

Supporting Information for Matthies et al. 2016.

The origin and evolution of assessment criteria for persistent, bioaccumulative and toxic (PBT) chemicals and persistent organic pollutants (POPs).

Environmental Science: Processes and Impacts

This supporting information provides additional information for the above paper.

Stockholm Convention

The Stockholm Convention on Persistent Organic Pollutants (POPs), adopted on 22 May 2001,¹ is a global agreement which is designed to protect human health and the environment from the negative effects of persistent organic pollutants (POPs) which can be transported long distances. It is capable of eliminating and/or restricting the production, use, release and unsafe disposal of the substances listed in the SC. POPs are chemical substances that have toxic properties, resist degradation in the environment, bioaccumulate through the food chain and are transported long distances through air, water and migratory species, within and across international boundaries. The SC entered into force in May 2004 and now has over 160 signatory countries. It initially listed twelve chemicals; however, ten more substances have been added to the banned and severely restricted annexes up to 2013. The 22 POPs belong to three groups (some substances are listed twice because they belong in more than one category, e.g., hexachlorobenzene, pentachlorobenzene, polychlorinated biphenyls).

Pesticides used in agricultural applications, for fungus control or for insect control: Aldrin, chlordane, chlordecone, dichlorodiphenyltrichloroethane (DDT), dieldrin, endrin, heptachlor, hexachlorobenzene (HCB), gamma-hexachlorocyclohexane (γ -HCH, lindane) and by-products of lindane [α -hexachlorocyclohexane (α -HCH) and β -hexachlorocyclohexane (β -HCH), mirex, Toxaphene.

Industrial chemicals used in various applications: tetra- and pentabromodiphenyl ethers (PBDEs), hexa- and heptabromodiphenyl ethers (PBDEs), hexabromobiphenyl, hexabromocyclododecane (HBCD), perfluorooctane sulfonic

acid (PFOS), its salts and perfluorooctane sulfonyl fluoride (PFOS-F), pentachlorobenzene (PeCB), polychlorinated biphenyls (PCBs).

Chemicals generated unintentionally as a result of incomplete combustion and/or chemical reactions: hexachlorobenzene (HCB), pentachlorobenzene (PeCB), polychlorinated biphenyls (PCBs) and polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs).

The Persistent Organic Chemicals Review Committee (POPRC) is a subsidiary body of the Conference of the Parties mandated to review proposals from Parties to the Convention to list new substances under the Convention's annexes (A, B and C). Upon the recommendation of the POPRC, the Conference of the Parties listed nine additional substances in May 2009:

Pesticides: chlordane, alpha hexachlorocyclohexane, beta hexachlorocyclohexane, lindane, pentachlorobenzene;

Industrial chemicals: hexabromobiphenyl, hexabromodiphenyl ether and heptabromodiphenyl ether, pentachlorobenzene, perfluorooctane sulfonic acid, its salts and perfluorooctane sulfonyl fluoride, tetrabromodiphenyl ether and pentabromodiphenyl ether; and

By-products: alpha hexachlorocyclohexane, beta hexachlorocyclohexane and pentachlorobenzene.

Upon the recommendation of the POPRC, the Conference of the Parties listed one additional substance in May 2009:

Pesticide: Endosulfan

Five substances have been proposed by Parties and are under review by the POPRC as of October, 2014

Hexabromocyclododecane, short-chained chlorinated paraffins, chlorinated naphthalenes, hexachlorobutadiene, and pentachlorophenol

Protection goals

The protection goals of the SC¹ and UNECE POPs Protocol² are summarized below:

1. *...health concerns, especially in developing countries.... impacts upon women and, through them, upon future generations.*
2. *...Arctic ecosystems and indigenous communities are particularly at risk because of the biomagnification of persistent organic pollutants
...contamination of their traditional foods is a public health issue.*
3. *...protect human health and the environment from the harmful impacts of persistent organic pollutants,...*

The EU's REACH (EC No. 1907/2006 as amended) ³ lists the following protection goals:

- *... with a view to ensuring a high level of protection for human health and the environment.*

The EU regulation for the Placing of Plant Protection Products on the Market (EC No. 1107/2009) ⁴ specifically addresses pesticides and the protection goal, which echoes the SC, is:

1. *...to ensure a high level of protection of both human and animal health and the environment and at the same time to safeguard the competitiveness of Community agriculture. Particular attention should be paid to the protection of vulnerable groups of the population, including pregnant women, infants and children. The precautionary principle should be applied and this Regulation should ensure that industry demonstrates that substances or products produced or placed on the market do not have any harmful effect on human or animal health or any unacceptable effects on the environment.*

The CMP of the Government of Canada uses similar language to describe protection goals for chemicals to be regulated under the Canadian Environmental Protection Act⁵ by identifying goals to not allow releases of chemicals into the environment that:

2. *have or may have an immediate or long-term harmful effect on the environment or its biological diversity;*
3. *constitute or may constitute a danger to the environment on which life depends; or*
4. *constitute or may constitute a danger in Canada to human life or health.*

The word “danger” is not defined in the CEPA, but legal precedent in Canada suggests that “danger” is not an expression of hazard but rather that it is risk in the sense of probability of harm.⁶

Deterministic categorization and probabilistic assessments of POPs and PBTs

In a tiered approach, deterministic categories are normally used in lower tiers. These are usually numerical criteria to which properties of the substance in question are compared. If the property of the substance exceeds the criterion, one action is taken, if not another. Deterministic approaches are useful for initial screening but often become more difficult to conduct when multiple values are available and clear guidance is not provided for selection of the most appropriate and relevant data. This is particularly relevant when the properties of the substance have values that are close to the criterion. The same applies to multiple scenarios of use, release, or exposure.

