided by 1,000,000 (1E+6) to derive the mass fraction value.

The sum of all unitless component mass fractions should be 1, or close to 1. This can provide a useful sense check on the unit conversions and laboratory mass fraction results to evaluate whether the NAPL composition has been fully characterised, as

most fuels/oils contain a significant proportion of unidentified components (CL:AIRE, 2014). Where mass fraction data indicates a large proportion of unidentified components, the analysing laboratory should be consulted to provide an indication of the likely possible reason, examples include the possible presence of high molecular weight resins or asphaltenes in the NAPL, or a NAPL derived from fuel comprising a large proportion of ethanol (eg petrol E10) or fatty acid methyl esters (FAME) (eg biodiesel B5 or B20). In conjunction with the laboratory, consideration should be given to scheduling additional analytical suites to provide further characterisation where necessary.

2.3.2 Molecular Weight of the Compound

The molecular weight[2] of the individual compound (MW_i) can easily be sourced from standard literature chemical databases (CL:AIRE 2010, EA 2008, TPHCWG 1997) and is a known value based on the molecular formula of the compound.

2.3.3 Molecular Weight of the Whole Hydrocarbon (NAPL) Mixture

This value is the approximate molecular weight of the hydrocarbon mixture as a whole (MW_0) and given the complex range of compounds that may be present between fresh and weathered NAPLs the average molecular weight can vary substantially.

CL:AIRE (2017) suggested that "*Molecular weights are unlikely to be derived from site-specific measurements and the use of literature values is generally required…Where molecular weights are not available, consider using a plausible range of values*"

Example molecular weights are given in Table 1.

Table 1 – Representative molecular weights of hydrocarbon sources

Hydrocarbon Product	Approximated molecular weight (g.mole[-1])
Petrol (gasoline)	105
Kerosene	165
Diesel (gas oil)	230

Notes
1. CLAIRE (2017) Table 4.1 after USEPA 2015

---

[2] The molecular weight is also called the molar mass and molecular mass and presented as g.mol^{-1}. For the calculations in this document the terms and unit notations are interchangeable, but for consistency purposes we have followed the CL:AIRE (2017) notation in g.mole[-1]

However, CL:AIRE (2014) suggested that "*Mean molecular mass estimates of bands of quantified hydrocarbon ranges may likewise be used*" to estimate MW_0.

A methodology for estimating MW_0. based on the carbon distribution is given in McAlexander (2015). Assuming the mass fraction data is based on a TPHCWG speciation, this can be calculated by using the molecular weight reported for each of the CWG carbon bands. The molecular weight of each of the carbon band is multiplied by the reported mass fraction for each band, and these calculated values are summed up to give the LNAPL molecular weight MW_0.

A molecular weight calculator has been included in the spreadsheet tool accompanying this document, and an example calculation of MW_0 using this tool is given in Box 3 overpage.

Box 3: An Illustration of Calculating MW_0 for an LNAPL

A sample of a suspected weathered petrol was collected from a monitoring well. This was submitted for laboratory analysis of the LNAPL for TPHCWG speciation. The reported % composition for each of the CWG carbon bands was converted to a mass fraction in g.g⁻¹.

The results were input into the NAPL molecular weight calculator provided in the spreadsheet tool. An extract of the tool is reproduced below

Determinand	Mass fraction	Molecular weight	Compenent Mass fraction x molecular weight
	g.g-1	g.mole-1	g.mole-1
i	MF_i	MW_i	MF_i x MW_i
Aromatics >EC5-EC7	0.08	78	6.24
Aromatics >EC7-EC8	0.08	92	7.36
Aromatics >EC8-EC10	0.4	120	48
Aromatics >EC10-EC12	0.039	126	4.914
Aromatics >EC12-EC16 (aq)	0.0068	145	0.986
Aromatics >EC16-EC21 (aq)	0.0045	168	0.756
Aromatics >EC21-EC35 (aq)	0.0012	239	0.2868

Aliphatics >C5-C6	0.018	81	1.458
Aliphatics >C6-C8	0.29	102	29.58
Aliphatics >C8-C10	0.035	130	4.55
Aliphatics >C10-C12	0.036	159	5.724
Aliphatics >C12-C16 (aq)	0.0089	200	1.78
Aliphatics >C16-C21 (aq)	0.0014	269	0.3766

Calculated NAPL molecular weight (MWo):			112	g.mole-1
Mass fraction total:	1.0008		

A NAPL molecular weight of 112 g.mole⁻¹ was calculated. This was higher than the literature value of 105 g.mole⁻¹ reported in Table 1 for fresh petrol, and likely reflects the weathered nature of the LNAPL sampled, which indicates it has been depleted of the lower molecular weight carbon bands

The method described in Box 3 is particularly relevant for mixed fuel NAPLs, where estimating a NAPL molecular weight from reported literature values for single fuel sources would be more problematic and uncertain. It should be noted that mixed fuel NAPL comprise the majority of uncontrolled releases.

The method described by McAlexander (2015) also includes an estimate to calculate a compound's mole fraction and effective solubility from soil laboratory analysis data, based upon certain assumptions. This approach may be suitable for scenarios where NAPL samples were unable to be collected, for example where no monitoring wells are

present, such as during excavation works. This method using soil analytical data described by McAlexander is not included within the SoBRA spreadsheet tool, but follows a similar approach, with the mass fraction calculated by dividing the compounds concentration in soil by the respective TPH concentration in the same soil sample. The source reference should be consulted for full details and limitations of this method.

2.4   Calculating Effective Solubility

The effective solubility C_i of a compound is a simple calculation as described in Box 1, where the derived mole fraction is multiplied by the compound's pure phase solubility, which is obtained from standard literature chemical databases. It should be noted that the solubilities for hydrocarbon fractions given by TPHCWG are approximations based on properties for a range of representative compounds present within each fraction and therefore are a source of uncertainty. Where literature sources report a wide range of solubilities for a compound, it is recommended that sensitivity analysis be completed to evaluate the effect this has on the effective solubility calculation.

2.5   Using Effective Solubility in Risk Assessment

2.5.1   Benefits of Effective Solubility Estimation

Calculating the effective solubility of a compound provides the following additional information to aid risk assessment:

- It allows estimation of the maximum dissolved phase source mass concentrations likely to be present in the source zone, where the presence of NAPL prevents the reliable collection of groundwater samples; and,

- It can be used to indicate the possible presence of a NAPL source where dissolved phase concentrations are present approaching the effective solubility limit (the variously reported rules of thumb).

It can also be used to demonstrate degradation and weathering of the NAPL source term. Dissolution and volatilisation of the more soluble and volatile components from a NAPL over time lead to a reduction in the effective solubility of those components in the NAPL, leaving behind a less soluble persistent residual NAPL. By reassessing the NAPL mass fractions and effective solubility periodically over time it can be demonstrated that the NAPL source term is declining for key COPC. This NAPL compositional evaluation is also one of the established methods that can be used to demonstrate natural source zone depletion (NSZD) is occurring.

2.5.2 Risk Assessment Models

Referencing effective solubility concentrations in risk assessment models will depend on the type of model used. Forward predicting models are typically used to predict future concentrations at a compliance point to compare with allowable concentrations or generic assessment criteria. Backward calculating models, start with the acceptable or allowable concentration at the compliance point (e.g., a water quality standard) and calculate back to derive a higher concentration at the source (the site-specific assessment criteria or SSAC[3]) that would not cause an exceedance of the acceptable concentration at the compliance point.

In forward predicting risk models (e.g., Consim) the effective solubility concentration may be used to represent the maximum groundwater concentration input into the model for the source zone where NAPL is present or suspected. Assuming equilibrium dissolution then this will give a more accurate representation of the likely true dissolved phase source term, rather than, for example, a groundwater sample recording positive bias from entrained sheen or NAPL. The latter can often significantly overestimate the dissolved phase source term by a factor of between 10 and 100 and thereby grossly over predicting risks.

In back calculating risk models (e.g., Remedial Targets Methodology - RTM) the effective solubility concentration can be used as the site representative concentration to compare to the derived SSAC.

