ECO54

# Developing a Tiered Modeling Framework in Support of Risk Assessment of Chemical Substances Associated with Mobility Concerns


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## Background

### Chemicals with "mobility" concerns are perceived as an emerging threat to aquatic environments and drinking water quality

- Ubiquitous in our daily life
  - Pharmaceuticals, personal care products, cosmetics, plant protection products, etc.
- Highly polar, soluble, and/or ionizable in water
  - A high propensity to be transported easily in the aqueous environment
- Highly efficient in transport from sources of release to groundwater, source water protection areas, or aquatic ecosystems

**LRI ECO54 Project seeks to develop a tiered modeling framework in support of the risk assessment of chemicals with mobility concerns**

### Policy focus #1: What do they look like?

Umweltbundesamt (UBA)'s "bright-line" cut-off criteria (2019) for screening chemicals with "mobile" concerns.

False positives (over-protection): Chemicals meeting the criteria may not be substantially present in the aquatic environments;
False negatives (under-protection): Chemicals failing to meet the criteria can also be substantially present in the aquatic environments.

### Policy focus #2: How well do we know their risks?

Models available for screening and assessing chemical exposure and risks.

Existing models have largely been developed and evaluated for "legacy" pollutants, i.e., hydrophobic neutral organic chemicals;
There is uncertainty as to the reliability of these models for simulating polar and/or ionizable organic chemicals.

## Research

### Promote mechanistic understandings of the mobility of chemicals

- **Assess the mobility of chemicals**
  - Screening of 112k+ of unique chemicals on national and regional inventories for their potential of mobility, dominant pathways of human exposure, and risks to aquatic ecological receptors and human drinking water
- **Evaluate the merits and limitations of existing comprehensive fate & exposure models in assessing the mobility of chemicals**
  - Model structure, algorithm, and applicability domain
  - QSAR tools for parameterizing the models

**260,883 chemical records on national and regional inventories**
(103,491 from NORMAN; 28,373 from Canada's DSL; 45,614 from China's IECSC; 68,168 from U.S.'s TSCA; 24,500 from EU's REACH registration)

**112,259 unique chemicals with structural information**
(94,156 from NORMAN; 12,628 from Canada's DSL; 15,579 from China's IECSC; 31,907 from U.S.'s TSCA; 8,390 from EU's REACH registration)

**84,825 chemicals meet the UBA "M" criterion**
log $D_{OC}$ (pH from 4 to 9) or log $K_{OC}$ lower than 4

**65,271 chemicals meet the UBA "vM" criterion**
log $D_{OC}$ (pH from 4 to 9) or log $K_{OC}$ lower than 3

### Refine and improve existing lower- and higher-tiered fate & exposure models developed previously by the research team

- **Improve the structure and algorithm in existing comprehensive fate and exposure models**
  - More sophisticated characterizations of surface water, groundwater, and soil runoff
  - Algorithms to accommodate polar and/organic chemicals
  - Removal efficiency during water treatment
- **Develop QSAR tools for parameterizing the comprehensive fate and exposure models**
  - Quantitative prediction: Half-lives of biodegradation and hydrolysis
  - Qualitative prediction: Susceptibility to photolysis (Yes or No)

Higher-tiered sophisticated assessments

PROTEX
(Li et al. *Environ. Sci. Technol.* 2018)

INTEGRA
(Sarigiannis et al. *ICEMS Proceedings*, 2014)

RAIDAR
(Arnot et al. *Environ. Sci. Technol*. 2006, 2008)

Lower-tiered high-throughput screening

### Explore conditions for screening the occurrence of chemical substances in aqueous environments

- **Develop a holistic modeling approach for assessing the risks of chemicals posed to aquatic ecological receptors and humans**
  - The interaction between persistent (P), bioaccumulation (B), and mobile (M) properties
  - Interpretation of the temporal trend in monitoring data
- **Develop a scoring "rubric" for ranking and prioritizing chemicals with mobility concerns**
  - A risk score as a combination of bins of chemical tonnage, use patterns, persistence, sorption capacity, and other properties.

### Organize dedicated workshops for communication and engagements with industrial, regulatory, and academic stakeholders


Cefic-LRI Programme
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