CEFIC Long-range Research Initiative
Request for Proposals (RfP)

Title and Code Number
Breakthrough developments in the characterisation of Long-Range Transport of chemicals – **LRI-ECO53**

Background
Atmospheric transboundary and intercontinental Long-Range Transport (LRT) of chemicals may influence air quality and contamination of areas far from the initial emission. Those chemicals transported long distance may have an impact on human health as well as on the environment in locations remote from the emission sources.

The need for coordinated actions among countries has been recognized and international cooperation was put in place through several agreements to combat the impact of such pollutants:
- The United Nations Economic Commission for Europe (UNECE) signed in 1979 is the first international legally binding instrument establishing a framework Convention on Long-Range Transboundary Air Pollution (LRTAP). It entered into force in 1983 and was extended by eight specific protocols.
- The United Nations Environment Programme's (UNEP) Stockholm Convention on Persistent Organic Pollutants was adopted in 2001. It entered into force in 2004 and initially covered 12 chemicals and families of compounds. 16 additional POPs have been added by the Parties as of 2017. The Conference of Parties in May 2019 will discuss additional proposals.

Under Annex D of the Stockholm Convention, an atmospheric half-life >2 days is recognised as a physicochemical criterion for Long-Range Transport Potential (LRTP) for migration through the air. Vapour pressure (<1000 Pa) could equally be considered by other parties for screening purposes. Half-lives in water are also relevant when considering transport via ocean currents.

The ability for a substance to undergo LRT is predicted using modelling and screening criteria in combination with monitoring data. Models should be able to accurately predict the concentration of a chemical in a certain medium that is remote from its emission source.

While monitoring data would be used as "post-evidence" evaluation, predictive models have been developed to predict how chemicals are transported, degraded and deposited in different compartments (Mackay *et al.*, 2001; Scheringer and Wania, 2003). Considering that the chemicals potentially subject to LRT processes could interact with different environmental media at the same time (air, particles, water, sediments…), the models that were developed are quite complex, using multimedia compartment-based equations (Mackay and Reid, 2008; Reid and Mackay, 2008), as well as 3-dimensional general circulation models (Suzuki *et al.,* 2004). For instance, the MSCE (Meteorological Synthesizing Centre East) POP model, a multi-compartment chemistry transport model, uses a benchmark approach to overcome model dependency of numerical values. It has already been used for the assessment of several POP candidates under the Stockholm Convention (Vulykh *et. al*., 2006).

In screening exercises and in the case of predictive assessment, multi-compartment based-models using the fugacity approach have been developed and are commonly used by technical agencies working in support for the implementation of international conventions like the European Monitoring and Evaluation Programme (EMEP). Several of these models are referred in Franklin (2006).

Ten years ago, the OECD developed a screening tool to evaluate overall persistence and LRTP, the OECD P_{OV}-LRT Tool (Wegmann *et al*., 2009). This modelling tool is currently accepted as a strong argument in the assessment of LRTP of POP candidates. The OECD tool is a multimedia model considering the characteristics of bulk compartments (air, water and soil) and the characteristics of the sub-compartments (aerosols, suspended sediments, pore water in soil, air in soil and solid particles in soil).

Using those predefined characteristics and the properties of chemicals related to adsorption potential (partition coefficients to the different compartments), specific kinetics of degradation in each sub-compartment as well as inter-compartment exchanges are calculated. However, the accuracy of the predictions will depend on the applicability domain for each prediction. In that respect, some families of compounds, such as chemicals predominantly present in their ionic form under environmental conditions, may require specific attention.

Although LRT occurs in both air and water, the flow velocities are much higher in the air and therefore semi-volatile substances are usually prioritized for LRT potential (both in the air and aerosols).

Objectives

By 2019, the European Chemical Agency (ECHA) has received new responsibilities under the recast of the POPs Regulation (EC) No 850/2004). However, the assessment of the LRTP is complex and not yet precisely described in EU regulatory documents. There is an urgent need to provide support for the development of such guidance, which would standardize and parameterize this evaluation. As such, one of the main outcomes of this project will be to provide scientific support to these future developments at the ECHA level. In addition, since the OECD screening tool was developed, dispersion models and analytical techniques have improved, access to large databases is easier, the 'big data' concept has emerged, and geo-localised and statistical tools (e.g., Spatial Analysis and Decision Assistance, SADA, US-EPA) have been further developed. Hence, and beyond the need to validate the tools with legacy contaminants, which remains crucial before applying to new chemicals, there is a need to integrate all latest scientific developments in future guidance for the assessment of LRTP of chemicals.