When the RTM back-calculated SSAC is above the effective solubility concentration for a particular compound, this indicates that no dissolved phase risk can be present for that compound for the modelled pathway.

Any conclusion from modelling should be re-evaluated over time to take account of potential changes in effective solubility. In practice however, for the more soluble (and often, more volatile) compounds that represent the key dissolved phase risk drivers, the effective solubility will reduce over time as the compound is depleted from the source NAPL and the mass fraction in the source NAPL reduces. Therefore, future dissolved phase migration risks will generally be lower.

Conversely, it is possible for the lower solubility, high molecular weight compounds to increase in mass fraction and therefore increase in effective solubility concentration over time as a NAPL weathers and degrades. However, again in practice, because these compounds generally have a low pure phase solubility concentration, an

---

[3] The SSAC is referred to as the "remedial target" in Remedial Targets Methodology (RTM)

increase in effective solubility over time often has little impact on the overall dissolved phase risk assessment.

2.5.3 GroundWater Spatiotemporal Data Analysis Tool (GWSDAT)

GWSDAT is a geo-statistical modelling tool for assessing groundwater plumes. For sample locations recording NAPL, the tool substitutes a user defined maximum solute concentration to enable contouring of dissolved phase concentrations. Using the calculated effective solubility will provide a more realistic representation of the maximum solute concentration in the presence of NAPL within GWSDAT.

2.6 Dealing with Groundwater Samples above Effective Solubility

Sometimes laboratory analysis of groundwater samples gives results where the concentrations are significantly above calculated effective solubility limits.

This "positive bias" can occur as a result of a number of factors, including:

- collecting groundwater samples from monitoring wells were measurable NAPL is present in the monitoring well. This should generally be avoided, particularly for LNAPL where sampling equipment has to be lowered through an LNAPL layer;

- collecting groundwater samples using high disturbance techniques (e.g., bailers, inertial pumps) or at high flow rates that can cause excessive drawdown and induce NAPL close to the well to be collected, or which can disturb NAPL saturated sediment in the base of a well and cause this to be collected and entrained within a groundwater sample; and,

- NAPL sheens, emulsions or NAPL droplets becoming entrained in a sample.

Additional consideration of when groundwater concentrations can be recorded above calculated effective solubility limits include where different NAPL sources with different compositions could be present across a site. In this case, the effective solubility associated with one NAPL source area may be significantly different to another area, which means that the recorded groundwater concentration may be a true reflection of the different NAPL sources. Consequently, the characterisation and hydrocarbon profile of each groundwater sample should be compared to the source NAPL used to derive the effective solubility calculation to ensure they are consistent.

Also, the presence of colloidal particles or a co-solvency effect (Ford et al., 2014) can lead to greater than expected dissolved phase contamination. In particular, alcohols present in groundwater can lead to an increased solubility of hydrocarbons. This is of

particular relevance given the introduction of 10% ethanol composition in petrol blends (E10 fuel) in the UK in September 2021.

For groundwater assessments where groundwater sample results have been demonstrated to be above the effective solubility limit for the respective source, the risk assessor should clearly identify these samples as likely suffering from positive sampling bias, explain the reason why they are not representative (by reference to other lines of field evidence such as presence of sheens on water or in soil samples) and either use the effective solubility concentration or other nearby groundwater sample results to characterise the groundwater quality.

Occasionally, the laboratory analytical method detection limit for a compound may also be higher than the calculated effective solubility limit. In this case, it is recommended that the effective solubility limit is used as the representative groundwater concentration.

Where NAPL phase is shown to be present, this should be assessed separately in accordance with existing guidance (ITRC LNAPL 3 2019; CL:AIRE, 2014) and the framework set out within the companion SoBRA NAPL sub group guidance documents.

One way to avoid positive bias in the collection of groundwater samples at sites with a significant NAPL source term is to design different sampling and investigation strategies to address NAPL and groundwater separately. For example, different well locations and well constructions can be used separately for:

- evaluating in-well NAPL accumulation, enabling NAPL sample collection and conducting NAPL transmissivity tests (e.g., larger well screens or diameters to maximise accumulation and volumes); and,

- allowing groundwater sample collection to obtain representative dissolved phase concentrations, allowing vertical profiling and to minimise purge volumes and enable low flow sampling techniques (e.g., multi-level or nested sampling wells, targeted short well screen lengths).

3 USING THE SPREADSHEET TOOL

3.1 Introduction

To provide a reliable estimate of effective solubility, SoBRA has produced a peer reviewed, cell protected spreadsheet tool in Microsoft Excel to accompany this guidance.

The tool includes the following features:

- NAPL Molecular Weight calculator;

- Effective Solubility calculator based on "TPHCWG" carbon banding;

- Effective Solubility calculator using the "Top 20" compounds present in a mixed NAPL; and,

- An example library of published fuel compositions and real composition analysis of a range of NAPL types collated from the SoBRA contributors, as well as a library of organic compounds and their physical properties used in the calculations.

The following sections provide a user guide to the tool and a work through calculation for different NAPL types.

3.2 User Guide & Example Calculations

The tool includes 5 key tabs:

1. Organic Compound Physical Properties Library;

2. Mass Fraction Library of Various NAPLs;

3. NAPL Molecular Weight Calculator;

4. Standard Effective Solubility Calculator (TPHCWG banding); and

5. Effective Solubility Calculator (Top 20 Compound Mixture).

Cells that are unlocked and require user input (either as a drop down or value inserted) are coloured in green. All other calculation cells are locked and unshaded. The calculated outputs tabs are locked and shaded in yellow.

3.2.1 TPHCWG Banding Calculator Example

Step 1 – Choose NAPL Type

When using the TPH banding calculator, in the first instance the user needs to determine whether they will be using site specific mass fraction data (preferred method) or an appropriate NAPL selected from the Mass Fraction Library of various fuel types.

This is selected in the "NAPL Type" dropdown coloured green in the "Standard Calculation" tab as shown below:

Step 2 – Input Site Specific Mass Fraction Data

If "Site Specific" is selected, the user needs to input the mass fraction data from your laboratory analysis for each of the relevant carbon bands in the green shaded cells in the "Mass Fraction Library" tab shown overleaf. For C16-35 Aliphatics, this should be the sum of the C16-21 and C21-35 carbon bands.

The tool assumes individual compounds are included within the relevant carbon bands and not assessed separately (eg ethylbenzenes, xylenes and trimethylbenzenes within the Aromatic EC8-EC10 carbon band, and naphthalene within the Aromatic EC10-EC12 band).

If individual compounds are to be assessed separately in addition to the TPHCWG carbon band approach, then the "Top 20 Mixtures Calculation" tab should be used. In this approach, the individual compound value should be subtracted from the relevant carbon band to avoid double counting. For example, if naphthalene is entered individually, the naphthalene value should be subtracted from the corresponding Aromatic EC10-EC12 mass fraction value.

Step 3 – Calculate NAPL Molecular Weight

To calculate a NAPL molecular weight, the appropriate TPHCWG determinands should be selected from the dropdown box in the "Molecular Weight Calculator" tab. The same lab mass fraction data as step 2 should be entered into the relevant cells in the "Molecular Weight Calculator" tab in the same way. The calculated NAPL Molecular Weight value reported in this tab in the yellow shaded cell should then be input into the relevant cell in the "Mass Fraction Library" tab as shown below:

The mole fraction and effective solubility values will then be calculated and reported automatically in the yellow shaded cells of the "Standard Calculation" tab. The data overleaf shows the output for a weathered petrol with a calculated NAPL molecular weight of 113 g.mole^{-1} and composition including 4% benzene, 12% toluene, 40% EC8-10 aromatics and 29% C6-8 aliphatics.

