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Development of a List of Potential POP Candidates for the Stockholm Convention and Refinement of the POP Criteria – Which Strategy is to be Adopted for a Successful Identification of potential POP candidates?

by

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Abstract

The Stockholm Convention on Persistent Organic Pollutants (POPs) regulates highly persistent and toxic chemicals at the global level. Currently, 22 chemicals are regulated as POPs under the Convention. A key question for the future work of the Convention is how many additional POPs are to be expected, given the fact that there are tens of thousands of chemicals on the market globally. The Convention does not lay down any particular obligation concerning addition of chemicals to it but allows any Party to propose new chemicals for inclusion in the Convention. Against this background, the German Federal Environment Agency (UBA) contracted Öko-Institut and ETH Zürich (ICB) to develop a strategy for identifying potential POP candidates and to evaluate the data, methods and procedures that were used in the identification of the 22 existing POPs. Established models for the calculation of relevant POP-properties, information on chemical databases and substance lists, and environmental monitoring programs related to the detection of POPs were assessed and evaluated. Most of the screening studies found in the literature searched for highly persistent and bioaccumulative chemicals, but did not include the long-range transport potential, which is a key criterion under the Stockholm Convention. The strategy is based on the findings of the status-quo evaluation and describes a stepwise approach to evaluating currently used chemicals in order to identify substances with POP characteristics for initial proposals of the Stockholm Convention process. The strategy includes two main steps, a screening of chemicals according to the Annex D criteria of the Stockholm Convention and the evaluation of additional information on uses, adverse effects and regulatory importance of potential POP candidates.

Kurzbeschreibung

Das Stockholmer Übereinkommen über persistente organische Schadstoffe (POPs) regelt hochpersistente und toxische Chemikalien auf globaler Ebene. Derzeit fallen 22 Chemikalien als POPs unter das Übereinkommen. Angesichts der Tatsache, dass sich weltweit Zehntausende von Chemikalien auf dem Markt befinden, spielt die Frage, mit wie vielen zusätzlichen POPs zu rechnen ist, eine zentrale Rolle für die zukünftige Arbeit des Übereinkommens. Das Übereinkommen ermöglicht jeder Vertragspartei, neue Chemikalien zur Aufnahme in die Stoffliste des Übereinkommens vorzuschlagen, enthält jedoch keine besondere Verpflichtung in Bezug auf eine Hinzufügung weiterer Chemikalien. Vor diesem Hintergrund beauftragte das deutsche Umweltbundesamt (UBA) das Öko-Institut und die ETH Zürich (ICB) mit der Entwicklung einer Strategie zur Identifizierung potenzieller POP-Kandidaten sowie der Evaluierung von Daten, Methoden und Verfahren, die zur Identifizierung der vorhandenen 22 POPs verwendet wurden. In diesem Zusammenhang wurden etablierte Konzepte zur Ermittlung der relevanten POP-Eigenschaften, Informationen über Chemie-Datenbanken und Stofflisten sowie Umweltmonitoringprogramme zur Erfassung von POPs geprüft und ausgewertet. Die meisten Screening-Untersuchungen, die im Rahmen der Literaturrecherche zu hochpersistenten und bioakkumulierbaren Chemikalien gefunden wurden, enthielten jedoch keine Informationen über das Potenzial zum weiträumigen Transport der Chemikalie in der Umwelt, welches im Stockholmer Übereinkommen ein wichtiges Kriterium darstellt. Die gewählte Strategie basiert auf den Ergebnissen der Auswertung des gegenwärtigen Zustands.

Sie enthält einen stufenweisen Ansatz zur Analyse der aktuell verwendeten Chemikalien sowie zur Identifizierung von Stoffen mit POP-Merkmalen im Hinblick auf die Unterbreitung erster Vorschläge im Rahmen des Aufnahmeverfahrens des Stockholmer Übereinkommens. Die Strategie umfasst zwei Hauptschritte: zum einen eine Überprüfung der Chemikalien im Hinblick auf die in Anhang D des Stockholmer Übereinkommens aufgeführten Kriterien und zum anderen die Auswertung weiterer Informationen über Einsatz, negative Auswirkungen und rechtliche Bedeutung der potenziellen POP-Kandidaten.

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List of abbreviations

AMAP	Arctic Monitoring and Assessment Programme
B	bioaccumulative
BAF	bioaccumulation factor
BCF	bioconcentration factor
CAS	Chemical Abstracts Service
ChV	Chronic value, a toxicity estimate of ECOSAR model
CMR	carcinogenity, mutagenity or reproductive effects
COP	Conference of the Parties
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECHA	European Chemicals Agency
ECOSAR	Ecological Structure-Activity Relationship model
EDC	endocrine disrupting chemicals
ELPOS	Environmental Long-Range transport and Persistence of Organic Substances model
EMEP	European Monitoring and Evaluation Programme
GMP	global monitoring programme for persistent organic pollutants
HPV	high production volume
HPVC	high production volume chemical
IPEN	International POPs Elimination Network
LPVC	low production volume chemical
LRT	long-range transport
LRTP	long-range transport potential

LOEC/LOEL	lowest observed effect concentration/level
Log Kaw	logarithim of the air-water partition coefficient
LogD	logarithm of the octanol-water distribution coefficient
LogP or log Kow	logarithm of the octanol-water partition coefficient log octanol-water partition coefficient
NOEC/NOEL	no observed effect concentration/level
OECD	Organisation for Economic Cooperation and Development
P	persistent
RBT	readybiodegradability tests
REACH	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)
P_{ov}	overall environmental persistence
PBT	persistent, bioaccumulative and toxic
PFC	perfluorochemicals
PUF	polyurethane foam plug
POP	persistentorganic pollutant
POPRC	Persistent Organic Pollutants Review Committee
QSAR	Quantitative Structure Activity Relationships
OSPAR	Oslo and Paris Conventions for the Protection of the Marine Environment of the North-East Atlantic
SETAC	Society of Environmental Toxicology and Chemistry
SMILES	Simplfied Molecular Input Line Entry System
SVHC	substances of very high concern
T	toxic
TMAP	Trilateral Monitoring and Assessment Program
TMF	trophic magnification factor
UBA	Umweltbundesamt (Federal Environment Agency), Dessau-Roßlau, Germany
UNECE	United Nations Economic Commission for Europe
UNEP	United Nations Environment Programme
UNIDO	United Nations Industrial Development Organization
US EPA	United States Environmental Protection Agency
vPvB	very persistent and very bioaccumulative

1 Background and objectives

1.1 Background

Persistent organic pollutants (POPs) are chemical substances that do not degrade in the environment, that bioaccumulate and have harmful effects on human health and the environment; furthermore, POPs have the potential for long-range transport. Once released, they spread around the globe via air and water, and also through the food chain, which means that they may have a toxic effect on man and the environment far from the place in which they were released. Thus, POPs pose a global risk to regions that do not generate any emissions themselves, particularly to Arctic areas and mountain regions, where a deposition of airborne POPs is facilitated by cold condensation.

The Stockholm Convention (hereinafter called Convention) on Persistent Organic Pollutants[1] is an international treaty devoted to POPs in order to protect human health and the environment from chemicals that remain intact in the environment for long periods, become widely distributed geographically, accumulate in the fatty tissue of humans and animals, and have adverse effects to human health or to the environment. The Convention requires all parties to eliminate or reduce releases of POPs. With 177 Parties[2], the Stockholm Convention is a unique global effort for the protection of human health and the environment beyond national interests.

When the Convention was adopted in 2001, 12 substances were listed in its Annexes. In 2009, nine more POPs were included in the Convention. At the last Conference of the Parties (COP 5) in April 2010, endosulfan, on a proposal of the EU, was included in the convention, thus being the 22nd substance listed there. In addition, five additional substances are currently under review by the POP Review Committee (POPRC) of the Convention. Currently there are no new proposals. These POPs are listed in Annex A (elimination; 18 chemicals), B (restriction; two chemicals), or C (unintentional production; five chemicals); three chemicals are listed in both Annex A and C.

Any Party may submit a proposal for listing a new chemical in the Convention. The Party has to prepare a dossier containing chemical screening criteria, defined in the Annex D of the convention (UNEP 2009). Before a chemical can be regulated under the Convention, it is assessed by the POP Review Committee (POPRC). A key question for the future work under the Stockholm Convention is how many additional POPs are to be expected, given the fact that there are tens of thousands of chemicals on the market globally.

Against this background, the German Federal Environment Agency (UBA) has contracted Öko-Institut and ETH Zürich to develop a strategy for identifying POP candidates including the evaluation of the status-quo with regard to current methods to evaluate POP-properties of chemicals. Subsequent to this work potential POP proposal candidates shall be named. The project is designated to enable Germany to support the EU in proposing new possible

[1] http://chm.pops.int/Portals/0/download.aspx?d=UNEP-POPS-COP-CONVTEXT.En.pdf, last accessed 13.1.2012

[2] http://chm.pops.int/portals/0/amMap/status_of_ratifications.html, last accessed 16.3.2012

candidates for POPs to the Convention and to actively take part in the assessment procedure for the nomination of new POPs.

1.2 Objectives of the study

The project is divided into three work packages: At first, an analysis of the current approaches to identifying POP candidates was performed, secondly a strategy for POP-candidate identification and thirdly a new possible POP-candidate list.

As part of the first work package a comprehensive literature review was conducted. Moreover, well-established models for the calculation of relevant POP-properties, information on chemical databases and substance lists, and environmental monitoring programs related to the detection of POPs have been assessed and evaluated

The report is structured as a top-down report, beginning with a general overview of the situation and of the criteria and procedures for adding new chemicals to the Convention in chapter 2, which introduces definitions and general issues. Furthermore, we consider the national, regional and international frameworks regulating of POPs, persistent, bioaccumulative and toxic (PBT) chemicals as well as of very persistent, very bioaccumulative (vPvB) substances.

In chapter 3 we put special emphasis on the methods for assessing the POP screening criteria persistence, bioaccumulation, toxicity and long-range transport. Chapter 4 provides the most widely-used models to assess the same criteria, and chapter 5 summarizes the most relevant monitoring programs with a view to PBT or POP substances. The benefits and limitations of different methods, models and monitoring programs are discussed in detail in a summary to each chapter.

Chapter 6 provides an overview of different existing approaches and strategies for the evaluation of POPs or PBTs. The methodological approaches and other information sources of the current projects and work on the identification of POPs are assessed and compared. In comparison of different approaches we examine, inter alia, which criteria / variables are used to identify substances with POP or PBT properties. All different approaches and information sources are finally listed in an overview MS Excel file (see section 1.3).

A second aspect presented in chapter 6 is the state of existing scientific screening lists of POP, PBT and vPvB substances. The lists were analysed in terms of the completeness of substance identification information and the registration dates.

In addition, an ex-post analysis of the decision-making process behind the inclusion of the new POPs in the Stockholm Convention was undertaken to reflect and understand the decision-making process undertaken to list POPs in Annex A, Annex B, and/or Annex C. The results are presented in chapter 7.

The results from the different steps from chapter 3 to 7 are evaluated concerning the suitability of different approaches, methods, screening models and monitoring programs so that their advantages and disadvantages can be compared.

Up to now no coordinated procedure for identifying new POP proposals that fall into the scope of the Stockholm Convention has been defined. Therefore, a methodical approach for the identification of potential POP candidates has been developed as part of the research project. With this method we hope to make a contribution for an increased use of these data for

current tasks under the Stockholm Convention and for a further harmonisation, interfaces and synergies between the chemical legislations. Chapter 9 summarises the developed approach.

Finally, in chapter 10, we compile exemplarily for twelve identified potential POP candidates information on the possible POP candidates in "compound profiles". These profiles present the substances by the name and CAS number, the properties of these substances as regards persistence, bioaccumulation, long-range transport and toxicity (adverse effects) and they also provide the criteria set which were described in the strategy in chapter 9.

1.3 Reference management

An MS Excel file (“Register Sheet”) was developed to compile the most relevant information from the studied literature. With this, structured data collection was possible and it was ensured that all information relevant for the later evaluation of the approaches was available at one access point. The resulting “Register Sheet” served as main working basis for the subsequent work packages of this project.

The following categorisation of the information assessed was set up as single excel sheets. Each reference was then allocated to one of the categories (single excel sheets) with an own entry.

- MS: Methods to detect relevant parameters to P, B, T and LRT
- A: Approaches and strategies for identifying POP candidates
- SL: Substance lists
- M: Models
- MP: Monitoring programs
- OP: Other scientific publications
- R: List of references as displayed by reference manager; this reference list does not include the substance lists (SL) and the monitoring programmes (MP) as they refer to internet links and webpages
- Abbreviations in the excel file.

More detailed information regarding the excel sheets of each categorisation is available as a separate Excel-file (“Register Sheet”).

A comprehensive list of abbreviations within this report can be found above (page VIII); a reference list in chapter 13, page 96 ff.).

1.4 Terms and definitions related to “POPs”

Distinction has to be made to the broad meaning of the terms “new POPs” and “POP candidates”. These general terms have been used in several studies and publications about POPs. In the context of this project we will use the following terms and definitions of POPs as commonly used under the Stockholm Convention:

- **New POPs** are the ten additional POPs that were listed after the initial twelve POPs (“dirty dozen”) on the Annexes of the Stockholm Convention
- **POP candidates** are currently under review by the POP Review Committee
- **POP proposals** are chemicals which have been proposed for listing under the Convention by a party. As soon as the proposal is being reviewed under the Convention it becomes a POP candidate.

- In this report we will identify chemical substances that have a potential to fulfil the POP characteristics according to the Convention. In subsequent chapters we will call these newly identified substances "p**otential POP candidates"**.

2 Legal framework

Two international agreements are devoted to POPs: The Stockholm Convention and the Protocol on POPs to the Convention on Long-Range Transboundary Air Pollution (CLRTAP) (hereinafter POP Protocol). The Stockholm Convention and the POP Protocol basically tackle the same substances by setting the same criteria for POP substances (see Table 1). The agreements differ with respect to their geographic coverage and some of the POPs listed (e.g. Endosulfan). The POP Protocol is a regional agreement of the United Nations Economic Commission for Europe (UNECE), which includes countries of Europe, North America and Central Asia. The Stockholm Convention on the other hand is a global agreement with members additionally from Africa, South America, Southern Asia and Oceania.

The following sections will describe the procedures of the two international agreements for adding new chemicals in more detail.

2.1 Procedures for adding new chemicals to the Stockholm Convention

Article 8 of the Convention describes the decision-making process for the listing of chemicals in Annex A (Elimination), Annex B (Restriction) or Annex C (Unintentional Production) of the Convention[3]. The information that is required for listing of chemicals in the Annexes A, B and C of the Convention are specified in Annex D (Information Requirements and Screening Criteria), Annex E (Information Requirements for the Risk Profile) and F (Information on Socio-Economic Considerations) of the Stockholm Convention.

The POPRC is the subsidiary body to the Convention established for reviewing chemicals proposed for listing in Annex A, B or C. The POPRC consists of 31 government-designated experts from Parties appointed by the Conference of the Parties (COP)[4]. Additionally government and non-governmental Observers, such as NGOs, invited experts and government representatives not currently holding a POPRC mandate, are allowed to attend the meetings of the POPRC.

The procedure for adding new chemicals to the Convention applies a five-phase approach for an inclusion:

In a f**irst phase**, a signatory State of the Stockholm Convention (in the following called "party") presents a proposal (Article 8, paragraph 1 and Annex D) for inclusion of a chemical in the Convention and submits its proposal to the Secretariat. The Secretariat verifies the proposal and if it is in accordance with Annex D it shall forward the proposal to the POPRC.

[3] http://chm.pops.int/Portals/0/download.aspx?d=UNEP-POPS-COP-CONVTEXT.En.pdf, last accessed 18.12.2012, Annex D on page 53; Annex E on page 55 and Annex F on page 57

[4] http://chm.pops.int/Convention/ConferenceofthePartiesCOP/AbouttheCOP/tabid/578/Default.aspx, last accessed 27.9.2012

The four screening criteria relate to persistence (P), bioaccumulation (B), the potential for long-range environmental transport (LRTP) of the chemical and its adverse effects (toxicity or eco-toxicity data; T). Table 1 shows the criteria and thresholds for the screening-criteria on the basis of Annex D of the Stockholm Convention.

As mentioned in Table 1, not only numerical thresholds values but also the non-numerical criteria are mentioned as possible evidence for P, B, LRT and T. Numerical criteria are defined for P, B and LRT but no such value is given for T. The non-numerical evidence is considered as important if not even more important (for instance monitoring data for LRT) than fulfilling of the numerical criteria. Furthermore, the Stockholm Convention emphasizes the precautionary principle: Lack of full scientific certainty is not a reason for preventing a proposal from proceeding through the screening and risk assessment phases.

Table 1 P, B, T and LRT criteria according the Stockholm Convention Annex D

Properties	Criteria and Thresholds
Persistence (P)	half-life in water > 2 months
	half-life in sediments > 6 months
	half-life in soils > 6 months
	• Evidence that the chemical is otherwise sufficiently persistent to justify its consideration within the scope of the Convention
Bioaccumulation (B)	aquatic BCF or BAF > 5000
	in the absence of such data, log Kow > 5
	• Evidence that a chemical presents other reasons for concern, such as high bio-accumulation in other species, high toxicity or ecotoxicity; or • monitoring data in biota indicating that the bio-accumulation potential of the chemical is sufficient to justify its consideration within the scope of this Convention
Toxicity (adverse effects) (T)	• Evidence of adverse effects to human health or to the environment that justifies consideration of the chemical within the scope of the Convention; or • Toxicity or ecotoxicity data that indicate the potential for damage to human health or to the environment
Long-range transport (LRT)	half-life in air > 2 days
	• Measured levels of the chemical in locations distant from the sources of its release that are of potential concern • Monitoring data showing that long-range environmental transport of the chemical, with the potential for transfer to a receiving environment, may have occurred via air, water or migratory species; or • Environmental fate properties and/or model results that demonstrate that the chemical has a potential for long-range environmental transport through air, water or migratory species, with the potential for transfer to a receiving environment in locations distant from the sources of its release. For a chemical that migrates significantly through the air, its half-life in air should be greater than two days

(Source: UNEP 2009)

In the s**econd phase** the POPRC examines the proposal and decides if the screening criteria are fulfilled for the proposed substance. If Annex D criteria are not fulfilled, the Secretariat informs the Parties and sets the proposal aside, unless a Party resubmits the proposal for additional consideration.

In the t**hird phase**, the POPRC brings the application and its evaluation to the attention of all Contracting Parties and invites them to provide the information concerning a risk profile, which is referred to in Annex E. Annex E requires information on

- production data and uses, releases into the environment,
- hazard assessment for the endpoint or endpoints of concern, including a consideration of toxicological interactions involving multiple chemicals,
- environmental fate,
- monitoring data,
- exposure in local areas and, in particular, as a result of long-range environmental transport,
- national and international risk evaluations, assessments or profiles and labelling information and hazard classifications, as available; and
- status of the chemical under international conventions.

Taking into account any relevant additional information received from the Parties, the POPRC prepares a draft risk profile and sends this draft once again to the Parties and observers for comments. After receiving the technical comments, the POPRC completes the Risk Profile.

Subsequently, the POPRC takes a decision on whether the chemical will probably lead to s**ignificant adverse effects on human health and/or the environment as a result of long-range environmental transport, such that global action is warranted**. This introduction text to Annex E takes up the objective of the Convention that is to protect human health and the environment from persistent organic pollutants (UNEP 2009, Article 1). However, this decision is not specified further by values, indicators, or similar. It is thus leading to discussion and comprises normative aspects.

If Annex E criteria are not fulfilled, the Secretariat informs the Parties and sets the proposal aside, unless the Conference of Party (COP) decides otherwise after collecting additional information

In the f**ourth phase** all Parties and observers can submit additional information in accordance with Annex F, relating to socio-economic considerations and implications of a ban on the substance. Subsequently the POPRC prepares a risk management evaluation (or also called social-economic analysis) that includes an analysis of possible control measures for the chemical in accordance with Annex F and recommends whether the substance should be included in Annex A, B and/or C.

In the f**inal phase**, the responsible body is the Conference of the Parties (COP), which decides on whether a chemical will be included in the Convention and specifies its related control measures in Annex A, B and/or C.

The decision-making process takes several years. At the minimum, three years are needed from introduction of the proposal to listing a chemical. The following Figure 1 displays the procedure for the inclusion of new substances according to Article 8, paragraph 1-9 of the Convention.

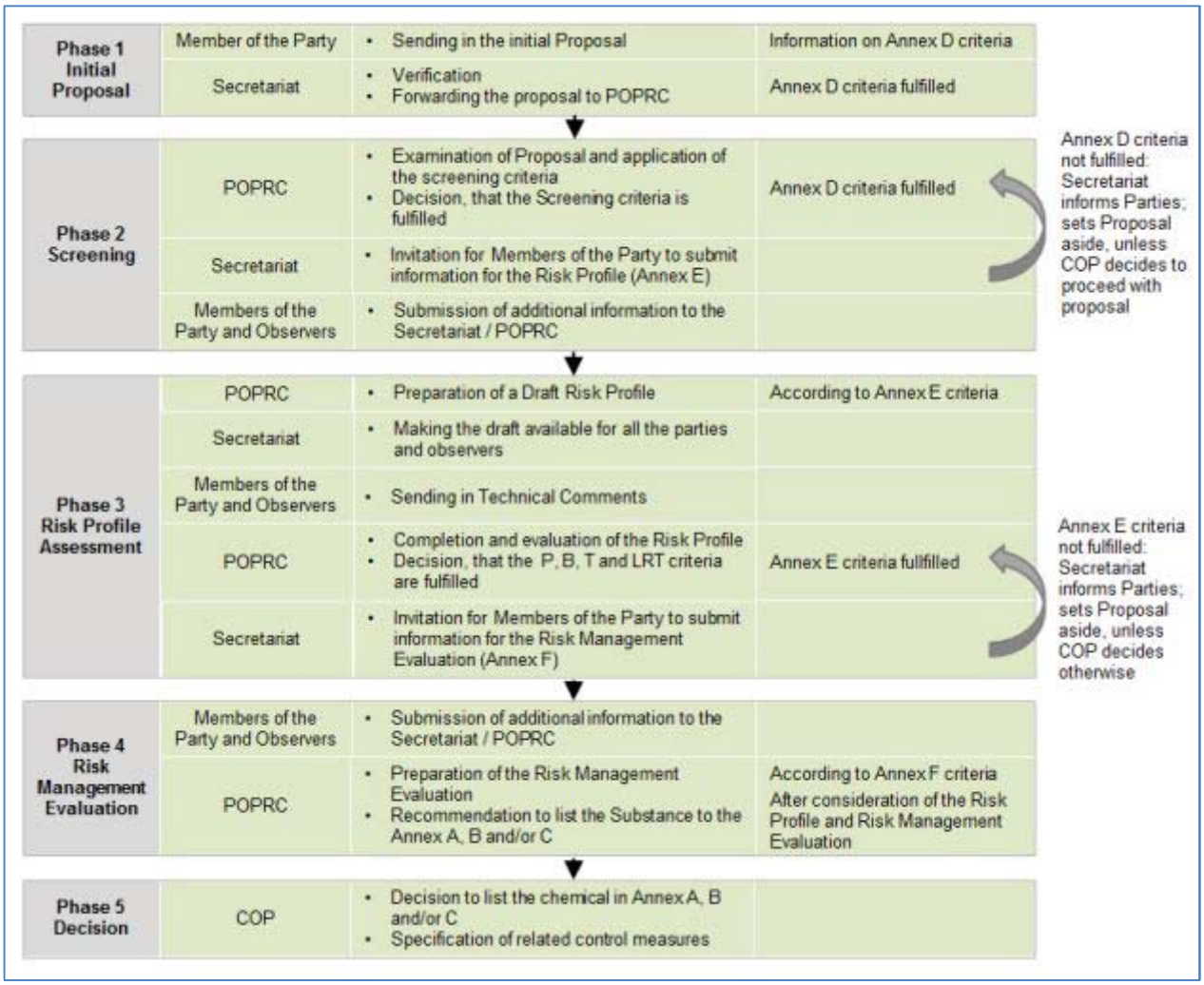

Figure 1 Procedure for the inclusion of new POPs according to Article 8 of the Convention (Source: Öko-Institut / ETH Zürich)

2.2 Procedures for adding new chemicals to the POP Protocol

The decision-making process for adding new chemicals to the POP Protocol demands fewer steps than the procedure under the Stockholm Convention.

The information to be submitted and the procedure for adding substances to annexes I, II or III to the POP Protocol are described in the Executive Body Decision 1998/2[5]: A proposal for adding new substances to the annexes shall provide the Executive Body with a risk profile that contains information on the substance characteristics: potential for long-range transboundary atmospheric transport, toxicity, persistence and bioaccumulation. Data about production, uses, substitutes, socio-economic factors etc. is required later in the process as well.

[5] http://www.unece.org/fileadmin/DAM/env/documents/2000/ece/eb/ece%20eb%20air.60.e.pdf, last accessed 18.4.2012

On the basis of this risk profile, the Executive Body decides by consensus how many (one or more) technical reviews of the proposal are conducted. These technical reviews shall evaluate, inter alia:

(a) The monitoring or equivalent scientific information suggesting long-range transboundary atmospheric transport; and

(b) Whether sufficient information exists to suggest that the substance is likely to have significant adverse human health and/or environmental effects as a result of its long-range transboundary atmospheric transport; and

(c) A list of the sources of the substance in the atmosphere, including the use of products estimates of the total emissions from these sources and the methodologies used; and

(d) Whether measures exist to reduce the risk of adverse effects on human health and/or the environment as a result of its long-range transboundary atmospheric transport, and whether they are technically feasible, as well as their associated effects and costs.

As in the Stockholm Convention, the conclusion has to be reached that the substance is likely to have significant adverse human health and/or environmental effects as a result of its long-range transboundary atmospheric transport. However, the Parties under the POP Protocol complete their evaluation of the proposal taking into account the objective of the protocol set out in article 2. The objective of the POP Protocol is to control, reduce or eliminate discharges, emissions and losses of persistent organic pollutants (Article 2). This objective of the POP Protocol is unambiguous and easier to interpret than the objective of the Stockholm Convention.

2.3 Other legal frameworks regulating PBT substances

National, regional and international bodies are developing ways to reduce the risk posed by chemicals substances of different concern, such as e.g. PBT or vPvB substances.

In order to improve environmental and public health and safety, some regulations have set up criteria for hazardous substances that cover persistence, bioaccumulation and toxicity in order to assess the potential risk to human health and the environment from the numerous chemicals industrially used and/or new on the market. The national scope usually does not consider the long-range transport potential of the substances (see Table 2).

The national regulations around the world differ in their approaches to the risk management of chemicals in the way they make reference to the precautionary principle, in the application of voluntary versus mandatory policy tools and in the way to generate the information for the assessments (burden of proof)[6]. It is beyond of the scope of this study to present these different approaches of the national and regional regulations.

In the following, the criteria of different frameworks for defining the corresponding hazardous chemicals are shown in Table 2:

[6] For a comparison of the US and European chemical legislation, see e.g. http://www.parl.gc.ca/Content/LOP/ResearchPublications/prb0629-e.pdf, accessed 18.4.2012

Table 2 Overview of POP and PBT/vPvB-criteria in different legislations

Definition by	Persistence (P)	Bio-accumulation (B)	Toxicity (T)	Long-range transport (LRT)
International agreements				
Stockholm Convention	Half-life in Water > 2 months, Soil and sediments > 6 months	BCF > 5 000 or log K_{ow} > 5 Other reasons of concern Monitoring data	Evidence of adverse effects (Eco-)toxicity data	Monitoring data from remote areas Half-life in air > 2 days
UNECE POP Protocol[7]	Half-life in Water >2 months or Soil and sediments > 6 months	BCF or BAF > 5 000 or log K_{ow} > 5	Potential to adversely affect human health or environment	Vapor pressure < 1000 Pa and half-life in air > 2 days or monitoring data in remote area
Regional agreement / regulation				
OSPAR[8] Criteria for PBT-Substances	Not readily biodegradable or half-life in water > 50 d	log Kow => 4 or => BCF 500	T_{aq} L(E)C50 =< 1 mg/L and long-term NOEC =< 0.1 mg/L or mammalian	n.a.
OSPAR additional criteria for hazardous substances	n.a.	n.a.	$T_{mammalian}$: CMR or chronic toxicity	n.a.
REACH: PBT	Half-life in Fresh- or estuarine water > 40 days, Marine water > 60 days, Marine sediment > 180 days, Fresh- or estuarine sediment or soil > 120 days	BCF > 2 000 L/kg	NOEC (long-term) < 0.01 mg/L for marine or freshwater organisms, or Classification as carcinogenic (category 1 or 2), mutagenic (category 1 or 2), or toxic for reproduction (category 1, 2 or 3), or Other evidence of chronic toxicity (see Classifications)	n.a.

