ECO54: Developing a tiered modelling framework in support of risk assessment of chemical substances associated with mobility concerns

1st Stakeholder workshop on mobility concerns for chemical substances

February 9, 2022, 14:00 – 17:00 CET

6:00 – 9:00 PT; 9:00-12:00 ET

Meeting link: https://global.gotomeeting.com/join/318897053

Time	***Topic***	***Facilitator***
14:00 – 14:05	Welcome	Denis Sarigiannis
14:05 – 14:20	Regulatory perspectives on mobility	
14:20 – 15:10	Moderated discussion topic 1: What are we really talking about when talking about the mobility of chemicals? A defined goal of protection is critical to assessments of environmental and health risks of substances with the mobility concern. This question seeks to solicit opinions about where and how the focus of protection should be placed in assessments of chemical mobility, e.g., the safety of drinking water, the threat posed to aquatic ecological acceptors, the capability of waterborne long-range transport to remote ecosystems, and/or others. 14:20 – 14:35 Overview of ECO54 provided by Li 14:35 – 15:05 Open discussion	Denis Sarigiannis
15:10 – 16:00	Moderated discussion topic 2: Is mobility a concern for hazard or risk? One can screen chemical substances for the mobility concern, based on bright line "hazard" criteria AND their "risk" (an integration of hazard and exposure) to humans and ecological acceptors. Exposure to "hazardous" chemicals in water is a function of several other parameters, not just mobility. This question seeks to solicit opinions about the desirable approach that should be used to assess the mobility of chemicals. 15:10 – 15:25 Presentation of preliminary results of ECO.54 on Hazard vs. Fate (Exposure-based) case study 15:20 -15:50 Open discussion	Jon Arnot

15:55 – 16:40	Moderated discussion topic 3: What data gaps did you encounter, or are you plagued with, when assessing the hazard (esp. mobility) of chemical substances? Gaps in chemical data hinder the ready application of developed models or approach methodologies in mobility assessment and this impacts both hazard and risk-based decision making. This question seeks to solicit opinions about the possible research needs, e.g., new data, new models, physicochemical properties, estimation tools, etc. for addressing the current data gaps in practices of hazard (esp. mobility) assessments. 15:50 – 16:05 Presentation by ARC on current data gaps related to M and fate parameters, and Steven T J Droge on K_{OC} and *Kd* 16:05 – 16:40 Open discussion	Trevor Brown
16:40 – 16: 55	Discuss next steps for addressing uncertainty in M assessment	Denis Sarigiannis
16:55 – 17:00	Closure	ALL

ECO54: Developing a tiered modelling framework in support of risk assessment of chemical substances associated with mobility concerns

1st Stakeholder workshop on mobility concerns for chemical substances

Workshop content

Moderated discussion topic 1: What are we really talking about when talking about the mobility (M) of chemicals?

According to the German Environmental Agency, a chemical is assessed to be "M" if it has a water solubility > 0.15 mg/L and a logKOC or logDOW (over the pH range of 4–9) < 4.0. Underlying this practice is an assumption that chemical substances fulfilling these individual criteria would have the potential to reach sources of drinking water. According to REACH, mobility can be qualitatively defined as "the potential of the substance (...), if released to the environment, to transport to groundwater or far from the site of release. Compounds with multiple ionic groups are particularly watersoluble. However, even molecules with a high solubility still may not be very mobile in water because of sorption. Solid phases, such as soils and minerals, can also contain dipoles and ionic charges that attract polar contaminants. This especially applies to cationic compounds, because most natural surfaces carry negative charges. Conversely, organic anions are expected to be poorly retained. Generally, the molecules most mobile in water are the ones in which solvation by water is more favorable (energetically) than sorption to environmental solids.

A defined goal of protection is critical to assessments of environmental and health risks of substances with the mobility concern. This question seeks to solicit opinions about where and how the focus of protection should be placed in assessments of chemical mobility, e.g., the safety of drinking water, the threat posed to aquatic ecological acceptors, the capability of waterborne long-range transport to remote ecosystems, and/or others. It has also to be mentioned that the interrelationship between the various factors that govern mobility (transport), occurrence in exposure media (such as air, water, sediment and soil) and occurrence in biota, is complex. For example, substances partition between different exposure media based on their physicochemical properties and may have a different persistence in each of these exposure media. It is important that persistence is related to the media in which the substance is considered mobile, or through which it is considered mobile. In this sense, more detailed environmental modelling of the fate, behaviour and transport potential are needed to fully understand the potential for a given substance to transport long-distances and to accumulate in water, sediment, soil and biota in remote regions. Furthermore, several types of interactions need to be considered, including physico-chemical processes of complexation and changes in solubility and sorption phenomena, but also chemical reactions between chemicals in the environment, including chemical-nutrient interactions.

Moderated discussion topic 2: Is mobility a concern for hazard or risk?

Various 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 One can screen chemical substances for the mobility concern, based on either bright line "hazard" criteria or their capability of posing "risk" (an integration of hazard and exposure) to humans and ecological acceptors. This question seeks to solicit opinions about the desirable approach that should be used to assess the mobility of chemicals. Also, regarding the models for estimating human exposure there is a lack of inclusion of scientific advancements in the field of exposure sciences in models currently used in support of chemical regulations. Chemicals on the market represent a wide range of chemistries and thus may not fit in the applicability domain of certain models (chemical space). The choice of the model also depends on the spatial and temporal scales of the evaluation. Although currently there is no "off the shelf" modeling tool available for screening, identification, and assessment for PMT substances, the ECO54 team has developed computational models (e.g., RAIDAR, PROTEX, INTEGRA), databases (e.g., databases of properties of >25k chemicals, toxicokinetics of >14k chemicals, and measured concentrations of >1k chemicals), and data prediction techniques (QSARs), which constitute a modular, tiered framework for fit-for-purpose assessments of ecological and human exposures through multiple pathways to chemicals in multiple environmental compartments released from multiple lifecycle stages.

Moderated discussion topic 3: What data gaps did you encounter, or are you plagued with, when assessing the hazard (esp. mobility) of chemical substances?

Gaps in data of chemicals may hinder the ready application of developed models or approach methodologies in mobility assessment. This question seeks to solicit opinions about the possible research needs, e.g., new models, physicochemical properties, estimation tools, etc. for addressing the current data gaps in practices of hazard (esp. mobility) assessments.

Although QSARs present an interesting option to address data gaps, at the moment, there is a lack of comprehensive or generic (as opposed to class-specific) QSAR models for predicting half-lives of biodegradation (HLbiodeg), hydrolysis (HLhydro), and photolysis (HLphoto), which are critical for addressing uncertainties associated with "M" assessment, fate and exposure modeling, and monitoring data interpretation. Thus, there is a need to develop databases by aggregating and curating measurements of biodegradation (half-life or rate constant), hydrolysis (half-life or rate constant), and photolysis (categoric result: susceptibility to photolysis or not) from the literature (e.g., peer-reviewed journal articles, technical reports, and training and test sets of existing QSAR models). A way to move forward, is the development of QSAR models for predicting biodegradation and hydrolysis predict half-lives, and qualitative classification QSAR models for predicting photolysis (susceptibility to photolysis or not).