Scientific concepts and methods for moving persistence (P) assessments into the 21st century

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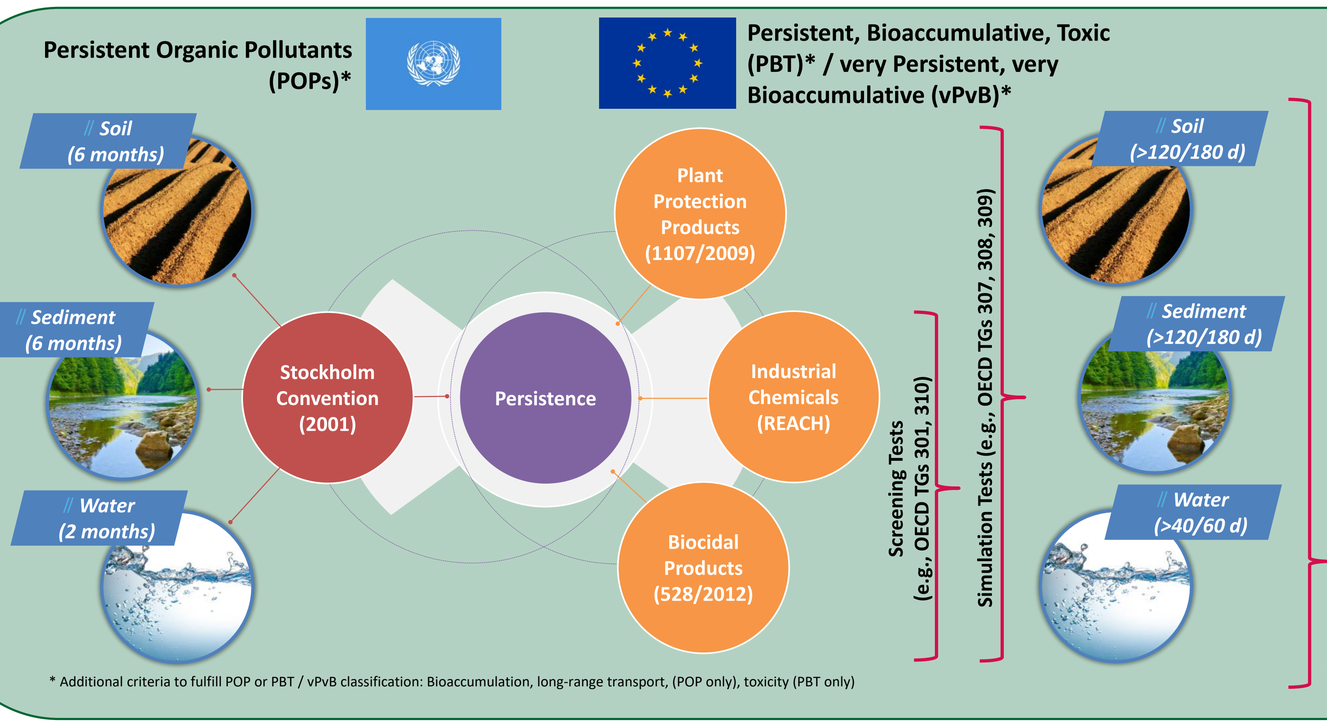


BACKGROUND

Persistence can be defined as the propensity for a chemical to remain in the environment before being transformed by chemical and/or biological processes, whatever the emission compartment (e.g. air, water, soil or sediment).

Current P assessment is based on methods developed >15 years ago and on a narrow range of chemical properties. A Task Force[a] was set-up to evaluate recent progress and future directions for improving such test methods.

CHALLENGES

Substrate-specific factors

Particles & poorly solubles: Need new testing procedures (problems: sedimentation, sorption, desorption)[1]

Non-extractable residues (NER): Methodology for differentiation of the three binding types not yet validated[2]

UVCBs: Difficult testing of complex substances (ecotox, biodegradability) without knowing each component[3]