[7] Under the Convention on Long-Range Transboundary Air Pollution (CLRTAP); http://www.unece.org/env/lrtap/pops_h1.html, last accessed 18.04.2012

[8] http://www.ospar.org, last accessed 26.9.2012

Definition by	Persistence (P)	Bio-accumulation (B)	Toxicity (T)	Long-range transport (LRT)
REACH: vPvB	Half-life in Marine, fresh- or estuarine water > 60 days, Marine, fresh- or estuarine sediment or soil > 180 days	BCF > 5 000 L/kg	n.a.	n.a.
National regulations				
US EPA PBT Chemical Program[9]	Half-life in soil, sediment and water: >2 months very persistent > 6 months Half-life in air: > 2 days -> very persistent	BCF > = 1,000 -> b BCF > 5,000 -> very b	Fish ChV[10] (mg/l) > 10 mg/l -> low concern 0.1 - 10 mg/l -> moderate concern < 0.1 mg/l -> high concern	n.a.
Canada Toxic Substances Management Policy[11]	Half life In air > 2 days in water >6 months or in sediment > 12 months or in soils > 6 months or subject to transport to remote areas	BAF/BCF => 5 000 or log Kow >5	acute and chronic toxicity to aquatic species (algae, invertebrates, fish): LC50(EC50) ✣ 1 mg/L NOEC ✣ 0.1 mg/L	The persistence criterion covers the half-life in air > 2 days, which is the criterion of long-range transport under the Stockholm Convention.
Japan Class I Specified Chemicals[12]	not likely to undergo a chemical transformation through natural processes (No precise criteria)	Bioacumulative (No precise criteria)	posing a risk of impairing human health if ingested continuously; posing a risk of interfering with the inhabitation and/or growth of animals at the top of the food chain, if ingested continuously	n.a.

n.a. = not applicable

[9] http://www.pbtprofiler.net/criteria.asp, accessed 18.4.2012

[10] Chronic value

[11] http://www.ec.gc.ca/Publications/2EE9E1E8-1DC4-4886-93B1-D67A085FBAA3/Toxic-Substances-Management-Policy.pdf; last accessed 26.4.2012, http://www.ec.gc.ca/substances/ese/eng/dsl/cat_criteria_process.cfm , accessed 18.4.2012

[12] Japan Chemical Substances Control Law ("Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc."): http://www.env.go.jp/en/laws/chemi/cscl/CSCL_law.pdf , accessed 18.4.2012

Table 2 shows that the thresholds related to P, B and T characteristics differ between the legislations (regulations, conventions). This means that a chemical may meet criteria in one geographic region, but fail to meet those criteria in another region. For example, several legislations use 60 days as the half-life threshold for persistence in water whereas half-life thresholds range from 60 to 360 days for sediment (see Table 2); for bioaccumulation a BCF range from 500 to 5000 is found. This observation has significant implications for the assessment of POPs and PBTs because substances that appear to qualify for action or listing under one legislation may not meet the criteria of another.

However, the persistence and bioaccumulation criteria of the Stockholm Convention are in the same range as the threshold values for vPvB-Substances under REACH and for PBT substances defined by the US EPA. The table above also demonstrates that the POP criteria as set up by the Convention and by the UNECE POP Protocol are the only frameworks that cover the criterion of long-range transport. The national regulations have mostly set up criteria for hazardous substances that cover persistence, bioaccumulation and toxicity. The criterion of long-range transport is not mentioned directly in any of the national regulations. However, the US EPA PBT Chemical Program as well as the Canadian Toxic Substances Management Policy includes half-life values in air for persistence, which is an indicator for long-range transport (but only as a criterion for “very persistent”).

The REACH regulation is dedicated to assessing and controlling chemicals in use. However, REACH can also be used to prevent the production and use of new chemicals exhibiting similar characteristics as POPs, i.e. PBTs and vPvBs as well as substances of equivalent concern by demanding an authorisation for every use. The Article 3(3) of the Stockholm Convention states that each party of the convention should aim to regulate and prevent the use of chemicals with POP characteristics with help of the existing national regulations. Within the EU this is implemented by the REACH Regulation (1907/2006/EC), the Regulation 1107/2009 for plant protection products and Regulation 528/2012 for biocidal products. Hence, if the authorities find an implication of POP-like characteristics, the Convention should be informed. The problem of using REACH as an information source for the Convention is nevertheless that the LRTP is not assessed under REACH. Also, depending on the tonnage trigger for registration, the data submitted to the authorities might not necessarily be sufficient for a POP assessment according to the Stockholm convention thresholds (lower P and B thresholds in REACH, see Table 2). Basically, the ECHA has a right to request further information from companies if it suspects that a substance might exhibit POP-like characteristics. Regulation (EC) No 1107/2009 concerning the placing of plant protection products on the market (PPP Regulation) prevents chemicals exhibiting POP characteristics from being used in plant protection products. Regulation (EC) No 528/2012 concerning the placing on the market and use of biocidal products (BPR Regulation) prevents chemicals exhibiting POP characteristics from being used in biocidal products. This is achieved by the provisions according to which an active substance cannot be authorised if it meets the criteria for PBT or vPvB according to Annex XIII to REACH Regulation. In addition, a substance shall be approved as a candidate for substitution if it meets two of the PBT criteria.

3 Methods for P, B, T and LRT assessment

In this chapter, methods for examining the screening criteria persistence, bioaccumulation, toxicity and long-range transport in context of the Annexes D and E of the Convention are introduced. Furthermore their advantages and limitations as well as measurement uncertainties are discussed. Later a detailed description of modelling (see chapter 4) and monitoring (see chapter 5) efforts as specific methods are given and discussed with regard to their benefits for completing the screening criteria.

The discussed methods, their key characteristics and sources for additional information are presented on the MS Excel file category sheet “MS”.

3.1 Persistence

Persistence describes the time that a substance remains in the environment. It can be described either for a specific environmental compartment (water, soil, sediment, air etc.) or for the environment as a whole (overall persistence, P_{ov}). Persistence of a compound is typically expressed as degradation half-lives or degradation rate constants. The compartment specific persistence is a sum of several degradation processes, and in an open system, loss processes due to transport from one environmental compartment to another.

The degradation processes are either abiotic chemical processes, or biologically mediated. The most important abiotic processes are photodegradation, hydrolysis and redox-reactions. Biodegradation is typically the main pathway in soils and sediments to mineralize xenobiotic organic compound, which makes it an important degradation process affecting the persistence of POPs. All degradation processes initially lead to primary degradation, i.e. transformation of the parent chemical to other (organic) transformation products (Pavan and Worth 2006, van Leeuwen and Vermeire 2007).

Transport processes from one environmental compartment to another are often expressed in terms of partition coefficients. These coefficients describe which fraction of the compound remains in which compartment under the condition of thermodynamic equilibrium. Alternatively the transport between compartments can be expressed in terms of volatility or solubility. In the water phase and in air, chemicals can adsorb to particles, which may further leave the original environmental compartment through sedimentation or deposition. Such transport processes can be described by the combination of partitioning to the solid phase and sedimentation rate constants. In the case of water, this means that the half-life of the compound is affected for example by photodegradation, biotransformation, hydrolysis, volatilization and sedimentation (Scheringer 2009a, van Leeuwen and Vermeire 2007). Other than compartment-specific half-lives, the P_{ov} accounts for the transport processes from one environmental media to another and the resulting effect on degradation in the receiving media.

The persistence thresholds are clearly defined in the Convention and in the POPs Protocol. However, in contrast to the European Chemicals Agency (ECHA) the Stockholm Convention provides no guidance on how to assess persistence[13]. The guidance by ECHA (2011) can be used

[13] This shall also apply for T, B and LRT

for POP assessment as well, with consideration of different threshold values. If the vP criteria is fulfilled according to REACH, the substance can also be considered persistent according to the Convention,

If any of the defined media-specific half-lives exceeds the thresholds set by the convention, a substance is classified as persistent. Further the convention adds that “other sufficient criteria” can also be used as a proof of persistence (see Table 1). This remark enables the use of overall persistence as an assessment criterion as well, even though it is not explicitly mentioned in the convention. P_{ov} analysis of the chemicals has been cited in several risk profiles of “new” POPs.

In the calculation of the Pov not only the degradation half-lives, but also the transport processes in the environment are taken into account. As a result, a substance that has low half-lives in all but one compartment (e.g. water) but is rapidly transported away from this compartment (e.g. through volatilisation), has a fairly low Pov, even though persistence in one compartment is high. High Pov on the other hand can be observed e.g. when high residence and degradation half-lives coincide in one compartment. The interplay between the compartments plays a key role in Pov assessment. As the persistence criteria of the convention do not mention the effect of transport processes, the main focus in this chapter is on the determination of the compartment-specific half-lives.

Even though the persistence criterion of the convention is clearly defined, the assessment of the persistence of chemical substances is not straightforward. This has mainly to do with the fact that the persistence is not a truly inherent property of a substance, but dependent on both, the chemical properties of the substance itself and environmental factors. Due to interplay of several environmental factors (pH, temperature, ability of microbial cultures to degrade specific chemicals) the experimental determination of environmental half-lives is challenging, and leads to large variability in the obtained data (Boethling 2009). Differences of up to three orders of magnitude have been observed for biodegradation half-lives of well-studied substances (Aronson et al. 2006). Standard test methods for determination of degradation processes are not available for all processes (Boethling et al. 2009). Interpretation of the measured half-lives in the context of real environment, with varying temperatures, redox conditions etc. represent a further challenge.

The determination of compartment-specific half-lives can be done in two ways. Either results from dissipation studies, which evaluate the degradation and removal of a substance from one specific compartment as a whole, can be used. Such simulation studies yield a degradation rate constant for a specific environmental compartment, but the results might be difficult to interpret or evaluate, as specific processes (biodegradation, hydrolysis, and volatilization) are not considered separately. The other method is to sum up the results from separately defined degradation processes. In this case, care should be taken that the measurement results do not overlap, e.g. that abiotic control is subtracted from biodegradation half-life, when it is summed up together with hydrolysis and photodegradation data (Boethling et al. 2009).

In soil, sediments and water biodegradation is often the most important degradation process (Pavan and Worth 2008, Aronson et al. 2006). Most of the biodegradation data is obtained with ready biodegradability tests (RBT), which indicate whether a substance is readily biodegradable or not. The measurement is done in stringent conditions with the tested chemical being the only carbon source for the microbial culture, the biomass density being relatively small and test duration 28 days. The analysis is done by measuring indirect indicators of biodegradation, such

as CO_2 production or O_2 consumption. This enables the use of RBT for several chemicals irrespectively of their physicochemical properties. If the compound is found to be readily biodegradable, it can be expected to degrade within 5 days. Chemicals passing the test and being categorized as "readily biodegradable" can be expected to biodegrade rapidly under environmental conditions (van Leeuwen and Vermeire 2007). The test does not deliver degradation rate constants and thus the determination of accurate degradation half-lives is not possible. Nevertheless, there are large uncertainties for chemicals being categorized as not-readily biodegradable. Many of these substances may, regardless of the classification, not be persistent in the environment (Aronson et al. 2006). Test results from more detailed simulation studies are rare for industrial chemicals. In simulation tests a compartment of interest is mimicked and typically indigenous biomass (of soil, water, sediment or sludge) is used. Low concentration of the chemical is then added to the system and the chemical's biodegradation is measured with ^{14}C radio-labelling techniques. Several OECD guidelines exist for the tests (van Leeuwen and Vermeire 2007).

Due to the lack of simulation test data determination of an actual biodegradation half-life is in many cases not possible. Experimental data on biodegradation has been collected in BIODEG and MITI-I databases (Pavan and Worth 2006, van Leeuwen and Vermeire 2007). The BIODEG database categorises the results as "biodegrades fast" "biodegrades fast with acclimation" etc. Additionally, it assigns each chemical with a reliability rating from 1 to 3. The best rating (1) is obtained, if the chemical is tested in three or more tests that deliver consistent results[14] (Boethling et al. 1994, Pavan and Worth 2006). Thus, the results found from the database with rating 1 can be assumed to be trustworthy, whereas for chemicals with the reliability rating 3 only one or ambiguous measurement data are available.

Biotic and abiotic degradation processes and the experimental determination of the related half-lives are described in van Leeuwen and Vermeire (2007). An overview of the experimental determination methods is given in the register sheet "MS". To sum up, determination of degradation rate constants and interpretation of the data is not trivial. Standardized testing methods exist only for hydrolysis and biodegradation measurements. The latter yields, due to use of microbial cultures and hence high sensibility to variances in environmental conditions, variable measurements results even with standardized protocols, (Aronson et al. 2006). Without use of protocols, comparison of the experimental data needs to be carried through for each individual case. In absence of experimentally determined half-lives screening models, such as HYDROWIN and BIOWIN of EPI SUITE, can be used for estimation of degradation rate constants (Scheringer et al. 2009a) (see chapter 4).

The concept of P_{ov} differs from the media-specific degradation half-lives. It measures the persistence of the substance as a whole in the environment, rather than in one single environmental compartment. It is a sum of the chemical's single-media half-lives weighted according to the chemical's partitioning behaviour (Scheringer et al. 2009a). Klecka et al. (2009) recommend assessing the overall environmental persistence P_{ov} in order to consider possible redistribution in a multimedia compartment. The P_{ov} is typically determined with model-based tools, for instance the OECD P_{ov} & LRTP Screening Tool (see chapter 4). The advantage of the P_{ov}

[14] http://www.srcinc.com/what-we-do/efdb.aspx, last accessed 26.4.2012

is that it enables comparison of several chemicals by use of one single persistence metric (Scheringer et al. 2009a). As no screening criteria are given for P_{ov}, its use for risk assessment can be questioned. Nevertheless, P_{ov} benchmarking of candidate-POPs with existing POPs has been cited several times in the risk profiles. Similar P_{ov} values for candidate and existing POPs have been evaluated as persistence indicator.

3.2 Bioaccumulation

Bioaccumulation describes a process of chemical uptake into living organisms from their environment. It leads to an increase of the chemical concentration within the organism in comparison to its environment. Like persistence, it is not only dependent on the intrinsic chemical properties, but also on environmental conditions and examined organisms. Exposure to the chemical can originate from different uptake routes: skin, respiratory surfaces and diet. Different elimination processes act against bioaccumulation. These include respiration, dermal diffusion, egestion, metabolism, reproductive losses and growth dilution. If chemical accumulates faster to the organism than it can be removed, bioaccumulation occurs (Arnot and Gobas 2006, Mackay and Fraser 2000).

Under laboratory conditions a simplified approach for assessment of the bioaccumulation potential is often used, namely bioconcentration. In the case of bioconcentration, only uptake via skin and respiratory system is accounted for. Accumulation of chemicals through food only is considered separately and described as biomagnification. Trophic magnification takes place if the concentration of the chemical increases within the food web from one trophic level to another. The opposite phenomenon, trophic dilution, occurs if the elimination processes exceed the uptake (Arnot and Gobas 2006). The last two cases are important when the chemical behaviour within food webs is assessed (Conder et al. 2011). Typical metrics for determination of the mentioned processes are described in Table 3.

Table 3 A list of typical bioaccumulation metrics (adjusted from Gobas et al. 2009)

Parameter		Formula	Description
Bioaccumulation factor	BAF	$BAF = C_{org}/C_w$ $[L/kg_{ww}]$	Ratio of the steady state chemical concentrations in an aquatic water-respiring organism (C_{org}) and the water (C_w). Organisms exposed to a chemical in the water and diet.
Bioconcentration factor	BCF	$BCF = C_{org}/C_w$ $[L/kg_{ww}]$	Ratio of the steady state chemical concentrations in aquatic water-respiring organism (C_{org}) and the water (C_w). Exposure via water only.
Biomagnification factor	BMF	$BMF = C_{org}/C_D$ $[kg_{dry}/kg_{ww}]$ or $BMF=C_{predator}/C_{prey}$	Ratio of the steady state chemical concentrations in aquatic water-respiring organism (C_{org}) and its diet (C_D). Exposure via diet only. Alternatively the concentrations of predator ($C_{predator}$) and prey (C_{prey}), either water or air-respiring, can be compared.
Trophic magnification factor	TMF	$TMF = 10^m$	The average factor by which the normalized chemical concentration in biota of a food web increases per trophic level. ("m" is the slope derived by linear regression from normalized chemical concentrations in biota and the corresponding trophic positions)
Octanol-Water partition coefficient	K_{ow}	$K_{ow}= C_o/C_w$	Ratio of the chemical concentrations in 1-octanol (C_o) and water (C_w) in chemical equilibrium
Octanol-Air partition coefficient	K_{oa}	$K_{oa}= C_o/C_a$	Ratio of the chemical concentrations in 1-octanol (C_o) and air (C_a) in chemical equilibrium

The Convention recognizes only the use of BAF or BCF in aquatic organisms, together with the log K_{ow}, as assessment criteria. Other bioaccumulation metrics are not explicitly mentioned by the convention, but "evidence that a chemical presents other reasons of concern" is defined as assessment criteria, justifying the use of other parameters as well. This addition is important especially for air-respiring organisms, as the BAF and BCF results for aquatic organisms (typical test species) as well as K_{ow} do not account for the chemical uptake from air. If a substance has been considered vB according to the REACH guidance (ECHA 2011) for the PBT assessment, it can be considered bioaccumulative also according to the Stockholm Convention.

Use of K_{ow} as a bioaccumulation criterion relies on the assumption that the bioaccumulating chemicals tend to accumulate specifically to the lipid fraction of the organisms and that octanol can be used as a surrogate for this fraction. For most organic chemicals this assumptions is accurate, but compounds partitioning to other parts of the organism, such as DNA or proteins, are neglected under this assumption (van Leeuwen and Vermeire 2007). The prediction accuracy of octanol as a lipid surrogate for diverse membrane lipids, consisting of lipid bilayer and embedded proteins is also limited (Müller and Nendza 2007). For organic chemicals that are mainly taken up by passive diffusion this assumption is nevertheless sufficient. Additionally, the K_{ow} describes the partitioning from water to lipid-phase, hence overlooking the possible accumulation directly from air. K_{ow} is not applicable for surface-active substances. The great advantage of K_{ow} as an assessment criterion is nevertheless, that no animal testing is required and the experimental data is easy to obtain (Gobas et al. 2009). There are large databases with experimental K_{ow} values. The experimental data is fairly accurate up to log K_{ow} = 6. For higher K_{ow} values, the measured data should be evaluated with care, as the effect of hydrophobicity of the compound becomes important. For such compounds the K_{ow} estimation is difficult due to limited water solubility, and hence inaccurate K_{ow} determination (Schwarzenbach et al. 2003).

BAF and BCF describe the initial uptake of a chemical from the environment to the food web (Conder et al. 2011). BCF is typically measured under laboratory conditions, whereas the BAF is usually based on field measurements. The accumulation via food is not considered in the BCF measurements. Arnot and Gobas (2006) stated that the monitored BAF values can be at least one order of magnitude larger than the laboratory derived BCF values and recommend the use of BAF rather than BCF in regulatory purposes. The uptake via food is increasingly important for high K_{ow} substances and on higher trophic levels, as the non-equilibrium in gastrointestinal tract enables the continuous uptake of the chemical. To make different BCF and BAF values from different organisms and studies comparable, they should be accordingly normalized. As many organic chemicals accumulate specifically on the fatty tissue, and the fraction of this tissue varies within different species, it is important to use lipid-normalized BCF and BAF when inter-species comparisons are made (Gobas et al. 2009). If preferred partitioning to other parts of the organism is evident, the normalization should be done accordingly. In the past most of the reported BCF and BAF values were nevertheless not normalized. Also, the Convention does not recognize a "lipid-normalized" BCF or BAF threshold. In this context reporting both, lipid (or other tissue)- and body-weight normalized values for new experimental results, would be justified so that both values could be taken into account in the chemical assessment accordingly.

Biomagnification and Trophic Magnification Factor (BMF and TMF) account explicitly for chemical update from the diet. The BMF nevertheless presents only one part of the food web

(predator-prey) whereas the TMF sums up the effect for the food web as a whole (several predator-prey relationships) (Conder et al. 2011). The BMFs from single predator-prey relationships can vary greatly due to different chemical uptake and metabolism processes in different organisms. The holistic view, which aggregates the uptake and removal features over several trophic levels, makes the TMF a conclusive bioaccumulation metric. Currently, the TMF is derived from measured field data, which makes it impossible to analyse the TMF for substances whose concentrations in the environment are not sufficiently high. Relevance of the food web investigated and the statistical uncertainties of the TMF determination should be considered when TMF is used for regulatory purposes. In general, a TMF > 2-3 is statistically significantly different from the threshold value of 1 (Conder et al. 2011).

For bioaccumulation evaluation, Gobas et al. (2009) suggested a framework with 5 steps for bioaccumulation assessment. The potential for bioaccumulation should at first be evaluated with TMF and BMF. TMF > 1 confirms already the bioaccumulation status of the chemical, whereas BMF > 1 indicates probable bioaccumulation. If data for these metrics are not available, experimentally determined BCF and BAF need to be considered. Physicochemical properties (K_{ow} and K_{oa}) and bioaccumulation models can imply possible bioaccumulation. K_{ow} might not be a conclusive metric for bioaccumulation assessment due to many false positives, but TMF > 1 is a good indicator for bioaccumulation in an ecosystem. This approach is nevertheless challenged by the fact that most bioaccumulation data is available in form of K_{ow}, followed by BCF and BAF. Only few BMF or TMF values are available.

The lack of data can be compensated with modelling data. K_{ow} and K_{oa} can be determined with the KOWWIN and KOAWIN programs of the EPI Suite package. BCF and BAF with on the other hand can be estimated with the BCFBAF program of the EPI Suite. All of the models are suitable for screening of large sets of chemicals with a minimum amount of information (see chapter 3.2).

Kitano et al. (2007) discussed the reasons why in some cases the BAF, BCF and logK_{ow} criteria were not fulfilled, but chemicals were still nominated as POPs in the Convention. They concluded that in some cases these concepts were not applicable for example due to protein-binding or if the main uptake route of the chemical was ingestion, as the case of PFOS demonstrates. The lack of evidence was compensated for by monitoring data from remote regions or higher trophic species, or measured levels of chemical in human blood or milk. Further, BMF was used as evidence of accumulation of the chemical through ingestion. In some cases high (eco)toxicity in comparison to the measured environmental values was used as sufficient bioaccumulation evidence as well.

3.3 Toxicity

Toxicity of a chemical describes the effect of a chemical within an organism after exposure, and is hence linked with bioaccumulation. It is dependent on the chemical and environmental conditions. Chemicals being strongly bioaccumulative often tend to be toxic as well due to triggered baseline toxicity.

The Convention does not define a toxicity threshold for the chemicals, but addresses only “adverse effects” or “toxicity and ecotoxicity data” as evidence of toxicity. Typically used toxicity data and endpoints are acute and chronic toxicity of aquatic organisms and mammals or evidence of carcinogenity, reproduction and developmental effects (Solomon et al. 2009). Toxic

effects can be measured on cellular, organism or population level. As the definition of adverse effects is so vague, the convention leaves a lot of room for interpretation. In their analysis of five POP risk profiles, Solomon et al (2009) further concluded that there is a lack of consistency in the endpoints used, as well as the amount and type of data included. Additionally, there is no consistent and generally accepted decision-making process to make the decision whether the adverse effects are likely or not. The guidance of ECHA for PBT assessment (ECHA 2011) can be applied to toxicity assessment under the Stockholm Convention as well. If the substance is considered T according to the guidance, it is also likely to pose significant adverse effects according to the Convention.

Typical experimental methods for toxicity determination on organism and population level are studies with aquatic species (algae, invertebrates or fish) within a controlled flow through system. The organisms are exposed to a certain chemical concentration in water for a defined period of time, and a predefined effect is measured as a function of time and different test concentrations. The evaluated effects are typically mortality, growth and effect on reproduction, but many other assessment endpoints also exist. Acute tests usually examine an effect of high exposure concentration during a short time period, whereas chronic studies often use lower concentrations for a period of time that typically covers most of the test-species life span. In the case of POPs it might be more important to use a test duration that refers to the half-life of a substance within an organism, rather than the organism lifetime, in order to enable observations at the equilibrium (Solomon et al. 2009). POPs are, per definition, persistent, which makes long-term and chronic studies particularly important for the toxicity assessment under the convention. From the experiments, median lethal or effect concentrations can be derived (LC_{50} and EC_{50}). These values describe the exposure concentration where 50% of the test organisms showed an effect. Alternatively, no-effect concentrations (NOEC) or lowest observed effect concentrations (LOEC) can be derived from the test data statistically (van Leeuwen and Vermeire 2007, Solomon et al. 2009).

The toxicological tests aim at finding the most sensitive species that represent the ecosystem. Therefore representative toxicity data should be obtained for many different taxonomic groups that have different abilities to cope with chemical substances and are hence more or less vulnerable for certain kinds of chemicals. Usually the lowest measured effect concentrations are used in the risk assessment (van Leeuwen and Vermeire 2007, Solomon et al. 2009). An assumption in interpreting the toxicity test is that the acute effects can be extrapolated to chronic effects. Due to this assumption, and the fact that acute tests are easier to conduct, more test results and more standard methods are available for acute toxicity tests than for chronic tests. For POPs the assumption of extrapolation is highly questionable: Typical test durations for acute toxicity tests is often only 24 to 96-h and does not enable a steady-state to occur, hence underestimating the toxicity of POPs. This caveat is also enhanced by the fact, that typically only the exposure concentration (concentration in water) is reported. It would nevertheless be more conclusive to know the actual exposure concentration within an organism and even at the target tissue, to be able to interpret whether a steady state has occurred and which environmental concentrations can truly cause harm for the organisms. As with bioaccumulation, the most relevant uptake route in toxicity tests for POPs might be food. If this is not taken into account, the test results might not be relevant. In tests with substances having poor water solubility (high K_{ow}), the solubility is sometimes enhanced with solvents. In such

cases care should be taken to recognize the difference of the toxic effect caused by the solvent and the chemical itself (Solomon et al. 2009, Vallack et al. 1998).

Even though the most toxicity data is available for the aquatic test species, it should be kept in mind that the most sensitive test species might be a terrestrial or sediment-dwelling organism as well. Specific guidelines for ecotoxicity testing of these species are available as well, and the results should be accounted for in the risk assessment. Very specific toxicity, such as carcinogenity, mutagenity or reproductive effects (CMR) is further a strong evidence of toxicity (van Leeuwen and Vermeire 2007, Solomon et al. 2009, Vallack et al. 1998).

Further considerations for toxicity test interpretation are that substances with the same mode of action have an enhanced toxicity, if present in mixtures. Such POPs are for example planar PCBs, which specifically bind to a certain cellular receptor. More often the POPs act as baseline toxicants. In both cases, if the mode of action is the same, the chemicals act as concentration additives causing larger toxicological effects for the organisms as a mixture than alone. In some cases the transformation products of the POPs should also be considered within the toxicity assessment. In most cases the transformation products are nevertheless less toxic than their parent products (Solomon et al. 2009).

Toxicity measurements are subject to uncertainties due to complexity of the biological systems and variability within the test systems and organisms. Standardized methods, such as those from OECD, deliver in the best-case comparable results within laboratories. Non-standardized toxicity tests should be considered with caution, and the test conditions should be evaluated before considering the toxicity data as valid.

3.4 Long-range transport

Long-range transport (LRT) describes the ability of a compound to travel long distances in the environment, causing potential harm in areas distant from their production and/or application areas. The LRT potential of a compound can be described with either transport or target oriented metrics. Transport oriented metrics measure the distance of substance transport in the mobile medium, mostly air, sometimes water. Target oriented metrics on the other hand describe typically the fraction of the chemical emissions that reach the surface media of a distant region, such as the Arctic (Fenner et al. 2005). An overview of different metrics is given in Table 4.