Determinand	Mass fraction	Pure phase solubility	Molecular weight	NAPL Molecular weight	Mole Fraction	Effective Solubility
		mg.L-1	g.mole-1	g.mole-1		mg.L-1
i	MF_i	C_i^0	MW_i	MW_0	x_i	C_i
Aromatics						
EC5-EC6 Benzene	0.04	1780	78	113	5.79E-02	1.03E+02
EC7-EC8 Toluene	0.12	590	92	113	1.47E-01	8.70E+01
EC8-EC10 (ethylbenzene, xylenes + others)	0.4	65	120	113	3.77E-01	2.45E+01
EC10-EC12 (includes naphthalene)	0.039	25	126	113	3.50E-02	8.74E-01
EC12-EC16	0.0067	5.8	145	113	5.22E-03	3.03E-02
EC16-EC21	0.0045	0.65	168	113	3.03E-03	1.97E-03
EC21-EC35	0.0012	0.0066	239	113	5.67E-04	3.74E-06
Aliphatics						
EC5-EC6	0.018	36	81	113	2.51E-02	9.04E-01
EC6-EC8	0.29	5.4	102	113	3.21E-01	1.73E+00
EC8-EC10	0.035	0.43	130	113	3.04E-02	1.31E-02
EC10-EC12	0.036	0.034	159	113	2.56E-02	8.70E-04
EC12-EC16	0.0089	0.00076	200	113	5.03E-03	3.82E-06
EC16-EC35	0.0014	0.000003	269	113	5.88E-04	1.76E-09
MTBE	0.0005	43000	88	113	6.41E-04	2.76E+01
Mass fraction total:	1.0012					

The example calculation shows a sum of the mass fraction data of 1, a calculated benzene effective solubility of 103 mg.L^{-1}, compared to a pure phase solubility of 1780 mg.L^{-1}, a toluene effective solubility of 87 mg.L^{-1} (pure phase 590 mg.L^{-1}) and EC8-10 aromatics effective solubility of 24.5 mg.L^{-1} compared to a pure phase of 65 mg.L^{-1}.

A pie chart showing the relative proportions of the calculated effective solubilities for the NAPL is also included.

3.2.2 Top 20 Compound Calculator Example

This calculator is designed to be used for mixed NAPLs where the composition may be less obvious. This could include for example a mixed multi component DNAPL comprising hydrocarbons, chlorinated solvents and benzene, toluene, ethyl benzene, toluene (BTEX). As an illustration we have used the example multi component DNAPL given in Table 5 of the DNAPL Handbook (EA, 2003).

Step 1 – Select the "Top 20" Compounds

The "Physical Properties Library" tab includes a range of organic compounds typically included in VOC and SVOC laboratory analysis suites. However, if the "Top 20" compound is not listed within the library, it can be added as a user defined compound.

In the "Top 20 Mixtures Calculation" tab, select each compound from the dropdown list, which links to the individual organic compounds listed in the Physical Properties Library tab.

Step 2 – Input Site Specific Mass Fraction Data

Enter the lab mass fraction data in the green cells for each selected compound

Step 3 – Calculate NAPL Molecular Weight

The same lab mass fraction data should also be entered into the relevant cells in the "Molecular Weight Calculator" tab in the same way. The calculated NAPL Molecular Weight value reported in this tab in the yellow shaded cell (cell "E43") should then be input into the relevant NAPL Molecular Weight cell in the "Top 20 Mixtures Calculation" tab.

Calculation sheet for effective solubility of site specific
NAPL mixtures - Top 20 Analysis

Based on Raoult's Law and methodology set out in CL:AIRE, 2017. Petroleum
Hydrocarbons in Groundwater: Guidance on assessing
petroleum hydrocarbons using existing hydrogeological risk assessment
methodologies. CL:AIRE, London. ISBN 978-1-905046-31-7
©SoBRA, 2021

☐ = Calculation outputs
🟩 = User defined value

NAPL Molecular Weight (site specific)
g.mole-1   231
Calculated outputs

Insert calculated
NAPL molecular
weight here

The mole fraction and effective solubility values will then be calculated and reported automatically in the yellow shaded cells of the "Top 20 Mixtures Calculation" tab.

The data below shows the output for the mixed solvent DNAPL example from the DNAPL handbook, comprising a NAPL, molecular weight of 231 g.mole^{-1}, mix of BTEX (7%), chlorinated solvents (19%), PCBs (47%) and some petroleum hydrocarbons (26%).

	Top 20	Mass fraction	Pure phase solubility mg.L-1	Molecular weight g.mole-1	NAPL Molecular weight g.mole-1	Mole Fraction	Effective Solubility mg.L-1
i		MF_i	C_i^0	MW_i	MW_0	x_i	C_i
1	1,1,1-Trichloroethane	0.007	1300	133	231	1.21E-02	1.58E+01
2	Trichloroethene	0.037	1370	131	231	6.51E-02	8.91E+01
3	Tetrachloroethene	0.143	225	166	231	1.99E-01	4.48E+01
4	Toluene	0.047	590	92	231	1.18E-01	6.95E+01
5	m-Xylene	0.003	200	106	231	6.53E-03	1.31E+00
6	p-Xylene	0.023	200	106	231	5.00E-02	1.00E+01
7	1,2,4-Trichlorobenzene	0.001	41.4	181	231	1.27E-03	5.27E-02
8	PCB congener 77	0.406	0.0663	292	231	3.21E-01	2.13E-02
9	PCB congener 123	0.071	0.0218	326	231	5.02E-02	1.10E-03
10	Aliphatics >C12-C16 (aq)	0.26	0.00076	200	231	3.00E-01	2.28E-04
11			---	---	231		
12			---	---	231		
13			---	---	231		
14			---	---	231		
15			---	---	231		
16			---	---	231		
17			---	---	231		
18			---	---	231		
19			---	---	231		
20			---	---	231		
	Mass fraction total:	0.998					

The calculation shows the sum of the mass fraction data of approximately 1, and calculated trichloroethene (TCE) and 1,1,1-trichloroethane (TCA) effective solubilities of 89 mg.L^{-1} and 15.8 mg.L^{-1} respectively, compared to pure phase solubilities 1370 mg.L^{-1} and 1300 mg.L^{-1}.

4 REFERENCES

CL:AIRE, 2010. The EIC/AGS/CL:AIRE Soil Generic Assessment Criteria for Human Health Risk Assessment. CL:AIRE, London. ISBN 978-1-905046-20-1

CL:AIRE, 2014. An Illustrated Handbook of LNAPL Transport and Fate in the Subsurface. CL:AIRE, London. ISBN 978-1-905046-24-9

CL:AIRE, 2017. Petroleum Hydrocarbons in Groundwater: Guidance on assessing petroleum hydrocarbons using existing hydrogeological risk assessment methodologies. CL:AIRE, London. ISBN 978-1-905046-31-7. Download at www.claire.co.uk/phg .

Environment Agency, 2003. An illustrated handbook of DNAPL transport and fate in the subsurface. R&D Technical Report 133. Bristol: Environment Agency. ISBN: 1844320669

Environment Agency, 2008. Compilation of data for priority organic pollutants for derivation of Soil guideline values. Science publication SC05002/ SR7 Bristol Environment Agency. Available from: http://publications.environment-agency.gov.uk/pdf/SCHO1008BOVO-e-e.pdf

Environment Agency, 2020. Land contamination risk management (LCRM). How to assess and manage the risks from land contamination. Environment Agency, 8th October 2020. Available at https://www.gov.uk/government/publications/land-contamination-risk-management-lcrm

Ford, R.G., Brooks, M.C., Ada, O.K., Enfield, C.G. and Kravitz, M., 2014. Evaluating potential exposures to ecological receptors due to transport of hydrophobic organic contaminants in subsurface systems. Available at https://clu-in.org/download/contaminantfocus/sediments/EPA-600-R-10-015.pdf

ITRC LNAPL-3: LNAPL Site Management: LCSM Evolution, Decision Process, and Remedial Technologies. https://lnapl-3.itrcweb.org/

McAlexander, B (2015). Calculating Mole Fractions from LNAPL and Soil Samples Applied NAPL Science Review (ANSR). Volume 5, Issue 1 | March 2015. Available at Calculating Mole Fractions from LNAPL and Soil Samples Volume 5, Issue 1 | March 2015 | Applied NAPL Science Review (naplansr.com)

