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Retrieval and scientific interpretation of ecotoxicological information

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Environmental Fate Modelling

Chemicals released into the environment interact according to various mechanisms in environmental media, e.g., adsorption and desorption of chemicals to or from soil or organic particles suspended in surface water bodies. Chemical substances can also migrate between media and may accumulate in specific environmental compartments (air, soil, water, animals etc) depending, amongst other factors, on the chemical and physical properties of the compound. Environmental fate modelling is the science of predicting the relative steady-state distribution of the compound in the various environmental compartments existing in a specific exposure scenario. Prediction of the distribution profile includes estimation of the residual chemical concentration in those compartments, which may subsequently be used for environmental health risk assessment.

Environmental fate modelling and analysis involve parameters such as water solubility, vapour pressure, fugacity, the octanol-water partition coefficient, bioconcentration factors, soil sorption constants, the water-air ratio, and degradation rate constants in water, air, soil, and biota. Fugacity is the pressure or chemical potential exerted by a substance in whichever phase or compartment it exists, and can also be described as the escaping tendency of a chemical from a medium. Fugacity is related to the concentration of the substance in the particular compartment or phase and is the basic concept applied in environmental fate models.

INFOTOX applies environmental fate modelling to assess the potential partitioning and fate of chemicals in environmental compartments, providing estimates of the steady-state concentration profile in the various compartments when comprehensive analytical data for the various media are not available. The results serve to define the most likely exposure pathways that are relevant in human health risk assessments and facilitate focused analytical surveys.

Artist: Edward Roworth