Table 4 Overview of common long-range transport metrics

Metric		Description
Characteristic travel distance	CTD	Transport oriented metric for LRTP. Describes the distance at which the concentration as a function of place has dropped to $1/e$ (≈0.37) of the concentration at the point of release.
Advective loss fraction	LF	Transport oriented metric for LRTP. Expresses how much of the chemical is transported out of the area where it was emitted. Mass flow through both, air and water, are considered.
Spatial range	SR	Transport oriented metric for LRTP. 95th percentile of the curve showing the concentration as a function of distance from the source.
Transfer efficiency	TE	Target oriented metric for LRTP. Ratio of the mass flux of net deposition from air to surface media in a

Metric		Description
		target region and the continuous release mass flux in the source region
Arctic contamination Potential	ACP	Target oriented metric for LRTP. Describes the amount of chemical present in the surface media in the Arctic region at a certain time, divided by the overall amount of chemical released globally until this time.
Half-life in air	$t_{1/2}$ air	Transport oriented metric for LRTP. Period of time that is needed for the chemical concentration of the substance to decrease by half in air.

(Sources: Scheringer 2009 and Scheringer et al. 2009a)

According to the Convention, LRT can be assumed when the chemical half-life in air exceeds 2 days. In this time, it is assumed that a chemical present in air can travel 778 km on an average wind speed of 4.5 m/s. The half-life in air is mainly influenced by the oxidation reaction with hydroxyl-radicals (chemical degradation), partitioning to aerosol particles and the subsequent dry deposition, as well as wet deposition with rain (Scheringer 2009).

Experimental data on atmospheric degradation of organic substances (reaction with OH-radicals) has been compiled by Klöpffer and Wagner (2007), but only few data can be found for semivolatile compounds, such as many POPs (Scheringer 2009). The reaction with OH-radicals can be estimated with the help of AOPWIN Software[15], a model based on group contribution method (see Models). The estimated results might nevertheless not be valid for complex molecules, such as POPs, and the program tends to underestimate the half-life for these chemicals. In general, the results are subject to large uncertainties (Scheringer 2009). Further challenges are met in the determination of the particle-bound fraction and the chemical degradation rate within this fraction. It is assumed that the degradation of the particle-bound fraction does not take place (as fast) as in the gaseous fraction. Furthermore, the aerosols are able to travel long distances in the atmosphere, contributing to the LRT. These topics are discussed by Scheringer (2009). It is important to understand that if the atmospheric half-life is determined only on the basis of chemical oxidation in the gas phase, not accounting for the low reaction rate constants of the particle-bound fraction, the half-life in air might be underestimated.

Experimental determination of LRT is challenging, as global measurement data or data from remote regions is needed. However, measured concentrations from remote regions as such are no direct evidence of LRT, but need to be evaluated further. It is necessary to know how the substance reached the region and which fraction of the emissions actually ended up in the region (Scheringer 2009a). Examples of monitoring programs contributing to this challenge are discussed in chapter 5. Generally, high-resolution global measurement data is scarce and measurement of low chemical concentrations in the environment presents a big challenge. Hence, models are often used for LRT estimations.

Other LRT metrics than half-life in air are mainly computed with help of models. For screening purposes CTD and TF can be estimated with the OECD P_{ov} and LRTP tool. The evaluation of the chemical risk profiles of the Convention shows that these metrics were the most often used LRT

[15] http://www.epa.gov/oppt/exposure/pubs/episuite.htm, last accessed 26.4.2012

metrics (see Models 4.1). As data of CTD and TF is available for many existing POPs, it is recommended to use the same metrics for further LRT estimations, to enable benchmarking of candidate POPs with existing POPs. The models for LRT estimation are discussed in section 4.2.1.

3.5 Conclusions methods

There are several methods available for P, B, T and LRT prediction and estimation. The availability of the experimental data is generally low, or the data quality varies a lot. Applicability of the methods as well as uncertainties and reliability of the published data should always be taken into account when new substances are being evaluated. Even often cited databases, such as BIODEG for biodegradation half-life information, contain highly variable data for the same chemical. For a conclusive identification of new candidate-POPs more experimental data needs to be created. For this purpose it is recommended to use well-established methods, such as those with acknowledged OECD protocols. In the absence of such methods, the experimental set up should be clearly documented.

Science often recommends the use of "more comprehensive" metrics for PBT and LRT evaluation, such as P_{ov} and TMF. These metrics are not explicitly mentioned in the Convention, but their use is enabled through the convention text.

Models are in some cases able to help in data generation. This possibility has the advantage of being typically less expensive and time consuming. Additionally no living organisms are needed for data generation.

If the substance has been analysed for its PBT potential according to the guidance of ECHA, this information can be used in the POP evaluation. However, the different threshold values of the regulations need to be addressed.

4 Models

4.1 Background

In the case of potential POPs, lack of reliable data that would enable accurate estimations of the P, B, T and LRT properties is common. Models provide means for estimating environmental properties of chemicals according to their structural and physicochemical properties.

Different estimation methods and models exist. Prevalent estimation methods, so-called quantitative structure-activity relationships (QSARs), are theoretical models that can be used for prediction of physicochemical, biological as well as environmental fate properties of molecules. Estimates of different properties are derived from input information about the chemical structure or other chemical properties. More than 20 000 QSARs have been reported in the scientific literature (van Leeuwen and Vermeire 2007). Typically QSARs and related models are used for the assessment of bioconcentration, toxicological properties as well as individual degradation processes affecting the persistence, whereas overall persistence and long-range transport are evaluated by using multimedia fate models.

Use of models for the estimation of the POP-characteristics of chemicals is mentioned in the Convention only once. Annex D states that the potential for LRT can be estimated in the screening phase with environmental fate properties, monitoring data or model results. The results should demonstrate the potential of the chemical for LRT through air, water or

migratory species. As the risk profile builds on the information acquired in the screening phase, it can be assumed that the use of modelling data in a similar manner is also adequate in the risk profile phase of the chemical assessment. In-depth modelling exercises with highly resolved models, rather than screening model exercises, may become increasingly important at the stage of the risk profile assessment.

During the ex-post analysis evidence of application of models in the risk profiles was found in 9 of the 10 cases of new POPs. Only for lindane, no clear reference to modelling was found. The most used modelling tool has been thus far the OECD P_{ov} and long-range transport potential (LRTP) Screening Tool, which is cited in 7 of the 10 risk assessments.

Even though modelling of B, P and T is not explicitly encouraged through the convention text, modelling was used in the risk profiles amongst others to estimate bioaccumulation, biomagnification, biodegradation and atmospheric half-life. Also research papers using tumor-modelling as means to evaluate toxicity are cited. In practice, the issue of using models in the risk assessment of the chemicals within the Convention is not straightforward. The Draft Risk Profile of endosulfan was discussed in the 5th POPRC Meeting in October 2009. After a presentation of the model-based study on the environmental persistence and LRTP of endosulfan, which was based on results from the OECD screening tool as well as a the global environmental fate model CliMoChem (Becker et al 2011), the views of the POPRC members diverged from finding the models useful tools for P and LRT prediction to cautious views towards model-based studies in general (UNEP POPRC 2009a).

A recent draft of the POPRC (Arndt 2011)[16] summarizes the agreed principles in the interpretation of the Annex E (Risk profile) according to the committee's past experience in preparing risk profiles. The draft highlights that use of environmental modelling is desirable if the measured environmental concentrations are very low, and thus the risk analysis according to the measured values is uncertain. Similarly, modelling was used if no measured environmental concentrations or concentrations in biota from remote areas are available due to withdrawal of the chemical from the global market. The same concept is proposed also for newly introduced chemicals with still very low environmental concentrations. The latter concept has not yet been fully agreed by the POPRC.

In the following, model tools for P, B, T and LRT assessment are discussed. The models are divided into two categories: Easy-to-use screening models are introduced as a way of screening several chemicals according to their POP characteristics. Highly resolved models for detailed analysis of specific chemicals are discussed. In each category we will focus to the most important modelling tool.

The documentation of the models is available in form of a separate excel file (cf. "Register Sheet")

[16] http://chm.pops.int/Portals/0/download.aspx?d=UNEP-POPS-POPRC7FU-E-PROP-1.En.pdf, last accessed 26.4.2012. Draft was later updated according to the comments of Party Members and observers (UNEP/POPS/POPRC.8/INF/9), http://chm.pops.int/Convention/POPsReviewCommittee/LatestMeeting/POPRC8/MeetingDocuments/tabid/2801/ctl/Download/mid/9135/Default.aspx?id=64&ObjID=14847, last accessed 29.10.2012

4.2 Screening models

4.2.1 OECD Pov and LRTP tool

The most often cited model in POP risk assessments, the OECD Pov and LRTP Screening Tool[17], is a standard tool for LRTP estimations. Other tools for LRTP assessment that have been cited in the risk profiles include Elpos (Environmental Long-Range transport and Persistence of Organic Substances model) and ChemRange. Description and comparison of these and other multimedia models can be found in Scheringer and Wania (2003) and Fenner et al. (2005)..

The OECD tool was developed by an OECD Expert Group for Multimedia Models after a study by Fenner et al. (2005). Nine different multimedia models for LRTP determination were compared with one another. The study showed that despite model differences, the chemical rankings provided by each model correlated strongly. For P_{ov} rankings eight of the nine models showed very high correlations with one another. For LRTP it was evident that the models using different LRT metrics delivered somewhat different results: The transport-oriented models correlated well with one another, as did the transfer-oriented models. The correlations between the two different model types nevertheless had only medium to low agreement with one another.

To improve the user-friendliness in the LRT-Model selection, the OECD Tool was developed as a consensus model, which reflects the basic properties of the compared models (Wegmann et al. 2009). The tool provides a LRTP estimation with both transport- and transfer oriented metrics (CTD and TF), together with the calculation of P_{ov}. Input parameters for the chemical half-lives in soil, air and water are needed, together with the partitioning constants K_{ow} and K_{aw} (Scheringer at al 2009b). From these inputs, the model calculates the chemical partitioning in the different environmental compartments in a generic environment. Compartments presented by the model are air, sea surface and soil surface layers. In water and air also partitioning to suspended particles and aerosols is taken into account and in the soil compartment the partitioning between the solid soil, pore water and soil air is considered (Wegmann et al. 2009).

The OECD Tool calculates P_{ov} at steady state as the total mass of a chemical in the model system is divided by the degradation flux from all model compartments (Scheringer et al. 2009b). As the residence time in each compartment strongly depends on the emission scenario, three different emission scenarios, total amount of emissions going directly to air, to water or to soil, are modelled. The most conservative values are presented as the P_{ov} (Scheringer et al. 2009b, Stroebe et al. 2004).

The LRTP results are given by the model in two metrics. First, a transport oriented LRTP metric, the characteristic travel distance (CDT) is used. The CTD is calculated in both air and water, according to the respective emission scenario. Secondly a target-oriented LRTP metric is given as transfer efficiency (TE) (Scheringer et al. 2009b).

Comparison of the OECD tool to other multimedia modelling tools for LRTP and P_{ov} showed that the results for the P_{ov} correlated highly with all the other models. Especially high

[17] http://www.oecd.org/document/24/0,3746,en_2649_34379_45373336_1_1_1_1,00.html; last accessed 18.04.2012

correlations were found for the P_{ov} results from Elpos and ChemRange. The LRTP correlated strongly as well when the rank correlation coefficients for CTD were compared with the results from other models with transport-oriented metrics (Wegmann et al. 2009).

Fenner et al. (2005) pointed out that the uncertainty between different LRT and P_{ov} estimation models was smaller than the uncertainty caused by the model parameters in 95% of the examined cases. For LRTP assessment, the model uncertainty nevertheless exceeded the parameter uncertainty in 70% of the cases. In 95% of these cases the effect of model uncertainty was nevertheless less than factor 2 larger than the effect of parameter uncertainty (Fenner et al. 2005). This highlights the importance of appropriate input data for the models. The OECD Tool incorporates as an additional feature Monte Carlo Analysis, which enables the evaluation of the parameter uncertainty for the analysed substances.

The OECD Tool has proven to be very efficient for screening level analysis and benchmarking of potential POPs. Some of its limitations are nevertheless that the screening is possible only for non-ionizing organic chemicals, but not for acids, bases or metals. The tool cannot be used for evaluation of environmental concentrations, but only for comparison and ranking of chemicals according to their P_{ov} and LRTP properties. As a screening tool, the model environment is also simplified and globally averaged values on the environmental parameters are used. The results are further highly dependent on good-quality input-parameters (Wegmann et al. 2009).

4.2.2 Toxicity estimation with ECOSAR

Ecological Structure-Activity Relationship Model (ECOSAR) is a QSAR based model for estimation of aquatic toxicology data of organic industrial chemicals. The underlying methodology has been developed with the support of the US EPA since 1970s, and the first computer based model version was developed in the early 1990s. ECOSAR is designed for chemical screening in absence of experimental data and is freely available (Mayo-Bean et al. 2001a).

ECOSAR estimates chronic and acute toxicity values for several aquatic species at different trophic levels from the chemical input data. This “standard toxicity profile” can be used for predicting general aquatic toxicity under the assumption that the surrogate species are representative for the whole aquatic community. The acute effects estimated for the standard toxicity profile consist of LC_{50} values for fish (96 h) and daphnia (48 h) and EC_{50} value (72 or 96 h) for algae. The chronic effects are estimated as chronic value (ChV), which is the geometric mean of LOEC/LOEL and NOEC/NOEL (Mayo-Bean et al. 2001a).

The only required input data is the SMILES[18] code for the chemical. From this information other input data, such as $\log K_{ow}$, water solubility and melting point of the chemical are estimated with other programs or from databases (KOWWIN and WSKOWWIN from US EPA EpiSuite[19] and the Physprop Experimental Database of Syracuse Research Corporation, SRC[20]). It is always

[18] Simplified Molecular Input Line Entry System; http://daylight.com/smiles/, last accessed 26.4.2012

[19] http://www.epa.gov/oppt/exposure/pubs/episuite.htm , last accessed 26.4.2012

[20] PHYSPROP, http://www.srcinc.com/what-we-do/product.aspx?id=133, last accessed 28.9.2012

possible to enter user-specified logK_{ow}, water solubility and melting point values, which is preferable if measured data are available for these properties (Mayo-Bean et al. 2011b).

The program (Version 1.1) consists of 709 QSARs for numerous endpoints and organisms. The decision about which QSAR is used for the effect estimation is made by an integrated expert decision tree that relates each chemical to its appropriate chemical class. The program recognizes altogether 111 chemical classes. The general classes of chemicals include neutral organics, organic chemicals with excess toxicity and surface-active organic chemicals (Mayo-Bean et al. 2001a).

Neutral organics act non-specifically and induce non-polar narcosis, or baseline toxicity. The group consists of non-ionisable and nonreactive chemicals. Organic chemicals with excess toxicity on the other hand have a more specific mode of action. Separate QSARs have been developed for different modes of action. The reactivity of the above mentioned chemicals is caused by the presence of reactive functional groups and the division to sub-classes is done according to the same principle. Surfactants, compounds with a polar functional group and a non-polar chain, present the third general class within ECOSAR. ECOSAR groups the surfactants further according to their charge (Mayo-Bean et al. 2001a).

The QSARs were developed by applying regression techniques to reliable experimental data (controlled pH, temperature, standard species etc.) and predicted K_{ow} values. Measured K_{ow} values were not used in order to minimize the variation caused by the experimental differences. The QSARs for neutral organics and organic chemicals with excess toxicity have generally a linear form and the toxicity is related to the K_{ow}. The QSARs for surfactants are either linear or parabolic and the toxicity is often related to the size of the hydrophobic component or the number of repeating hydrophilic functional groups (Mayo-Bean et al. 2001a).

Even though ECOSAR is able to deliver useful toxicity data for many compounds, it has some limitations. Inorganic and organometallic compounds are out of the domain of ECOSAR. The training set of the ECOSAR affects the reliability of the estimated results. It consisted mainly of chemicals with molecular weight < 1000. Estimation of the chemical properties for larger chemicals might lead to wrong estimations (Mayo-Bean et al. 2001a and b).

In general, the estimated acute toxicity data is most reliable if the logK_{ow} values of the chemicals are 5.0 for fish and daphnia and 6.4 for green algae. For chronic value estimations reliable results are delivered when the logK_{ow} is 8.0. The decreased reliability is due to decreased water solubility of lipophilic compounds. The larger the lipophilicity and the lower the water solubility of a compound, the longer reaction time is required for an effect to occur. If the water solubility of the compound is lower than the estimated effect concentration, the toxicity results might not be relevant. The program gives a notification for the user, if this is the case (Mayo-Bean et al. 2001a). However, it is important to note that Mayer and Reichenberg (2006) challenge the above-mentioned theory of ECOSAR developers: They found that hydrophobic substances with high K_{ow} (>6) were able to exert considerable toxicity in tests with different aquatic species.

The limitations of K_{ow} as a surrogate for lipid partitioning, mentioned in section 3.2, should also be recognized. The toxicity of chemicals partitioning preferably to other parts of the body, such as proteins or DNA, might be underestimated when K_{ow} is used as the only input parameter for the toxicity estimations. Some class-specific QSARs for specific toxicity are derived from a very

small experimental data set (e.g. 5 experimental values in case of QSAR for the group of haloketones), which decreases the reliability of these specific estimations.

4.2.3 Persistence estimation with BIOWIN

As described in section 3.1, persistence describes how long a substance stays in the environment. Persistence in different environmental compartments is influenced by the transformation of the chemical to other chemicals. Biodegradation is in many cases the most important transformation process governing the removal of a chemical in soil, sediment and water phases. Moreover, it is usually the only way in which a complete mineralization of an organic compound can be reached (Pavan and Worth 2008, Aronson et al. 2006).

Early biodegradation modelling concentrated on class-specific quantitative structure bioavailability relationships. The majority of these models used molecular properties, such as K_{ow}, or molecular connectivity indices as model descriptors. Even though the models generally delivered good correlations between the physicochemical properties and degradation rates, they had the disadvantage of being class specific and thus not useful for screening a large set of molecules (Pavan and Worth 2008). Additionally, only few of over 80 evaluated QSBR (Quantitative Structure Bioavailability Relationship) models provided acceptable levels of agreement between estimated and experimental data (Pavan and Worth 2006).

Establishment of more reliable, large databases with information about measured biodegradeability of chemical compounds has enabled development of further biodegradation models with advanced modelling approaches (Pavan and Worth 2008). In these models the biodegradability is related to sub-structures of molecules, such as the type and amount of substituents, chain length and branching of the molecule. The models have the advantage that they are applicable to a large set of structurally diverse chemicals (van Leeuwen and Vermeire 2007, Pavan and Worth 2008). Other types of models and approaches for persistence evaluation are described in detail by Pavan and Worth (2006).

BIOWIN is a broadly used biodegradability estimation program developed by the Syracuse Research Corporation in collaboration with the US EPA. It is a part of US EPA's EPI Suite[21], a collection of models for estimation of physical and chemical property data, as well as environmental fate of chemicals. BIOWIN contains seven different biodegradation models. The program is intended for chemical screening and priority setting only. The degradability estimate is derived from the SMILES codes, from which the program derives all the needed information (molecular weight and substructures) (van Leeuwen and Vermeire 2007).

All BIOWIN models were developed by means of linear or non-linear regression. Regression coefficients for preselected molecular structures (descriptors) are defined against indicator variables. Molecular weight is used as a continuous descriptor in all models. The indicator variables differ in different models. BIOWIN 1 and 2 describe whether a substance is rapidly biodegradable or not. The models were developed with data on aerobic biodegradation that were obtained from BIODEG database. BIOWIN 5 and 6 are re-calibrations of BIOWIN 1 and 2. The calibration was done by using data of 884 organic compounds from MITI-I database. The

[21] http://www.epa.gov/oppt/exposure/pubs/episuite.htm; last accessed 26.4.2012

MITI-I test is a biodegradation screening test in aerobic aquatic medium and describes whether a compound is readily biodegradable or not (van Leeuwen and Vermeire 2007). The development of the models BIOWIN 1-4 is described by Boethling et al. (1994). BIOWIN 7 is a model for methanogenic anaerobic biodegradation (Boethling et al. 2010).

BIOWIN 3 and 4 are the only models that enable a semi-quantitative, rather than binary (biodegradable yes/no) estimation of the biodegradation. The development of BIOWIN 3 and 4 was based on expert survey data. 17 Experts evaluated aerobic primary and ultimate biodegradation of 200 chemical substances. The given values for the biodegradation time were hours, days, weeks, months and longer than months. Later these values were assigned integers from 5 to 1, 5 presenting the fastest biodegradation. An average value of all the estimations was used for the modelling. BIOWIN 3 describes ultimate and BIOWIN 4 primary biodegradation (mineralization, resp. transformation to organic derivates) (van Leeuwen and Vermeire 2007, Pavan and Worth 2006).

The BIOWIN models are generally applicable to many organic chemicals. Even if none of the molecular fragments exist in the molecule, an estimation of biodegradation can theoretically be made by using the molecular weight as a descriptor. The model developers nevertheless warned that the reliability of such estimations might be low (Boethling et al. 1994). Applicability domain study confirmed this assumption (Boethling et al. 2010). Hence, the screened chemicals should present at least one of the molecular fragments used in the models (fragments used in BIOWIN1-4 are listed in Boethling et al. 1994). Also large and complex chemicals, such as pharmaceuticals are often out of the applicability domain of the model (Boethling et al. 2010).

The expert survey models BIOWIN 3 and 4 were better able to predict degradation half-lives of rapidly biodegrading compounds than compounds with slow biodegradation. The half-lives of very persistent chemicals were in many cases underestimated by BIOWIN 3. The classification accuracy of 77 to 83.5% has been reported, depending on the threshold used for “rapid” or “ready” biodegradation (Boethling et al. 1994, Aronson et al. 2006). The reported accuracy appears low, but if compared with the accuracy of the experimental data that was used in the model development (mainly obtained from the BIODEG database) the results are plausible and more accurate predictions cannot be expected (van Leeuwen and Vermeire 2007, Aronson et al. 2006).

Due to the limited prediction accuracy of the model it is clear that the modelling results from BIOWIN should not be used as such for estimating degradation half-lives. The models can nevertheless deliver useful information for chemical screening when chemicals should be prioritized or binned. The use of estimated BIOWIN-derived biodegradability half-lives or degradation rate constants as an input for multi-media modelling should be considered carefully (Aronson et al. 2006 van Leeuwen and Vermeire 2007). BIOWIN represents nevertheless one of the few models that can be used for screening a large set of chemicals and several chemical classes. Its usage in several attempts to screen BPT chemicals and POPs (see separated “Register Sheet”, category “MS”) points out that no significantly better models for screening purposes are available.

4.2.4 Bioaccumulation and bioconcentration estimation with BCFBAF

Mechanistic modelling of BCF is simpler than the BAF modelling, as the former takes into account the substance uptake only from water. For fish, the uptake through skin and gills can be described according to chemical partitioning using K_{ow} values as modelling parameters. Thus, bioconcentration QSARs are often fairly straightforward relationships of BCF and logK_{ow}, which are derived by regression methods from measured BCF values for different chemicals. In such models, the octanol is assumed to be a model for the lipids present in the organism and the mechanisms of uptake and elimination are summed up and not considered separately (Arnot and Gobas 2003, van Leeuwen and Vermeire 2007).

Bioaccumulation additionally takes into account chemical uptake via diet. For a complete mechanistic model also elimination processes through gills, fecal egestion, metabolism and growth should be accounted for. When the uptake of the chemicals through diet is predicted, factors of biomagnification and trophic dilution within the food web also need to be accounted for (Mackay and Fraser 2000). These factors greatly depend on environmental factors and not only on the physicochemical characteristics of the chemicals (Arnot and Gobas 2003). Especially the prediction of metabolism rates is difficult, as these are also organism specific. In most bioaccumulation screening models the biotransformation rates are assumed to be negligible. Disregarding this process nevertheless leads to overestimation of the BAF and can strongly influence the screening results (Arnot et al. 2009).

Specific BAF models that take into account all these mechanisms exist, but development of a BAF model that is applicable for a large number of chemicals and generally valid for screening purposes is difficult. Use of BAF rather than BCF as a parameter for chemical screening is nevertheless important, as the BCF often underestimates the chemical uptake when logKow > 4 and the uptake through diet becomes increasingly important (Arnot and Gobas 2003).

The BCFBAF model of EpiSuite[22] tackles the problem of bioaccumulation screening models. The model describes the bioaccumulation potential of organic chemicals in aquatic food webs. Prediction of both BCF and BAF is possible. The model consists of two parts, a mechanistic bioaccumulation QSAR (Arnot-Gobas model) and a QSAR describing biotransformation in fish (Boethling and Costanza 2010). The mechanistic QSAR describes the bioaccumulation with all previously mentioned uptake and elimination pathways, apart from biotransformation. The rate constants for different processes are assessed with linear and non-linear relationships using K_{ow} together with weight and lipid concentrations of organisms as descriptors. Trophic dilution is assessed to be dependent of the generic biotransformation rate constant. Additionally, a general biomagnification estimate was derived from measured BCF and BAF data (Arnot and Gobas 2003). To account for the biotransformation, the model is combined with a fish biotransformation model (Arnot et al. 2009). The biotransformation model was developed similarly as the BIOWIN model: Multiple linear regressions were performed with preselected molecular substructures, molecular mass and K_{ow} as independent variables. A dataset of estimated biotransformation rate constants was derived from measured BCF and total elimination rate constant data, which were converted to biotransformation half-lives. 421 $t_{1/2}$

[22] http://www.epa.gov/oppt/exposure/pubs/episuite.htm, last accessed 26.4.2012

values were used for model development and 211 $t_{1/2}$ values for model validation. The model presents the first biotransformation model for fish that is applicable for the screening purposes when no measured biotransformation rates or BCF and BAF data is available.

The only input parameters needed for the BCFBAF model is the SMILES code from which K_{ow}, molecular substructures and molecular weight are derived from. For environmental parameters, such as water temperature, lipid content and weight of the organisms present in the modelled food web, preselected values are used.

The BCF estimation of the Arnot-Gobas model tends to overestimate the bioconcentration potential of substances (true in 80% of the cases in model calibration data). This is nevertheless acceptable for screening purposes, when the chemicals are assessed conservatively according to their BCF potential. If BCF shows bioaccumulation potential, the chemical characteristics are ideally evaluated with more refined methods. The results of the BCF estimations are similar to those from its predecessor BCFWIN. The threshold value of BCF > 5000 is exceeded when the substance log K_{ow} is 4.5-8. The Arnot-Gobas model also shows that the BAF estimates are clearly higher than the BCF predictions. Additionally the logK_{ow} range, where the threshold of BAF > 5000 is exceeded, is larger (log Kow 4.0-12.2). Also here, the model overestimates the actual values. Only 2.5% of the measured BCF are above the predicted values (Arnot and Gobas 2003).

The large differences between BCF and BAF estimations imply that the BCF based QSARs, models and empirical data should preferably not be used for evaluation of the bioaccumulation potential (Arnot and Gobas 2003). The biotransformation model gives the best predictions for slowly biotransformed chemicals (82% correct predictions), which is the relevant chemical category in POP assessment. The poorest performance is given for moderate biotransformation rates (67% correct predictions) (Arnot et al. 2009).

The BCFBAF model provides the first available screening tool for both BCF and BAF estimation for aquatic organisms. The models helps to screen large amount of substances, but the applicability of the model should be taken into account. Charged or ionic compounds, together with surface-active chemicals are most likely not well estimated by the model. The model development set for fish biotransformation did not contain organometals or large molecules, and thus estimations for such substances (molecular weight > 600) should be used with caution. Both of the models used in the BCFBAF tool still contain substantial uncertainties. As the models were developed to be applicable for a large amount of chemicals, specific mechanisms of uptake or biotransformation are neglected. Additionally, the models cannot deliver more reliable estimations, than the underlying measured data. For screening purposes of BCF and BAF the BCFBAF model of EpiSuite is nevertheless the best model available.

4.3 Highly resolved models

Thus far the risk profiles of the Convention have relied mainly on measured environmental data on the exposure analysis. Some screening models have been used as an additional assessment tool. Due to simplified approach and inherent uncertainties, these models can mainly be used for chemical ranking and screening, but not to obtain reliable concentration estimates. Highly resolved environmental fate models, which are able to deliver detailed information about the chemical behaviour in the environment, have barely been used in the risk assessment. The case of endosulfan shows nevertheless that such global models can play an important role in the risk assessment of the POP candidates. The modelling results were able to

confirm the long-range transport even though the half-lives in different environmental media showed large uncertainties. The model results correlated with monitoring data, giving thus evidence for the LRTP of endosulfan and its transformation products (UNEP POPRC 2009b).

