Department for Environment Food & Rural Affairs

1. Purchase Order Number	To be confirmed once contract is in place. **Technical development for assessing the mobility of chemical substances**
2. Customer	Environment Agency Horizon House Deanery Rd Bristol BS1 5AH
3. Contractor(s)	WCA Environment Ltd Brunel House, Volunteer Way Faringdon Oxfordshire SN7 7YR Registration number: 5451320 WCA ENVIRONMENT LIMITED overview - Find and update company information - GOV.UK (company-information.service.gov.uk)
4. Co-Funder(s)	N/A
5. Defra Group Members	The following Defra Group members will receive the benefit of the Deliverables: Environment Agency
6. The Agreement	This Order is part of the Agreement and is subject to the terms and conditions appended at Appendix 1 and shall come into effect on the Start Date. Unless the context otherwise requires, capitalised expressions used in this Order have the same meanings as in the terms and conditions. The following documents are incorporated into the Agreement. If there is any conflict, the following order of precedence applies (in descending order): a) this Order; b) the terms and conditions at Appendix 1; and c) the remaining Appendices (if any) in equal order of precedence.
7. Deliverables	**Goods:** None
	Services: See Appendix 2 – Specification/Description
8. Milestone Delays (Clause 18.2.10)	N/A
9. Start Date	26th August 2024
10. Expiry Date	31st March 2025

11. Extension Period (Clause 5.2)	Option to extend for 3 months (1st April to 30th June 2025), to cover the delivery of Phase 3.
12. Charges	The Charges for the Deliverables shall be as set out below in Appendix 3 – Charges. Unless and to the extent otherwise expressly stated in Appendix 3, the Charges are fixed for the duration of the Agreement.
13. Payment including Payment by Co-funder(s)	Payments will be made in pounds (GBP) by BACS transfer using the details provided by the supplier on submission of a compliant invoice. It is our preference that all invoices are sent electronically, quoting a valid Purchase Order number to [redacted] Any invoices that are submitted that do not meet the following criteria will not be processed: • 1 PDF per invoice (no larger than 4mb in size) – all supporting documentation must be included in that PDF (no additional separate supporting documentation as a separate file). • Multiple invoices can be attached to one email; however, as above we can only accept 1 invoice per PDF (and no additional supporting files). • Invoices must be dated • Invoices must quote a valid Purchase Order • Invoices must have a breakdown of what is being billed • Invoices must include the total before and after VAT
14. Customer's Authorised Representative(s)	For general liaison your contact will continue to be [redacted]
15. Contractor's Authorised Representative	For general liaison your contact will continue to be: [redacted]
16. Co-funder's Authorised Representative	N/A
17. Optional Intellectual Property Rights ("IPR") Clauses	The Customer has chosen Option B in respect of intellectual property rights provisions for the Agreement as set out in the terms and conditions.
18. Contractor's general liability cap	The liability of the Contractor as set out in Clause 16.2.1 of the terms and conditions is limited to the greater of: (a) an amount equal to 150% of the Charges paid or payable to the Contractor; and (b) £5,000,000

19. Progress Meetings and Progress Reports	• The Contractor shall attend progress meetings with the Customer every month
20. Address for notices	**Customer:** [redacted] Attention: [redacted] Email: [redacted] **Contractor:** [redacted] Attention: [redacted] Email: [redacted]
21. Key Personnel of the Contractor	**Key Personnel Role:** **Contractor's Project Manager** **Key Personnel Name:** [redacted] **Contact Details:** [redacted]
22. Procedures and Policies	For the purposes of the Agreement: The Customer's security / data security requirements are: Contractor must comply with all UK legal requirements regarding GDPR, and data security and commercial confidentiality where applicable The Customer's additional sustainability requirements are: Environment Agency quality policy and commitment to sustainable business - GOV.UK (www.gov.uk) The Customer's equality and diversity policy/requirements and instructions related to equality Law [and] environmental policy is: Equality and diversity - Environment Agency - GOV.UK (www.gov.uk) The Customer's health and safety policy is: Contractor must comply with all UK Health and Safety legal requirements
23. Commercial Exploitation (Clause 11)	Clause 11 (Commercial Exploitation) shall apply to this Agreement: **No**
24. Special Terms	N/A
25. Additional Insurance	N/A
26. Further Data Protection Provisions	The further data protection provisions as contained at Annex 1 of the Terms and Conditions are applicable to this Agreement where indicated below: **Yes:** ☐ **No:** ☒

