**MODELING CHEMICAL MOBILITY IN THE ENVIRONMENT FOR PERSISTENT, MOBILE AND TOXIC (PMT) COMPOUNDS**

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**ABSTRACT**

Persistent, mobile, and toxic (PMT) chemicals, are perceived as an emerging threat to aquatic environments and drinking water quality due to (a) their high polarity and water solubility, that enables them to be transported efficiently from sources of release to groundwater or remote ecosystems; and (b) the relatively low removal efficiencies during water treatment. The goal of the current study, performed in the frame of the CEFIC LRI ECO54 project, is to develop a tiered modeling framework in support of risk assessment of (PMT) chemicals. Such a modeling framework couples (i) a comprehensive fate model simulating the transport, transformation, and accumulation of chemicals of interest in various environmental compartments, and (ii) an external and internal human exposure module to chemicals of interest. The current state of the art in chemical mobility modelling includes our in-house model (INTEGRA), another four comprehensive fate and exposure models RAIDAR/RAIDAR-ICE, PROTEX, EUSES and USEtox, and two soil-groundwater models FOCUS and PRZM-GW. An intercomparison exercise on these models focused on (a) the domain of applicability of algorithms or equations (coverage of ionogenic organic chemicals), (b) the fate and transport processes considered for the water environment, with a special focus on elimination processes (e.g., biodegradation, hydrolysis, photolysis), (c) routes of exposure, (d) spatial segmentation. From this comparison, it has been concluded that the applicability domain (AD) of a fate and exposure model is constrained by the following three considerations: (a) the AD of tools used for parameterization of fundamental properties, e.g., QSARs, used to generate equilibrium partition coefficients in the tertiary octanol-water-air system (KOW, KOA, and KAW), as well as biodegradation and biotransformation half-lives; (b) the range of the fundamental properties of chemicals the experimental measurements of which are used to develop built-in empirical relationships for parameterization of partitioning or mass transfer inputs; and (c) assumptions adopted by model algorithms. Most fate and exposure models assume well-mixed, homogeneous environmental compartments, and equilibrium partitioning between phases within a compartment (i.e., sub-compartments). High-throughput screening models additionally assume the steady-state of mass distribution in the modeled region. Ideally, a suitable fate and exposure model should be used to make predictions falling within this AD by interpolation, not extrapolation and it should be able to capture the complex temporal and spatial dynamics of chemical mobility in the environment.

**KEYWORDS:** PMT chemicals, multimedia environmental fate, exposure modeling