Highly resolved multimedia models provide a tool for understanding many aspects of POP-specific behaviour. They can help interpret the effect of the past emissions and anticipate the future behaviour of the POPs. The presence of POPs in all environmental media highlights the importance of the multimedia approach. Due to their low degradation rates, long-time perspective is necessary to account for the continuous cycling of POPs between different environmental media. The persistence of the chemicals leads also to contaminant dispersion far from the emission source. Therefore a regional or global perspective is needed (Scheringer and Wania 2003).

Multi-media models provide detailed information for the user about the mass balances of the chemical in different environmental compartments. From these mass flows and mass contents within the compartments can be determined. The mass distribution between different media and different geographical regions can be estimated, as well as elimination rates in different environmental media, the mobile fraction leaving the emission source and further characteristics can be estimated as well. The obtained data and its resolution depend on the model used. Indicator values, which enable better comparison of the chemical behaviour, can be determined from the model output. Such indicator values are for example P_{ov}, spatial range, CTD and arctic accumulation potential.

Global multimedia models and their application in the context of POPs are described in detail by Scheringer and Wania (2003).

Highly resolved models are divided in two categories: global multimedia box models and atmospheric dispersion models. In both model types different environmental compartments (soil, water, air etc.) are described. The models can be refined through addition of more processes (e.g. partitioning to aerosols with related wet and dry deposition or degradation) and compartments (e.g. ice, freshwater, vegetation) for better depiction of the environment (Scheringer and Wania 2003).

Multimedia box models are described by mass-balance equations. The equations are solved for each compartment and all spatial boxes within the model. Different processes and compartments play a key role in these models, but the spatial resolution of the models is typically limited as one box can describe several thousand square kilometres. Typically the transport of POPs is described only in the north-south direction and the latitudinal mixing is assumed to be instantaneous. These models are easier to interpret, understand and refine through additional processes and compartments than the atmospheric dispersion models. They also require less computational effort, but are nevertheless suitable for investigation of long-term dynamics of POP concentrations in the environment (Scheringer 2009)..

Atmospheric dispersion models were developed for calculating detailed atmospheric deposition and transport of pollutants. Hence the processes in the atmosphere play a key role. The atmospheric distribution is described with help of detailed meteorological data. Other environmental compartments are typically not described explicitly. For POP modelling, the processes taking place between the different environmental media need to be added to the model. The spatial and temporal resolution of the atmospheric dispersion models is very high in comparison to the global multimedia box models. This nevertheless requires high

computational effort, and long-term calculations become difficult. Detailed emission data for the application time of the model needs to be available together with the chemical background concentrations. Typically time ranges of 1-2 years are modelled.

Typical input parameters needed for the models are related to the chemical properties and emission data:

- Partitioning coefficients between different environmental compartments, possibly information about their temperature dependence
- Degradation rate constants
- Actual emission pattern
- Historical emission data

The models themselves account for the environmental parameters, such as precipitation and aerosol deposition rates and wind speed. In more detailed models these can vary as a function of time, space and/or temperature. In some models the user can also specify certain parameters himself, if more detailed information is available.

The input parameters provide the biggest challenge for the application of highly resolved models. Compilation of large amount of data is very time consuming, especially when the reliability of the data needs to be ascertained. Empirical data on partitioning coefficients and degradation rate constants is often limited and/or large deviations in measured values are encountered. It is especially difficult to find partitioning constants for specific compartments, such as ice or snow. Generally, more information is found about the partitioning behaviour and degradation in temperate regions, but the effects in other regions are unknown. Temperature dependence of partitioning data is many times not known. Often similar QSAR estimations, as were described for screening models, need to be used to define partitioning coefficients between different compartments, such as aerosols and air.

A further challenge is the emission data. To evaluate today's emissions historical data is needed, and for future scenarios actual emission patterns should be obtained. Finding reliable data with adequate temporal and regional resolution is challenging. This is even more the case, when atmospheric dispersion models with very detailed resolution are being used. Emission estimates might be available only for some parts of the world and the production and usage figures are reported for country or continental level. Extrapolation and surrogate measures are needed to overcome these limitations. Detailed information of emission data can be omitted in case of benchmarking efforts. Here same theoretical emission pattern can be used for different chemicals, and their behavioural differences are analysed. Simplified or idealized emission scenarios are also sufficient if the basic environmental behaviour of a single chemical is being analysed.

Several global high-resolution models exist, see model comparisons by Scheringer and Wania (2003) and Hollander et al. (2008).. A global multi-media box model, CliMoChem, was used for the environmental fate assessment of endosulfan, and the modelling results were acknowledged in its risk profile (UNEP POPR 2009b). The model was able to reproduce the measured environmental concentrations in Arctic air with two seasonal peaks and the LRT potential of endosulfan. Further, the model was able to distinguish between α- and β-endosulfan, which are emitted as a mixture, and predict the concentrations of their degradation product endosulfan sulphate. From the point of view of risk assessment this was relevant information, as the parent products did not exceed the P criteria of the convention, but the

endosulfan sulphate did. The joint persistence of these chemicals was estimated to be 620 days. The largest uncertainties were caused by the emission-specific parameters and substance properties. The parameterization of the model itself did not have a major influence on the uncertainties (Becker et al. 2011).

As the application of highly resolved models is considerably more labour-intensive than the application of screening models, it is advisable to take advantage of these models only after initial chemical screening. After compiling the appropriate chemical properties, these models can be used for benchmarking with other existing POPs. Such models can be used for interpretation of the existing emission and monitoring data, as recommended by Cowan-Elseberry et al. (2009).

4.4 Conclusions models

Measured chemical property and monitoring data are limited compared to the large number of chemicals requiring assessment. Mass balance and QSAR based models can help in screening of chemicals, and prioritizing these chemicals for further detailed assessment in inexpensive and efficient way. Several models for P, B, T and LRTP characterization exist. The estimation models developed by US EPA have been widely used and are regarded as valuable tools among the scientific community. The OECD P_{ov} and LRTP Tool on the other hand have been cited in most of the POP risk profiles, indicating its importance as a POP-modelling tool. With minimal input data, typically only CAS-number and SMILES-code, the models enable rapid screening organic chemicals. These methods are nevertheless designed to be robust for evaluating large amounts of chemicals, leading to uncertainties in prediction accuracy and neglecting of specific mechanisms of B and T for instance.

More highly resolved models can support risk evaluation in creating a picture of the global environmental fate of the chemical according to its emission patterns, partitioning and transport behaviour. The model results can be used among others for confirmation of existing environmental data, benchmarking or understanding the long-time behaviour of the chemical in the environment.

The uncertainties of the modelled data and caveats of the models should always be taken into account when predicted values are used in chemical risk assessment. It should nevertheless be noted that the models predictions can only be as precise as the measured data used for the model development. Hence, for further model improvements more high quality measurement data for P, B, T and LRTP should be created.

5 Monitoring

Environmental monitoring is the repeated surveillance of environmental media (air, water, sediment, soil, sewage sludge, biota, etc.) for the presence and quantity of – in the case of the Convention - POP substances. It also includes human biomonitoring which describes the measurement of pollutants in human, e.g. blood, breast milk or tissues

Under the Convention, monitoring is foreseen to evaluate the effectiveness of the Convention (UNEP 2009, Article 16). Additionally, monitoring data can be used for the assessment of chemicals in order to define substances as POPs.

As for the effectiveness evaluation according to Article 16, the Parties are responsible for the monitoring of the presence of the chemicals listed in Annexes A, B and C as well as their regional and global environmental transport by using existing monitoring programmes.

To give guidelines for the implementation, the Conference of the Parties adopted in May 2007 the Global Monitoring Plan for Persistent rganic Pollutants (UNEP COP 2007a; annex II), the implementation plan for the Global Monitoring Plan (UNEP COP 2007b) and the Guidance on the Global Monitoring Plan for Persistent organic Pollutants[23] (GMP) that has been prepared by a technical working group mandated by the Conference of the Parties. As for the core media, the Conference of the Parties decided on air monitoring and human exposure through breast milk or blood for the first evaluation. The Guidance recommends a sampling frequency of at least once a year.

The Parties are required to report on the effectiveness evaluation four years after the date of entry into force of the Convention and regularly thereafter. The first GMP Report UNEP COP 2009 was released in 2009 and based on five Regional Monitoring Reports from Africa, Latin America and the Caribbean (GRULAC), Asia and the Pacific, Central and Eastern Europe (CEEC) and Western Europe and other States Group (WEOG)[24]. These first regional respectively global monitoring reports provide support for the effectiveness evaluation of the Convention and the baseline for future evaluations and decisions.

The second option for the use of monitoring data under the Convention is the support of the identification of POPs as the information according to Annex D of the Convention required on bioaccumulation and long-range transport can also rely on monitoring data (see Table 1).

Article 11 of the Stockholm Convention on research, development and monitoring explicitly requires the Parties that they should - within their capabilities and where relevant - monitor alternatives to POPs and candidate POPs. For example the chemical sources, environmental concentrations, effects on human health and environment and transport should be monitored.

The aim of this section is to compile a comprehensive overview on existing environmental monitoring programmes on international and regional levels of POPs, PBTs, potential POPs and emerging substances. Particular attention was put on the research whether these monitoring programmes regularly take up new chemicals on their agenda or have basically the capacity to monitor new substances. The conclusions give an estimate on which programmes could strategically be used for the identification of new POPs as well as on the strategic and infrastructural needs therefore.

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[23] United National Environmental Program (UNEP) (2007): Guidance on the Global Monitoring Plan for Persistent Organic Pollutants Preliminary version, February 2007, amended in May 2007. http://www.pops.int/documents/meetings/cop_3/meetingdocs/inf14/GMP%20Guidance%20CD/Guidance.pdf, last accessed 17.04.2012

[24] The Global Monitoring Report UNEP COP 2009 as well as the five Regional Monitoring Reports from 2008 resp. 2009 are available at: http://chm.pops.int/Implementation/GlobalMonitoringPlan/MonitoringReports/tabid/525/Default.aspx, last accessed 17.4.2012

5.1 Data collection

The starting points of the investigation were two detailed reports that provide comprehensive listings of past and current environmental monitoring programs: Swackhamer et al. (2009) and the latest report of hemispheric transport of air pollution (Dutchak and Zuber 2010). Another main source for information about existing monitoring programs was the Regional Monitoring Reports for the UNEP Global Monitoring Plan from 2008 and 2009.

These reports were the basis for an intensive internet research for more detailed information on the listed programs as well as a search for other monitoring activities. The main focus during the data gathering process was to cover as many programmes and information on programmes as possible. Therefore, during this process not only classical environmental monitoring programmes have been screened, but also networks or single studies.

The information collection was based on an intensive internet research taking into account data available from

- national and federal authorities in Germany (UBA) or other countries (e.g. Defra (UK), EPA (USA)
- national, European and international organisations and Commissions (e.g. HELCOM, OSPAR, etc.),
- web pages from existing (monitoring) projects and programmes (AMAP, MONARPOP, EMEP, TMAP, etc.),
- search platforms (e.g. ISI Web of Science) to identify relevant monitoring reports scientific journals (cf. Annex 12.1)
- databases (PortalU, Environmental Specimen Bank, Dioxin Database, MUDAB, STARS, EEA Air Pollution Data Centre and Water Data Centre, etc.),
- information from working groups and networks (e.g. NORMAN),

The monitoring programmes and activities have been compiled in an excel sheet (“MP”) as part of the overall excel file (cf. “Register Sheet”) according to the reference management. The monitoring results are described according to the following parameters:

- detailed name of the programme / monitoring activity,
- short name of the programme / monitoring activity,
- monitored compounds,
- region of interest,
- media,
- frequency/archives (sampling frequency, duration of the programme,...),
- information source (reference / internet link, as the monitoring programmes are not included in the reference list),
- additional comments on the public available information on the programme.

The programmes were classified according to their geographic coverage to global, regional and national programs. Further, a class “single studies” was created to account for monitoring efforts which do not result in time trends. By entering the data in the excel file, a first quality check of the data and programmes took place and remaining data gaps were filled as far as possible by additional research.

The final step in the evaluation was an estimate of which programmes respectively activities already monitor new POPs, emerging pollutants or are capable of monitoring new POPs.

5.2 Results

A total of 61 programmes, activities, networks or single studies have been identified and are listed in the separated data collection sheet (c.f. "Register Sheet"). Only few monitoring programs or activities could be identified beyond the programmes and activities already listed in Swackhamer et al. (2009), the HTAP report (2010) and the Regional Monitoring Reports for the UNEP Global Monitoring Plan 2008 and 2009. The existing monitoring programmes are already well documented and integrated in the global POP monitoring in order to evaluate the effectiveness of the Stockholm Convention. Thus, these monitoring programmes are focused with their activities on the legacy POPs of the Convention.

Of the 61 programmes and activities, seven programmes monitor globally or hemispheric. They include also umbrella programmes that compile and evaluate data from other programs without conducting measurements, like the UNEP global monitoring programme (GMP), or national programmes in Arctic regions (for example AMAP). 10 programmes operate regionally or continentally. These programs comprise programmes such as OSPAR, HELCOM and EMEP. 28 programmes conducted by national authorities have been identified including also activities like specimen banks. The list of national programmes is certainly not exhaustive but this relies also on the access to (comprehensible) information.

The majority of all these programmes (26) monitor air (only or among other media); the second most analysed media are biota (activities and programmes on human biomonitoring not included): Overall 17 activities and programmes monitor biota. However very different species are covered thereby.

Monitoring of the abiotic media water, soil and sediment are marginal: seven programmes monitor water (freshwater, surface water, sea water) and four programmes cover soil and sediment.

A major problem during the data collection was the access to relevant data, especially on which exact substances were observed/monitored. To obtain this information, the research in publications and reports was often necessary. Most programs observe all or some of the substances that are already restricted by the Stockholm Convention, specified as legacy POPs.

The number of monitoring activities, which observe pollutants other than legacy POPs, is limited and conducted by the North American and European countries:

- AMAP, the Arctic Monitoring and Assessment Program, is the umbrella for national programmes in Arctic regions of the USA, Canada, Norway, Sweden, Finland, Russia, Denmark (Faroe Islands), Greenland, and Iceland; every 5 years a POP report and additionally a large number of single studies are released. In AMAP, all kind of environmental media are covered (air, seawater, sediments, soils, lichens, plants as well as terrestrial, freshwater and marine biota).
- NCP, the Northern Contaminants Program (Canada), which is a part of AMAP, currently does not monitor POP candidates; however NCP started in 2002 monitoring of polybrominated diphenyl ethers (PBDEs) and in 2006 the monitoring of perfluorinated

compound (PFCs); thus NCP supported the upcoming debate on PBDEs and PFOS. NCP monitors arctic air and biota.

- Global Atmosphere Passive Sampling (GAPS); comparable to NCP, GAPS monitored PBDEs before the regulation under the Stockholm Convention and monitors PFCs since 2009; besides, GAPS monitors polychlorinated naphthalene (PCN). GAPS samples air on 65 sites on seven continents.
- OSPAR, the Convention for the Protection of the marine Environment of the North-East Atlantic, observes within the Joint Assessment and Monitoring Programme substances that are restricted by the OSPAR Convention, this list is more wide-ranging than the Stockholm Convention. For OSPAR purposes, PBT substances, and substances with equivalent level of concern, such as substances with identified effect for hormone system of organisms, are recognized (see Table 2). Within OSPAR; the Environmental Monitoring Programme monitors sediment and biota and the Comprehensive Atmospheric Monitoring Programme air and precipitation as well rivers[25].
- IADN, the Integrated atmospheric deposition network, already monitored in 2008 the former candidate POPs endosulfan and PBDEs, thus is comparable to NCP and GAPS. IADN monitors air or precipitation samples at the Great Lakes (USA and Canada).
- The US EPA Great Lakes Fish Monitoring Program covers new chemicals, such as e.g. Octachlorostyrene, Cis-nonachlor, Trans-nonachlor, Oxychlordane and Dacthal; it monitors fish in the Great Lakes.
- Some of the “smaller” programmes that focus on specific biota or are have a national scope but that also monitor new and candidate POPS are: the Mussel Watch Contaminant Monitoring (US coastal waters, including the Great Lakes), the Environment Canada Great Lakes herring gull monitoring (Great Lakes), the Denmark: Greenland (Danish National Environmental research Institute), which is however linked to AMAP

NORMAN[26]is the European network of reference laboratories, research centres and related organisations for the monitoring and biomonitoring of emerging environmental substances and develops sampling and analysis methodology, which both are a prerequisite for monitoring. It was taken up in the list, even though it is not a monitoring program because the availability of analytical methods is a prerequisite for monitoring.

Within a research project on the effective control of SVHC under REACH by Führ et al. (2011), the authors identified environmental monitoring as an important element for an effective control of SVHC. As part of the project, they developed a proposal for a new Guidance Document "Monitoring of SVHC".

[25] http://www.ospar.org/content/content.asp?menu=00170301000000_000000_000000, last accessed 12.11.2012

[26] http://www.norman-network.net/index_php.php, last accessed 16.04.2012

Lambert et al. (2011) listed substances that may undergo long-range transport and detected in the Arctic or Antarctic environment. More than 100 monitoring studies were reviewed in the Arctic and Antarctic published between 2005 and September 2011.

5.3 Conclusions monitoring

Globally, significant efforts are made to monitor many of the acknowledged POPs, other POP-like substance and various current-use pesticides in various matrices (water, air, biota, soil, human milk, etc.) as a consequence of legislation, national and international initiatives and scientific curiosity. The monitoring activities dedicated to the Stockholm Convention focus on the legacy POPs as their aim is the effectiveness evaluation under the Convention.

Thus, on the other hand, there is no monitoring programme or activity that is explicitly dedicated to identify potential POP candidates. The need to continue screening efforts - based among others on monitoring activities – in order to identify substances with POP characteristics for further consideration is also raised as an issue in Dutchak and Zuber (2010). The latter report (2010) considers monitoring programs to play a key role in identifying chemicals that are persistent and undergo long-range transport.

Generally, the concept of a monitoring programme depends largely on its objectives.. Thus, if the identification of new POPs were specified as the monitoring aim of a programme, this would need some adaptation of the concept. In the following, some requirements for adaptation of the monitoring are discussed.,

Sampling and analytical techniques:

Substance properties influence the relevant environmental media to be monitored, the sampling conditions as well as the analytical methods. Thus, a prerequisite for the monitoring of new POPs is the presence of sampling and analytical methods. HTAP 2007 provides information to laboratories and clients how to produce reliable data for concentrations of POPs in various matrices.

Different substance properties might necessitate the adaption of current sampling techniques as the example of the new POPs taken up in the Stockholm Convention in 2010 shows: Some of the new POPs are more polar and/or have higher tendencies to bind to particles compared to the old POPs. “For instance, current passive and active air monitoring programs that use polyurethane foam plugs (PUFs) as a vapour-phase sampling medium will have to adapt with the inclusion of [highly absorbent] XAD resins or other high capacity sorbents to capture more polar and/or volatile chemicals such as PFCs. Also, high volume air sampling is required to distinguish particle-bound versus gas-phase pollutants, which is important for understanding the transport of particle-bound PBDEs, other flame retardants, and PFCs” (HTAP report 2010).

In this regard, the NORMAN Network of reference laboratories, research centres and related organisations for the monitoring and biomonitoring of emerging environmental substances

could be used for the identification of POPs. The NORMAN list of emerging substances as of March 2011 contains more than 700 substances.[27]

Need of information sharing

Besides information on sampling and analytical methods, further valuable data and information are production quantities, application patterns and exposure pathways. The ECHA collects key data on physical and chemical properties and production volumes of industrial chemicals under REACH. Exchange of such data with the ECHA will be helpful for the identification of potential POP candidates. Furthermore, an exchange of information and experiences between REACH and monitoring programme experts should be continued.

A clear political commitment is required for the use of monitoring data in chemical evaluations – and for a harmonisation of the existing monitoring activities and data bases – as it has been made for human biomonitoring.

At the EU level and in the better case, worldwide a single access point for monitoring programmes (e.g. in form of a central database) needs to be established that would ensure a coordinated and integrated approach to collecting, storing, accessing and assessing of monitoring data.

Use and evaluation of individual studies for first screenings – networking with research institutions

With most programs observing the restricted substances, a promising way to find information on pollutants not yet restricted by the Stockholm Convention is to evaluate individual studies by scientists or institutes. Unfortunately, these data are spatially and temporally limited. Analysis of this information is often tedious, because a central source for summarized information is often not available and one has to evaluate the publications published by the scientists or institutes. Thus, there is also a need for sharing information on publications on the detection of certain contaminants in remote regions.

A first large-scale attempt to recognize hazardous substances or POP candidates from the ECHA pre-registration list was performed by Öberg and Iqbal (2012). They identified 68 potential POP candidates among approximately 50 000 pre-registered chemicals. Nevertheless in their screening exercise the list of hazardous chemicals was compiled with the help of modelled data rather than detailed information from the registration. P_{ov} rather than compartment specific half-lives and CTD rather than half-life in air were used as P and LRT indicators.

A closer networking with scientific institutions is also necessary for minimizing duplication of efforts. In the following, research groups and institutions are compiled that work on the detection of new pollutants or emerging substances in remote regions:

[27] http://www.norman-network.net/index_php.php?module=public/about_us/emerging&menu2=public/about_us/about_us, last accessed 27.09.2012

Table 5 Important research and official institutions in the field of monitoring possible POP candidates

University / Institution	Chair	Senior Researcher	Link
Environment Canada	Hazardous Air Pollutants (HAPs) Laboratory	Tom Harner, Hayley Hung	http://www.ec.gc.ca/scitech/default.asp?lang=En&n=F97AE834-1&formid=B55A281E-BBA8-49C5-912E-714E118D9010&xsl=scitechprofile
Environment Canada	Canada Centre for Inland Waters	Derek Muir	http://www.ec.gc.ca/scitech/default.asp?lang=En&n=F97AE834-1&formid=A694B5F5-F8D2-4017-A38F-FFF62D82FF60&xsl=scitechprofile
Lancaster University, UK	The Lancaster Environment Centre	Kevin Jones	http://www.lec.lancs.ac.uk/people/Kevin_Jones/publications
Norwegian Polar Institute, Norwegian Institute for Air Research	-	Geir Wing Gabrielsen	http://www.npolar.no/en/; http://www.nilu.no/Forskning/Miljøkjemi/Miljøgifter/Miljøgifteripolareområder/tabid/159/language/en-GB/Default.aspx
Oregon State University	Environmental & Molecular Toxicology	Staci Simonich	http://emt.oregonstate.edu/stacisimonich
Masaryk University, Czech Republic	Faculty of Science - Research Centre for Toxic Compounds in the Environment (RECETOX)	Ivan Holoubek, Jana Klanova	http://www.muni.cz/sci/313060; http://www.recetox.muni.cz/
Ehime University, Japan	Center for Marine Environmental Studies (CMES)	Shinsuke Tanabe	http://www.ehime-u.ac.jp/~cmes/e/cmese.htm
Tsinghua University, Beijing, China	Division of Environmental Chemistry	Gang Yu	http://www.tsinghua.edu.cn/publish/enven/6309/2011/20110216000043281742822/20110216000043281742822_.html
Institute of Chemical and Environmental Research (CSIC-IIQAB)		Jordi Dachs	http://www.cid.csic.es/

6 Approaches and strategies for POP identification

In the recent years, numerous approaches have been published that present lists of potential PBT/vPvB and POP substances. This chapter provides a comprehensive overview of the recently published approaches and strategies for POP identification and of different substance lists.

6.1 Data collection and evaluation matrix

The aim of the data collection was to find approaches to screen a set of chemicals for PBT/vPvB or POP substances. Thus, the authors have performed a comprehensive internet research and provide an overview of the currently available literature and studies on approaches and strategies for PBT/vPvB and POP identification. Major efforts were invested to cover the most relevant information sources. The results were divided into two data sets each put in an own excel sheet within the overall excel file:

- Approaches and Strategies for the Identification of POP or PBT Substances (excel sheet A) and
- Substance Lists that reflect a certain approach and represent the results of a screening process (excel sheet SL); the term SL has to be generally distinguished from the term databases.

The approaches and lists were evaluated according to the methods used, their consideration to identify P, B, T and LRT properties of the chemicals and the criteria used for the identification. In addition, limitations and advantages in comparison to other approaches were recognised and the amount of identified substances was listed.

Care was taken especially to extract the criteria used for the identification of substances of concern. The approaches and substance lists greatly differ in this matter. Thus, the usefulness of the approaches with regard to identifying potential POPs was evaluated according to the number of criteria and the thresholds of the Stockholm Convention (Table 6). This matrix should help to clearly distinguish substance lists meeting all POP criteria according to Annex D of the Stockholm Convention from lists that cover some of these criteria and possibly with different P, B and T values. If only two criteria are covered as laid down in REACH for vPvB substances or only one criterion is used e.g. P or a specific toxic property like endocrine disruption, CMR etc., the approaches or lists have to be considered as not useful for a further consideration in our context.

Table 6 Matrix used for evaluating the approaches and substance lists

Evaluation	Description
All POP criteria	The criteria as laid down in the Stockholm Convention on persistence, bioaccumulation, toxicity and long-range transport are considered for assessing substances. The thresholds of Annex D are exceeded
POP criteria	The criteria as laid down in the Stockholm convention are evaluated but lower threshold values are used..
PBT criteria as laid down in the Canadian Toxic Substances Management Policy	The criteria of the Canadian Toxic Substances Management Policy are used; the criterion for P and B are equivalent to the REACH vPvB criteria; besides evidences for LRT via half-life in air is assessed. These criteria are the same thresholds as laid down in the Stockholm
PBT criteria, no criteria / data on long-range transport	PBT criteria as laid down in REACH or by US EPA are used; the values for P and B are lower than under the Stockholm Convention; the potential for long-range transport is not considered.
P and B criteria used as laid down for vPvB substances under REACH	The criteria von vPvB under REACH are the same values as for P and B under the Stockholm Convention; however, T and potential for LRT are not considered.
Two criteria used as laid down in REACH for PBT substances.	These approaches miss too many criteria as for being useful for identifying POP candidates.
One criteria used e.g. P or a specific toxic property like endocrine disruption, CMR etc.	These approaches miss too many criteria as for being useful for identifying POP candidates.

6.2 Results

The research conducted in the course of this project identified 18 approaches and 14 substance lists. The approaches are summarized in Table 7 and the substance lists in Table 8.

6.2.1 Approaches

Generally, the existing approaches in the scientific literature differ in their context and details but at the same time also show much similarity within their procedure that can be described by three phases (see also Figure 2):

- Starting point of a screening, the choice of databases (hereinafter called p**reparation phase**), is not always considered in the scientific literature (e.g. Klecka et al. 2009), however it determines the resulting list,
- **Screening phase** of the selected basic set of chemicals can be described as the priority-setting phase, because here the criteria for the substance screening are defined and applied; based on the evaluation matrix described in Table 6 we assessed the usefulness of different screening approaches for our purpose.
- **Assessment phase** is an in-depth phase,that aims to assess the properties and risks of prioritized substances and their resulting potential for adverse effects on human health and the environment.