Signed for and on behalf of the **Customer**	Signed for and on behalf of the **Contractor**
[redacted]	[redacted]

Appendix 1: R&D Terms and Conditions

The terms and conditions applicable to this requirement can be found on the website below

Research and development terms and conditions - GOV.UK (www.gov.uk)

Appendix 2: Specification/Description

Background to the Environment Agency

Who is the Environment Agency?

We are an Executive Non-departmental Public Body responsible to the Secretary of State for Environment, Food and Rural Affairs. Our principal aims are to protect and improve the environment, and to promote sustainable development.

Further information on our responsibilities, Corporate Plan and how we are structured can be found on our website.

https://www.gov.uk/government/organisations/environment-agency/about

What do we spend our money on?

We are a major procurer of goods and services within the UK, spending circa £600M per annum, our major spend areas are:

- Flood and Coastal Risk Management (design, construction and maintenance)
- ICT and Telecommunications
- Vehicles and Plant
- Environmental Consultancy and Monitoring
- Temporary Staff and Contractors
- Facilities Management, Energy and Utilities
- Flood Management and Water Related Services

What do we need from our suppliers?

Suppliers are vital in supporting the delivery of our corporate plan. We aim to support the economy and society whilst delivering more environmental outcomes for every pound we spend. In many areas we are leading the way on environmental and technical developments. It is our role to ensure that suppliers clearly understand our corporate aims and objectives and know that we are committed to delivering the best value most sustainable solutions, taking into account the whole life cost of our procurement decisions. We promote diversity and equality and treat all of our suppliers fairly.

Our procurement strategy may be of interest to you as a potential supplier. It sets out our priorities and key commitments in a range of areas such as delivering our corporate plan, Government policy, supplier management and sustainable procurement:

https://www.gov.uk/government/organisations/environment-agency/about/procurement#procurement-strategy

Government changes and collaboration

Since 1 April 2013, the Environment Agency is no longer responsible for delivering the environmental priorities of Wales. This is now the remit of Natural Resources Wales (NRW). Further information can be found here:

http://naturalresources.wales/splash?orig=/

By bidding for this requirement, you may also be approached by other members of the Defra network, NRW or other government departments that are specifically named in the tender document.

Further information

For further information and to see our commitments to Diversity and Equality, please visit our website.

https://www.gov.uk/government/organisations/environment-agency/about/procurement

https://www.gov.uk/government/organisations/environment-agency/about/equality-and-diversity

Background to the specific work area relevant to this purchase

The Chemicals Assessment Unit (CAU) in the Chief Scientist's Group of the Environment Agency supports the UK Chemicals Agency (the Health and Safety Executive, HSE) on the environmental aspects of the UK Registration, Evaluation, Authorisation and restriction of Chemicals (REACH) regulation. CAU assess environmental hazards and risks from the manufacture, use and disposal of industrial and consumer chemicals, and produces formal regulatory documentation.

Members of the United Nations are discussing criteria to identify chemicals that are "persistent, mobile and toxic" (PMT) or "very persistent and very mobile" (vPvM). These proposed new environmental hazard categories fill a regulatory gap to identify substances that have a high potential to accumulate in water resources over long timescales and can be very difficult to remove using conventional treatment methods (Neumann and Schliebner, 2019). The Environment Agency agrees with the purpose of the PMT / vPvM criteria, which is to prioritise action on relevant substances to protect drinking water and freshwater ecosystems for future generations and avoid high remediation costs.