Total Petroleum Hydrocarbons Criteria Working Group (TPHCWG) 1997. Volume 3: Selection of Representative TPH Fractions Based on Fate and Transport

Considerations. MA: Amherst Scientific Publishers. Available from: http://www.aehsfoundation.org/Amherst-Scientific-Publishers.aspx

United States Environmental Protection Agency (USEPA), 2015. EPA On-line Tools for Site Assessment website. https://www3.epa.gov/ceampubl/learn2model/part-two/onsite/es.html

Zemo, D. A. (2009). Suggested Methods to Mitigate Bias from Non-dissolved Petroleum in Ground Water Samples Collected from the Smear Zone. Ground Water Monitoring & Remediation 29, no. 3: 77-83

APPENDIX 1

Example NAPL Analysis Reports

SVOC/ VOC & TPHCWG Product Report

April 2016

FINAL ANALYTICAL TEST REPORT
SUPPLEMENT TO TEST REPORT 16/02128/2

Envirolab Job Number: ▮▮▮▮▮▮▮

Issue Number: 3   **Date:** 06 June, 2016

Client: ▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮

▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮

Order No: N/A
Date Samples Received: 12/04/16
Date Instructions Received: 12/04/16
Date Analysis Completed: 25/04/16

Prepared by: **Approved by:**

▮▮▮▮▮▮▮▮   ▮▮▮▮▮▮▮▮

▮▮▮▮▮▮   ▮▮▮▮▮

UKAS
TESTING
1247

Lab Sample ID									Units	Method ref
Client Sample No										
Client Sample ID	BH213	BH211	BH207	BH206	WA3-R1	WA2-R1				
Depth to Top										
Depth To Bottom										
Date Sampled	05-Apr-16	08-Apr-16	06-Apr-16	07-Apr-16	07-Apr-16	06-Apr-16				
Sample Type	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil				
Sample Matrix Code	N/A	N/A	N/A	N/A	N/A	N/A				
Product (Oil) Density$_A$	1.020	1.056	1.043	1.013	1.117	1.033			g/ml	A T 018

Envirolab Job Number: ▮▮▮▮▮▮

										Units	Method ref
Lab Sample ID	▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮										
Client Sample No											
Client Sample ID	BH213	BH211	BH207	BH206	WA3-R1	WA2-R1					
Depth to Top											
Depth To Bottom											
Date Sampled	05-Apr-16	08-Apr-16	06-Apr-16	07-Apr-16	07-Apr-16	06-Apr-16					
Sample Type	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil					
Sample Matrix Code	N/A	N/A	N/A	N/A	N/A	N/A					
Product (Oil) SVOC											
Hexachlorobenzene_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Diethyl phthalate_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Dimethyl phthalate_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Dibenzofuran_A	989000	<25000	2130000	2060000	2000000	1480000				µg/kg	A T 052s
Carbazole_A	551000	<25000	305000	364000	619000	161000				µg/kg	A T 052s
Butylbenzyl phthalate_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Bis(2-ethylhexyl)phthalate_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Bis(2-chloroethoxy)methane_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Bis(2-chloroethyl)ether_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
4-Nitrophenol_A	<25000	<25000	572000	621000	482000	<25000				µg/kg	A T 052s
4-Methylphenol_A	61200	<25000	<25000	<25000	36500	<25000				µg/kg	A T 052s
4-Chloro-3-methylphenol_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2-Nitrophenol_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2-Methylphenol_A	119000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2-Chlorophenol_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2,6-Dinitrotoluene_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2,4-Dinitrotoluene_A	<25000	<25000	969000	973000	<25000	1190000				µg/kg	A T 052s
2,4-Dimethylphenol_A	231000	<25000	<25000	<25000	627000	<25000				µg/kg	A T 052s
2,4-Dichlorophenol_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2,4,6-Trichlorophenol_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2,4,5-Trichlorophenol_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2-Chloronaphthalene_A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
2-Methylnaphthalene_A	2670000	<25000	14300000	11700000	3710000	5430000				µg/kg	A T 052s
Acenaphthylene_A	2770000	<25000	6550000	6140000	3350000	1860000				µg/kg	A T 052s
Acenaphthene_A	583000	<25000	1690000	1940000	974000	6840000				µg/kg	A T 052s
Anthracene_A	1980000	<25000	3470000	3410000	2190000	4660000				µg/kg	A T 052s
Benzo(a)anthracene_A	1040000	<25000	1780000	1750000	1430000	1750000				µg/kg	A T 052s
Benzo(b)fluoranthene_A	680000	<25000	1040000	1050000	1030000	928000				µg/kg	A T 052s
Benzo(k)fluoranthene_A	275000	<25000	437000	1510000	419000	420000				µg/kg	A T 052s
Benzo(a)pyrene_A	732000	<25000	1420000	1290000	910000	1330000				µg/kg	A T 052s
Benzo(ghi)perylene_A	308000	<25000	416000	416000	368000	409000				µg/kg	A T 052s
Chrysene_A	1030000	<25000	1740000	1750000	1310000	1740000				µg/kg	A T 052s

Lab Sample ID	████████									Units	Method ref
Client Sample No											
Client Sample ID	BH213	BH211	BH207	BH206	WA3-R1	WA2-R1					
Depth to Top											
Depth To Bottom											
Date Sampled	05-Apr-16	08-Apr-16	06-Apr-16	07-Apr-16	07-Apr-16	06-Apr-16					
Sample Type	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil					
Sample Matrix Code	N/A	N/A	N/A	N/A	N/A	N/A					
Fluoranthene A	3650000	<25000	6210000	6310000	4070000	6520000				µg/kg	A T 052s
Fluorene A	1050000	<25000	5550000	5640000	2740000	5880000				µg/kg	A T 052s
Indeno(1,2,3-cd)pyrene A	287000	<25000	452000	462000	434000	360000				µg/kg	A T 052s
Phenanthrene A	5490000	<25000	11500000	11800000	4860000	13500000				µg/kg	A T 052s
Pyrene A	4100000	<25000	7300000	7660000	2580000	9770000				µg/kg	A T 052s
Naphthalene A	18600000	79200	47900000	39200000	17800000	28000000				µg/kg	A T 052s
Dibenzo(ah)anthracene A	62300	<25000	99900	87200	92600	88400				µg/kg	A T 052s
Bis(2-chloroisopropyl)ether A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Phenol A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Pentachlorophenol A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
n-Nitroso-n-dipropylamine A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
n-Dioctylphthalate A	132000	<25000	109000	122000	134000	116000				µg/kg	A T 052s
n-Dibutylphthalate A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Nitrobenzene A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Isophorone A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Hexachloroethane A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Hexachlorocyclopentadiene A	<25000	<25000	<25000	<25000	<25000	<25000				µg/kg	A T 052s
Perylene A	143000	<25000	200000	188000	224000	171000				µg/kg	A T 052s

Envirolab Job Number: ▮▮▮▮▮

Lab Sample ID	▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮								Units	Method ref
Client Sample No										
Client Sample ID	BH213	BH211	BH207	BH206	WA3-R1	WA2-R1				
Depth to Top										
Depth To Bottom										
Date Sampled	05-Apr-16	08-Apr-16	06-Apr-16	07-Apr-16	07-Apr-16	06-Apr-16				
Sample Type	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil				
Sample Matrix Code	N/A	N/A	N/A	N/A	N/A	N/A				
Product (Oil) VOC										
Dichlorodifluoromethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Chloromethane$_A$#	<37500	<37500	<37500	<37500	<37500	<37500			µg/kg	A T 006s
Vinyl Chloride$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Bromomethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Chloroethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Trichlorofluoromethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,1-Dichloroethene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Carbon Disulphide$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Dichloromethane$_A$	<18750	<18750	<18750	<18750	<18750	<18750			µg/kg	A T 006s
trans 1,2-Dichloroethene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,1-Dichloroethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
cis 1,2-Dichloroethene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
2,2-Dichloropropane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Bromochloromethane$_A$#	<18750	<18750	<18750	<18750	<18750	<18750			µg/kg	A T 006s
Chloroform$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,1,1-Trichloroethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,1-Dichloropropene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Carbon Tetrachloride$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,2-Dichloroethane$_A$#	<7500	<7500	<7500	<7500	<7500	<7500			µg/kg	A T 006s
Benzene $_A$#	292000	<3750	115000	44500	104000	32700			µg/kg	A T 006s
Trichloroethene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,2-Dichloropropane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Dibromomethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Bromodichloromethane$_A$#	<37500	<37500	<37500	<37500	<37500	<37500			µg/kg	A T 006s
cis 1,3-Dichloropropene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Toluene $_A$#	496000	<3750	358000	220000	195000	9220			µg/kg	A T 006s
trans 1,3-Dichloropropene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,1,2-Trichloroethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,3-Dichloropropane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Tetrachloroethene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Dibromochloromethane$_A$#	<11250	<11250	<11250	<11250	<11250	<11250			µg/kg	A T 006s
1,2-Dibromoethane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s