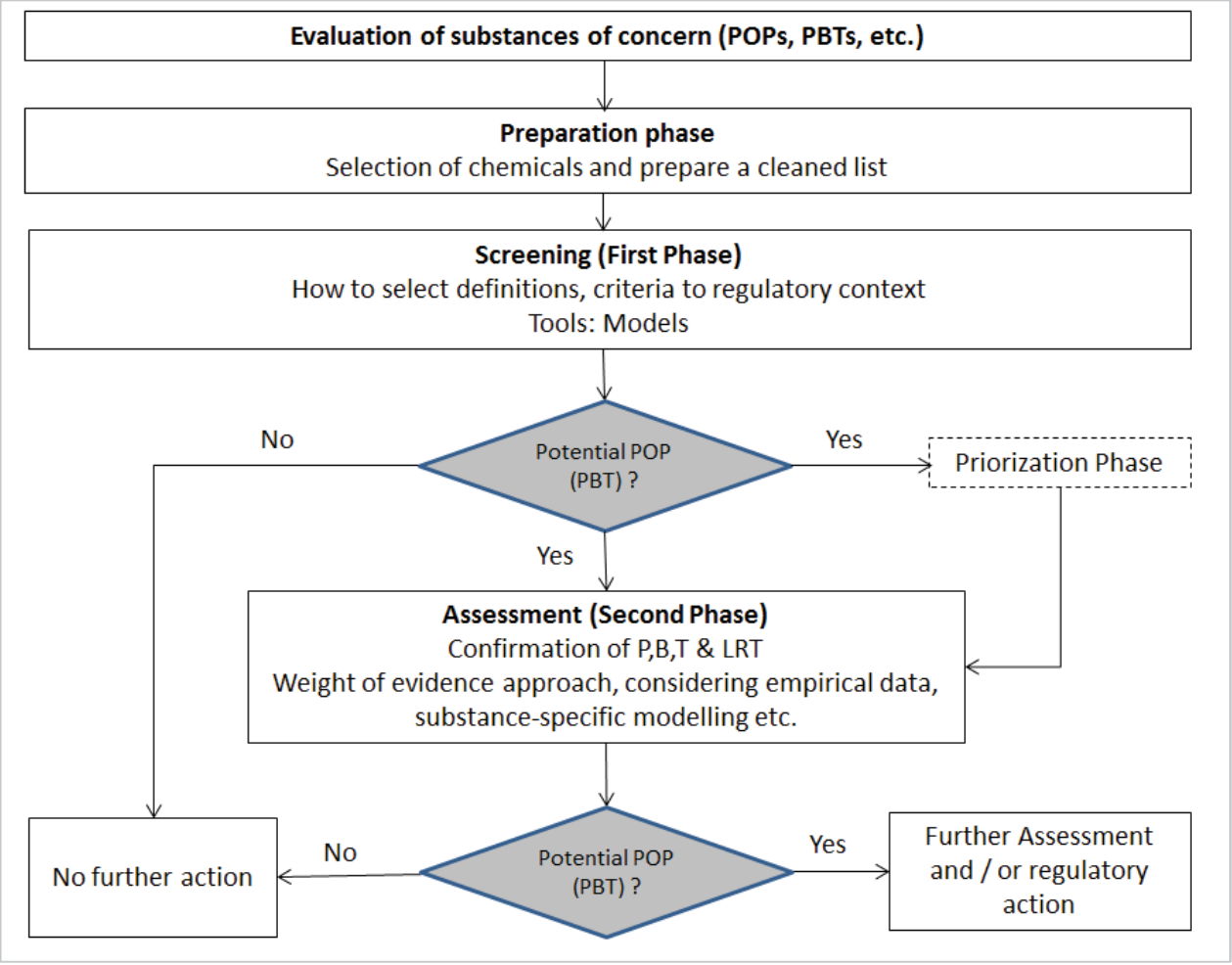

Figure 2 Most common evaluation of chemical substances with regard to POP properties (Source: Öko-Institut / ETH Zürich based on Van Wijk et al. 2009)

In the following, these phases will be analysed in more details discussing how they were implemented in the approaches.

Starting Point of a Screening: Databases or Lists

The first step within the approach consists in the choice of a basic set of chemicals that will be subject to the screening. Substance identification data can be searched and verified in large

databases mostly publically available. Most of the databases provide information about chemicals (physical and chemical characteristics, structure and more). Such databases differ in information about chemicals and contain records up to hundred thousands of chemicals. The databases are analysed in terms of the completeness of substance identification information and the registration dates.

The minimum information about a chemical that is needed for such a screening exercise based on estimated property data is the CAS number[28] and the SMILES code[29]. Steps made in the preparation phase are:

- confirmation of the chemical identity (CAS number) and molecular structure information (SMILES code); deletion of ambiguous entries and substances out of applicability domain of the models (if they are being used for in the screening phase); validation of the generated substances,
- collection of experimental data for the chemical characterization,
- generation of predictions of physicochemical properties for the chemical characterization.

The choice of the database has an impact on the screening results. Many databases contain a considerable number of entries that are ambiguous or unclear, for example because they represent mixtures rather than single substances. In some cases individual congeners of chemicals (such as > 200 PCB congeners) give high weight to acknowledged POPs. Missing chemical name or registration number can, on the other hand, lead to underestimations of potential POPs.

The databases with the largest number of entries are the CAS / SMILECAS databases. However only three approaches of our comprehensive literature review based their screening on CAS / SMILECAS (Howard and Muir 2010a; Brown and Wania 2008; Strempel et al. 2012).

According to the CAS website, there are 63,803,475 commercially available chemicals and 293,736 are reported to be inventoried/regulated chemicals.[30] The SMILECAS Database contains SMILES notations, chemical names, and CAS numbers for 103,000 records (as of February 2012)[31]. The active compounds of biocides, pesticides and pharmaceuticals are also registered with a CAS No.

In Europe, the maintenance of the European chemical Substances Information System (ESIS) is ensured by the European Commission. The information system provides the following chemical inventories:

[28] http://www.cas.org/expertise/cascontent/35 registry/regsys.html, last accessed 27.9.2012.

[29] http://www.daylight.com/dayhtml/doc/theory/theory.smiles.html, last accessed 27.9. 2012.

[30] http://www.cas.org/cgi-bin/cas/regreport.pl, last accessed 16.4.2012

[31] http://www.srcinc.com/what-we-do/product.aspx?id=135, last accessed 16.4.2012

- The European Inventory of Existing Commercial Chemical Substances (**EINECS**) contains 100,204 substances .[32]
- ELINCS (European List of Notified Chemical Substances),
- The ESIS HPVC-list provides information on the HPVCs (High Production Volume Chemicals) and the LPVCs (Low Production Volume Chemicals); the content has been extracted from the IUCLID (International Uniform Chemical Information Data Base), where data have been reported by Industry; the current HPVCs list contains 2 782 substances and the LPVCs list contains 7 825 substances (as of February 2012). [33]

Some other applied databases for high production volume chemicals are:

- The TSCA Chemical Substance Inventory of the US EPA contains 67,013 substances (as of February 2012).[34]
- The US EPA high production volume (HPV) list contains chemicals produced or imported in the United States in quantities of 1 million pounds or more per year[35].
- The status of all HPV (High Production Volume) chemicals within the process of investigation in the OECD HPV Chemicals Programme is recorded in the OECD Existing Chemicals Database. It contains the list of all OECD HPV chemicals together with any chemical specific annotations that have been provided by Member countries to the Secretariat. Each chemical is identified as to exactly which stage it is at in the assessment process, and for those chemicals, which have been assessed; a link is provided to internet pages where completed assessments can be downloaded.
- The Canadian Domestic Substances List (DSL) is an inventory of approximately 23,000 substances manufactured in, imported into or used in Canada on a commercial scale. It is based on substances present in Canada, under certain conditions, between January 1, 1984 and December 31, 1986."[36] The DSL for the additional screening is only used by Muir and Howard (2006) and Howard and Muir (2010a).

The databases above vary very much in their number of records with a maximum of 200,000 substances used for a screening (Lerche et al. 2002) and the amount of information available for the substances. For instance, Rorije et al. (2011) used a set of 65,000 industrial chemicals and Strempel et al. (2012) a set of 95,000 industrial chemicals for the screening.

The Canadian Domestic Substances List (DSL) is an inventory of approximately 23,000 substances manufactured in, imported into or used in Canada on a commercial scale. It is based on substances present in Canada, under certain conditions, between January 1, 1984 and

[32] http://esis.jrc.ec.europa.eu/index.php?PGM=ein, last accessed 18.4.2012

[33] http://esis.jrc.ec.europa.eu/index.php?PGM=hpv, last accessed 18.4.2012

[34] http://www.epa.gov/oppt/existingchemicals/pubs/tscainventory/howto.html, last accessed 18.4.2012

[35] http://www.epa.gov/HPV/, last accessed 18.4.2012

[36] http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1, last accessed 18.4.2012

December 31, 1986."[37] The DSL for the additional screening is only used by Muir and Howard (2006) and Howard and Muir (2010a).

REACH-focused approaches, e.g. Daginnus 2010 and Öberg and Iqbal 2012, used the list of **pre-registered substances** (PRS)[38] **under REACH** as the basic set of chemicals. The PRS does not include information on chemical structures. Besides, active ingredients of pesticides and biocides as well as pharmaceuticals are not covered by the PRS. The PRS list (version March 2009) contains 143 000 pre-registered REACH substances.

In order to include pesticides, biocides and pharmaceuticals if e.g. the CAS database was not used, some approaches used the following "small" databases:

- **Pesticides:** PAN pesticide Database,[39] Alanwood database, US-EPA pesticide database, WHO list of current use pesticides,
- PPDB (2012) Pesticide Properties DataBase, University of Hertfordshire,[40]
- **Biocides:** Annex I of Regulation 1451/2007[41],
- **Pharmaceuticals:** international non-proprietary names as reported by regulation 1031/2008,[42]
- EU Endocrine Disruption Database (2012)[43],
- **Other databases with ecotoxicological and environmental data**, e.g. US EPA ECOTOX Database, TOXNET: Hazardous Substances Data Bank (HSDB), Chemical Risk Information Platform (CHRIP), PTB database (created by HASKONING Consulting Engineers and Architects).

The Chinese approach by Ma and Zhang (2011) used the Existing Chemical Substances in China 2009 (IECSC).

Four approaches (Nendza et al. 2010, BIOIS and INERIS 2010 (unpublished) and Van der Veen and Knacker 2011) did not start with chemicals derived from a database but chose lists of chemicals that already meet some criteria of concern. Thus, the starting number of substances was much smaller compared to the other approaches that screened e. g. all high production volume chemicals. Lambert et al. (2012) compiled an own list with substances with measured environmental data in remote regions.

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[37] http://www.ec.gc.ca/lcpe-cepa/default.asp?lang=En&n=5F213FA8-1, last accessed 18.4.2012

[38] The PRS published by the European Chemicals Agency includes chemicals that industry may to register in accordance with the deadlines specified in the REACH legislation.

[39] http://www.pesticideinfo.org/, last accessed 27.9.2012

[40] http://sitem.herts.ac.uk/aeru/footprint/en/, last accessed 27.9.2012

[41] http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2007:325:0003:0065:EN:PDF, last accessed 27.9.2012

[42] http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2008:291:0001:0894:en:PDF, last accessed 27.9.2012

[43] http://ec.europa.eu/environment/endocrine/strategy/short_en.htm, last accessed 27.9.2012

Screening Phase

Most of the approaches applied non-testing methods in the screening phase. Non-testing methods for assessing persistence, bioaccumulation, toxicity, and long-range transport are presented and discussed in chapter 3.

The substances were checked for chemical characteristics of the regulatory purpose (e.g. Annex D criteria as defined under Stockholm Convention or other criteria to regulatory context such as REACH). Either measured data, screening models or both were used for this purpose. One reason for using estimation tools is to ensure a rapid review of substances in an in-expensive way.

The approaches greatly differ in the criteria and the thresholds they applied. Basically, non-testing methods are available for all criteria of the Stockholm Convention. However, not all approaches covered persistence, bioaccumulation, toxicity and long-range transport. There are only two approaches covering all POP criteria. These are in order of publication date Lerche et al. (2002) and Lambert et al. (2011).

The other approaches mostly screened PBT substances by using the REACH criteria. In some cases the approaches aimed to address PBT and POP substances at the same time, but did not cover all POP criteria. For example, Rorije et al. (2011) solely assessed persistence and bioaccumulation criteria. Many of the approaches did not cover the POP criteria with the values set up by the Annex D of the Stockholm Convention as in Howard and Muir (2010a).

The results in the number of possible substances of concern are very different. For instance, Rorije et al. (2011) identified almost 2 000 substances that may fulfil the persistence and bioaccumulation criteria of the Stockholm Convention. Similarly, Strempel et al. (2012) identified 3 000 potential PBT chemicals. These high numbers indicate that the number of potential POPs may be higher than the top 30 substances screened according to the Stockholm Convention P, B and LRT criteria reported by Muir and Howard (2006).

Öberg and Iqbal (2012) identified 68 potential POPs by modelling the overall persistence (P_{ov}) and LRTP with the OECD P_{ov} and LRTP Tool. The threshold values were set at 195 d for P_{ov} and more than 5 000 km for the characteristic travel distance. Both of the criteria have no threshold values within the convention, but if average wind speed of 4 m/s is assumed, the half-life of more than 2 days in air results to an environmental transport of > 690 km. Thus, the applied LRT criteria are more stringent than that in Annex D of the Stockholm Convention. Furthermore, toxicity was not included as a screening criterion

Finally, Lambert et al. (2011) used a different approach and searched for potential POPs in a list of 83 chemicals that have been detected in field samples from the Arctic and Antarctic. To this end, they applied a scoring system that combines various properties of the chemicals. The 17 substances presented on their list of “potential POP candidates” were selected according to a score which sums up the P, B, T and LRT properties of the chemicals. Closer investigation of the selected chemicals shows nevertheless that in several cases not all four criteria are fulfilled, as required by the convention, but some criteria scores compensate for low scores of the others.

The mechanism of the DYMAMEC process by OSPAR (2006) constitutes a screening process of 315 substances of possible concern and picked out those hazardous substances on the basis of their numerical cut-off values for persistence, bioaccumulation and toxicity or CMR properties resulting in the list of substances of priority action. These substances were divided into three

groups: part A, part B and part C substances. This list includes also a variety of POPs and POP candidates. Some of these substances have already been phased out of production such as pentachlorophenol, but others are still produced and released to the environment on a daily basis.

The second and much less applied screening is performed by sorting the substances according to quantitative and qualitative criteria or categories of concern as done by BIO IS and Ineris (so far unpublished). This means that the studies did not perform own calculations. These studies compiled a POP candidate list by summarizing, comparing and prioritizing different substance lists but they did not check the substances according to the POP criteria by own methods.

Prioritization Phase

An important step that cannot clearly be assigned to the screening phase or the assessment phase is a prioritization or ranking phase of the screening results that reduces the number of substances of concern that are deemed most critical and practical to address to a manageable quantity. The prioritization consists of a ranking, cross-checking with other data, assessment or scoring. It is important to keep in mind what the regulatory context or the protection goals are. Prioritization or ranking provides the basis for a more specific identification of potential POPs; for the chemicals that rank highest after the screening phase it is probably not contentious that they exceed the respective screening criteria of concern. Another option for prioritization is to compile additional information on uses and emissions in order to identify a smaller set of high-priority potential POPs; for these substances, the estimates for P, B, LRTP and T need to be refined by inclusion of more measured data.

Here we present three examples of prioritization:

- The OSPAR process is highly complex: OSPAR (2006) prioritize the Substances of Possible Concern resulting from the screening phase, the chemicals according to concerns due to the amount produced, and the degree of hazardous properties and/or the actual occurrence in the marine environment. Based on the result of the first three steps, the OSPAR Commission will make a decision on a List of Substances for Priority Action with the advice from experts. The latest OSPAR List, for instance, consists of 42 chemicals/groups of chemicals that the parties to the Convention have committed to eliminate by the year 2020.
- According to Ma and Zhang 2011, the China list was cross-checked with several existing lists of hazardous chemical that are either promulgated by regulatory authorities in other countries or proposed by leading academics in the field.
- Howard and Muir (2010a) selected top priority chemicals according to production volume, bioconcentration factor and persistence as well the absence of environmental measurements as the aim of the study was to feed in chemical candidates so far not considered in current contaminants measurement programmes.
- Rorije et al. (2011) developed a methodology for a combined persistence and bioaccumulation score based on the calculated P and B-properties giving both identical weights; the substances were ranked according to this score. The outcome was a top 30 list of substances according to their combined PB-score, the highest P-scores and the highest B-scores were discussed in more detail.

- Nendza et al. (2010) assessed 130 lists, among them 32 PBT lists and no definite list of POP substances, according to the REACH PBT/vPvB criteria in order to identify SVHC, which means that the assessment did not apply all criteria of the Stockholm Convention (the potential for long-range transport is not considered) respectively, the values for P and B are lower than under the Stockholm Convention.
- Muir and Howard (2006) scored substances meeting P and B as well as the LRT criterion as very high priority substances; however, they did not take into account the T characteristics of the substances

It is often not explicitly mentioned in which studies the prioritization process was carried out. It is important that the ranking or prioritization is documented accurately, i.e. with a clear explanation of the criteria applied, databases used etc.

Overview

An overview of the results of approaches and strategies of the literature review and an evaluation of steps according to the matrix are presented in the upper part of Table 7. The number of substances selected, the description of the respective criteria and the prioritization are also briefly presented. For an extensive description of the approaches and strategies, see the MS Excel data sheet. Not all studies had the aim to create a substance list of concern, thus not all studies from the Excel-data sheet are included in the table.

Table 7 Summary and evaluation of selected screening approaches according to Table 6

#	Source	Database	No. of substances selected	Description of the criteria	Most relevant results (number of substances)	Prioritization phase
A1	Howard and Muir 2010	DSL, CAS	22 263	Criteria of the Stockholm convention are applied but lower values are used	610 potential P&B chemicals	Yes
A2	Rorije et al. 2011	EINECS additionally sources for pesticides, biozides and pharmaceuticals	64 721	P and B criteria according to the Stockholm Convention / vPvB under REACH	1 986 meet the P and B and vPvB criteria based on their calculated properties; top 30 substances according to their combined PB-score	Yes
A3	Nendza et al. 2010	130 information sources such as inventories, substance lists etc.	3 700	PBT criteria according to REACH	234 SVHC candidates	Yes
A5	Brown and Wania 2008	CAS/SMILES, HPV databases; list of Arctic contaminants	105 584	Criteria of the Stockholm convention are applied, but lower values are used	4 291 potential Arctic contaminants 120 HPV chemicals	Yes
A6	OSPAR 2006	No database, industry information	n.a.	PBT OSPAR criteria, no criteria of long-range transport	42 substances of priority action	Yes

#	Source	Database	No. of substances selected	Description of the criteria	Most relevant results (number of substances)	Prioritization phase
A7	Brooke and Burns 2010	IUCLID, LPV substances	8 000	PBT criteria but lower values than REACH	103 PBT substances	Yes
A9	Strempel et al. 2012	SMILECAS, EINECS and ELINCS	95 000	PBT criteria of REACH	2 889 PBT, 755 vPvB substances	No
A10	Muir and Howard 2006	DSL	11 317	PB and criteria on long-range transport	30 substances	Yes
A11	Ma and Zhang 2011	IECSC	45 311	P and B criteria as laid down in REACH for PBT substances	163 PB substances that are on the Chinese market	Yes
A14	BIOIS and INERIS 2010 (unpublished)	Substance lists	911	n.a.	Check of the agreement of the lists	Yes
A15	Van der Veen and Knacker 2011	Databases with ecotoxicological and environmental data	144	Criteria as laid down in the Stockholm convention are met but lower values are used	13 PBT, 16 vPvB substances	No
A16	Lerche et al. 2002	PTB database	200 000	The criteria as laid down in the Stockholm Convention on P,B,T and LRT	12 potential POPs	No
A17	Öberg and Iqbal 2012	REACH pre-registered substances	48 782	P and LRT criteria differ from the Stockholm Convention, T not taken into account	68 substances fulfilling the P, B and LRT criteria	No
A18	Lambert et al. 2011	Contaminants detected in Arctic and/ or Antarctic	84	Criteria as laid down in the Stockholm Convention on P,B,T and LRT	15 potential POPs	Yes
A19	Scheringer et al. 2012	SMILES, EINECS	93 144	Criteria as laid down in the Stockholm Convention on P,B, LRT; T criteria as laid down in REACH	574 chemicals that exceed the Annex D thresholds; 193 high potentials POPs; 10 highly potentials POPs	Yes

Assessment Phase

Results from the screening lists evaluated in the Excel file cannot be further corroborated without experimental data. Thus, potential PBTs or POPs substances identified by the process described above usually represent starting points for more detailed assessments.

This phase will generally involve more robust data (e.g. through substance-specific modelling) to determine whether the substances do meet PBT or POP criteria (confirmation of P,B,T & LRT) and to assess their impact on environmental or human health by considering empirical data. This more detailed assessment involves additional consideration of other factors relevant to

decision-making process (depending of the purpose), such as risk characterization or the weight of evidence approach.

Thus results of the screening and prioritization process of chemicals depend on the purpose of the assessment phase and the regulatory action of concern.

None of the approaches delivers a detailed assessment of the result of the screening phase.

According to Van Wijk et al. (2009) additional or robust data should be used in the assessment phase. Alternatively, the assessment phase may involve using the same data used for the screening criteria but in a more robust analysis or evaluation

Often there are separate assessments for each defined chemical property (e.g. persistence, bioaccumulation, toxicity and/or long-range transport) There may be a priori legislative, scientific, or policy reasons for detailed evaluation of a substance even without an earlier screening phase. For example, POP evaluation may be part of established or mandated regulatory assessments of new or existing chemicals, monitoring in polar regions may reveal the presence of hitherto unsuspected substances, or knowledge about the bioaccumulation of a chemical may focus attention on analogous classes of substances.

6.2.2 Substance lists

There are numerous substance lists that result from approaches as described above and that are publically available. A compilation of lists was already provided by Nendza et al. (2010) and BIO IS and Ineris (unpublished). Out of these studies, information sources and lists have been extracted, however lists covering fewer than two criteria have not been considered here.

Table 8 compiles and evaluates the most important substance lists covering P, B and T, respectively vPvB criteria. Long-range transport is generally not considered with two exceptions: The US and the Canadian Environmental Protection Agencies also consider the half-life in air among other half-life thresholds in different environmental media that is the criterion for long-range transport under the Stockholm Convention (see Table 2 for the criteria of the US EPA PBT Chemical Program and the Canada Toxic Substances Management Policy).

The combination of persistence, bioaccumulation and toxicity is addressed as concern by all the lists. All lists refer to numerical criteria. The lists mostly refer to the PBT criteria of the respective regulation. The toxicity parameters used represent a wide variety of effects on humans and the environment: ranging from aquatic EC50, to NOEC, CMR, EDC and neurotoxicity etc. For instance, the SIN list – besides substances passing the PBT and vPvB thresholds – also contains substances that are carcinogenic, mutagenic and toxic to reproduction (CMR) and also includes substances that raise an equivalent level of concern, e.g. as endocrine disruptors. Also the OSPAR List of Chemicals for Priority Action applies the PBT criteria and additional criteria for hazardous substances, such as CMR or chronic toxicity for mammals. Strempel et al. (2012) found that the SIN list of 2011 contains only 5% of potential PBT chemicals according to REACH thresholds, whereas in the list of priority substances of the OSPAR convention (OSPAR 2011), almost 50% are potential PBT substances. This is most likely due to the different underlying P, B and T criteria and thresholds of these lists.

The REACH regulation only considers P, B and T properties but not LRT, and in addition applies lower thresholds for PBT-substances than the Convention Therefore, the different lists of the ECHA such as the list of substances proposed for the adoption to the Candidate List or Registry

of Intentions, the list of substances of very high concern (SVHCs) or Candidate List and the recommendations of substances for Annex XIV or Authorisation List, cannot be used for the identification of POP proposals directly; instead chemicals in these lists need to be evaluated for the POP criteria according to the thresholds of the Convention in the same way as the other lists.

Table 8 Evaluation of various substance lists according to the POP criteria

#	Name	P-criteria	B-criteria	T-criteria	LRT-criteria
L1	ECHA candidate list of SVHC	According to REACH	According to REACH	According to REACH	Not applied
L2	ESIS: European Chemical Substances Information System / PBT List	According to REACH	According to REACH	According to REACH	Not applied
L3	OSPAR List of Chemicals for Priority Action	According to OSPAR	According to OSPAR	According to OSPAR	Not applied
L4	SIN List 2.0	According to REACH	According to REACH	According to REACH, additionally CMR and endocrine disrupting substances	Not applied
L5	"Trade Union Priority List for REACH Authorisation"	According to OSPAR	According to OSPAR	According to OSPAR, CMR, known and suspected endocrine disruptors, neurotoxic substances, sensitizers.	Not applied
L6	US-EPA: Extremely Hazardous Substance List	Not applied	Not applied	Animal lethality, human toxicity or clinical effects other than death	Not applied
L7	TRI PBT Chemical List	According to US EPA	According to US EPA	According to US EPA	According to the Stockholm Convention, but not necessarily to be fulfilled
L8	CEPA list	According to the Stockholm Convention	According to the Stockholm Convention	Acute and chronic aquatic toxicity	According to the Stockholm Convention, but not necessarily to be fulfilled
L9	Washington State list	According to US EPA	According to US EPA	According to US EPA	Not applied
L10	Priority Substances, Norway	According to REACH	According to REACH	According to REACH	Not applied
L11	List of Potential Substances of Concern to be considered by HELCOM	According to REACH	According to REACH	According to REACH	Not applied
L12	PRIO database	According to REACH	According to REACH	According to REACH, additionally CMR and endocrine disrupting substances	Not applied
L13	List of undesirable substances (LOUS 2009)	According to REACH	According to REACH	According to REACH	Not applied
L14	Finnish Environment Institute: Proposal for a Selection of National Priority Substances	Own P value	According to OSPAR	Own T value	Not applied

#	Name	P-criteria	B-criteria	T-criteria	LRT-criteria
L15	PBT Profiler	According to US EPA	According to US EPA	According to US EPA	According to the Stockholm Convention, but not necessarily to be fulfilled

The POP Protocol lists some more substances than the Stockholm Convention, which are HCBD – hexachlorobutadiene, PCN (polychlorinated naphthalenes), SCCPs (short chain chlorinated paraffins) and polycyclic aromatic hydrocarbons (PAHs). However, the short-chained chlorinated paraffins, the chlorinated naphthalenes as well as hexachlorobutadiene are already under review of the POPRC (see Table 9). PAHs comprise a group of over 100 different chemicals that are produced during the incomplete burning of fuels, garbage or other organic substances. They are short-lived in air, but can be very persistent in soil. PAHs can be detected in many parts of the world, but this is probably because they are released from many local sources. Their potential for airborne long-range transport is probably not high when they are present in the gas phase; this may be different when PAHs are incorporated into soot particles released from combustion processes, but in this case, the PAH problem is related to the health risks of fine particulate matter.

6.3 Conclusions

It is necessary to clearly define the aim for screening a list of substances to identify substances that possibly meet POP or PBT criteria.

From our knowledge gained within the literature research, we conclude that chemical screening is not a new insight tool for determining substances of concern. It has been performed and carried out many times before using various approaches and strategies. A selection of chemicals is the starting point for the screening activities. The screening activity is always part of the identification process of possible substances of concern. Several approaches consist of two subsequent phases, the screening and prioritizing phase focusing on identification of the substances of concern.

The following recommendations for the different phases will focus on how current knowledge can be applied to improve the identification of POP substances.

It makes sense to carry out a pre-evaluation of several databases. Furthermore, it should to be assured that active compounds of pesticides, biocides and pharmaceuticals are included in the screening by a combination of databases (see Rorije et al. 2011). The minimum information for the basic set of chemicals is the CAS registry number, molecular formula, and chemical structure.

The first main phase of the evaluation of the potential substances of concern is the screening step. Through the implementation of the REACH Regulation, the EU will eventually be in the possession of a large amount of chemical property data. This data could be used to assess any further candidates for the inclusion into the Stockholm Convention and the POP Protocol. Pesticides, biocides and pharmaceuticals have to be included to the initial data set as well.

Several approaches identify chemicals of concern such as PBT, vPvB, P&T or others but which do not fully meet criteria of Stockholm Convention. Taken together they are also very diverse in terms of scope, criteria, design and method. Identification of POPs and the evaluation of their

impact are more complicated than those for other chemicals and remain a challenge. The main reason for this is that POP assessment generally requires more data and includes a further property, LRT. Although it has been internationally recognized since quite some time that there is a need for strict control of POPs, hardly any study has made substantial effort to create a POP candidate list that includes all the four POP criteria, P, B, T and LRT, according to the Stockholm Convention threshold values.

One disadvantage of many lists is that the number of the potential substances of concern is too high to be processed by the following assessment procedure. Hence, a further prioritization of the mentioned substance lists could be a useful extension and possibly a better starting point for the assessment procedure of the Stockholm Convention.

7 Ex-post analysis

In the ex-post analysis the decision-making process dealing with inclusion of new chemicals in the Annexes of the Stockholm Convention was analysed. Scientific, socio-economic and political decision-making aspects were considered. Especially the fulfilment of the screening criteria from the Annex D was examined. Here the most important questions to answer were whether the numerical B, P and LRT criteria (Table 1) were fulfilled. If this was not the case, the compensating evidence was analysed. The consistency of the decision-making process was thus evaluated. In some cases socio-economic aspects of the decision-making were evaluated together with the stakeholder influence on the decision-making process. The focus was set on how controversial points within the screening, risk profile and socio-economic assessment were overcome. Some of the results of the Ex-Post analysis have already been cited above (see chapter 4, Models).