There are significant concerns with the proposed metrics to assess mobility (M). The standard laboratory screening methods proposed to measure M are not applicable for a significant sub-group of substances (i.e., surface active substances, highly polar substances, and organic acids/bases). Currently recommended methods (laboratory and estimated predictions) will lead to incorrect screening decisions for such substances. This will in turn lead to unnecessary testing and regulatory management.

An Environment Agency evidence review from 2023/2024 (in publication) explored whether the properties of soils (including sediments) that influence the movement of substances could be replicated using different solid stationary phases of high-performance liquid chromatography (HPLC) columns. The most promising solid phases were identified as 'mixed mode' (specifically, reverse phase ion exchange; RP-IEX). These could be used as a relatively quick and cheap method to generate standardised "mobility metrics" in the laboratory. The evidence review recommended practical testing and generation of primary data as the next steps in this research. The current project aims to fulfil this need.

The key objective is to perform a comprehensive assessment into the use of HPLC columns containing mixed mode RP-IEX solid stationary phases to understand the retention of substances with low log K_{OC} metrics (< 3).

This project has been split into three phases:

- Phase 1: Method development.
- Phase 2: Data collation.
- Phase 3: Data examination and reporting.

This work is relevant to a range of UK legislation relating to chemical safety. It will support the Defra policy position development on the use of PMT criteria in hazard identification; risk management under UK REACH; and Health & Safety Executive (HSE) discussions of the same topic at the United Nations.

We anticipate that this project will run from August 2024 through to June 2025.

Phase 1 and 2 will be delivered by 10th March 2025. A possible extension will be awarded for Phase 3 to cover 1st April 2025 - 30th June 2025.

Requirement

The proposed mobility criteria for the assessment of the M / vM are built on the organic carbon normalised adsorption coefficient (K_{OC}), as a measure of the partitioning of substances between water and either soil, sediment, or sludge.

The use of K_{OC} to assess M assumes that adsorption is directly related to the quantity of organic matter in a soil (Jarvis, 2016). Organic matter can be the dominant adsorption surface, but this may not always be the case (Ghafoor et al., 2013; Jarvis, 2016). Sorption to inorganic components, such as clays, becomes significant in the following situations:

When the test substance is highly polar or ionisable / ionised.

When the soil, sediment, or other environmental matrix is low in organic matter. In this situation, not only is there less organic matter, but the organic matter that is present is not going to block inorganic adsorption sites on clays and other mineral components.

Both of these situations are relevant to potential PMT / vPvM substances:

Many substances that are candidates for identification as M / vM are going to be highly polar or ionisable / ionised under environmentally relevant conditions.

PMT / vPvM substances may enter the environment through:

- the discharge of effluents from sewage treatment works into surface waters. Following this, their movement to remote waters, such as groundwater by filtration through riverbeds or riverbanks, is quite likely to involve movement through environmental matrices with relatively low organic matter content (for example, some types of soil, sediment, and sub-surface groundwater associated soils).
- the exposure of agricultural soils, for example, via irrigation water, direct deposition, or sludge amendment. Although topsoil in general is relatively high in organic matter, the inherent mobility of PMT / vPvM substances means that they are quite likely to move by hydraulic transport to sub-surface layers, which are generally low organic matter environmental matrices.

One example where K_{OC} is not going to be an adequate measure of adsorption is for substances with cationic functional groups. If the organic matter content of the environmental matrix is low, binding to organic matter by van der Waals forces, dipole-dipole interactions, and possibly anion exchange will be limited, but adsorption to anion exchange sites on clays and other minerals present could still occur. This may not be reflected in the K_{OC} values obtained from the Organization for Economic Cooperation and Development (OECD) test guideline (TG) study typically used for K_{OC} determination (e.g., OECD TG

121) under REACH. The relevance of K_{OC} as a metric for specific substance chemistries and for assessing mobility beyond surface soils has previously been questioned for both plant protection products and REACH substances (e.g., see: Doucette, 2000; Ghafoor et al., 2013; Pawlowski et al., 2023; Strawn, 2021).

