

Evaluating the Environmental Persistence of Organic Pollutants from Laboratory Tests, Monitoring and Modelling

R.S. Boethling¹, J.R. Snape², K. Fenner³, P. Howard⁴, T. Madsen⁵ & M. Whelan⁶,

¹Office of Pollution Prevention and Toxics, US EPA, Washington, DC; ²AstraZeneca, Brixham, United Kingdom; ³EAWAG, Dübendorf, Switzerland; ⁴Syracuse Research Corporation, Syracuse, NY; ⁵DHI Water & Environment, Horsholm, Denmark; ⁶Cranfield University, Cranfield, United Kingdom

jason.snape@astrazeneca.com (download from <http://www.brixham-lab.com/>)

Introduction & Aims

Environmental persistence is an important property that can enhance the potential of a chemical substance to exert adverse effects and be transported to remote environments. The persistence of organic compounds is governed by the rates at which they are removed by chemical and biological processes such as biodegradation, hydrolysis, atmospheric oxidation and photolysis. The persistence workgroup focused on evaluating persistence of organic compounds in environmental media (air, water, soil, sediment) in terms of their single-medium degradation half-lives. The findings build upon the results of a previous Pellston workshop, as well as recent guidance developed for other assessment programs. The primary aim was to provide guidance to authors and reviewers of chemical dossiers in government and the private sector. A second objective was to provide a summary of the current state of the science with respect to fate assessment for POPs. Assessing the persistence of chemical substances in the environment is not straightforward. A common misconception is that like many chemical properties, environmental persistence is an inherent property of the substance and can be readily measured. This is not the case. Rates of degradation of a substance in the environment are determined by a combination of substance-specific characteristics and environmental conditions. This presentation considers how persistence can be evaluated based on an assortment of supporting information including the results of laboratory degradation tests, monitoring, multimedia environmental modelling and QSARs. In addition to identifying information that a risk profile should contain, special attention is given to several critical issues including degradation products, bound residues, and treatment of uncertainty and conflicting data as part of a 'weight of evidence' assessment.

Why is Persistence Important?

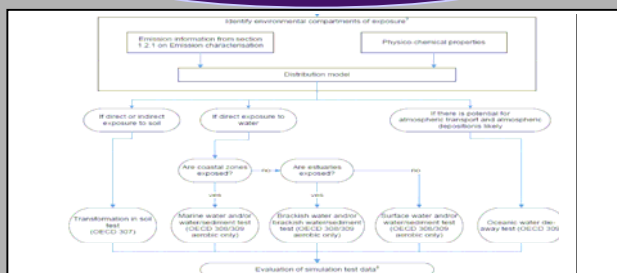


Assumes 10 kg substance released per day for 100 days

Weight of Evidence

- Recommend tiered approach: chemical is first examined at the screening level, then in more depth in the confirmatory phase when certain conditions are met
- Should involve careful analysis of all relevant data and a comparison of the relative merits of studies, to determine where the "weight of evidence" lies
- In principle, results from higher tier studies (simulation tests) have greater environmental relevance. Therefore, they should have more weight
- No single half-life value can adequately describe degradation in the environment or any environmental compartment. Where a range of half-lives has been reported, it is not appropriate to use the slowest or most conservative half-life
- We recommend using a half-life in the higher end of the observed range or a measure such as geometric mean, median or upper 95% confidence limit
- It is generally acceptable to calculate a combined-process rate constant for an environmental compartment from the sum of process-specific first-order rate constants for that compartment. This summed rate constant can be used to derive a half-life for comparison with persistence criteria or input to models
- Multi-media models should be used at the screening level, to identify the types of persistence data that would be most useful; thus testing, if additional testing is needed
- In the confirmatory phase, multi-media models can help in evaluating the relative importance of half-lives from different environmental compartments. This is crucial in determining where the weight of experimental evidence lies

Confirmatory Testing



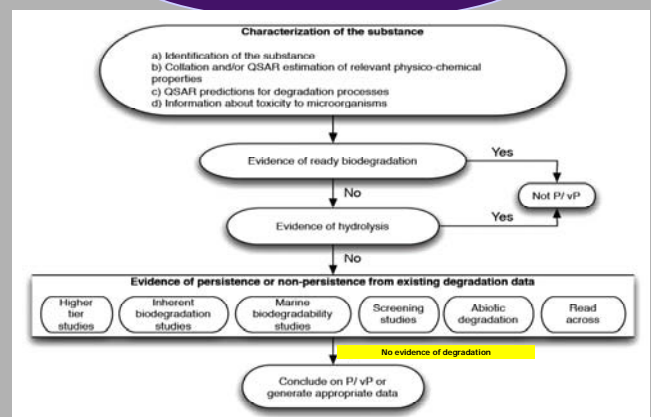
Degradation Products

- Substances that degrade in screening tests can be considered non-persistent. However, it may be necessary to demonstrate that no persistent degradation products are formed
- It should be standard practice to include in the evaluation any degradation product(s) formed at a level of 10% or more relative to the initial mass of parent
- If stable products are formed, it is justified to regulate or control the parent substance based on an assessment of its degradation products

Inconsistency in Persistence

UNEP	UNECE	CEPA	US EPA PBT Profiler	US EPA TSCA ¹	US EPA TSCA ²	EU REACH P	EU REACH vP
Water T _{1/2} >60 d	Water T _{1/2} >60 d	Water T _{1/2} >182 d	Water T _{1/2} >60 d	Aquatic env T _{1/2} >60 d	Aquatic env T _{1/2} >180 d	Fresh water T _{1/2} >40 d	FW or MW T _{1/2} >60 d
Sediment T _{1/2} >180 d	Sediment T _{1/2} >180 d	Sediment T _{1/2} >365 d	Sediment T _{1/2} >60 d			Marine water T _{1/2} >60 d	FW or MW sediment T _{1/2} >180 d
Soil T _{1/2} >180 d	Soil T _{1/2} >180 d	Soil T _{1/2} >182 d	Soil T _{1/2} >60 d			FW Sediment T _{1/2} >120 d	Soil T _{1/2} >180 d
Or sufficient concerns	Or sufficient concerns					MW Sediment T _{1/2} >180 d	
						Soil T _{1/2} >120 d	

Types of 'Screening' Data



Data Quality

- Step 1: determine acceptability of available data
 - Only valid data should be used
 - It should be possible to trace information in risk profiles back to the original sources
- Step 2: evaluate acceptable studies with awareness of the intended use
 - When a conflict arises, assessors should try to understand why
 - Normally, it is not necessary to adjust half-lives for pH and temperature at the screening level
 - It is not sound science to use the Arrhenius equation ("Q10 rule") to adjust biodegradation rate constants to a representative environmental temperature

Dissipation vs Degradation

- Disappearance or dissipation of a compound does not necessarily mean that the compound has been degraded (dissipation includes actual degradation but also physical removal)
- Physical removal includes transfer to other compartments (e.g. volatilization) and formation of non-extractable residues (NER) in soil or sediment
- Physical removal by sorption often observed in soil and sediment studies; e.g. OECD 307/308
- NER: the fraction of original test substance (and metabolites) that is not degraded but also not recovered by extraction of the solid phase. Extraction can be exhaustive but must not substantially change the compounds themselves or the structure of the matrix
- It is important to distinguish between time for 50% dissipation (DT50) and 50% degradation time (DegT50)
- Key issue: are NER bioavailable, or can they become so again over time?