7.1 The initial twelve POPs

The initial 12 POPs ("dirty dozen") were considered for the Stockholm Convention without a risk profile and consideration of the socio-economic effects, as foreseen in the Article 8 of the Convention. The substances were included to the convention as initial substances because of the uncontroversial acceptance unwanted properties of these substances and the threat to the environment caused by them. The "dirty dozen" were already heavily regulated and/or banned in many countries and were no longer protected by patents (Olsen 2003). The distribution of these substances was also limited, as they were mainly used in agricultural applications as pesticides. The chemical industry was not strongly involved in the Convention negotiations, because the substances of concern were largely considered to be non-marketable. They were either no longer in widespread use or production, and had even been replaced in the market by more profitable alternatives (Kohler and Ashton 2010). The Convention negotiations were characterized by a strong participation of different NGOs. Over 100 NGOs were participating in important negotiation steps and were able to affect the final outcome of the convention (Olsen 2003). A clear representation of all the facts of the decision-making process upon including the first twelve chemicals into the Stockholm Convention is untraceable or not identifiable. However, a document from 1995 (Ritter et al. 1995) has compiled a summary of the available information on the chemistry, toxicology, relevant transport pathways and the origin, transport and disposition of the substances concerned. The twelve POPs were characterized by their persistence, their ability to biomagnify and bioconcentrate under typical environmental conditions, potentially toxicological effects and to long-range transport. Even though Risk

profiles were not compiled for the first twelve substances, risk estimates for certain "dirty dozen" chemicals are available.

7.2 New POPs and POP candidates under review

At the fourth meeting of the COP held from 4th to 8th of May 2009, nine more substances (so-called "9 new POPs") were added of the annexes of the Convention. Another substance, endosulfan, was considered by the COP at its fifth meeting in April 2011. Currently five chemicals are still under review. The inclusion of these new POPs in the Convention relied predominantly on the science-based criteria, but was also based on the innovative approach of taking into account socio-economic considerations later in the assessment (Olsen 2003).

There are some strong differences between the "new POPs" in comparison to the initial twelve POPs. The new POPs are typically used for many different applications and as components of a variety of different products in many different industrial branches (Kohler and Ashton 2010). Due to this fact more industry branches are conflicted with the restrictions that inclusion of these substances in the Stockholm Convention would bring about. The participation of the chemical industry in the negotiations of inclusion of new chemicals in the convention has risen since the "dirty dozen", as the chemicals in question are still in widespread use (Kohler and Ashton 2010).

Moreover, for the recent chemicals (10 new POPs and 5 POP-candidates) only 4 Parties (EU, Norway, Sweden and Mexico) submitted proposals to the Secretariat for inclusion in Annexes A, B or C of the Convention. About half of these proposals originate from the EU (Table 9). This indicates that the EU is a strong actor and a key player when it comes to the inclusion of new chemicals to the convention. The EU took a demanding position already in the negotiations preceding the Stockholm Convention adoption. This is due to the fact that when it became clear that only the 'dirty dozen' would be included in the Convention, it was more important for the EU to make progress in the negotiations, and the EU then strived for a flexible procedure to add new chemicals to the list afterwards. POPs management was already covered by EC legislation at the time of the negotiations (Delreux 2009) and the new POPs have already been subject to prohibition or severe restrictions in the EU.

Considering the large number of members of the COP (more than 150 signatories), that have the right to make proposals for POP candidates, only few actors have been interested in or are capable of proposing new chemicals for regulation by the Convention: In June 2010, the Stockholm Secretariat invited Parties and observers to provide information related to application of Annex D criteria in the regulatory and assessment schemes of chemicals (Article 3, paragraph 3 on the prevention of the production and use of new chemicals exhibiting characteristics of POPs and paragraph 4 on assessing and controlling chemicals in use).[44] Among the 47 submissions, 18 respondents have no regulatory framework for chemicals with POP characteristics. With reference to chemicals with characteristics of POPs, 23 respondents had regulatory systems for new pesticides, and 18 for new industrial chemicals. Similarly, 21 respondents have regulation for existing pesticides and 20 for existing industrial chemicals in

[44] http://chm.pops.int/Convention/POPsReviewCommittee/POPRCMeetings/POPRC6/POPRC6Followupcommunications/RegulatoryandAssessmtSchemesArt3p3and4Request/tabid/1193/Default.aspx; last accessed 27.9.2012

place respectively. Furthermore, 14 respondents[45] have regulatory systems in place for all of the abovementioned four categories, of which, except for the United States of America, all are parties to the Convention (UNEP COP 2011). These countries would basically be in the position to bring forward POP proposals. In Canada, for example a systematic hazard assessment is performed within the regulatory assessment scheme (see also section 2.3): PBT characteristics and even long-range transport are taken into account. Japan as well assesses persistence and bioaccumulation, however, a systematic risk assessment is not performed.

Controversies in chemical risk assessment, especially in not fulfilling the screening criteria, were assessed. These controversies are further referred to as "scientific controversies". If the screening criteria according to the Annex D were not fulfilled, we analysed which findings were important in compensating for the inadequate results. In 7 of the 10 cases of new POPs at least one of the numerical screening criteria was not fulfilled according to the risk profiles; examples thereof are listed in Table 9. For possible POP candidates the evaluation is more difficult, as many of them do not yet have an accepted risk profile[46]. As most of the lists screening PBT and LRT substances use this or similar kind of screening criteria, it can be concluded that some potential POPs might not pass the screening, if only the numerical criteria are used.

All substances that have been examined to date with reference to the criteria in Annex D have been evaluated to fulfil the numerical or the alternative criteria and consequently passed on to the next step in the process, the development of the risk profile.

Table 9 Evaluation of the ex-post analysis. The parentheses () indicate in the case of pentachlorophenol that PCP itself does not fulfil the full set of Stockholm Convention thresholds, but its transformation product pentachloroanisole does fulfil the criteria.

Substance	Annex	Proposal submission by	Meets numerical Annex D criteria	Meets alternative Annex D criteria
Alpha hexachlorocyclohexane (-HCH)	A	Mexico		✓
Beta hexachlorocyclohexane (-HCH)	A	Mexico		✓
Lindane	A	Mexico		✓
Chlordecone	A	EU		✓
Hexabromobiphenyl (HBB)*	A	EU	✓	✓
Endosulfan	A	EU		✓
Hexabromodiphenyl ether and heptabromodiphenyl ether	A	EU		✓
Pentachlorobenzene	A	EU	✓	✓
Tetrabromodiphenyl ether and pentabromodiphenyl ether	A	Norway	✓	✓

[45] Bulgaria, Canada, EU, Finnland, India, Japan, Latvia, Netherlands, New Zealand, Norway, Philippines, Poland, Romania, Thailand

[46] State of September 2012

Substance	Annex	Proposal submission by	Meets numerical Annex D criteria	Meets alternative Annex D criteria
Perfluorooctane sulfonic acid, its salts and perfluorooctane sulfonyl fluoride (PFOS)	B	Sweden		✓
Short chain chlorinated paraffins (SCCPs)	under review	EU		✓
Hexachlorobutadien HCBD	under review	EU	✓	✓
Polychlorinated naphthalenes (PCN)	under review	EU	✓	✓
Pentachlorophenol (PCP), penta-chloroanisole and other derivates	under review	EU	(✓)	✓
Hexabromocyclododecane (HBCDD)	under review	Norway		✓

Kitano et al. (2007) reported that five substances (PFOS, -HCH, -HCH, Lindane and octabromo diphenyl ether[47]) did not fulfil the screening criteria for bioaccumulation.. According to their statement other reasons for concern compensating for the insufficient of numerical BAF, BCF or K_{ow} were

- long half-life,
- mechanistic explanation why K_{ow} is not applicable or why BCF and BAF not fulfilled,
- evidence of biomagnification,
- risk analysis: comparison of detected environmental concentrations and the strength of (eco)toxicity,
- detections in biota and human body,
- exposure on developmental stage.

Due to the surface-active properties of PFOS, the K_{ow} cannot be determined for PFOS. Reported BCF values for bluegill sunfish and rainbow trout were around 3000 L/kg_{ww}, clearly below the set limit of 5000 L/kg_{ww}. In the risk profile it was stated that the BCF, which accounts only for the uptake of chemicals via water, clearly underestimates the bioaccumulation of PFOS, as the main uptake source of the chemical is diet. The insufficient numerical criteria were compensated for by results that demonstrated low elimination rates of the substance, as well as developmental effects on mammals at low levels. Additionally, monitoring data from Arctic and other places demonstrated the bioaccumulation potential.

Endosulfan did not pass the bioaccumulation criteria of the Convention either. The bioaccumulation was observed to occur mainly in terrestrial species. K_{ow} was hence an insufficient bioaccumulation descriptor. If K_{oa} values were taken into account, under the assumption that the threshold would be the same as for K_{ow}, the endosulfan showed a clear evidence of bioaccumulation. BCF and BAF results typically refer to measured bioaccumulation in aquatic species. In those species the measured values were under the convention threshold.

[47] Octabromodiphenyl ether is not added to the Convention, but its congeners hexa- hepta-, tetra- and pentabromodiphenyl ether are listed to Annex A of the Convention

Nevertheless the modelled BMF of endosulfan for terrestrial food webs showed a strong bioaccumulation potential (UNEP POPRC 2009b).

For chlordecone the LRT criteria, $t_{1/2}$ air > 2 d, could not be evaluated. There were also no environmental measurements of chlordecone from remote regions. The assessment of the LRTP was done with environmental modelling and through assessment of the physico-chemical characteristics of the chemical. The modelling results with the OECD P_{ov} and LRTP Tool indicated that LRT is likely to occur. As lack of scientific evidence does not prevent substance from proceeding in the Stockholm Convention decision-making process, chlordecone passed thus the screening criteria (UNEP POPRC 2007). Listing chlordecone on Annex A was nevertheless easier than for PFOS, due to the decreasing production in earlier years (Wang et al. 2009).

In case of PFOS, the former world's largest producer delivered the POPRC with PFOS relevant data, which enabled balanced evaluation of the chemical properties and usage patterns, including the adverse effects of the chemical (UNEP POPRC 2006). As it is difficult get information about such data, the co-operation of industry helped greatly in forming the risk profile and socio-economic assessment of PFOS. Such support finally made it possible, that the PFOS was added to the Annex B of the convention, even though many other industrial groups still using PFOS in various products were against its addition to the convention.

7.3 Conclusions from ex-post-analysis

When a Party intends to submit a POP proposal care should be taken that the information on the substance is comprehensive, relevant and reliable; a good portfolio of scientific evidence is very important. To make the assessment process more robust, additional information such as measurement data is necessary. If the thresholds are not met, a conclusive discussion about the reasons needs to be included. If the proposed chemicals tend to bind to other than lipid tissue, have surface-active properties or are taken up by the organisms rather by diet than by adsorption, many traditional measurement and estimation methods for bioaccumulation do not deliver conclusive results. Due to these reasons it is also possible that in screening exercises some potential POPs are not identified.

Parties to the Convention are able to influence the decision-making process by proposing new chemicals for inclusion. The countries with already strict chemical legislation are more likely to propose new candidates, if their national regulation or other binding agreements already covers these candidates. In case of EU this seems to be the case (see also Table 9).

Dynamics of the interest groups (parties or observers) are also able to form the decision-making process: The interest groups are able to deliver information about the substance and its usage, the possibilities to replace the substance, its adverse effects, and the regulations today etc. This information enters the Risk assessment of the POPRC. The case of PFOS shows the importance of participation of different actors to the decision-making process. For a party which intends to propose a POP candidate, it might be of importance to build alliances in order to find as much support for the substance substitution or replacement as possible. Importantly, industry can, in the role of observers, affect the perception of the matter.

8 Summary of the of the first working package

A key question for the future work under the Stockholm Convention is how many additional POPs are to be expected, given the fact that there are tens of thousands of chemicals on the market globally. In other words, concepts and tools are needed that make it possible to screen large numbers of chemicals for substances with POP properties. The Convention does not lay down any particular obligation concerning addition of chemicals to it but allows any Party to propose new chemicals for inclusion in the Convention. Here we summarize the results from the different steps and evaluate the suitability of different approaches for identification of potential POP candidates focusing on two questions:

- Why are there only few POP candidates that have been identified recently? What are the difficulties that may impede identification of new POP candidates?
- What alternatives or other methodologies are used to identify new POPs candidates?

For the estimation of P, B, T and LRT properties, there are generally several **methods** available. The availability of experimental data is generally low, or the data quality varies a lot. Mostly, data are available for "simple" methods such as $\log_{Kow}$ for estimating bioaccumulation and for acute toxicity. However, these data only provide limited information on the POP characteristics. Generally, screening-methods have a high potential for false positive results. For conclusive identification of new candidate-POPs more experimental data needs to be created. For this purpose it is recommended to use well established methods, such as those with acknowledged OECD protocols, which are however more extensive expensive and time-consuming.

Models may in some cases help in data creation. This possibility has the advantage of being typically less expensive and time consuming; additionally no living organisms are needed for data creation:

- Mass balance and QSAR-based models can be used to screen chemicals, and to prioritize these chemicals for further detailed assessment. Several models for P, B, T and LRTP characterization exist. The models developed by the US EPA have been widely used and are regarded as valuable tools among the scientific community. The OECD P_{ov} and LRTP Tool has been cited in most of the POP risk profiles, indicating its importance as a POP-modelling tool. These models only need CAS-number and SMILES-code and make possible an evaluation of large amounts of chemicals, but are always associated with uncertainties.
- Highly resolved environmental fate models can further support risk evaluation by creating a picture of the global environmental fate of the chemical according to its emission patterns, partitioning and transport behaviour. The model results can be used among others for confirmation of existing environmental data, benchmarking or understanding the long-term behaviour of the chemical in the environment.

The evaluation of the m**onitoring programmes** clearly showed that there is no programme or activity explicitly dedicated to identifying new POPs. However, monitoring programs play a key role in identifying chemicals that are persistent and capable of long-range transport. However, most programs only observe already restricted substances.

A monitoring programme that aims to identify new POPs requires the sampling and analytical techniques for the suspected substances to be available, because the substance properties influence the environmental media to be monitored, the sampling conditions as well as the

analytical methods. Different substance properties might necessitate the adaptation of current sampling techniques. The need of information sharing furthermore covers data and information on production quantities, application patterns and exposure pathways. Thirdly, a promising way to find information on pollutants not yet restricted by the Stockholm Convention is to evaluate individual studies published in the scientific literature.. Unfortunately, these data are often spatially and temporally limited. The research for this information is quite elaborate, because a central source for summarized information is often not available and one has to evaluate the individual papers published in the scientific literature.

In order to compile and coordinate the information input, further activities are needed in order to involve information of the ECHA, the NORMAN network etc. and the data of individual studies. Therefore, knowledge and resources should be concentrated and coordinated in the best case by an international body or within the Convention.

Numerous s**creening activities** have already been performed mostly with the focus on identifying potential PBT substances. Rarely, the LRT criterion was considered. The screening activities comprise firstly the choice of a basic set of chemicals that should also include the active compounds of pesticides, biocides and pharmaceuticals. As for the screening step, the criteria and thresholds applied determine the type and number of chemicals identified.. Identification of POPs and the evaluation of their impact are more complicated than those of other chemicals because this requires more data and includes a further property, LRT. One disadvantage of many lists is that the number of the potential substances of concern is too high to be processed by the following assessment procedure. Hence, a further prioritization of the substance lists is in some cases performed by adding criteria such as HPV chemicals, ranking, setting up thresholds, etc.

The e**x post analysis** of the decision-making process dealing with inclusion of new chemicals in the Annexes of the Stockholm Convention showed that for submitting a possible POP, care should be taken that the information on the substance is comprehensive, relevant and reliable; a good portfolio of scientific evidence is very important. To make the assessment process more robust, additional information such as measurement data is necessary. If the thresholds for the given substance are not met, a conclusive discussion of the reasons needs to be included. If the proposed chemicals tend to bind to other than lipid tissue, have surface-active properties or are taken up by the organisms via by diet rather than by adsorption, many traditional measurement and estimation methods for bioaccumulation do not deliver conclusive results. Due to these reasons it is also possible that in screening exercises some potential POPs are missed.

Parties to the convention can influence the decision-making process by proposing new chemicals for inclusion. Countries with strict chemical legislation are most likely to propose new candidates, if their national regulation or other binding agreements already cover these candidates (one example is the EU, who proposed nine of the 15 POPs evaluated in the ex-post analysis).

For each chemical, the entire process takes several years. Yet, there are many thousands of unevaluated chemicals on the market. Therefore, a key question for the future identification and regulation of POPs under the Stockholm Convention is how many potential POPs exist and how they can be identified.

The results summarised above were subject of a brainstorming meeting (Cf. Annex 12.2) in order to support with the development of a strategy that helps to identify possible POP candidates.

9 Development of a strategy for identifying potential POP candidates

9.1 Contents and structure of the strategy

In the following chapters, we propose a strategy for identifying potential POP candidates. The strategy describes a methodological approach to evaluating currently used chemicals in order to identify substances with POP characteristics for initial proposals to the P**hase 1** of the Stockholm Convention process (cf. Figure 1, page 7). The strategy includes activities to support SC-phases 2–5 (cf. and activities to find data for individual substances referring to annex E and F criteria)

Thus the strategy is intended to enable the German Federal Environmental Agency to take part in the assessment procedure for the nomination of new POPs and to assist the EU with possible further POP proposals..

The strategy also includes activities to support SC-phases 2–5 (cf. and activities to find data for individual substances referring to annex E and F criteria]. Socio-economic aspects are addressed to a minor extent only. Such aspects are treated in detail within the socio-economic analysis, which takes place after screening (Annex D) and Risk Profile (Annex E) are completed (see Figure 1, page 7). Likewise, the “strategy” does not aim to give an assessment method resulting in information for a risk profile//management dossier.

The aim of the strategy is to identify chemicals for a proposal as POP candidates. The proposed chemicals should be “living” chemicals, which means that they are being used today, preferably in high quantities so that their restrictions will be of high ecological benefit.

The strategy is based on the findings of the first work package in this project where existing approaches and strategies for POP identification were analysed.

We recommend a stepwise approach:

1. Screening: Evaluation of chemical substances with regard to POP properties and indication of environmental and/or socio economical relevance.
2. Use of interfaces and synergies to collect additional information for substances passing the first step and to further evaluate their POP status

In more detail, these two steps include

1. Screening
    a. Preparation Phase: Selection of chemical databases
    b. Screening Phase: Screening of the selected basic set of chemicals according to their PBT and LRT properties with selected thresholds
    c. Filtering Phase:
        – Check of more stringent POP threshold value

- Check of HPVC, High Production Volume Chemicals
- Check of REACH-preregistered and registered substances and substances identified by industry to be registered by 31 May 2013

2. Use of interfaces and synergies (Additional Recommendations)
    a. Check of toxicity data
    b. Check of monitoring data
    c. Cross-Checking to regulations
    d. Cooperation with other Stakeholders (Additional Recommendations) (e.g. determination of planned activities of other parties and NGOs with regards to POPs and POP proposals)
        - Interconnection of the implementation agencies
            - PBT Group (e.g., upgrade of the chemicals on the PBT list with LRT, P&B assessment according to Annex D (SC) thresholds, updating of methods and criteria etc.)
            - Pesticides, Biocides, Pharmaceuticals
            - EU Water Framework Directive (WFD) etc.
        - Institutional cooperation
            - Stockholm Secretariat, Basel and Rotterdam Convention
            - EU, EEA, NGOs, developing countries etc.

Figure 3 illustrates how the strategies for identifying potential POP candidates are interlinked.

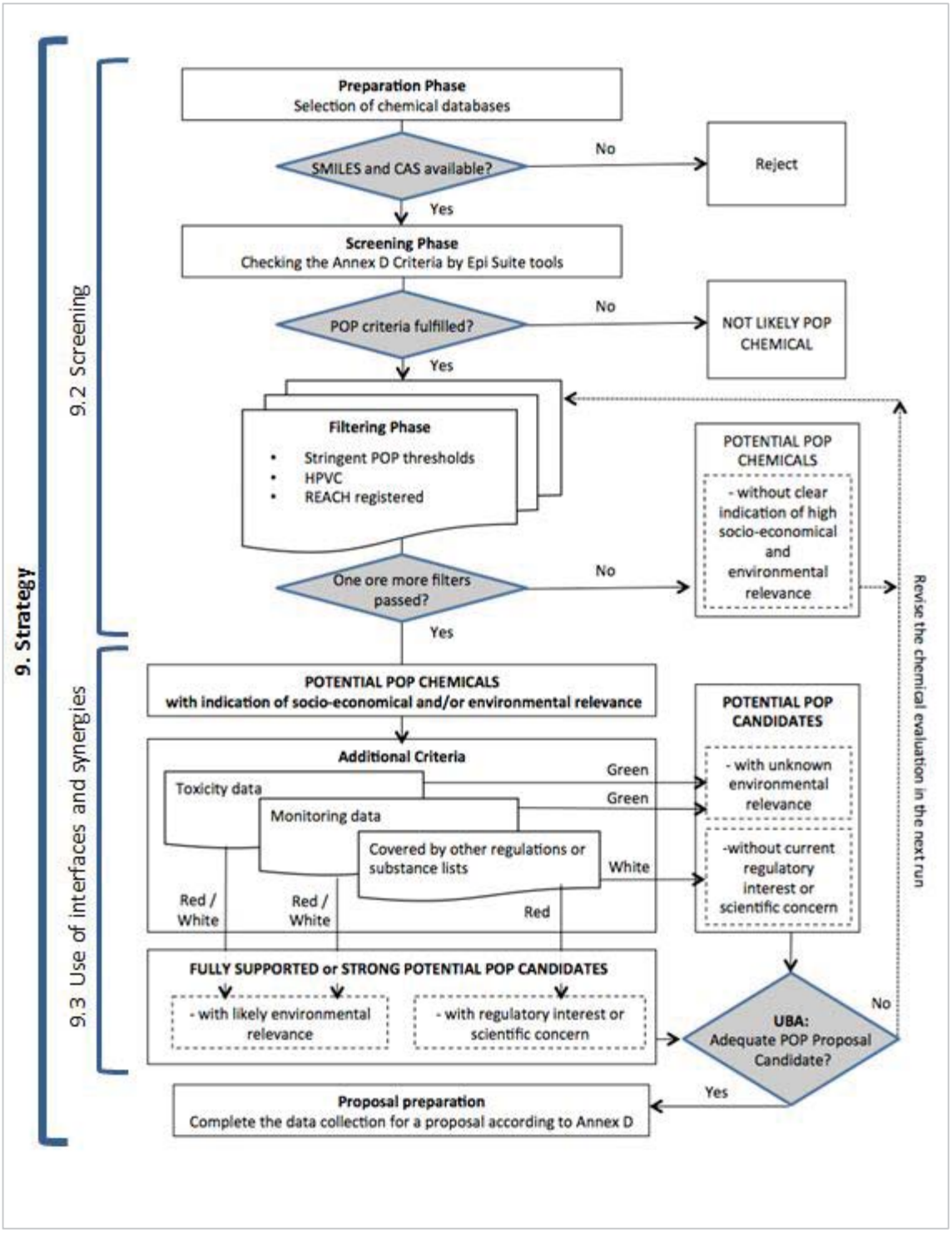


Figure 3 The strategy for identifying potential POP candidates. The decision-making and meaning of the colour labelling (red/white/green) within use of interfaces and synergies is discussed in chapter 9.3 (Source: Öko-Institut / ETH Zürich)

9.2 Screening

9.2.1 Preparation phase: selection of chemical databases

A selection of chemicals is the first step and the starting point for the screening. The screening is usually part of the identification process of possible substances of concern.

The minimum information about a chemical that is needed for a screening exercise based on estimated property data is the CAS number and the SMILES code (see also 6.2.1, page 40). The CAS number specifies the identity of the chemical and the SMILES code describes the chemical structure. The database should be as comprehensive as possible, so that as many chemicals are covered by interest.

The preparation phase "Selection of chemical databases" is evaluated using table 10. "Yes" should be given if the CAS number and the SMILE code of the substance have been identified and the substance will go to the next step. If these conditions are not fulfilled then their substances will no longer to be considered. Ambiguous CAS numbers (e.g. mixtures) or chemicals outside of the applicability domains of the modelling tools should not proceed to the next step either.

Table 10 Summary of the essential information required for the preparation phase

Info Box Preparation Phase (selection of chemical databases)		
Applicability	CAS number and the SMILES code	
Relevance	Confirmation of the chemical identity (CAS number) and molecular structure information (SMILES code); deletion of ambiguous entries and substances out of applicability domain of the models (if they are being used for in the screening phase).; validation of the generated data	
Sources of information	The recommended databases are publicly accessible. For instance, the SMILECAS database included in the EPI Suite software; the existing chemicals database provided by the JRC in EINECS. As some of them are regularly updated, no current summary of the lists is provided. Databases on pesticides, biocides and pharmaceuticals. Property estimation with tools included in the EPI Suite software. Links to the web pages on chemical databases (as well for pesticides, biocides and pharmaceuticals) are compiled in Annex 12.1, p. 92 in Table 21	
Evaluation	Are CAS number and the SMILES code available and adequate?	
	"**Yes**" should be given if the CAS number and the SMILE code of the substance have been identified.	"**No**" should be given if • the CAS number of the substance has not yet been identified. • the CAS is ambiguous, e.g. refers to mixture of chemicals • the chemical is a congener or isomer of one of the acknowledged POPs. • chemicals are outside the applicability domains of the property estimation methods, for example inorganic and metal organic substances and salts (EPI Suite)

9.2.2 Screening phase of the selected basic set of chemicals

As the first priority, the substances are checked for chemical characteristics of all four Annex D criteria as defined under Stockholm Convention. In Annex D of the Stockholm Convention, threshold values are defined for three of the four screening criteria, namely, for persistence, bioaccumulation and long-range transport. For toxicity, Annex D refers to evidence of adverse effects to human health or the environment but does not specify a threshold value. We recommend using the toxicity thresholds from the REACH regulation (EU 2006) and referring to marine or freshwater species (aquatic toxicity) in the screening phase. According to REACH, a substance fulfils the toxicity criterion if the long-term no-observed effect concentration (NOEC) or EC50 for marine or freshwater organisms is less than 0,01 mg/l or if the short-term toxicity value (LC_{50} or EC_{50}) is less than 0,1 mg/l.

As for the property estimation methods, we recommend to use the collection of estimation tools of Epi Suite, which is software package from the US EPA which contains several modules for the estimation of physicochemical properties, environmental fate and ecotoxicity and which are freely available. BIOWIN3, ECOSAR, BCFBAF and AOPWIN cover all properties needed for the assessment of POP properties (P as biodegradability t1/2 in water (d), T as NOEC/ChV and LC50/EC50 (mg/L), B as BCF or BAF and LRT as t1/2 in air (d)). The estimation methods and their implication are described in more details in section 4.2, page 23.

Substances pass the screening if the thresholds for P, B and LRT properties exceed the threshold value and T property is below the threshold value (yes). If one or more POP properties fail to pass the threshold, the substance does not pass the screening (no).

Table 11 Summary of the essential information required for the screening phase

Info Box Screening Phase				
Applicability	Annex D of the Stockholm Convention and toxicity thresholds from the REACH regulation			
Relevance	The substances are checked for chemical characteristics of all four Annex D criteria as defined under Stockholm Convention.			
Sources of information	EPI Suite screening-level tool (Estimation Programs Interface Suite for MS Windows, v4.10). Links to the web pages on tools are compiled in Annex 12.1, page 92 in Table 21			
Evaluation	Do the chemicals meet the POP criteria according to The Annex D?			
	"**Yes**" should be given if all criteria are fulfilled "**No**" should be given if only some or none of the criteria is fulfilled			
	Persistence (P)	Bioaccumulation (B)	Long-range-transport (LRT)	Toxicity (T)
	half-life in water > 2 months	aquatic BCF or BAF > 5000	half-life in air > 2d	NOEC (long-term) or ChV[48] < 0.01 mg/L or EC50 or LC50 < 0.1 mg/L for marine or fresh-water organisms

[48] Chronic Value – estimated with ECOSAR, see section 4.2.2, page 24

It is important to note that Annex D of the Stockholm Convention provides the option that for all four properties other evidence can also be used for the assessment of whether or not a chemical exceeds the screening criteria (section 7.2, page 53). If the proposed chemical tends to bind to other than lipid tissue, has surface-active properties or is taken up by the organisms rather by diet than by adsorption, many traditional measurement and estimation methods for bioaccumulation do not deliver conclusive results (see also section 7.3, page 56). Due to these reasons and other limits of the screening models (section 4.2, page 23) it is also possible that in screening exercises some potential POPs are ignored (cf. chapter 7). If the thresholds are not met due to known limitation of the screening models and if other evidence exists that the POP criteria are fulfilled, the substances should proceed to the filtering phase.