POSSIBLE OPTIONS

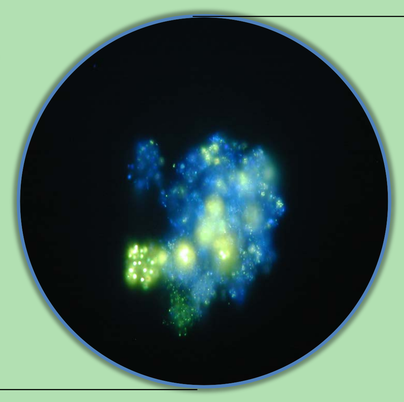
- Poorly solubles: Passive dosing allows realistic and constant exposure concentrations[9]
- NER: Isotope-label studies allow to distinguish primary vs ultimate degradation, types of binding, and establish mass balance and remobilisation potential[2]
- UVCB: Whole substance ecotox testing, biodegradability testing (based on carbon balance approach), read-across and further *in-silico* tests, ´omics´ analyses (targeted and non-targeted)[3]

Microbial-specific factors

Sample sizes are small (up to 10,000 × less cells) leading to large variability in outcomes[4] and half-lives[5] in biodegradation tests, which has an impact on diversity

Diversity, biogeography & lifestyles: Chance inclusion of relatively rare catabolic functions[4] influenced by environmental compartment/location/redox

Adaptation is currently excluded from biodegradation screening tests[6]



- Increased number of total cells can improve screening test accuracy[10].
- Biomass measurements for normalization of tests[10] and/or degradation rates across test formats[11].
- Microbial community analyses ('omics) to contextualize, normalize and understand biodegradation rate variations[12].
- New adaption tests improve the accuracy of screening outcomes[13]

Testing format & abiotic environmental factors

Photolysis is rarely studied[7] (except for PPPs[8]), but is important for a complete understanding of potential persistence

Temperature: Testing is usually done at a single temperature[7,8], but degradation processes are often temperature-dependent (e.g., biotransformation)

- Performance of tests on abiotic processes (e.g., hydrolysis (OECD 111[14]), photolysis (OECD 316[15])
  Inclusion of abiotic processes in simulation tests (e.g., irradiation in OECD 309 tests)[16]
- Inclusion of abiotic data in weight-of-evidence approach

ADDITIONAL GENERIC TOOLS AND APPROACHES

Benchmarking

Benchmark chemicals for assessing biodegradation relative to a reference chemical(s).[17]

Modelling

- High-quality biodegradation rate database to include metadata[18]
- Inverse modelling of rates from degradation/dissipation data[11]
- Further development of QSBRs grouping chemicals by reaction type[12]

Biochemical assays

Screening for specific transformation types: hydrolysis, redox, substitutions with/without enzymes (cf plant metabolism[19])

NEXT STEPS

- ECETOC Task Force[a] is on-going and will draft two publications for researchers and practitioners on: i) a conceptual framework for persistence Poster 3.17P.7 and ii) introduce more recent improvements in test methods.
- A workshop for academia, industry and regulators is scheduled for September 2020 to further discuss our findings.

[a]http://www.ecetoc.org/taskforce/moving-persistence-p-assessments-into-the-21st-century/

References: 1. Schmidt & Mayer (2015) *Chemosphere* 120, 305. **2.** Schäffer *et al.* (2018) *Environmental Sciences Europe* 31, 21 **3.** Sauer *et al.* (2020) *Regulatory Toxicology and Pharmacology* 111, 104583. **4.** Kowalczyk *et al.* (2015) Ecotoxicology and Environmental Safety, 111, 9. **5.** Latino *et al.* (2017) *Environmental Science: Processes and Impacts*, 3, 449. **6.** Poursat *et al.* (2019) *Critical Reviews in Environmental Science and Technology*, 49, 2220. **7.** ECHA (2017) **8.** EC, 213. EC 283/2013, **9.** Stibany *et al.* (2017), *Chemosphere*, 167, 551. **10.** Martin *et al.* (2017) *Environmental Science and Technology*, 51, 3065. **11.** Honti *et al.* (2016), *Environmental Science and Technology*, 50, 6865. **12.** Achermann *et al.* (2020), *Environmental Science and Technology*, 54, 235. **13.** Poursat *et al.* (2020), *Chemosphere*, 242, 125102. **14.** OECD TG 111, 2004, **15.** OECD TG 316, 2008, **16.** OECD TG 309, 1994, **17.** McLachlan *et al.* (2017), *Environmental Science and Technology,* 51, 4. **18.** Wang *et al.* (2018) *Chemosphere*, 209, 430. **19** OECD TG 501/502, 2007.