Given that the adsorption of a polar or ionised substance to the components of soil, sediment or subsurface environmental matrices may not be fully accounted for by a K_{OC} value, this means that the mobility concern may be over-estimated. This has significant implications; a 2010 survey of the EU REACH registration database identified that approximately 50% of registrations are substances that contain functional groups that are ionisable or polar (Franco et al., 2010). It is possible that a large proportion of substances will meet the P / vP criteria, thereby triggering assessment of mobility (M). How M is assessed is important, because any substance that fulfils the P and M criteria will require toxicity (T) characterisation (with animal welfare implications for any new testing).

The variables that may influence sorption processes between substances and soils/sediments were reviewed in the Environment Agency 2023/34 evidence review (in publication), which considered:

- the suitability of the current OECD TG 121 (OECD, 2001), which uses a readily available HPLC column with a standard stationary phase and reflects only interaction with organic matter, and
- the feasibility of using other available stationary phases to act as surrogates for soils and sediments.

A combination of mixed-mode HPLC column solid phases (specifically RP-IEX) were identified as having the greatest potential to reflect likely partitioning of substances between organic and the inorganic components of soils and sediments.

The main outcome from the evidence review was the need for practical testing using the RP-IEX stationary phases to generate data and demonstrate the proof of concept. Hence, the requirement of this project is to perform this primary research. The method development and data generated from these investigations would allow us to build a better understanding of how substances with different chemistries partition between surrogate organic and inorganic components of soils and sediments. The results will be interrogated and modelled to understand whether correlations can be derived from the variables.

The detailed objectives for each phase of the project are described below.

Objectives

The principal aim of the pilot study is to perform a comprehensive assessment into the use of HPLC columns containing mixed mode RP-IEX solid stationary phases to understand the retention of substances with low log K_{OC} metrics (< 3). The pilot study will comprise three key phases: method development, data collation, and data examination and reporting, with objectives as described in the following bullets.

Phase 1: Method development stage

- Identify and purchase mixed mode RP-IEX solid stationary phase HPLC columns (henceforth RP-IEX column) including the four sub-types recommended in the evidence review from 2023/2024 (i.e., strong cation exchange, SCX; weak cation exchange, WCX; strong anion exchange, SAX; weak anion exchange, WAX). These columns should be commercially available (or have the potential to be so at a later date).

- Identify an appropriate detector. The merits of using a spectrophotometer, evaporative light scattering detector, radio detector or mass spectrometer should be considered. The proposed detector should be:

    - compatible with the proposed test substances.
    - readily available in commercial laboratories.

- Identify (an) appropriate HPLC mobile phase(s). The HPLC mobile phase(s) should be:

    - compatible with the proposed HPLC column and detector.
    - representative of the environmental compartment of interest (i.e., subsurface soils).

- Identify the appropriate pH(s) for the mobile phase of the HPLC system. This should consider the pH range of environmental relevance, including those of sub-surface environments. We propose pH 5.5 to 8.5 but would like this to be considered further by the contractor at the method development stage.
- Identify the composition of the buffer salts / acids / bases required to maintain the appropriate pH(s) of the mobile phase of the HPLC system and whether the solubilised constituents will adversely interact with components of the stationary phases.
- Identify 30 appropriate test substances (we suggest these should be drawn from: Arp et al., 2023; Droge and Goss, 2013; Franco and Trapp, 2008; OECD, 2001), which should:

    - cover a range of low K_{OC} values (0 to 3).
    - cover the key substance chemistries identified, that is, ionic (cation/anionic) and highly polar. Preferably each substance would have one dominant functional group to enable easier data interrogation. *If surface active / ion-pairing substances could be considered this would be beneficial. They are out of scope of the original OECD TG 121 (OECD, 2001), and it may not be appropriate to consider them at this time.*
    - be commercially available and abiotically stable.
    - have historical OECD TG 121 (OECD, 2001) data. *If OECD TG 106 (OECD, 2000) data are available this would be beneficial.*
    - be compatible with the proposed study design and detector.