9.2.3 Filtering phase (reasons for high concern)

If the Screening Phase identifies POP-like substances, these should be evaluated according to additional criteria that make it possible to identify "living" chemicals and to identify lack of information such as monitoring data that are important for an initial proposal under the Stockholm Convention.

For the evaluation of possible POP chemicals, the following three priority substance-specific criteria should be checked:

1. Check of stringent POP threshold value
2. Check of HPVC, High Production Volume Chemicals
3. Check of REACH-registered substances

All filtering criteria "Stringent POP threshold value", "High Production Volume Chemicals" and "REACH-registered substances" are equally important.

Potential POP candidates identified in this work have passed the screening and are additionally either HPVCs, identified for registration under REACH or pass the Stringent POP threshold values. The aim of the filtering phase is to identify potential POP candidates with an indication of socio-economical and/or environmental relevance.

For chemicals which have passed more than one filter, a clear indication of high socio-economical or environmental relevance is given. Such chemicals will go to the next step. Chemicals which do not pass any of the three filtering criteria can be set aside until the next chemical evaluation (see Figure 3).

This approach is based on a strict division between substances that do fulfil the criteria and those that do not.

The application of the filtering criteria to chemicals evaluated as "yes" or "no" may be helpful in the prioritising of action needs. Substances which are exceeding all criteria with "yes" is given highest priority. The result is a filtering profile of the substance.

Table 12 Filtering profile for a substance

Chemical		Stringent Pop	HPVC	REACH	fulfills "X" criteria which are set
CAS	name				
Example.....	*####*	*(yes)*	*(no)*	*(no)*	*(1 from 3)*
....	....				

In the following, these three filtering criteria are described.

Stringent POP threshold value

When a Party submits a possible POP, care should be taken that the information on the substance is comprehensive, relevant and reliable; a good portfolio of scientific evidence is very important. The models used as screening tools are robust enough for screening large amount of chemicals but also lack sensitivity of more refined models. To avoid cases where the Annex D criteria are only slightly exceeded and the obtained results possibly controversial, we recommend a more stringent POP threshold as the first filtering criteria to prioritize the screened substances. This criteria presented by the authors is aimed at giving greater importance to possible candidates and greater objectivity to the choices made.

A suggested set of more stringent thresholds comprises biodegradation half-life in water exceeding 180 days, a BCF or BAF exceeding 20 000, and a half-life in air exceeding 10 days; the toxicity thresholds remains unaltered (Scheringer et al. 2012).

Table 13 Summary of the essential information required for "Stringent POP threshold value"

Info Box Criterion "Stringent POP threshold value"				
Applicability	Giving greater importance to possible candidates and greater objectivity			
Relevance	Less controversial screening			
Evaluation	Does the chemical meet the Stringent POP threshold value?			
	"Yes" should be given if all criteria are fulfilled		"No" should be given if only some or none of the criteria is fulfilled	
	Persistence (P)	Bio-accumulation (B)	Long-range-transport (LRT)	Toxicity (T)
More stringent POP threshold value	> 180 days	> 20 000	>10 days	NOEC or ChV[49] < 0.01 mg/L or EC50 or LC50 < 0.1 mg/L for marine or freshwater organisms,

Check of HPVC, High Production Volume Chemicals

There are no harmonized definitions of which amounts are a "high" or "low" amount. Under REACH, registration requirements distinguish between amounts of 1 to 10, 10 to 100, 100 to 1 000 and above 1 000 t/a. The amounts should be considered in relation to the dangerous properties: for a substance of very high concern (SVHC) an amount of 1 t/a may already be very high.

High use amounts can enhance the importance of some substance-specific criteria. The higher the resource consumption of a substance, the higher the weight of these criteria in the overall evaluation is. In particular if large amounts of the substance are produced or used. Vice versa, if a substance is used in small amounts, the importance of the criteria "resource consumption" should be decreased. The use of amount as an isolated indicator is fairly meaningless.

[49] Chronic Value – estimated with ECOSAR, see section see section 4.2.2, page 24

However, the check whether the substance is a high production volume chemical makes it possible to identify "living" chemicals that are used in high quantities. Additionally, for substances which are according to the screening fulfil the POP properties, high production volumes present an ever larger risk of global contamination. If HPVC are found to exert unwanted environmental effects, restriction of their usage would have a high environmental relevance. There are lists of h**igh production volume chemicals** of the OECD, ESIS and the U.S. that are publically available.

The lists apply the same or similar volume thresholds such as production of 1 000 tonnes per year in at least one member country/region according to the OECD HPV list, or production or import volume in excess of 1 000 tonnes per year according to the ESIS HPVCs list; the High Production Volume Information System (HPVIS) of the US EPA challenges companies to make this data publicly available on chemicals produced or imported into the United States in quantities of 1 million pounds or more per year, which is about 450 tonnes.

Table 14 Summary of the essential information required for "HPVC"

Info Box Criterion HPVC		
Applicability	High production volume chemicals	
Relevance	Living chemicals. Restrictions lead to large environmental impact. High use amounts can enhance the importance of substance-specific criteria.	
Sources of information	OECD HPV list; ESIS HPVCs list; HPVIS of the US EPA. Links to the web pages on chemical databases are compiled in Annex 12.1, page 72 in Table 19	
Evaluation	Is the substance a high production volume chemical?	
	"Yes" should be given if the substance is mentioned in one or more lists	**"No"** should be given if the substance is not mentioned in any list

Check of REACH-registered substances

The registration under REACH or the identification for registration[50] is another indicator that the substance is currently used in considerable amounts. Till now (as of June 2010), substances have to be registered that are manufactured or imported at 1000 tonnes or more per year. Carcinogenic, mutagenic or toxic to reproduction substances need to be registered above 1 tonne per year, and substances dangerous to aquatic organisms or the environment above 100 tonnes per year. REACH registration is an indication of use in high amounts or cause of considerable adverse effects and thus, as for HPVC, an indication of higher socio-economical and/or environmental importance.

Besides, the **registration is an indicator** that additional information to the substance is basically available. For registered substances, additional information is available e.g. at the ECHA database for information on registered substances. Detailed information on exposure and risk should be given in the Chemical Safety Report. These are not publically available. However, the Federal Environment Agency as the German REACH competent authority can have access to this information.

[50] Substances identified by industry to be registered by 31 May 2013.

Table 15 Summary of the essential information required for "REACH"

Info Box Criterion REACH		
Applicability	REACH registration status	
Relevance	Substances which are • **registered substances**, or • substances identified by industry to be registered by 31 May 2013	
Sources of information	European Chemicals Agency ECHA The candidate list[51] for authorisation under REACH, by virtue of Annex XIV. Links to the web pages on chemical databases are compiled in Annex 12.1, page 72 in Table 19	
Evaluation	Is the substance registered under REACH?	
	"Yes" should be given if the substance is REACH-registered	**"No"** should be given if the substance is not REACH-registered

9.3 Use of interfaces and synergies

9.3.1 Additional criteria

For substances found to fulfil the POP threshold and filtering criteria, additional information should be collected in order to be able to make a choice for appropriate p**otential POP candidates.** This additional information serves as verification of the already obtained screening results and as a checkpoint for need for generation of more (measurement) data.

Critical information to collect includes toxicity and monitoring data. This data can be used to assure the correctness of the screening results. On the other hand data gaps indicate the need of further research in this field, as both, monitoring and toxicity data are essential at the latest in the risk profile compilation according to the convention. From acceptance point of view substances that are covered by other regulations have most likely the greatest chances to be accepted as new POPs in the Stockholm Convention. Also, most likely crucial information is available for substances already regulated. A third additional criterion we recommend to check for the synergies with other regulations as well as synergies with other scientific substance lists or legislations:

- check of toxicity data,
- check of monitoring data,
- check of other regulations (synergies) or covered by scientific substance lists

With regard to the two substance-specific criteria "Toxicity" and "Monitoring" the authors recommend a further additional check. This is only possible by making some rather rough elaborations. Evaluation of "Toxicity" and "Monitoring" is not as straightforward as the evaluation of the filtering criteria. Instead of clear "yes" and "no" answers, the collected information should be assessed in a more qualitative way, as described below, for each additional criteria. We introduce colour labelling for the evaluation of additional criteria (Table 16).

[51] Not all of the chemicals in the EU candidate list have POPs characteristics in accordance with Annex D, Stockholm Convention

Table 16 Profile for additional information

Chemical		Toxicity data	Monitoring data	Synergies	Evaluation "X/X/X" red/white/green
CAS	name				
Example.....	*.....*	*red/white /green*	*red/white /green*	*red/white*	*(x/x/x)*
e.g. 50-29-3	*DDT*	*red*	*red*	*red*	*3/0/0*

Red label indicates that the substance is most likely POP-like according to additional evidence. **Green** label indicates the opposite, whereas a w**hite** label indicates lack of information or (adequate) scientific evidence.

A **fully supported or strong potential POP candidate** (Figure 3) acquires the label "red" in all three additional criteria categories. Such candidates are found to be toxic according to experimental information; they are found in remote regions and regulated in other legislations.

Even though additional evidence would not be found in all fields (i.e. all or some fields are white, whereas others might be red) the POP proposal candidate can be considered strong due to passing of the POP screening and filter criteria. S**trong potential POP candidates** still lack scientific evidence, and more research is needed to confirm the POP status. A higher number of red labels indicate a stronger potential of the substance for being a POP candidate...

If one or two fields are labeled green, the screening results have been contradicted for toxicity and/or long-range transport. The substance is still considered as p**otential POP candidate** (see Figure 3), due to the passed screening and filtering phases. The UBA can consider to set the candidate should be aside until the next chemical evaluation or to propose it for the Convention (Figure 3). In the meanwhile more research should be done in order to determine the POP status and an expert opinion should be consulted to clarify the contradicting points.

Fully supported and strong potential POP candidates are suitable for submission to the Stockholm Convention. The decision which chemical(s) are the most adequate POP proposal candidate(s) lies finally on UBA. If adequate candidate(s) are found, the data collection for the proposal according to Annex D needs to be completed.

Check of toxicity

Additional information on toxicity should be assessed to check whether the substance leads to "significant adverse human health and/or environmental effects such that global action is warranted" (Article 8 of the Stockholm Convention). In the screening phase, aquatic toxicity was considered by reference to marine or freshwater species. Here, it should be additionally checked whether measured data, also for other species, are available. Toxicity check is of relevance due following reasons: It is essential to present measured toxicity test results or "other reasons of concern" for POP proposals according to Annex D. With measured data the screening results can be either confirmed or contradicted.

As no toxicity thresholds are defined within the Convention, all toxicity-related information from literature and/or databases can be used. The most common toxicity values are LC50 and EC50 for acute toxicity, NOEC and LOEC for chronic toxicity and carcinogenity, mutagenity and reproduction toxicity (See section 3.3, page 17). If possible, ecotoxicological test results should be presented for as many different groups of species at different trophic levels to detect the

most vulnerable organism. Long term testing results should be preferred over short-term tests. Effects on terrestrial species should also be reported if possible.

If good quality data of several trophic levels is available, the confirmation of screening results can be indicated with “red”. If good quality data contradicts the screening results “green” evaluation colour can be given. If only limited amount or no information can be found, it implies that more research should be done in this field to be able to support potential POP candidates and white field code chosen. In uncertain cases white colour code should be chosen as well. The evaluation of the toxicity data and the corresponding colour codes can be found in Table 16. Toxicity information can be searched for in different Databases and publications, e.g. ECHA CHEM, OECD eChemPortal etc.).

Table 17 Summary of the essential information required for “Toxicity”

<table>
<tr><td colspan="4">Info Box Toxicity</td></tr>
<tr><td>Applicability</td><td colspan="3">Availability of toxicity data</td></tr>
<tr><td>Relevance</td><td colspan="3">Control the toxicity of the substance according to (eco)toxicological test results. Check the need for additional measurement data.</td></tr>
<tr><td>Sources of information</td><td colspan="3">Sources of information: ECHA; OECD eChemPortal; JRC Publications Repository; Restricted and Priority Substances Database; IUCLID Chemical Data Sheets.
Links to the web pages on chemical databases are compiled in Annex 12.1, page 92, Table 21</td></tr>
<tr><td rowspan="5">Evaluation</td><td colspan="3">Is good quality data available and are enough trophic levels taken into account?</td></tr>
<tr><td>In accordance with screening</td><td>Contradicting screening</td><td></td></tr>
<tr><td colspan="2">Yes</td><td>No</td></tr>
<tr><td>RED</td><td>GREEN</td><td>WHITE</td></tr>
<tr><td>Red means, that substance presents an environmental concern</td><td>Green means that based on available information, it can be excluded that the substance is toxic. Substance can be set aside until the next chemical evaluation. Expert knowledge should be used for the evaluation.</td><td>White means that the substance has an unknown environmental relevance, more data needed</td></tr>
</table>

Check of Monitoring Data

Detection in remote regions (Monitoring Data): This criterion comprises a check whether there are scientific publications on the detection in the Arctic or Antarctic environment, either in living organisms or the environment (air samples, water, sediment, etc.). Monitoring data are of high importance for the identification of a POP substance. Measured levels of the chemical in locations distant from the sources of its release that are of potential concern indicate the potential for long-range environmental transport. Monitoring data in biota can be used as evidence for bioaccumulation.

If a substance that is characterized as a POP substance in the screening phase and that also fulfils all other additional criteria but lacks monitoring data, it is recommended that the Federal Environmental Agency launches field experiments respectively a measurement campaign. It could be possible that COP would be launched with measurement programme for serious POP proposals.

A check of the availability of monitoring data not necessarily in remote areas but also e.g. in the EU is useful to find out whether the substance is considered as an emerging pollutant/contaminant. The substance thus should also be checked for the presence in the NORMAN database EMPODAT, a database of geo-referenced monitoring / occurrence data on emerging substances and EMPOMASS, a database of mass spectra of unknown or provisionally identified substances. Information exchange and cooperation with NORMAN, the network of reference laboratories for monitoring of emerging environmental pollutants, should further be used if the substance has already been considered by NORMAN.

A monitoring programme that aims to identify new POPs requires the sampling and analytical techniques for the suspected substances as the substance properties influence the relevant environmental media to be monitored, the sampling conditions as well as the analytical methods.

Substance presents an environmental concern if it has been detected in good quality measurement data in arctic regions. The environmental relevance is unknown, if the substance has not been detected in remote regions, but can be expected to be an emerging contaminant, which has not yet reached the remote regions, but has possibly been detected in other monitoring programs. The environmental relevance is also unknown if no monitoring data can be found. The substance is not of environmental relevance if it has been monitored in remote regions, but not detected there a**nd** if the substance is not likely an emerging contaminant (Table 18).

The gathered data is of good quality if there is evidence of certification or documented quality assurance on all stages of the data gathering process. Questionable data quality refers to unknown environmental relevance (label white). In such data some parts of quality assurance process can be documented (but may not be fully described in e.g. published reports). If no evidence of quality assurance or of data compatibility is provided for the monitoring data, the data should not be considered.

Table 18 Summary of the essential information required for "Monitoring"

<table>
<tr><td colspan="5">Info Box Monitoring</td></tr>
<tr><td>Applicability</td><td colspan="4">Monitoring programme that aims to identify new POPs</td></tr>
<tr><td>Relevance</td><td colspan="4">Monitoring data are of high importance for the identification of a POP substance.</td></tr>
<tr><td>Sources of information</td><td colspan="4">ECHA; OECD eChemPortal; NORMAN databases; scientific databases for peer reviewed publications; study of Lambert et al. 2011.
Links to the web pages on chemical databases are compiled in Annex 12.1, page 92, Table 21</td></tr>
<tr><td rowspan="5">Evaluation</td><td colspan="4">Is good quality data and data from remote regions available?</td></tr>
<tr><td colspan="3">Yes</td><td>No</td></tr>
<tr><td>Detected</td><td colspan="2">Not detected: Discuss why</td><td>WHITE</td></tr>
<tr><td>RED</td><td>WHITE</td><td>GREEN</td><td rowspan="2">Unknown environmental relevance, more data needed</td></tr>
<tr><td>Substance presents an environmental concern</td><td>Emerging contaminant, not yet present in remote regions (monitoring data from other regions available) or not analysable with current methods. Unknown environmental relevance</td><td>Most likely not a POP, not of environmental relevance</td></tr>
</table>

The action requirement is highest for red and lowest for green. In case of "white" additional monitoring data is needed. An expert evaluation should be performed always if contradicting (green or yes/white) information is found.

Cross-Checking to regulations

Substances with particularly dangerous properties for man and the environment may already be regulated in different contexts (e.g. legislation or conventions, such as the Helsinki or Stockholm Convention). Corporate instruments may exist for managing these substances as well, such as the "Global Automotive Declarable Substance List" of the automotive industry. Legislation, conventions and private instruments may contain lists of substances to which they refer. If substances are included in any of these regulations, it is a strong indication that it is not sustainable. Additionally, substances, which are already regulated in other conventions or legal frameworks, are more likely to find support in the evaluation process of the Stockholm Convention due to present national, regional or global restrictions.

Unfortunately, there is no universally valid list, but several lists exist. For the evaluation of substances we recommend to use the following lists according to Table 8, page 50. They originate from European or international regulations and conventions.

It is to be noted that the lists are developed for a particular purpose (e.g. environmental protection) or from a particular perspective. Therefore, certain properties may dominate whether or not a substance is included and consequently, the lists are not complete regarding sustainable decisions. They have been thoroughly discussed by experts and politically agreed.

It should also be noted, that none of the list uses the PBT and LRTP properties, as defined in the Stockholm Convention, as criteria. Hence, it is recommended to perform the cross-checking after chemical screening only for those chemicals, which seem to fulfil POP properties as defined in the Stockholm Convention.

To distinguish between synergies with other regulations and compound lists (regulatory interest and environmental concern), the synergies indicated "red" are colored either deep red (regulatory interest; substance is found on one or more of the list described in Table 2, Table 7 and Table 8) or light red (environmental concern; substance is listed in Table 7.

Table 19 Summary of the essential information required for "Regulations"

Info Box Regulations		
Applicability	Substance Lists The use of these lists should be easy as soon as the CAS numbers of the substances have been identified.	
Relevance	Indication of environmentally hazardous properties and intention of national/regional/global regulation.	
Sources of information	The recommended lists are publicly accessible. As some of them are regularly updated, no current summary of the lists is provided. Links to the web pages on regulations are compiled in Table 2, Table 7 and Table 8	
Evaluation	Does the substance appear on regulations?	
	YES	NO
	"**Red**" should be given if the substance is mentioned in one or more lists	"**WHITE**" should be given if substance is not mentioned in any list

9.3.2 Cooperation with other stakeholders (additional recommendations)

Many chemical substances are currently on the market, and only a limited number of those substances have been evaluated on their PBT and POP characteristics. This is because, until recently, placing new and existing substances on the market did not necessitate a comprehensive investigation of the substance PBT or POP characteristics. Thus, for many of these existing substances it is not known if they potentially fulfil the criteria for being considered a POP or PBT chemical.

Besides the additional criteria described above that sets a focus on substances currently in use, the following section lists some additional recommendation that however cannot be implemented all in the short term:

a. We recommend assessing the regulatory and assessment scheme for new industrial chemicals, substances developed for plant protection purposes or biocides. Further evaluation has shown that the PBT evaluation under REACH respectively the registration dossiers are not of adequate quality. Thus the prevention of POP substances to be newly introduced onto the market is not effectively fulfilled.

b. If the regulatory assessment results in the identification of a POP substance into a proposal to the Stockholm Convention, it is not clear how this case proceeds further on the European

c. Generally, further institutional cooperation would substantially support the identification of new POP candidates (as a source of expert knowledge and additional information and validation of the data gathered in the different steps of the strategy). We see possible interfaces with activities and working groups from other legislation, e.g. REACH and the ECHA (incl. PBT expert Group), Pesticides, Biocides, Water Framework Directive, Basel and Rotterdam Conventions. These steps address the national, European and international level and require long-term activities.

- For instance, the ECHA has established a PBT Expert Group. The first meeting of the expert group took place 21.-22. February 2012. Second meeting is scheduled for 13.-15. November 2012. Further meetings are scheduled for 2013. The expert group provides informal and non-binding scientific advice on questions related to identification of PBT and vPvB properties of chemicals and, in particular, on:
    i. questions related to screening methods/activities to identify PBT/vPvB candidates (e.g. for the substance evaluation activities and the candidate list);
    ii. questions related to the development of integrated testing strategies (including specific test methods) for PBT/vPvB properties;
    iii. feedback and recommendations on complex (generic/specific) scientific issues related to information and (tiered) testing needs for potential PBTs/vPvBs (e.g. during development of draft decisions under dossiers or substance evaluation)
    iv. specific question on the interpretation of test data in relation to the identification of PBT/vPvB properties (e.g. during the development of an SVHC dossier).
- The focus of the scientific work of the group is on PBT and vPvB identification. However, the discussions can also cover REACH Art 57(f) cases of equivalent concern.
- Two main elements of the work of this group can be of great interest for the identification of new POP candidates: the discussion of specific substances and the development of specific guidances to identify substances with PBT or vBvP properties. An information exchange between the PBT Expert Group and authorities involved in the identification of news POPs would be of high value for both sides.

d. The key principle of paragraphs 3 and 4 in Article 3 of the Convention is that the national authorities responsible for the approval of existing chemicals must take the POPs criteria specified in Annex D of the Stockholm Convention into consideration whenever decisions have to be made on the approval of new industrial chemicals and pesticides for use, marketing and production. EU member states must also initiate any other measures needed to prevent the production, marketing and use of chemicals with similar characteristics to POPs. Legislation on chemicals and pesticides needs to be developed with regard to taking into account POP characteristics as set out in Annex D of the Convention. At present, the marketing of new chemicals exhibiting POPs characteristics can be prohibited based on chemical properties on authorization scheme set out in the Biocide Directive (98/8/EC, implemented in Finland through amendment of Chemicals Act 1198/1999) and Regulation (EC) 1107/2009 placing the plant protection products on the market. The biocidal product legislation is currently being reviewed as described in the EU submission.

e. The EU but as well Germany should be aware of the special situation of the developing countries when it comes to the proposal of new POPs; Germany should evaluate the

possibilities to support developing countries in detecting relevant POPs and fix these provisions in their legislative frameworks and provide technical and financial assistance.

f. Effective enforcement cannot be ensured without constructive cooperation between the Commission and the EU Member States respectively its institutions. This is also recommended in order to minimize duplication of efforts. A closer networking with scientific institutions is also necessary for minimizing duplication of efforts.

g. Also the cooperation with NGOs, which have been involved in the POPRC as observers in past and provided statements on the substances under review could be improved. The approach of most of the NGOs has been thus far reactive and they have not been directly involved in the proposal submission:

   - The International POPs Elimination Network (IPEN)[52]
   - International Chemical Secretariat (ChemSec)[53]
   - World Wildlife Foundation (WWF)
   - Inuit Circumpolar Council[54] or
   - Pesticide Action Network (PAN)[55]
   - General monitoring measurements should take into account all substances on the candidate list of REACH by virtue of Annex XIV.

h. General monitoring measurements should take into account all substances on the candidate list of REACH by virtue of Annex XIV.

i. Recommendations for future activities to support the further use of environmental monitoring data for the Convention.
   - the implementation of a central European data base (“Chemical Data Centre”) to ease the access to available monitoring data;
   - the harmonisation of environmental monitoring activities on EU level with regard to programme concepts , i.e. sampling, analysis, data evaluation, quality requirements as well as presentation / publication of data;
   - the improvement of administrative and organisational structures with regard to data exchange between different authorities in order to eliminate existing information barriers;

j. Furthermore it was concluded that the exchange between chemical (risk) assessment experts under REACH on the one hand and environmental monitoring experts on the other hand needs to be intensified. With respect to existing administrative and organisational barriers in data exchange between different authorities, the regulatory framework established in the context of the Aarhus Convention on the European,

[52] http://www.ipen.org, last accessed 27.9.2012

[53] http://www.chemsec.org/, last accessed 27.9.2012

[54] http://www.inuitcircumpolar.com, last accessed 27.9.2012

[55] http://www.pan-international.org/panint/?q=node/33, last accessed 27.9.2012

national and regional level providing, i.a., the active dissemination of environmental data, might support activities in order to simplify the availability and accessibility of monitoring results.

k. Dynamics of the interest groups (parties or observers) are also able to form the decision-making process: The interest groups are able to deliver information about the substance and its usage, the possibilities to replace the substance, its adverse effects, and the regulations today etc. This information enters the Risk assessment of the POPRC. The case of PFOS shows the importance of participation of different actors to the decision-making process. For a party who intends to propose POP candidate, it might be of important to build alliances in order to find as much support for the substance substitution or replacement as possible. Importantly, industry can, in the role of observers, affect the perception of the matter in the similar manner as the NGOs. Building alliances with the industry supporting the restrictions for certain chemicals (like 3M in case of PFOS) can be of relevance in the negotiations.

10 Creating a list of possible POP candidates

The strategy presented in chapter 9, page 59 ff. was applied in order to create a list of potential POP candidates. The preparation phase, screening and filtering were done as described in a recent paper published by the Institute for Chemical and Bioengineering, ETH Zürich (Scheringer et al. 2012).

The screening was performed with the modelling tools suggested in section 4.2. 574 chemicals that exceed the Annex D thresholds for P, B and LRT as well as the REACH threshold for T were found. Among them were most of the known POPs. 510 substances, not regulated under the Convention can be considered as potential POPs. The list of these chemicals can be found in the supporting material of Scheringer et al. 2012. 98% of these chemicals are halogenated; frequent types of chemicals are halogenated aromatic compounds, including polychlorinated diphenylethers, tetrachloro benzyltoluenes, brominated and fluorinated naphthalenes and biphenyls; and highly or fully chlorinated and fluorinated alkanes (Scheringer et al. 2012).

According to the filtering phase, the chemicals registered in REACH, HPV chemicals and chemicals exceeding the more stringent POP thresholds were separated. Approximately 45% of the substances in the POP group have been pre-registered in the EU (ECHA 2010).

Three chemicals not currently regulated or under review by The Convention are intended to be registered under REACH by 2013. A total of 15 substances in the POP group are listed as high-production-volume chemicals (HPVCs), five of these are acknowledged POPs or POP candidates currently under review (DDT, HCB, PFOSF, HBCD, octa-BDE). The other 12, together with the REACH registration intentions, are listed in Table 20

There were 193 substances fulfilling the more stringent POP filtering criteria. These can be found in the supporting material of Scheringer et al. 2012. In the summary Table 20 fulfilment of the three filtering criteria is indicated for all REACH registered and HPV chemicals which are not acknowledged POPs or under review by the POPRC (Scheringer et al. 2012).. Due to the large amount of substances fulfilling the more stringent POP criteria, the further analysis concentrates only on the chemicals, which passed either the REACH or HPVC filter

Substances identified in Table 20 are identified as potential POP candidates.. For these chemicals compound profiles are compiled. Each profile exhibits for each substance: the name

of substance, the CAS number and the criteria set which was described in the strategy in chapter 9 (P, B, T and LRT screening results, as well as status of HPVC, REACH and more stringent POP threshold criteria). Furthermore, the compound profiles are complemented with additional criteria (toxicity and monitoring data and synergies with other regulations and compound lists) described in section 9.3. To ease the chemical identification information about the chemical usage was added to the profiles wherever possible.

10.1 Compound lists

The list of potential POP candidates is the result of a screening exercise and the filtering phase and provides starting points for more detailed assessments. Table 20 presents the POP proposal candidates together with a summary of the filtering criteria status and labeling according to the additional criteria. In the following also separate compound profiles with detailed information are presented.

Some additional lists where the substances appear, but which are not included in Tables 2, 7 or 8 are added in section “other information” of the compound profiles.

Evaluation 1 refers to the sum of “Yes” answers in categories REACH, HPVC and Stringent POP. Evaluation 2 Refers to amount of different Colour Labelling’s of the chemical (Red / White / Green)

Table 20 Present in the group of 12 potential POPs identified in this work.