Envirolab Job Number: ▮▮▮▮▮▮

	BH213	BH211	BH207	BH206	WA3-R1	WA2-R1			Units	Method ref
Lab Sample ID	▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮▮									
Client Sample No										
Client Sample ID	BH213	BH211	BH207	BH206	WA3-R1	WA2-R1				
Depth to Top										
Depth To Bottom										
Date Sampled	05-Apr-16	08-Apr-16	06-Apr-16	07-Apr-16	07-Apr-16	06-Apr-16				
Sample Type	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil				
Sample Matrix Code	N/A	N/A	N/A	N/A	N/A	N/A				
Chlorobenzene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,1,1,2-Tetrachloroethane$_A$	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Ethylbenzene$_A$#	315000	<3750	216000	270000	103000	350000			µg/kg	A T 006s
m & p Xylene$_A$#	1430000	<3750	853000	703000	444000	246000			µg/kg	A T 006s
o-Xylene$_A$#	649000	<3750	325000	272000	168000	172000			µg/kg	A T 006s
Styrene$_A$#	<3750	<3750	318000	209000	111000	<3750			µg/kg	A T 006s
Bromoform$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Isopropylbenzene$_A$#	24900	<3750	20300	22200	9870	7370			µg/kg	A T 006s
1,1,2,2-Tetrachloroethane$_A$	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,2,3-Trichloropropane$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
Bromobenzene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
n-Propylbenzene$_A$#	102000	<3750	64600	57100	36600	48700			µg/kg	A T 006s
2-Chlorotoluene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,3,5-Trimethylbenzene$_A$#	378000	<3750	240000	225000	117000	204000			µg/kg	A T 006s
4-Chlorotoluene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
tert-Butylbenzene$_A$#	<7500	<7500	<7500	<7500	<7500	<7500			µg/kg	A T 006s
1,2,4-Trimethylbenzene$_A$#	730000	<3750	467000	453000	266000	472000			µg/kg	A T 006s
sec-Butylbenzene$_A$#	14600	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
4-Isopropyltoluene$_A$#	12900	<3750	28400	26200	19300	58900			µg/kg	A T 006s
1,3-Dichlorobenzene$_A$	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,4-Dichlorobenzene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
n-Butylbenzene$_A$#	82700	<3750	84300	76300	6340	<3750			µg/kg	A T 006s
1,2-Dichlorobenzene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,2-Dibromo-3-chloropropane$_A$	<7500	<7500	<7500	<7500	<7500	<7500			µg/kg	A T 006s
1,2,4-Trichlorobenzene$_A$	<11250	<11250	<11250	<11250	<11250	<11250			µg/kg	A T 006s
Hexachlorobutadiene$_A$#	<3750	<3750	<3750	<3750	<3750	<3750			µg/kg	A T 006s
1,2,3-Trichlorobenzene$_A$	<11250	<11250	<11250	<11250	<11250	<11250			µg/kg	A T 006s

Envirolab Job Number: ███████

Lab Sample ID	███████								Units	Method ref
Client Sample No										
Client Sample ID	BH213	BH211	BH207	BH206	WA3-R1	WA2-R1				
Depth to Top										
Depth To Bottom										
Date Sampled	05-Apr-16	08-Apr-16	06-Apr-16	07-Apr-16	07-Apr-16	06-Apr-16				
Sample Type	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil	Liquid - Product / Oil				
Sample Matrix Code	N/A	N/A	N/A	N/A	N/A	N/A				
Product (Oil) TPHCWG										
Ali >C5-C6$_A$#	53	<7.50	36	125	77.6	12.6			mg/kg	A T 022s
Ali >C6-C8$_A$#	555	14	800	614	611	138			mg/kg	A T 022s
Ali >C8-C10$_A$#	5130	42.3	2040	1490	1350	525			mg/kg	A T 022s
Ali >C10-C12$_A$#	18600	<35.0	13600	11200	9210	7870			mg/kg	A T 023s
Ali >C12-C16$_A$#	11400	<35.0	26800	25500	16100	22400			mg/kg	A T 023s
Ali >C16-C21$_A$#	3380	<35.0	12300	15300	10900	18000			mg/kg	A T 023s
Ali >C21-C35$_A$#	1150	<35.0	6760	9340	15500	4710			mg/kg	A T 023s
Total Aliphatics$_A$	34500	56.3	59500	61400	51800	53000			mg/kg	A T 022+23s
Aro >C5-C7$_A$#	2350	<7.50	817	229	681	231			mg/kg	A T 022s
Aro >C7-C8$_A$#	5070	<7.50	3300	1440	1400	46.1			mg/kg	A T 022s
Aro >C8-C9$_A$#	11300	9.75	11700	6940	4300	3350			mg/kg	A T 022s
Aro >C9-C10$_A$#	13300	8.23	10600	10400	6290	7990			mg/kg	A T 022s
Aro >C10-C12$_A$#	54100	<35.0	68000	70900	27600	41600			mg/kg	A T 023s
Aro >C12-C16$_A$#	56200	<35.0	132000	136000	53400	137000			mg/kg	A T 023s
Aro >C16-C21$_A$#	78400	<35.0	86100	97600	71700	136000			mg/kg	A T 023s
Aro >C21-C35$_A$#	67700	<35.0	51400	71900	76900	84500			mg/kg	A T 023s
Total Aromatics$_A$	256000	<35.0	338000	376000	230000	398000			mg/kg	A T 022+23s
TPH (Ali & Aro)$_A$	291000	74.3	397000	438000	281000	451000			mg/kg	A T 022+23s
BTEX - Benzene$_A$#	2350	<7.50	817	229	681	231			mg/kg	A T 022s
BTEX - Toluene$_A$#	5070	<7.50	3300	1440	1400	46.1			mg/kg	A T 022s
BTEX - Ethyl Benzene$_A$#	1270	<7.50	1180	1410	540	1540			mg/kg	A T 022s
BTEX - m & p Xylene$_A$#	5670	<7.50	4990	3820	2560	901			mg/kg	A T 022s
BTEX - o Xylene$_A$#	3880	<7.50	2130	1690	1130	815			mg/kg	A T 022s
MTBE$_A$#	<7.50	<7.50	<7.50	<7.50	<7.50	<7.50			mg/kg	A T 022s

REPORT NOTES

Notes - Soil chemical analysis
All results are reported as dry weight (<40°C).
For samples with Matrix Codes 1 - 6 natural stones and brick and concrete fragments >10mm are removed or excluded from the sample prior to analysis and reported results corrected to a whole sample basis. For samples with Matrix Code 7 the whole sample is dried and crushed prior to analysis.

Notes - General
This report shall not be reproduced, except in full, without written approval from Envirolab.
Subscript "A" indicates analysis performed on the sample as received. "D" indicates analysis performed on the dried sample, crushed to pass a 2mm sieve, unless asbestos is found to be present in which case all analysis is performed on the sample as received.
All analysis is performed on the dried and crushed sample for samples with Matrix Code 7 and this supersedes any "A" subscripts.
All analysis is performed on the sample as received for soil samples which are positive for asbestos and/or if they are from outside the European Union and this supercedes any "D" subscripts.
Superscript "M" indicates method accredited to MCERTS.
If results are in italic font they are associated with an AQC failure. These are not accredited and are unreliable.
A deviating samples report is appended and will indicate if samples or tests have been found to be deviating. Any test results affected may not be an accurate record of the concentration at the time of sampling and, as a result, may be invalid.