Deterministic procedures are binary and do not consider likelihood or probability. Although the concept of probability has been used in mathematics since the mid-1600s,⁷ it has only recently been more widely incorporated into the consideration of environmental risks.⁸ Probabilistic approaches allow better characterization of uncertainty and avoid the need for arbitrary uncertainty factors or best guesses when conducting assessments. These approaches have been applied in ecotoxicology⁸ but are only infrequently used in identification or characterization of POPs and PBTs.^{9, 10}

Bioaccumulation

The different and complex patterns involved in the uptake of chemicals from the environment to biota and the transfer in the food web may be defined as follows:

- **Bioconcentration** is the uptake of a chemical as a result of direct exposure to the surrounding medium (e.g., water, air). It is a physical-chemical process involving potential metabolism and equilibrium partitioning between the organism and the environmental medium. It may be quantified through the bioconcentration factor (BCF) that is defined as the ratio of a contaminant

concentration in biota (C_b) to its concentration in the surrounding medium (C_m) at steady state:

$$BCF = C_b/C_m$$

- **Bioaccumulation** is defined as the accumulation of chemicals in the tissue of organisms through any route, including respiration, ingestion, or direct contact and is measured through a bioaccumulation factor (BAF).
- **Biomagnification** is the result of the process of bioaccumulation and biotransfer by which concentrations of chemicals in organisms at one trophic level exceed tissue concentrations in organisms at the next lower trophic level. It is conceptually different from bioconcentration and bioaccumulation in that it involves chemical transport against the thermodynamic gradient from the prey to the predator, i.e. from a low fugacity in the prey to a higher fugacity in the predator ¹¹. It is usually reported as the biomagnification factor (BMF), i.e., a ratio of the concentration in one trophic level to a lower trophic level.
- **Trophic magnification** is characterized by the slope of the regression of lipid-normalized concentration vs. trophic level when biomagnification occurs through a series of prey-predator relationships covering several trophic levels in a food chain (e.g., plankton to polar bears) and is often reported as the trophic magnification factor (TMF).

Abbreviations and acronyms

ARET: Accelerated Reduction/Elimination of Toxics (Canada)

BAF: Bioaccumulation Factor

BCF: Bioconcentration Factor

BMF: Biomagnification Factor

CEC: Commission on Environmental Cooperation

CEG: Criteria Expert Group (of UNEP)

CEPA: Canadian Environmental Protection Act

CLP: Classification, Labelling and Packaging of Substances and Mixtures

CMP: Chemical Management Plan of Environment Canada

CMR: Carcinogenic, Mutagenic, Toxic for Reproduction

CNG: Swedish Committee on New Guidelines on Chemicals Policy

EC: Environment Canada

EC₁₀: Effect Concentration for 10% of the Test Species Population in a Defined Period of Time

EC₅₀: Lethal Concentration for 50% of the Test Species Population in a Defined Period of Time

ECHA: European Chemicals Agency

EFSA: European Food Safety Authority

EL_{0.5}: Elimination Half-life

FIFRA: Federal Insecticide, Fungicide, and Rodenticide Act of the USA

GHS: Globally Harmonized System of classification and labelling of chemicals

GLWQA: Great Lakes Water Quality Agreement

HC: Health Canada

IJC: International Joint Commission

INC: Intergovernmental Negotiating Committee (of UNEP)

K_{OW}: Octanol/Water Partition Coefficient

LC₅₀: Lethal Concentration for 50% of the Test Species Population in a Defined Period of Time

LD₅₀: Lethal Dose for 50% of the Test Species Population in a Defined Period of Time

LRAT: Long Range Atmospheric Transport

LRT(P): Long Rang Transport (Potential)

LRTAP: Long Range Transboundary Air Pollution

NAAEC: North American Agreement on Environmental Cooperation

NOEC: No Observed Effect Concentration

NOEL: No Observed Effect Level

OECD: Organization of Economic Cooperation and Development

OME: Ontario Ministry of the Environment

OMEE: Ontario Ministry of the Environment and Energy

OSPAR: Oslo Paris Convention for the Protection of the Marine Environment

PBT: Persistent, Bioaccumulative and Toxic

PCB: Polychlorinated biphenyls

PCPA: Pest Control Product Act (of Canada)

PCDD/Fs: Polychlorinated dibenzo-*p*-dioxins and -furans

PEC (is it predicted environmental concentration?)

POP: Persistent Organic Pollutant

P_{OV}: Overall persistence

REACH: Registration, Evaluation, Authorisation and Restriction of Chemicals (EU)

SC: Stockholm Convention

SETAC: Society of Environmental Toxicology and Chemistry

SMOC: Sound Management of Chemicals

SOC: Semi-volatile Organic Chemicals

STOT RE: Specific Target Organ Toxicity after Repeated Exposure

TGD: Technical Guidance Document

TMF: Trophic Magnification Factor

TRI: Toxics Release Inventory

TSCA: Toxic Substances Control Act (US)

TSMP: Toxic Substances management Policy

UNECE: United Nations Economic Commission for Europe

UNEP: United Nations Environment Programme

US EPA: United States Environmental Protection Agency

UVCB: Unknown or Variable Composition, or of Biological origin

vB: Very Bioaccumulative

vP: Very Persistent

WoE: Weight of Evidence

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