Phase 2: Data collation stage

- Analyse the selected substances according to OECD TG 121 (OECD, 2001).
- Analyse the selected substances through each of the RP-IEX columns (and potentially at different pHs). This stage should incorporate decisions made during the method development stage.

Possible Extension

Phase 3: Data examination and reporting stage

- Report on details of the method development, study design, justification of decisions, detailed analytical methodology and the generated data. *Whether surface active / ion-pairing substances are analysed or not, the issue surrounding them should be summarised.*
- The pilot study results should be used to:

- evaluate how different substances are retained on each RP-IEX column type and compare the results with those obtained according to OECD TG 121 (OECD, 2001).
- evaluate how pH affects the data (for example, for ionisable substances, it may be that two tests should be performed with both ionised and non-ionised forms in appropriate buffer solutions where at least 10% of the test compound is dissociated within the pH range 5.5–7.5).
- evaluate the robustness, reproducibility, and applicability of the approach.
- identify the most appropriate parameter(s) to describe the environmental mobility of substances with low K_{OC} values.
- analyse how parameters identified correlate with known variables like functional group $pK_{a/b}$ or polarity, water solubility, and OECD TG 121 K_{OC}. If feasible, a principal component analysis should be undertaken.
- propose a route map forward with potential use for substance evaluation in mind, including considering at which point the results of an OECD TG 121 may trigger further testing on the RP-IEX HPLC columns and how those results could be used to screen for mobility.

Deliverables

Deliverables for the pilot study have been designed to show fulfilment of the key milestones.

Phase 1: Method development stage

Deliverable 1: Findings, including any uncertainties or issues, will be presented to the Environment Agency following the method development stage.

Phase 2: Data collation stage

Deliverable 2: Data and results will be provided and presented to the Environment Agency following the data collation stage. Raw data will be supplied to the Environment Agency in the form of an excel workbook.

Possible extension

Phase 3: Data examination and reporting stage

Deliverable 3: A draft report will be produced and provided to the Environment Agency for review and comment that fulfils the objectives defined in the data examination and reporting stage. The draft report will be prepared using MS Word using the Environment Agency Chief Scientist's Group reporting template.

Deliverable 4: A final report will be produced in a format that is suitable for publication as an Environment Agency report to be shared externally. The final report will incorporate and address comments from the Environment Agency review of the draft report.

Artificial Intelligence

If artificial intelligence (AI) is proposed to be used to produce any part of the report or to perform any tasks contributing to the project, this shall be made clear in your tender response, along with any relevant quality assurance. We would ask for you to cost all aspects of AI separately as an itemised item within your costings, so we can clearly see what makes up the AI component and associated cost

thereof. If the AI component is taken up, this will be agreed within the Contract Award between the supplier and the Project Manager, before any works commence.

Sustainability

The Environment Agency protects and improves the environment and is committed to reducing the sustainability impacts of its activities directly and through its supply chains. We expect the Contractor to share this commitment and adopt a sound, proactive sustainable approach in keeping with the UK Government 25 Year Environment Plan and our commitments compliant with all applicable legislation. This includes understanding and reducing direct and indirect sustainability impacts and realising opportunities, including but not restricted to; resilience to climate change, reducing greenhouse gas emissions, water use and quality, biosecurity, resource efficiency and waste, reducing the risk of pollution, biodiversity, modern slavery and equality, diversity & inclusion, negative community impacts.

As a delivery partner, the successful contractor is expected to pursue sustainability in their operations, thereby ensuring the Contracting Authority is not contracting with a supplier whose operational outputs run contrary to the Contracting Authority's objectives. The successful contractor will need to approach the project with a focus on the entire life cycle of the project

Outputs and Contract Management

We anticipate a start-up meeting between the contractor and the Environment Agency project staff in the week commencing 2nd September 2024. Thereafter, monthly teleconferences should be factored in, in addition to teleconferences at completion of each milestone.