TPH analysis of water by method A-T-007
Free and visible oils are excluded from the sample used for analysis so that the reported result represents the dissolved phase only.

Asbestos in soil
Asbestos in soil analysis is performed on a dried aliquot of the submitted sample and cannot guarantee to identify asbestos if present as discrete fibres/fragments. Stones etc. are not removed from the sample prior to analysis.
Quantification of asbestos is a 3 stage process including visual identification, hand picking and weighing and fibre counting by sedimentation/phase contrast optical microscopy if required. If asbestos is identified as being present but is not in a form that is suitable for analysis by hand picking and weighing (normally if the asbestos is present as free fibres) quantification by sedimentation is performed. Where ACMs are found a percentage asbestos is assigned to each with reference to 'HSG264, Asbestos: The survey guide' and the calculated asbestos content is expressed as a percentage of the dried soil sample aliquot used.

Predominant Matrix Codes:
1 = SAND, 2 = LOAM, 3 = CLAY, 4 = LOAM/SAND, 5 = SAND/CLAY, 6 = CLAY/LOAM, 7 = OTHER, 8 = Asbestos bulk ID sample.
Samples with Matrix Code 7 are not predominantly a SAND/LOAM/CLAY mix and are not covered by our BSEN 17025 or MCERTS accreditations.

Secondary Matrix Codes:
A = contains stones, B = contains construction rubble, C = contains visible hydrocarbons, D = contains glass/metal, E = contains roots/twigs.

IS indicates Insufficient Sample for analysis.
US indicates Unsuitable Sample for analysis.
NDP indicates No Determination Possible.
NAD indicates No Asbestos Detected.
N/A indicates Not Applicable.
Superscript # indicates method accredited to ISO 17025.
Analytical results reflect the quality of the sample at the time of analysis only. Opinions and interpretations expressed are outside the scope of our accreditation.

Please contact us if you need any further information.

Envirolab Deviating Samples Report

Units 7&8 Sandpits Business Park, Mottram Road, Hyde, SK14 3AR
Tel. 0161 368 4921
email. ask@envlab.co.uk

Client:

Project No:

Date Instructions Received: 12/04/2016 (am)

NO DEVIATIONS IDENTIFIED

TPHCWG Product Report

April 2019

Exova Jones Environmental

Unit 3 Deeside Point
Zone 3
Deeside Industrial Park
Deeside
CH5 2UA

Tel: +44 (0) 1244 833780
Fax: +44 (0) 1244 833781

Attention :

Date :

Your reference :

Our reference :

Location :

Date samples received :

Status :   Final report

Issue :   1

Eleven samples were received for analysis on 26th April, 2019 of which one were scheduled for analysis. Please find attached our Test Report which should be read with notes at the end of the report and should include all sections if reproduced. Interpretations and opinions are outside the scope of any accreditation, and all results relate only to samples supplied.
All analysis is carried out on as received samples and reported on a dry weight basis unless stated otherwise. Results are not surrogate corrected.

Compiled By:

Project Manager

Please include all sections of this report if it is reproduced
All solid results are expressed on a dry weight basis unless stated otherwise.
QF-PM 3.1.1 v16   1 of 8

Exova Jones Environmental

											LOD/LOR	Units	Method No.
J E Sample No.	4-5												
Sample ID													
Depth	3.749												
COC No / misc													
Containers	V												
Sample Date	25/04/2019												
Sample Type	Product												
Batch Number	1												
Date of Receipt	26/04/2019												
Whole Oil Trace	See Attached											None	TM1/PM0
TPH CWG													
Aliphatics													
>C5-C6 #	1.8										<0.01	%	TM1/PM0
>C6-C8 #	29										<0.01	%	TM1/PM0
>C8-C10 #	3.5										<0.01	%	TM1/PM0
>C10-C12 #	3.6										<0.01	%	TM1/PM0
>C12-C16 #	0.89										<0.01	%	TM1/PM0
>C16-C21 #	0.11										<0.01	%	TM1/PM0
>C21-C35 #	0.03										<0.01	%	TM1/PM0
Aromatics													
>EC6-EC8 #	16										<0.01	%	TM1/PM0
>EC8-EC10 #	40										<0.01	%	TM1/PM0
>EC10-EC12 #	3.9										<0.01	%	TM1/PM0
>EC12-EC16 #	0.68										<0.01	%	TM1/PM0
>EC16-EC21 #	0.45										<0.01	%	TM1/PM0
>EC21-EC35 #	0.12										<0.01	%	TM1/PM0

Please see attached notes for all abbreviations and acronyms

Please include all sections of this report if it is reproduced
All solid results are expressed on a dry weight basis unless stated otherwise.
QF-PM 3.1.2 v11   2 of 8

Exova Jones Environmental

Client Name:
Reference:
Location:
Contact:
JE Job No.:

VOC Report :   **Product**

	J E Sample No.	4-5														
	Sample ID															
	Depth	3.749														
	COC No / misc															
	Containers	V														
	Sample Date	25/04/2019														
	Sample Type	Product														
	Batch Number	1														
	Date of Receipt	26/04/2019									LOD/LOR	Units	Method No.

Please see attached notes for all abbreviations and acronyms

			LOD/LOR	Units	Method No.
VOC MS					
Methyl Tertiary Butyl Ether	<0.05		<0.05	%	TM124/PM0
Benzene	0.36		<0.01	%	TM124/PM0
Toluene	12		<0.01	%	TM124/PM0
Ethylbenzene	5.0		<0.01	%	TM124/PM0
m/p-Xylene	14		<0.01	%	TM124/PM0
o-Xylene	7.5		<0.01	%	TM124/PM0

Please include all sections of this report if it is reproduced
All solid results are expressed on a dry weight basis unless stated otherwise.

Client Name:			**JE Job No.:**	
Reference:			**JE Sample No.:**	
Location:			**Sample Identity:**	
Contact:			**Depth:**	3.749

Description:	Burnt Amber Oil	**% Diesel:**	-
Carbon Range:	5-21	**% Petrol:**	-
Boiling Point Range (°C):	36-356	**Estimated % Weathering of Petrol:**	-
Pristane/Phytane Ratio:	N/A	**Toluene/nC$_8$ ratio of Petrol:**	-
nC$_{17}$/Pristane Ratio:	N/A	**Age of Petrol (years) (schmidt et al 2002):**	-
Age of Diesel (+/- 2 years)*:	N/A		

