LRI ECO69: IMPROVING UNDERSTANDING OF SORPTION MECHANISMS BEYOND ORGANIC CARBON PARTITIONING: DEVELOPMENT OF METRICS AND SCREENING METHODS FOR CHEMICALS OF LOW-HYDROPHOBICITY

Background

The European Commission published the Delegated Regulation (EU) 2023/707 amending the CLP (Classification, Labelling and Packaging) Regulation, which entered into force on April 20th, 2023. This defined new hazard classes for substances and mixtures in the European Union (EU) including for PMT (persistent, mobile in the water cycle, toxic) and vPvM (very persistent, very mobile in the water cycle) substances.

Mobility, in the CLP, is described as a function of the organic carbon-water partitioning coefficient (log Koc). This captures solely one sorption mechanism and disregards other possibilities where electrostatic interactions may be dominant (e.g., in the presence of clays, for ionisable chemicals, and where organic carbon content of the environmental matrix is low). This is likely to be highly relevant for a high proportion of industrial chemicals, where ionisables constitute >50% of all REACH dossiers.

Whereas the Koc may be used for non-polar chemicals at a screening level, the K_{OC} remains a simplistic metric not considering the complex sorption behaviour that substances can undergo in soils and sediments. This may lead to the mobility of the substances being overestimated as it not able to bind to organic carbon and thus, not adsorbing to an environmentally relevant degree in the HPLC column used in the OECD TG 121.

Hence, the Koc does not permit efficient prioritisation for further regulatory consideration for all substances. In addition, for hydrophilic and ionisable chemicals, the Koc is inappropriate, particularly (but not exclusively) for soils with low organic carbon contents. Research is therefore needed to develop suitable descriptors which take in to account interactions amongst these types of chemicals and the complex soil/sediment matrices where multiple sorption mechanisms are likely to occur.

An adequate suitable standardized tool to determine relevant sorption properties to improve assessment of chemical mobility under various conditions is urgently needed. This project aims to investigate which mechanisms are the most relevant for substances that cannot be properly assessed using log Koc. Chemical selection, sorbent selection and experimental feasibility assessment is critical for this project to demonstrate the importance of sorptive mechanisms, other than hydrophobicity based, related to Koc, which are prevalent and representative of environmental matrices.

According to the current HPLC method, this is performed on analytical columns packed with a commercially available cyanopropyl solid phase containing lipophilic and polar moieties. A moderately polar stationary

phase based on a silica matrix is used. Presently, log K_{OC} values ranging from 1.5 to 5.0 can be determined. In the context of this project, the method should be updated and extended and/or a new method developed, including the definition of new standard references. For calibration, the novel method developed in LRI ECO62 could be used. It is the goal that the method could be proposed to improve the existing method or lead to a new OECD TG.

A better understanding of the sorption mechanisms of these substances and defining relevant metrics to characterise them would allow for a better environmental exposure assessment of mobile and very mobile substances since the most relevant parameters would be used as an input. This would support the current proposals for an effective assessment of PMT and vPvM chemicals using risk assessment (e.g. Gouin et al. 2024, Janer et al. 2025, Whelan et al. 2025).

Objectives

The project's objectives are to:

1. Review existing data and based on the acquired knowledge, expand the range of sorption mechanisms considered for the determination of soil mobility as well as define the relevant associated metrics.
2. Determine soil mobility parameters precisely and establish most relevant sorption mechanism for specific chemistries as well as the metrics needed to characterize these mechanisms.
3. Propose new or updated test method fit-for-purpose for the assessment of non-organic carbon sorption mechanisms.

Scope

This project aims to address the evaluation and assessment of substances for which adsorption to organic carbon is not the main mechanism driving mobility in soil. To this date, there is a lack of metrics and methods to adequately define the behaviour of such substances in the environment.