Reference	Deliverable	Responsible Party	Date of completion
	Kick off meeting with contractor	Environment agency	W/C 2nd September 2024
	Monthly meeting updates (via MS Teams or a similar platform)	Contractor	At least monthly and more frequently if required on matters arising
	Deliverable 1: Presentation following the method development stage.	Contractor	14th October 2024
	Deliverable 2: Presentation following the data collation stage. Raw data in the form of an excel workbook.	Contractor	10th March 2025
	Deliverable 3: Draft report following the data	Contractor	12th May 2025

Reference	Deliverable	Responsible Party	Date of completion
	examination and reporting stage.		
	Comments on the draft report.	Environment Agency	2nd June 2025
	Deliverable 4: Final report.	Contractor	30th June 2025

References

Arp, H. P. H., Hale, S. E., Borchers, U., Valkov V., Wiegand, L., Zahn, D., Neuwald, I., et al. (2023). A prioritization framework for PMT/vPvM substances under REACH for registrants, regulators, researchers and the water sector. [22/2023]. Umweltbundesamt. Dessau-Roßlau, Germany. Available at: https://www.umweltbundesamt.de/publikationen/a-prioritization-framework-for-pmtvpvm-substances

Doucette, W. J. (2000). Soil and sediment sorption coefficients. In: Mackay, D. & Boethling, R. (eds.) Handbook of property estimation methods for chemicals. 1st ed. Boca Raton: CRC Press. https://doi.org/10.1201/9781420026283

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Franco, A., Ferranti, A., Davidsen, C. & Trapp, S. (2010). An unexpected challenge: Ionizable compounds in the REACH chemical space. The International Journal of Life Cycle Assessment, 15(4), 321-325. 10.1007/s11367-010-0165-6

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Ghafoor, A., Jarvis, N. J. & Stenstrom, J. (2013). Modelling pesticide sorption in the surface and subsurface soils of an agricultural catchment. Pest Management Science, 69(8), 919-929. https://doi.org/10.1002/ps.3453

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OECD (2000). Test no. 106: Adsorption -- desorption using a batch equilibrium method. OECD Guidelines for the Testing of Chemicals, Section 1. OECD Publishing. Paris. https://doi.org/10.1787/9789264069602-en

OECD (2001). Test no. 121: Estimation of the adsorption coefficient (Koc) on soil and on sewage sludge using high performance liquid chromatography (HPLC). OECD Guidelines for the Testing of Chemicals, Section 1. OECD Publishing. Paris. https://doi.org/10.1787/9789264069909-en

Pawlowski, S., Aicher, L., Berends, A., Curtis-Jackson, P., Haner, A., Hollender, J., Jene, B., et al. (2023). Mobility in the context of exposure-based assessment of chemicals for drinking water resource protection. Integrated Environmental Assessment and Management, 19(3), 775-791. https://doi.org/10.1002/ieam.4705

Strawn, D. G. (2021). Sorption mechanisms of chemicals in soils. Soil Systems, 5(1). 10.3390/soilsystems5010013

Appendix 3: Charges & Tender Submission

Costing tables:

Table 1

Job Role	Day rate
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]

Table 2

Contract Year	Task / Milestone	Delivery Date	Number of days input for each project member	Each staff cost (ex VAT) (£)	Travel & Subsistence / Equipment & Material Cost	Total Price (ex VAT) (£)
[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]

[redacted]

			[redacted]	[redacted]	[redacted]	
	[redacted]					
					Total Cost for FY 24/25:	**£78,042.75**

[redacted]

[redacted]

Technical responses:

E01 - Technical expertise and experience to successfully deliver the pilot study

E02 - Approach and methodology to complete the pilot study

E03 - Consideration of sustainability and social value

Appendix 4: Processing Personal Data

Authorised Processing Template

N/A