Interpretation: Degraded Petrol

Chromatogram:
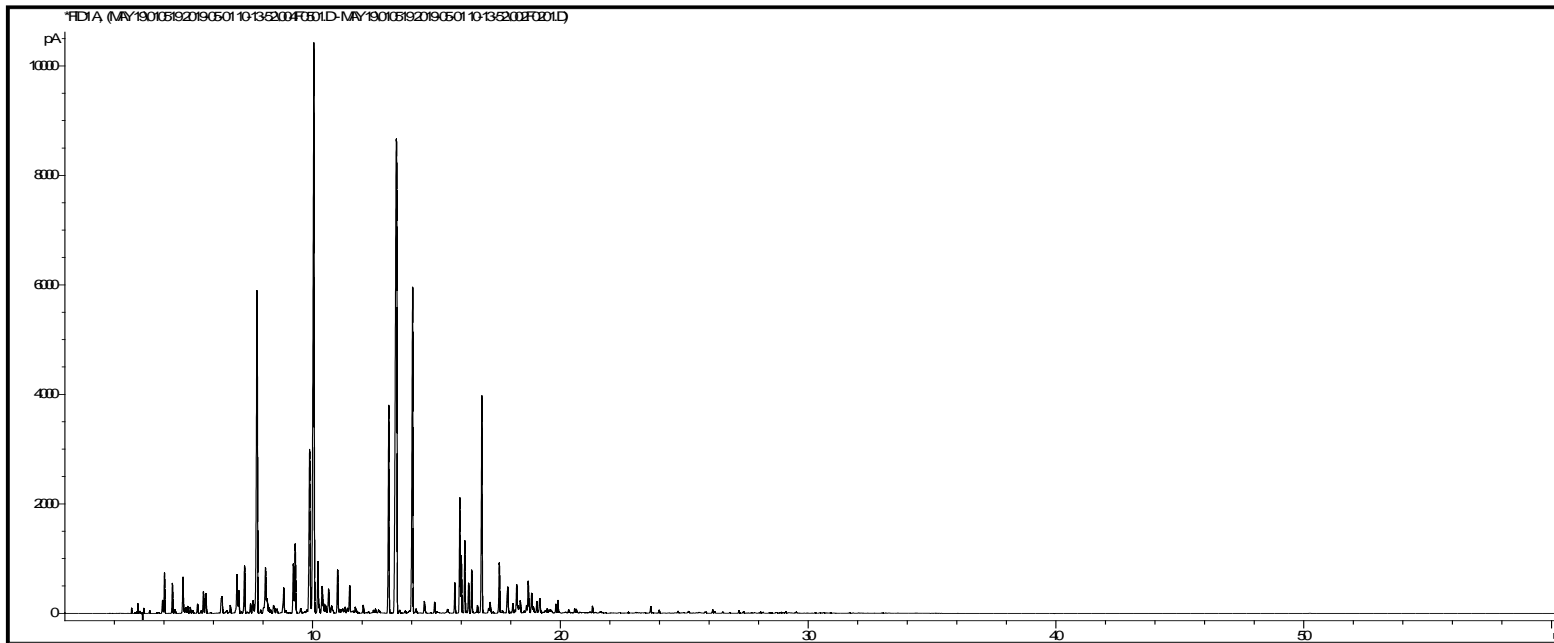
*The age of release estimated in this report is based on the nC17/pristane ratio only as prescribed by Christensen and Larsen (1993) and Kaplan, Galperin, Alimi et al., (1996).

Age estimation should be treated with caution as it can be influenced by site specific factors that the laboratory are not aware of.

Client Name:

Reference:

Location:

Contact:

J E Job No.	Batch	Sample ID	Depth	J E Sample No.	Analysis	Reason

Please note that only samples that are deviating are mentioned in this report. If no samples are listed it is because none were deviating.

Only analyses which are accredited are recorded as deviating if set criteria are not met.

NOTES TO ACCOMPANY ALL SCHEDULES AND REPORTS

JE Job No.:

SOILS

Please note we are only MCERTS accredited (UK soils only) for sand, loam and clay and any other matrix is outside our scope of accreditation.

Where an MCERTS report has been requested, you will be notified within 48 hours of any samples that have been identified as being outside our MCERTS scope. As validation has been performed on clay, sand and loam, only samples that are predominantly these matrices, or combinations of them will be within our MCERTS scope. If samples are not one of a combination of the above matrices they will not be marked as MCERTS accredited.

It is assumed that you have taken representative samples on site and require analysis on a representative subsample. Stones will generally be included unless we are requested to remove them.

All samples will be discarded one month after the date of reporting, unless we are instructed to the contrary.

If you have not already done so, please send us a purchase order if this is required by your company.

Where appropriate please make sure that our detection limits are suitable for your needs, if they are not, please notify us immediately.

All analysis is reported on a dry weight basis unless stated otherwise. Results are not surrogate corrected. Samples are dried at 35°C ±5°C unless otherwise stated. Moisture content for CEN Leachate tests are dried at 105°C ±5°C.

Where Mineral Oil or Fats, Oils and Grease is quoted, this refers to Total Aliphatics C10-C40.

Where a CEN 10:1 ZERO Headspace VOC test has been carried out, a 10:1 ratio of water to wet (as received) soil has been used.

% Asbestos in Asbestos Containing Materials (ACMs) is determined by reference to HSG 264 The Survey Guide - Appendix 2 : ACMs in buildings listed in order of ease of fibre release.

Negative Neutralization Potential (NP) values are obtained when the volume of NaOH (0.1N) titrated (pH 8.3) is greater than the volume of HCl (1N) to reduce the pH of the sample to 2.0 - 2.5. Any negative NP values are corrected to 0.

The calculation of Pyrite content assumes that all oxidisable sulphides present in the sample are pyrite. This may not be the case. The calculation may be an overesitimate when other sulphides such as Barite (Barium Sulphate) are present.

WATERS

Please note we are not a UK Drinking Water Inspectorate (DWI) Approved Laboratory .

ISO17025 accreditation applies to surface water and groundwater and usually one other matrix which is analysis specific, any other liquids are outside our scope of accreditation.

As surface waters require different sample preparation to groundwaters the laboratory must be informed of the water type when submitting samples.

Where Mineral Oil or Fats, Oils and Grease is quoted, this refers to Total Aliphatics C10-C40.

DEVIATING SAMPLES

All samples should be submitted to the laboratory in suitable containers with sufficient ice packs to sustain an appropriate temperature for the requested analysis. The temperature of sample receipt is recorded on the confirmation schedules in order that the client can make an informed decision as to whether testing should still be undertaken.

SURROGATES

Surrogate compounds are added during the preparation process to monitor recovery of analytes. However low recovery in soils is often due to peat, clay or other organic rich matrices. For waters this can be due to oxidants, surfactants, organic rich sediments or remediation fluids. Acceptable limits for most organic methods are 70 - 130% and for VOCs are 50 - 150%. When surrogate recoveries are outside the performance criteria but the associated AQC passes this is assumed to be due to matrix effect. Results are not surrogate corrected.

DILUTIONS

A dilution suffix indicates a dilution has been performed and the reported result takes this into account. No further calculation is required.

BLANKS

Where analytes have been found in the blank, the sample will be treated in accordance with our laboratory procedure for dealing with contaminated blanks.

NOTE

Data is only reported if the laboratory is confident that the data is a true reflection of the samples analysed. Data is only reported as accredited when all the requirements of our Quality System have been met. In certain circumstances where all the requirements of the Quality System have not been met, for instance if the associated AQC has failed, the reason is fully investigated and documented. The sample data is then evaluated alongside the other quality control checks performed during analysis to determine its suitability. Following this evaluation, provided the sample results have not been effected, the dcata is reported but accreditation is removed. It is a UKAS requirement for data not reported as accredited to be considered indicative only, but this does not mean the data is not valid.
Where possible, and if requested, samples will be re-extracted and a revised report issued with accredited results. Please do not hesitate to contact the laboratory if further details are required of the circumstances which have led to the removal of accreditation.

REPORTS FROM THE SOUTH AFRICA LABORATORY

Any method number not prefixed with SA has been undertaken in our UK laboratory unless reported as subcontracted.

ABBREVIATIONS and ACRONYMS USED

#	ISO17025 (UKAS Ref No. 4225) accredited - UK.
SA	ISO17025 (SANAS Ref No.T0729) accredited - South Africa.
B	Indicates analyte found in associated method blank.
DR	Dilution required.
M	MCERTS accredited.
NA	Not applicable
NAD	No Asbestos Detected.
ND	None Detected (usually refers to VOC and/SVOC TICs).
NDP	No Determination Possible
SS	Calibrated against a single substance
SV	Surrogate recovery outside performance criteria. This may be due to a matrix effect.
W	Results expressed on as received basis.
+	AQC failure, accreditation has been removed from this result, if appropriate, see 'Note' on previous page.
++	Result outside calibration range, results should be considered as indicative only and are not accredited.
*	Analysis subcontracted to an Exova Jones Environmental approved laboratory.
AD	Samples are dried at 35°C ±5°C
CO	Suspected carry over
LOD/LOR	Limit of Detection (Limit of Reporting) in line with ISO 17025 and MCERTS
ME	Matrix Effect
NFD	No Fibres Detected
BS	AQC Sample
LB	Blank Sample
N	Client Sample
TB	Trip Blank Sample
OC	Outside Calibration Range

Please include all sections of this report if it is reproduced
All solid results are expressed on a dry weight basis unless stated otherwise.

