In environmental exposure assessment, the mobility of chemicals presents two different types of concerns. Initially, mobility was associated with the protection of water resources used as a source in the preparation of drinking water. In this context, PMT (persistent, mobile, toxic) / vPvM (very persistent, very mobile) criteria have been proposed to identify substances that may pose a hazard to drinking water sources under the EU REACH Regulation ((EC) No 1907/2006) (Neumann and Schliebner, 2019). Mobility is also associated with the transport of chemicals by water, where there is the potential for mid-field to far-field (often referred to as pristine water resources) exposure which could also have implications for ecological and human health. It has been hypothesized that due to persistence, the exposure to mobile chemicals in a given environmental compartment might increase with time also referred to as “potential accumulation” (groundwater, bank water filtrates,
or far-field ecological and human exposure). Regulatory actions, in particular, recent nominations for Substances of Very High Concern (SVHC) under the REACH regulation, have raised the profile of these issues associated with mobile substances in water.

Recent reviews have pointed to the lack of specificity of the proposed PMT/vPvM criteria in proactively identifying chemicals of concern, thus pointing to a need for effective and efficient screening level and higher-tier risk assessment models to identify chemicals of potential concern to drinking water (ref. ECETOC Task Force ‘Persistent chemicals and water resources protection’). A quantitative approach to evaluate concern for increasing exposure over time is not readily available. Finally, contaminants are increasingly detected in all environmental compartments, due to growing knowledge of exposure routes leading to greater exploration, and advances in the field of analytical chemistry improving detection limits. However, the interpretation of monitoring data for evaluating risk has not yet reached a consensus agreement.

Whereas initial discussions involved soil leaching, river-bank filtration is now considered by UBA (Umweltbundesamt; German Environment Agency) as the main entry path for mobile substances into the groundwater. The UBA PMT classification scheme uses the organic carbon normalised adsorption coefficient \(K_{OC}\) as a measure for mobility. Whereas the \(K_{OC}\) may be used for non-polar chemicals at a screening level, it should not be used for a definitive regulatory classification purpose. The \(K_{OC}\) is simplistic and does not consider the complex sorption behaviour that chemicals can undergo in soils and sediments nor the hydraulic conditions in river-banks, where water transits over multiple years. Hence, it does not permit efficient prioritisation for further regulatory consideration. For hydrophilic and ionisable chemicals, the \(K_{OC}\) is inappropriate, particularly (but not exclusively) for soils with low organic carbon (OC) contents. Research is therefore needed to develop suitable descriptors which take into account interactions amongst these types of chemicals and the complex soil/sediment matrices.

The most relevant parameter for expressing the binding strength of a chemical to soil is the water-to-soil distribution coefficient at a given temperature \(K_d\), mostly expressed as the non-linear, concentration-dependent, Freundlich isotherm, where the \(K_d\) value becomes a Freundlich factor \(K_f\) value and the Freundlich exponent \((1/n)\) describes the degree of non-linearity. \(K_d\) is both soil and chemical-specific, and can therefore be used to compare the relative mobility of different chemicals in similar soils.

Existing test methods to assess sorption to soils such as OECD’s Adsorption - Desorption Using a Batch Equilibrium Method (OECD 106) and OECD’s Leaching in Soil Columns (OECD 312) are using a 0.01 M solution of calcium chloride (CaCl\(_2\)) in deionised water as the aqueous solvent
phase to minimise cation exchange. Hence, for ionisable chemicals, 0.01 M CaCl$_2$ will block cation exchange and other ionic partitioning and may partly erroneously suggest that organic carbon partitioning is the principal partitioning mechanism.

Moreover, OECD’s Leaching in Soil Columns (OECD 312) is using percolation of artificial rainwater through soil columns whereas river-bank filtration would require fully saturated conditions.

The aim of the project is therefore to design and evaluate suitable test methods to assess the mobility of chemicals in sediment columns under fully saturated conditions thereby using realistic environmental concentrations.

The results from this test method may then be used to adapt existing leachability in silico tools available to assess the soil leachability of chemicals (vertical transfer from topsoil to groundwater) as recommended by the chemical industry in light of the EU COM proposal for the introduction of new hazard classes (i.e., for PMT/vPvM) within Regulation (EC) No 1272/2008 on the classification, labelling and packaging of substances and mixtures (CLP Regulation) and within the classification as substances of very high concern for Authorisation (SVHC) in the context of Article 59(10) of the REACH Regulation.

Leaching tests as described by the Swiss authorities for the evaluation of contaminated sites (Office fédéral de l’environnement OFEV (2017): Méthodes d’analyse dans le domaine des déchets et des sites pollués) could be used as a basis for the development of a leaching test for river-bank with the following modifications: instead of using material from contaminated sites standard sediments as described in OECD 308 may be used; instead of leaching by deionised water, a solution of the test substance in environmental concentrations is pumped from the bottom to the top through the test sediments. The scheme of the test system as proposed by OFEV (2017) is as follows:

The following specifications have to be met:
Objectives

This project is looking to evaluate suitable laboratory tests to assess the mobility of chemical substances during river-bank filtration under fully saturated conditions. As a follow up, parameters may be identified to improve/adapt the existing in silico tools available to assess soil leachability (vertical transfer of substance) so that they can also be used for river-bank filtration (horizontal transfer from surface water to nearby wells).

The project’s objectives are:

1. Literature review of existing adsorption/desorption tests
2. Proposal of a test method to assess river-bank filtration
3. Performance of testing of selected contaminants under environmental conditions
4. Proposal for round-robin testing in view of a future potential acceptance as e.g., ISO or OECD test guideline
5. Elaboration on how existing in silico tools for soil leachability can be improved to fit for river-bank filtration assessments.

Scope

Deliverables

The final report shall contain 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 a suitable scientific conference(s).

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:** September 1st, 2023 at 11:59 PM.

**Timing:** Start in Q4 2023, 12 months

**LRI funding:** €200,000

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**LRI research programme overview**

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