**Problems when assessing the persistence of ionic or ionisable organic chemicals under REACH**

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For the protection of humans and the environment, the identification and regulation of chemicals with persistent (P), bioaccumulative (B) and toxic (T) properties are a central element within the environmental assessment. The criterions for the identification of PBT‑substances under REACH (Registration, Evaluation and Authorization of Chemicals) and the guidance for the PBT-assessment have been developed for neutral organic molecules, whereas positively or negatively charged chemicals were not considered. Therefore, ionic and ionisable compounds could not be currently evaluated by the methodical approaches of the PBT‑assessment.

The persistence is the first criterion to be assessed prior to identifying substances with PBT-properties and includes the investigation of abiotic and biotic degradation processes in surface water, soil or sediment. For the conduction of surface water, soil or sediment simulation studies, standardized test guidelines of the OECD are available (OECD 307, 308 and 309). The decision, which test to use depends on physico‑chemical properties as well as exposure routes of the substance in the environment (ECHA R.11, 2014). Besides the water solubility, vapor pressure and partioning coefficient n-octanol/water (log Pow), the adsorption behavior of the substance should be considered. While the first three physico‑chemical properties are requested as standard information requirements in the registration of substances with a production or import volume of > 1 t/a under REACH, data on adsorption of a substance have to be delivered not until a tonnage of 10 t/a or more is reached (REACH Annex VII, 7.5; 7.7.; 7.8.).

The estimation of the adsorption of a substance to soil or sediment could either be done using the batch-equilibrium method (OECD 106) or the HPLC method (OECD 121) obtaining carbon normalized adsorption coefficients (Koc). However, if the physico‑chemical properties of the substance indicate a low adsorption potential, e.g. a low Pow, the adsorption behavior of a substance to soil organic and mineral particles must not be further experimentally proofed (REACH Annex VIII, 9.3.1.).

Due to the structural complexity of polar and ionic chemicals, the easy relationship between the hydrophobicity of a chemical (log Pow) and their affinity to soil organic and mineral surfaces (Kd, Koc) may fail in these cases. The effect of pH, soil properties, mineral surfaces and other factors influencing the adsorption and the fate of ionic and ionisable substances in the environment will not be sufficiently considered even if the log Pow is used. These circumstances will be illustrated on different ionic and ionisable substances belonging to different substance classes (pharmaceuticals, biocides, pesticides). Consequences of false estimations of the adsorption potential of ionic substances with respect to the assessment of their persistency under REACH will be discussed.

Literature:

European Chemical Agency (2014): Guidance on informations requirements on chemical safety assessment, Chapter R11: PBT/vPvB-Assessment; Version 2.0.

OECD-Guideline 121 for testing chemicals (2001): Estimation of the Adsorption Coefficient (Koc) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC).

OECD-Guideline 106 for testing chemicals (2001): Adsorption - Desorption Using a Batch Equilibrium Method

OECD-Guideline 308 for testing chemicals (2002): Aerobic and Anaerobic Transformation in Aquatic Sediment Systems.

OECD-Guideline 307 for testing chemicals (2002): Aerobic and Anaerobic Transformation in Soil.

OECD-Guideline 309 for testing chemicals (2004): Aerobic Mineralisation in Surface Water‑Simulation Biodegradation Test.

REACH (2012): Regulation (EC) No 1907/2006 of the European parliament and the council of 18 December 2006.