QF-PM 3.1.9 v34   7 of 8

JE Job No:

Test Method No.	Description	Prep Method No. (if appropriate)	Description	ISO 17025 (UKAS/S ANAS)	MCERTS (UK soils only)	Analysis done on As Received (AR) or Dried (AD)	Reported on dry weight basis
TM1	Modified USEPA 8015B method for the determination of carbon banding in oil and product samples by GC-FID.	PM0	No preparation is required.			AR	
TM1	Modified USEPA 8015B method for the determination of carbon banding in oil and product samples by GC-FID.	PM0	No preparation is required.	Yes		AR	
TM124	Modified USEPA 8260. Semi- Quantitative Determination of Volatile Organic Compounds (VOCs) by Headspace GC-MS.	PM0	No preparation is required.			AR	

SVOC Product Report

March 2021

To:

xxx

Non–routine Analysis Report

9 MARCH 2021

Our Reference:	21–xxx (SDG: 21xxxx–xx)
Quote Reference:	NRWXXX
Your Reference:	Not Specified
Location:	Not Specified

One product sample was received on XXth March 2021 for SVOC analysis.

We are pleased to enclose our non–routine analysis report.

SIGNED:

XX

ALS HAWARDEN

www.alsglobal.eu

Contents

Right Solutions · Right Partner   www.alsglobal.eu

1. Summary

One product sample was received in a 40ml EPA vial for determination of semi-volatile components (SVOC). Client sample references are displayed in Table 1. All analyses within this report are outside our accreditation status and were conducted on the 'As Received' sample.

Lab SDG	Lab Sample Event	Customer Sample Ref
21XXXX-XX	SE 20XXXXX	BHXXX

Table 1: Client Identification and Sample References

2. Sample Analysis

A small portion of sample was serially diluted in dichloromethane and placed in a vial with known amounts of analytical reagent. The sample was introduced into the gas chromatograph and the components were separated by gas chromatography before being detected by the mass selective detector.

Identification of target semi-volatile compounds was performed via retention time and qualifier match against a known reference standard. Quantification was performed against 5-point calibration curves generated using standards of known concentration containing all target analytes.

The reporting limits quoted are based on the calculated LOD for the routine SVOC soils method, the dilutions needed and the density obtained.

A full scan SVOC chromatogram of sample BHXXX (20XXXXXX) is displayed in Figure 1, below.
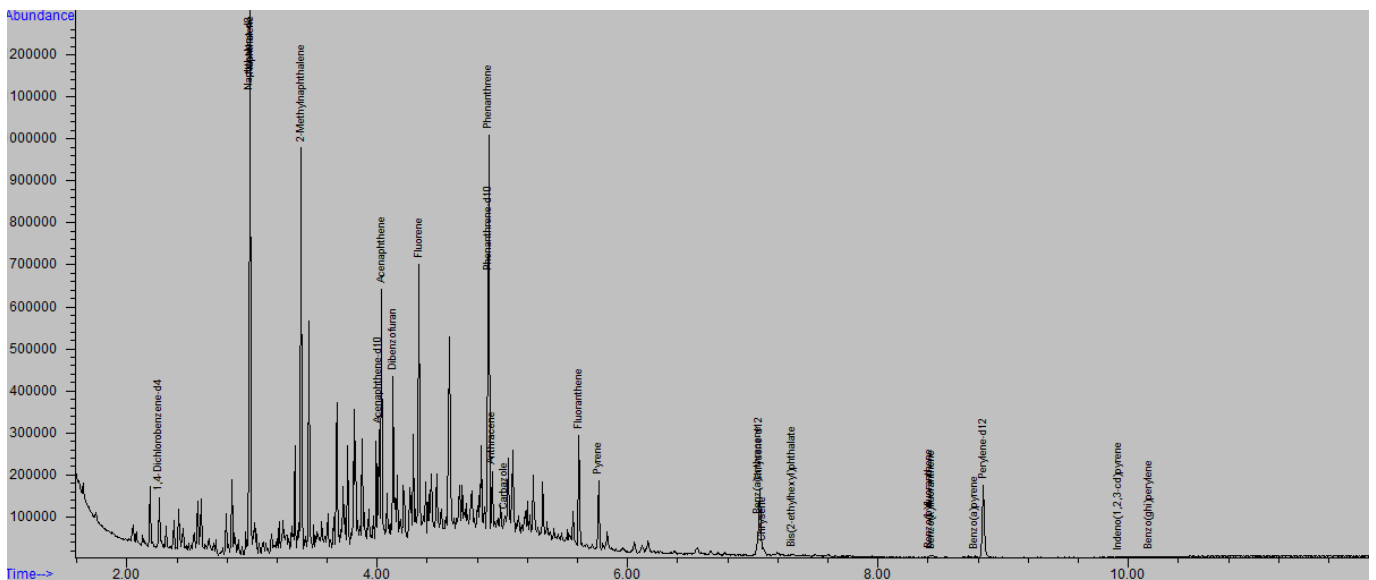

Figure 1: Full-scan chromatogram of sample BHXXX (20XXXXXX)

3. SVOC Results

Target Compounds	Concentration (mg/kg)	Target Compounds	Concentration (mg/kg)
Phenol	<10.0	Acenaphthylene	<10.0
Bis(2-chloroethyl)ether	<10.0	3-Nitroaniline	<10.0
2-Chlorophenol	<10.0	Acenaphthene	<10.0
1,3-Dichlorobenzene	<10.0	4-Nitrophenol	<10.0
1,4-Dichlorobenzene	<10.0	Pentachlorobenzene	<10.0
1,2-Dichlorobenzene	<10.0	2,4-Dinitrotoluene	<10.0
Benzyl Alchohol	<10.0	Dibenzofuran	<10.0
2-Methylphenol	<10.0	Diethyl phthalate	<10.0
Bis(2-chloroisopropyl)ether	<10.0	4-Chlorophenylphenylether	<10.0
4-Methylphenol	<10.0	Fluorene	<10.0
N-nitrosodi-n-propylamine	<10.0	4-Nitroaniline	<10.0
Hexachloroethane	<10.0	Azobenzene	<10.0
Nitrobenzene	<10.0	4-Bromophenylphenylether	<10.0
Isophorone	<10.0	Hexachlorobenzene	<10.0
2-Nitrophenol	<10.0	Pentachlorophenol	<10.0
2,4-Dimethylphenol	<10.0	Phenanthrene	<10.0
Bis(2-chloroethoxy)methane	<10.0	Anthracene	<10.0
2,4-Dichlorophenol	<10.0	Carbazole	<10.0
1,2,4-Trichlorobenzene	<10.0	Di-n-butylphthalate	<10.0
Naphthalene	<10.0	Fluoranthene	<10.0
4-Chloroaniline	<10.0	Pyrene	<10.0
Hexachlorobutadiene	<10.0	Butylbenzylphthalate	<10.0
4-Chloro-3-methylphenol	<10.0	Bis(2-ethylhexyl)phthalate	<10.0
2-Methylnaphthalene	<10.0	Benz(a)anthracene	<10.0
Hexchlorocyclopentadiene	<10.0	Chrysene	<10.0
2,4,6-Trichlorophenol	<10.0	Di-n-octylphthalate	<10.0
2,4,5-Trichlorophenol	<10.0	Benzo(b)fluoranthene	<10.0
Biphenyl	<10.0	Benzo(k)fluoranthene	<10.0
2-Chloronaphthalene	<10.0	Benzo(a)pyrene	<10.0
2-Nitroaniline	<10.0	Indeno(1,2,3-cd)pyrene	<10.0
Dimethyl phthalate	<10.0	Dibenzo(a,h)anthracene	<10.0
2,6-Dinitrotoluene	<10.0	Benzo(ghi)perylene	<10.0

Table 2: Sample results in mg/kg reported to 3 significant figures