The project will derive efficient approaches permitting rapid and accurate screening of chemical entities of broadly differing chemical classes and is likely to require the proposal of suitable and well characterised reference substances relevant to corresponding sorption mechanisms to serve as benchmarks. The approach to be developed should be not only fit-for-purpose for each designated sorption mechanism but should also be reproducible and easily transferable to other testing facilities.

With the experimental procedure(s) developed, it is expected that the procedure can undergo a validation process to ensure the potential of OECD adoption.

Out of scope

Neutral organic / hydrophobic chemicals / inorganics.

Deliverables

This project is expected to deliver:

- Substantial database of adsorption data to adequately define the relevant sorption mechanisms and metrics, and to appropriately define reference substances to be used in the proposed method,
- Technical method to appropriately measure the relevant metrics, including a draft protocol and a proposal for an inter-laboratory ring trial,
- A guidance document discussing the relevance of the proposed method and metrics for the application in regulatory assessments.

A final report containing an executive summary (2 pages max), a main part (max. 50 pages) and a detailed bibliography. It is expected that the findings will be developed into at least one peer reviewed publication, following poster(s) and presentation(s) at suitable scientific conference(s) as well as the aforementioned guidance document.

Cost and Timing

Start in Q4 2025, duration 2-3 years

Budget in the order of €300,000

Partnering / Co-funding

Applicants should provide an indication of additional partners and funding opportunities that can be appropriately leveraged as part of their proposal. Partners can include, but are not limited to industry, government/regulatory organizations, research institutes, etc. Statements from potential partners should be included in the proposal package.

Fit with LRI objectives / Possible regulatory and policy impact involvements / Dissemination

Applicants should provide information on the fit of their proposal with LRI objectives and an indication on how and where they could play a role in the regulatory and policy areas. Dissemination plans should also be laid down.

DEADLINE FOR SUBMISSIONS: June 27th , 2025 at 11:59 PM (Central European Time).

Please see www.cefic-lri.org/funding-opportunities/apply-for-a-grant/ for general LRI objectives information, project proposal form and further guidance for grant applications. Please note that, if awarded the project, the institute must be able to accept Belgian Law (or an equivalent European legal framework) in the contract. If there are questions, please email .

Related links

- *Collard M., Camenzuli L., Lyon D., Saunders D., Vallotton N., Curtis-Jackson P., 2023. Persistence and mobility (defined as organic-carbon partitioning) do not correlate to the detection of substances found in surface and groundwater: Criticism of the regulatory concept of Persistent and mobile substances. Science of the Total Environment, 865: 161228.*
- *ECETOC, 2021 - Technical Report 139 : Persistent chemicals and water resources (https://www.ecetoc.org/publication/tr-139-persistent-chemicals-and-water-resources-protection/)*
- *Gouin T., Bitsch A., van Duursen M., Escher S.E., Hamers T., 2024. Informing the decision-making process for potential PMT/vPvM chemicals through the adoption of a risk-based prioritization*

framework: the ZeroPM approach. Environmental Sciences Europe, 36:208.

- *Janer G., Elmoznino J., Häner A., Bramke I., 2025. PBT/PMT assessment of active pharmaceutical ingredients. Regulatory Toxicology and Pharmacology, 156: 105772.*
- *LRI ECO62 – STREAM: Substance testing for river-bank filtration and mobility. https://cefic-lri.org/projects/eco62-stream-substance-testing-for-river-bank-filtration-and-mobility/*
- *OECD TG 121, 2001. Estimation of the Adsorption Coefficient (Koc) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC)*
- *Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006*
- *Whelan M.J., Pemberton E., Hughes, C.B., Swansborough C., Goslan E.H., Gouin T., Bell V.A., Bird E., Bull S., Segal L., Cook S.H., Jephcote C., Fane S., 2025. A tiered assessment of human health risks associated with exposure to persistent, mobile and toxic chemicals via drinking water. Science of the Total Environment, 958: 177868.*

Timing: Q4 2025, duration 2-3 years

LRI funding: €300,000

LRI research programme overview

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LRI Toolbox for your needs

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