The project's objectives are to:

1. Provide a good understanding of the state of the art in transportation models (including dispersion models) developed to estimate LRTP of chemicals, with the associated applicability domain and some references of their use in a regulatory context (including how to avoid false positives for LRTP simply due to wrong assumptions being made upfront and input values not carefully aligned when considering the compartment of main exposure, fate behaviour, etc). The case of chemicals predominantly present in their ionic form under environmental conditions and metals will need to be investigated as they are not within the applicability domain of the OECD Pov – LRT Tool. A large number of models would need to be investigated and analysed according to their domain of applicability, advantages, drawbacks and usefulness for LRT estimations.
2. Analyse available databases and existing monitoring programs for the concentrations of chemicals in the environment and their possible use to address LRTP. A critical review of the monitoring data with regards to the quality of the monitoring information (representativeness and analytical accuracy), its sources (local vs LRT) and the associated emission rate should also be conducted. The purpose of this analysis should be to test the validity of the LRT models to see how the predictions may be compared with the monitored concentrations including the concentrations in the remote surface media. Special consideration should be given to distinguishing exposure resulting from local sources vs. exposure from LRT and deposition.
3. Depending on the outcome of Objective 1 (usefulness, and other criteria to be determined during the project), a selection of models will have to be proposed for further evaluation. For example, the evaluation of the selected models could include the sensitivity/uncertainty analyses. One of the main objectives would be to determine the key parameters that are important or influential, and to what extent these may influence critical characteristics (half-lives, partition coefficients etc.).
4. Assess other possible screening criteria apart from the atmospheric half-life (and vapour pressure) to predict LRTP of chemicals in the environment (e.g. log K_{aw}, log K_{oa} could be considered key parameters).
5. Propose a tiered approach, with associated flow diagram including weight-of-evidence considerations, to assess LRT of chemicals, from the use of screening criteria and simple models to the use of more complex models and field data. In this same scheme, make proposals for how long a distance must be to be considered as LRT, in what direction the transport must take place (longitude vs latitude) etc.

Scope

- Semi-volatile substances are the priority chemicals in this project as they are targeted as having the highest propensity for long distance dispersion. In addition, the case of water-soluble compounds and their transportation will need to be investigated as well for all above objectives.
- In this project, there might be first steps dedicated to reviewing literature, existing models and databases, followed by identification of further steps to improve the models.
- Transport associated with microplastic in the water compartment is not in scope

Deliverables

The final report shall contain an executive summary (2 pages max.), a main body of text (50 pages max.) and a detailed bibliography.

It is expected that the findings will be developed into at least one peer-reviewed publication, following poster and oral presentation(s) at suitable scientific conference(s). At least one publication shall be open-access.

Cost and Timing

Start in Q1 2020, duration 2 years

Budget in the order of €280 000

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 of study results should also be outlined.

References

- Franklin J, 2006. Long-Range Transport of Chemicals in the Environment, Eurochlor Science Dossier n°17, 71p; http://www.eurochlor.org/media/14954/sd10-long_range_transport-final.pdf
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- Vulykh N., S. Dutchak, E. Mantseva, V. Shatalov, 2006. EMEP contribution to the preparatory work for the review of the CLRTAP Protocol on persistent organic pollutants. New substances: Model assessment of potential for long-range transboundary atmospheric transport and persistence of PentaBDE, Endosulfan, Dicifol, HCBD, PeCB, PCN. EMEP/MSC-E Technical Report 1/2006. Available at: http://msceast.org/reports/1_2006.pdf
- Wegmann F, Cavin L, MacLeod M, Scheringer M, Hungerbühler K, 2009. The OECD software tool for screening chemicals for persistence and long-range transport potential. Environmental Modelling & Software **24**, 228 – 237; http://www.oecd.org/chemicalsafety/risk-assessment/oecdpovandlrtpscreeningtool.htm

DEADLINE FOR SUBMISSIONS: September 1st, 2019

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.