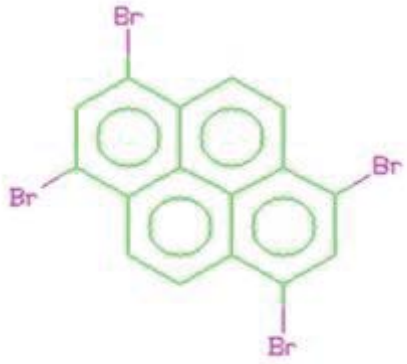
CAS	Name	REACH	HPVC	Stringent POP	Toxi-city	Moni-toring	Synergies	Evaluation	
								1	2
128-63-2	1,3,6,8-Tetrabromopyrene	Yes	Yes	No	White	White	Red	2	1/2/0
115-32-2	dicofol	Yes	Yes	No	Red	White	Red	2	2/1/0
133-49-3	Pentachlorothiophenol	Yes	Yes	No	Red	WHITE	Red	2	2/1/0
77-47-4	Hexachlorocyclopentadiene	YES	Yes	No	Red	White	Red	2	2/1/0
95-94-3	1,2,4,5-tetrachlorobenzene	Yes	Yes	No	White	Red	Red	2	2/1/0
2043-53-0	1-iodo-1H,1H,2H,2H-perfluorodecane	Yes	Yes	Yes	White	White	Red	3	1/2/0
2043-57-4	1-iodo-1H,1H,2H,2H-perfluorooctane	Yes**	Yes	Yes	White	White	Red	3	1/2/0
678-39-7	8:2 fluorotelomer alcohol	Yes	Yes	No	White	Red	Red	2	2/1/0
311-89-7	Perfluoro tri-N-butylamine	Yes	Yes	Yes	White	White	Red	3	1/2/0
52184-19-7	6-[(2-nitrophenyl)azo]-2,4-di-tert-pentylphenol	Yes	No	No	White	White	White	1	0/3/0
338-83-0	Perfluorotripropylamine	Yes**	No	Yes	White	White	Red	2	1/2/0
375-45-1	1,2,3,4-tetrachlorohexafluorobutane	Yes*	No	No	White	White	White	1	0/3/0

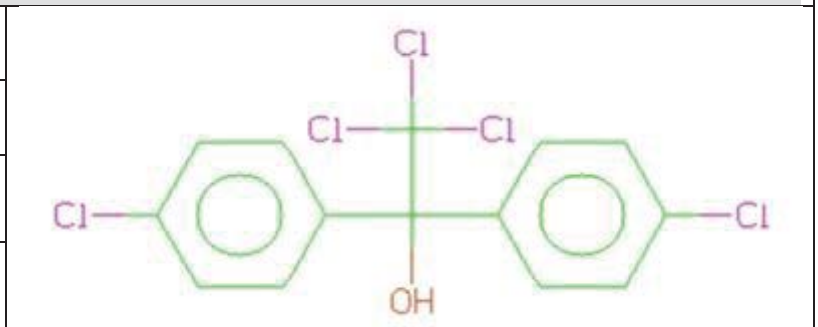
* the registration follows in 2013.

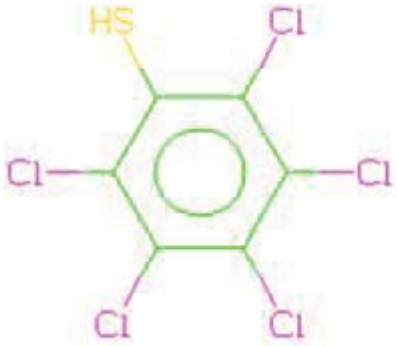
** Diverging information on the registration status. Substances have according to REACH either an envisaged registration date in 2010 or are foreseen for registration in 2012

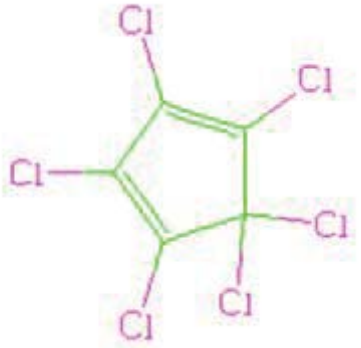
The overall evaluation of the compound profiles according to Table 20 reveals following

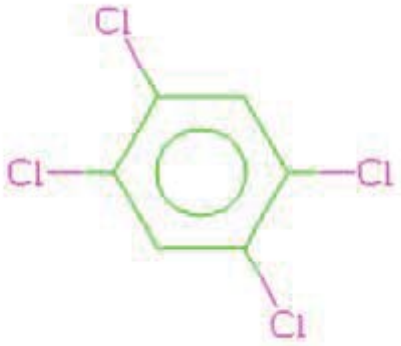
- Three of the POP candidates fulfill all three of the screening criteria: iodo-perfluoro-decane and –octane and perfluorotributylamine
- Seven of the candidates fulfill two of the tree criteria, and one only one criteria. The possible candidates fulfilling only one criterion is nevertheless larger, when the complete "very-POP" group fulfilling the more stringent POP thresholds is considered (193).
- Most of the color labels given were white. This highlights the lack of toxicity and monitoring data among the POP proposal candidates
- No green color labels were given – thus the screening results were not contradicted by scientific evidence. This is nevertheless to be expected when the relevant data is scarce
- No "fully supported" potential POP candidates were found (i.e. color labeling (3/0/0)
- All of the potential POP candidates qulify as "strong" as they are characterized by red and white labeling (no green labels)
- Two red labels, indicating elevated environmental concern among the "strong" candidates were found for (dicofol), pentachlorotiophenol, hexachlorocyclopentadiene, tetrachlorobenzene and fluortelomer alcohol
- Different substances presented the highest concern among the POP candidates in the filtering phase and according to the additional criteria.
- The synergies were mostly found among compound lists, which used a similar initial screening as a starting point of their studies. Synergies were found in ten of twelve cases
- Regulatory interest was evident only in case of dicofol

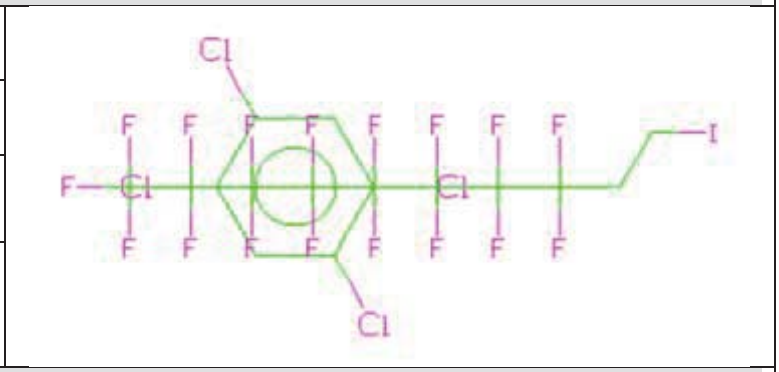
Identification			
Name(s)	1,3,6,8-Tetrabromopyrene		
CAS	128-63-2		
EINECS	204-900-6		
SMILES	Brc1cc(Br)c2ccc3c(Br)cc(Br)c4ccc1c2c34		
General information			
Chemical formula	$C_{16}H_6Br_4$	Molecular weight	517.83 g/mol
Usage	Laboratory chemicals, Manufacture of substances, used as a chemical intermediate in liquid chrystal display (LCD) production		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	670	T	9.47×10^{-8} and 7.50×10^{-6}
B	9 520 and 555	LRT	6.57
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity (White)	Almost no Toxicity Data available LD50 12 000 mg/kg, mouse, intravenous >10 000 mg/kg, rat		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) Not monitored in the Great Lakes monitoring Programme According to Howard and Muir (2010) not well monitored		
Synergies with other regulations (substance lists) (RED)	Howard and Muir 2010 (in List of 610 potential P&B chemicals)		
Other information			
TSCA	Toxic Substance Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
Howard and Muir 2010	High priority chemical according to P and B screening		
Howard and Muir 2010	The substance is analysable with existing analytical methods		

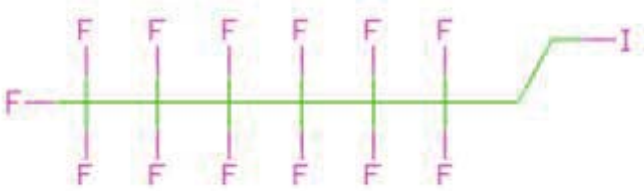
Identification			
Name(s)	Dicofol		
CAS	115-32-2		
EINECS	204-082-0		
SMILES	ClC1ccc(cc1)C(O)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl		
General information			
Chemical formula	$C_{14}H_9Cl_5O$	Molecular weight	370.48 g/mol
Usage	organochlorine pesticide (Insecticide) that is chemically related to DDT 5 500 t/a worldwide		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	390	T	9.00×10^{-3} and 8.00×10^{-3}
B	7 270 and 47 200	LRT	3.12
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity (Red)	Sub-Chronic toxicity, NOEC 0.019 mg/l, rainbow trout, 21 d Chronic toxicity, EC50 0.073 mg/l, algae, 96 h Acute Toxicity, LC50 0.06 mg/l, mysid shrimp, 48 h Acute toxicity, LC50 0.51 mg/l, bluegill-sunfish, 96 h		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) A Review of current use pesticides in Arctic media in 2000-2007 (Hoferkamp et al. 2009), did not find evidence of measured dicofol concentratons in arctic environmental media Dicofol was found in sea-water and air samples in South-East Asia and the Arctic. The occurrence in the arctic could be caused by riverine transport from Russia not necessarily by LRT via air Zhong et al (2012)..		
Synergies with other regulations (substance lists) (Red)	PBT Group	Identified as POP by PBT Working Group; see PBT Information System by the JRC (http://esis.jrc.ec.europa.eu/index.php?PGM=pbt)	
	UNECE	UN ECE (2009) Report by the Co-chairs of the Task Force on Persistent Organic Pollutants, ECE/EB.AIR/WG.5/2009/7, (http://www.unece.org/fileadmin/DAM/env/documents/2009/EB/wg5/wgsr45/ece.eb.air.wg.5.2009.7.e.pdf, 2012-04-16)	
	Brown and Wania (2008)	List of 120 potential arctic contaminants	
	OSPAR	List of substances for priority action	
Other information			
UNECE (POP Protocol)	Risk profile of Dicofol: http://www.unece.org/fileadmin/DAM/env/lrtap/TaskForce/popsxg/2008/Dicofol_Addendum%20to		
Becker et al 2012	DDT is used in Dicofol production and is found as impurities within commercial Dicofol. Becker et al reported that average DDT impurities in Dicofol produced in china were 244 g/kg dicofol, whereas impurities in other countries are typically regulated, and max 0.1%. Between 1988 and 2002 40 000 t of dicofol were produced in china, leading thus to DDT releases of approximately 9.7 tons.		

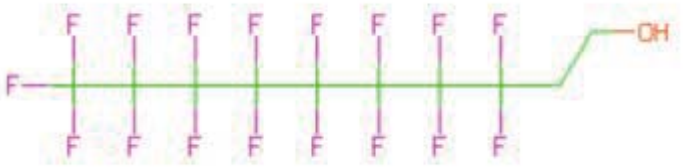
Identification			
Name(s)	Pentachlorothiophenol		
CAS	133-49-3		
EINECS	205-107-8		
SMILES	Clc1c(S)c(Cl)c(Cl)c(Cl)c1Cl		
General information			
Chemical formula	C_6HCl_5S	Molecular weight	282.4 g/mol
Usage	No production, import or use of pentachlorobenzenethiol occurs at the present in the EU.		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	158	T	8.00×10^{-3} and 4.00×10^{-3}
B	3 670 and 13 500	LRT	76.7
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity (RED)	Acute toxicity algae EC50, 0.019 mg/l		
	Acute toxicity daphnia EC50, 0.248mg/l		
	Acute toxicity fish LC50, 0.084mg/l		
	Chronic toxicity daphnia NOEC, 0.009mg/l		
	Chronic toxicity fish NOEC, 0.008mg/l		
Monitoring Data (white)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) Not monitored in the Great Lakes monitoring programme, not well monitored (Howard and Muir 2010)		
Synergies with other regulations (substance lists) (Red)	Brown and Wania (2008) – List of 120 potential arctic contaminants		
	Howard and Muir (2010) - List of 610 potential P&B chemicals		
Other information			
TSCA	Toxic Substance Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
Howard and Muir 2010	High priority chemical according to P and B screening		
Howard and Muir 2010	The substance is analysable with existing analytical methods		

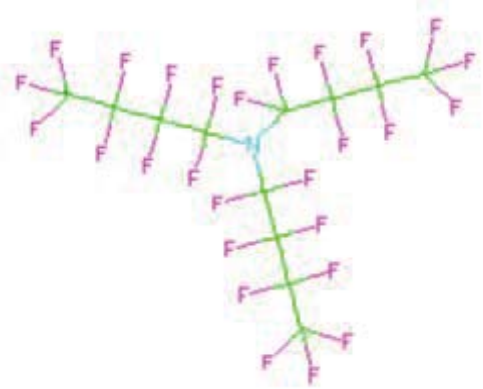
Identification			
Name(s)	Hexachlorocyclopentadiene		
CAS	77-47-4		
EINECS	201-029-3		
SMILES	ClC1=C(Cl)C(Cl)(Cl)C(=C1Cl)Cl		
General information			
Chemical formula	C_5Cl_6	Molecular weight	272.77 g/mol
Usage	Raw material in manufacturing other chemicals, including pesticides (aldrin, dieldrin, chlordane and heptachlor, endosulfan), flame retardants, resins, dyes, pharmaceuticals, plastics, synthetic lubricants etc. Has no end use of its own. In 1988, production volume 15 000 tonnes worldwide		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	223	T	6.00×10^{-3} and 2.03×10^{-2}
B	43.1 and 6 500	LRT	27.2
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity (Red)	Acute oral toxicity LD50 505 mg/kg, rat Acute NOAEL 150 mg/kg, rat Acute NOAEL 300 mg/kg Acute inhalation toxicity LC50 3.06 mg/kg, rat, 4 Hrs Chronic NOAEL 10 mg/kg, rat NOAEL of 0.1 mg/m3, mice (inhalation) LOAEL of 0.4 mg/m3, mice (inhalation)		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) Has been found in the atmosphere above the Great Lakes, but is not being analysed on the Great Lakes monitoring programme (Howard and Muir 2010) Monitored and regulated by EPA National Primary Drinking Water Regulations		
Synergies with other regulations (substance lists) (Red)	Brown and Wania (2008) - List of 120 potential arctic contaminants		
	Howard and Muir (2010) - List of 610 potential P&B chemicals		
Other information			
TSCA	Toxic Substanc Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
Howard and Muir 2010	High priority chemical according to P and B screening		
Howard and Muir 2010	The substance is analysable with existing analytical methods		

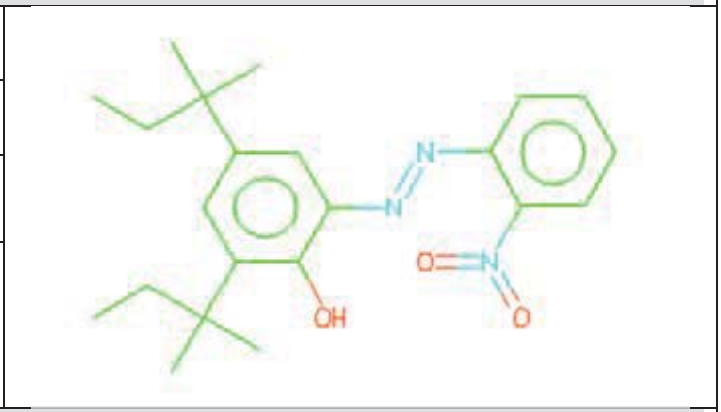
Identification			
Name(s)	1,2,4,5-tetrachlorobenzene		
CAS	95-94-3		
EINECS	202-466-2		
SMILES	Clc1cc(Cl)c(Cl)cc1Cl		
General information			
Chemical formula	$C_6H_2Cl_4$	Molecular weight	215.89 g/mol
Usage	Synthesis of Chlorophenoxyalkanoic Acids (herbicides, such as mecoprop, insecticides and defoliants). It is also used to make other chemicals		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	85.6	T	6.00×10^{-3} and 1.45×10^{-1}
B	1 970 and 9 640	LRT	130
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity (White)	LD50 1500 mg/kg, rat oral LD50 1035mg/kg, mouse oral LD50 1500mg/kg, Rabbit oral NOEL 30 mg/kg for rats NOEL 300 mg/kg for mice		
Monitoring Data (Red)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) Analyzed in the Great Lakes Monitoring Programme, well monitored Found at the Canadian Arctis (http://www.ec.gc.ca/ese-ees/default.asp?lang=En&n=3A77B3BF-1) List on ground water monitoring program in Ohio (http://codes.ohio.gov/oac/3745-27-10)		
Synergies with other regulations (substance lists) (Red)	CEPA - Listed in the Canada Priority Substances List		
	Brown and Wania (2008) - List of 120 potential arctic contaminants		
	Howard and Muir (2010) - List of 610 potential P&B chemicals		
Other information			
TSCA	Toxic Substanc Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
Howard and Muir 2010	High priority chemical according to P and B screening		

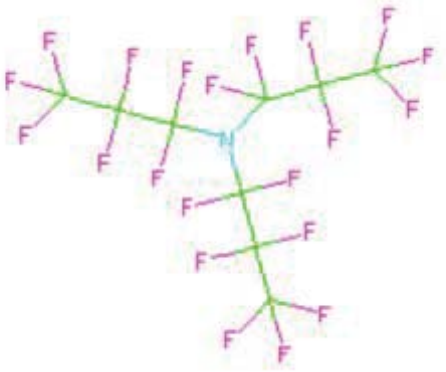
Identification			
Name(s)	1-iodo-1H,1H,2H,2H-perfluorodecane		
CAS	2043-53-0		
EINECS	218-053-5		
SMILES	ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		
General information			
Chemical formula	$C_{10}H_4F_{17}I$	Molecular weight	574.02 g/mol
Usage	Intermediate in perfluortelomer synthesis as well as in oil and water repellant, surfactant and fire-extinguishing foam manufacture. intermediate in the polymerproduction processes in addition to the synthesis of FTOH		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	2 590	T	5.14×10^{-7} and 3.49×10^{-5}
B	4 460 and 1.56×10^{6}	LRT	17.3
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	yes
Reasons for further concern (see additional criteria)			
Toxicity (White)	no data		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) Not monitored in the Great Lakes monitoring programme (Howard and Muir 2010) According to Howard and Muir (2010) this substance is not analysable with existing methods		
Synergies with other regulations (substance lists) (Red)	Howard and Muir (2010) - List of 610 potential P&B chemicals Brown and Wania (2008) - List of 120 potential arctic contaminants		
Other information			
TSCA	Toxic Substanc Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
IECSC	China Inventory of Existing Chemical Substances		
NDLS	Canadian Non-Domestic Substances List		
ENCS	Japan Existing and New Chemical Substances		
Howard and Muir 2010	High priority chemical according to P and B screening		

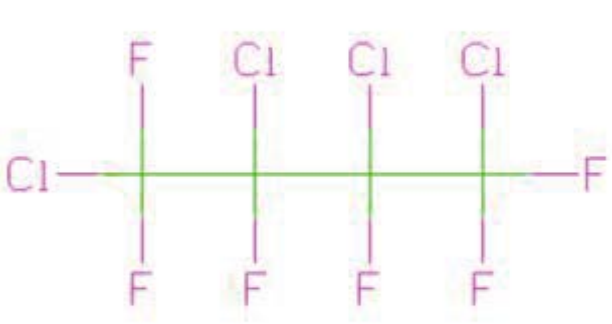
Identification			
Name(s)	1-iodo-1H,1H,2H,2H-perfluorooctane		
CAS	2043-57-4		
EINECS	218-056-1		
SMILES	ICCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		
General information			
Chemical formula	$C_8H_4F_{13}I$	Molecular weight	474.00 g/mol
Usage	Intermediate of perfluortelomer synthesis, processing as a reactant		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	845	T	2.47×10^{-5} and 1.13×10^{-3}
B	11 000 and 114 000	LRT	17.3
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	Expected by 31/05/2013
HPVC	yes	Stringent POP	yes
Reasons for further concern (see additional criteria)			
Toxicity (White)	No data		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) Not monitored in the Great Lakes monitoring programme (Howard and Muir 2010) According to Howard and Muir (2010) this substance is not analysable with existing methods		
Synergies with other regulations (substance lists) (Red)	Howard and Muir (2010) - List of 610 potential P&B chemicals Brown and Wania (2008) - List of 120 potential arctic contaminants		
Other information			
TSCA	Toxic Substance Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
NDLS	Canadian Non-Domestic Substances List		
Howard and Muir 2010	High priority chemical according to P and B screening		

Identification			
Name(s)	8:2 fluorotelomer alcohol		
CAS	678-39-7		
EINECS	211-648-0		
SMILES	OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		
General information			
Chemical formula	$C_{10}H_5F_{17}O$	Molecular weight	464.12 g/mol
Usage	Intermediate, Impregnating agent, used in coating of textiles, paper and carpets to achieve oil, stain and water repellent properties, cleaning agents and is present as residual raw materials		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	1290	T	3.55×10^{-4} and 1.20×10^{-2}
B	2 230 and 39 700	LRT	2.56
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity (White)	LD50 Female rats 500 mg/kg; males 2000 mg/kg No further toxicity was reported		
Monitoring Data (Red)	Stock et al (2007) detected the compound in air samples at canadian Arctic Analyzed in Great Lakes monitoring programme, but not well monitored (Howard and Muir 2010)		
Synergies with other regulations (substance lists) (Red)	Howard and Muir (2010) - List of 610 potential P&B chemicals Brown and Wania (2008) - List of 120 potential arctic contaminants		
Other information			
TSCA	Toxic Substanc Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
ENCS	Japan Existing and New Chemical Substances		
Howard and Muir 2010	High priority chemical according to P and B screening		
CLH REPORT (2010)	Proposal for harmonised classification and labelling http://echa.europa.eu/documents/10162/13626/clh_axvrep_norway_ftoh_en.pdf		

Identification			
Name(s)	Perfluoro tri-N-butylamine		
CAS	311-89-7		
EINECS	206-223-1		
SMILES	FC(F)(N(C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F		
General information			
Chemical formula	$C_{12}F_{27}N$	Molecular weight	671.10 g/mol
Usage	E.g. isolation fluid, insulating medium and demulsifier. It can also be mixed with tetrafluoroethylene for the preparation of fluoride ester.		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	145 533	T	121 655 and 2.43×10^{-4}
B	3 441 and 6.0×10^{6}	LRT	1.00×10^{6}
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	yes
Reasons for further concern (see additional criteria)			
Toxicity (White)	LD50 12 000 mg/kg, mouse intravenous >10 000 mg/kg, rat oral No data found on other species apart from other rodents		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011) Not analysed in the Great lakes monitoring programme, Analyzalbe with existing methods (Howard and Muir 2010)		
Synergies with other regulations (substance lists) (Red)	Howard and Muir (2010) - List of 610 potential P&B chemicals		
	Brown and Wania (2008) - List of 120 potential arctic contaminants		
Other information			
TSCA	Toxic Substance Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
Howard and Muir 2010	High priority chemical according to P and B screening		

Identification			
Name(s)	6-[(2-nitrophenyl)azo]-2,4-di-tert-pentylphenol		
CAS	52184-19-7		
EINECS	257-716-3		
SMILES	CCC(C)(C)c1cc(N=Nc2ccccc2N(=O)=O)c(O)c(c1)C(C)(C)CC		
General information			
Chemical formula	$C_{22}H_{29}N_3O_3$	Molecular weight	383.48 g/mol
Usage	Pigment for cosmetic product (more research necessary)		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	166	T	1.79×10^{-5} and 1.34×10^{-6}
B	6.00 and 20 100	LRT	2.42
Reasons for high concern (see filtering criteria)			
Preregistration REACH	yes	Registration REACH	30/11/2010
HPVC	yes	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity (White)	No data		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011)		
Synergies with other regulations (substance lists) (White)	Not known		
Other information			
TSCA	Toxic Substance Control Act (USA)		
IUR	Inventory Update Reporting of US EPA (http://cfpub.epa.gov/iursearch/)		
Persistent Pollutant Science Workgroup (PPSWG)	Identified as persistent Pollutant in a screening by PPSWG in Oregon, US. http://www.deq.state.or.us/wq/sb737/docs/DraftTechnicalReportAttachments.pdf		

Identification			
Name(s)	Perfluorotripropylamine		
CAS	338-83-0		
EINECS	206-420-2		
SMILES	FC(F)(C(F)(F)F)C(F)(F)N(C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F		
General information			
Chemical formula	$C_9F_{21}N$	Molecular weight	521.07 g/mol
Usage	Cleaning Electronic, compact disc, precision instrument. anticorrosive driving isolating liquid for apparatus & Instruments. dielectric insulating oil. Leak detecting liquid of electronic devices. Oxidation-resistant lubricant.		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	13 500	T	7.00×10^{-3} and 5.70×10^{-2}
B	5 650 and 438 000	LRT	$1.00e \times 10^{6}$
Reasons for high concern (see filtering criteria)			
Preregistration REACH	No	Registration REACH	Expected by 31/05/2013
HPVC	no	Stringent POP	yes
Reasons for further concern (see additional criteria)			
Toxicity (White)	R36/37/38 Irritating to eyes, respiratory system and skin. no further data		
Monitoring Data (White)	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011)		
Synergies with other regulations (substance lists) (Red)	Rorije et al. 2011		
Other information			
TSCA	Toxic Substance Control Act (USA)		

Identification			
Name(s)	1,2,3,4-tetrachloro-hexafluorobutane		
CAS	375-45-1		
EINECS			
SMILES	FC(F)(Cl)C(F)(Cl)C(F)(Cl)C(F)(F)Cl		
General information			
Chemical formula	$C_4Cl_4F_6$	Molecular weight	303.85 g/mol
Usage	no further details about data		
POP properties either measured or estimated with EpiSuite of US EPA: BIOWIN3, ECOSAR, BCFBAF and AOPWIN: P as biodegradability $t_{1/2}$ in water (d), B as BCF and BAF, T as NOEC/ChV and LC_{50}/EC_{50} (mg/L), LRT as $t_{1/2}$ in air (d)			
P	416	T	7.96×10^{-4} and 2.50×10^{-2}
B	1 550 and 13 100	LRT	1.00×10^{6}
Reasons for high concern (see filtering criteria)			
Preregistration REACH		Registration REACH	Expected by 31/05/2013
HPVC	no	Stringent POP	no
Reasons for further concern (see additional criteria)			
Toxicity	Draize test, rabbit, eye: 100 mg/24H Moderate; Oral,mouse: LD50 = 300 mg/kg; Oral, rabbit: LD50 = 3200 mg/kg; Oral, rat: LD50 = 980 mg/kg.		
Monitoring Data	No monitoring studies from Arctic or Antarctic in 2005-2011 (Lambert et al. 2011)		
Synergies with other regulations (substance lists)	Not Known		
Other information			
TSCA	Toxic Substance Control Act (USA)		
DSL	Domestic Substances List		
	Registered in RTESC Registry of Toxic Effects of Chemical Substances http://www.cdc.gov/niosh/rtechs/		

11 Discussion and outlook

The Stockholm Convention can be considered a success story: 177 Parties worldwide committed themselves to eliminating or reducing the releases of 22 POPs. In order to continue this success story, new POPs need to be included in the Convention. Five substances are currently under review. It is important to note that the procedure for including new POPs in the Annexes to the Convention needs substantial efforts and normally takes three to five years: First, a Member state has to compile and submit a proposal; then the POPRC, after having examined the proposal and decided to proceed, compiles a risk profile by consulting the Parties to the Convention. From a scientific and technical point of view, the compilation of such a dossier is a big project and requires considerable effort. Thus, only substances should undergo this procedure that are “relevant” chemicals, which means that they are used in high quantities and that their restrictions will be of ecological benefit.

In order to identify candidates for new POP proposals, we developed a methodological approach to screening a high number of chemicals that are currently in use. The strategy is based on a screening exercise on property estimation of the four criteria laid down in Annex D of the Stockholm Convention.

Previous studies have also performed similar screening exercises. They all concluded that there are a considerable number of potential POP-like and PBT-like chemicals. However, this screening exercise is the first one that applies without prior weighting or scoring all four POPs criteria of the Stockholm Convention because this specific set of criteria defines which chemicals are relevant. Based on the four criteria, we derived a list of 12 possible POP candidates and compiled their substance profiles.

However, there are two groups of substances that are not detected as POPs by our approach:

Substances that are not presented in the compound profiles might still be categorized as POPs (in the future), because Annex D of the Stockholm Convention specifies for all four properties that other evidence can also be used for the assessment of whether or not a chemical exceeds the screening criteria. The Stockholm Convention explicitly mentions the possibility that substances may be considered as POPs because of additional evidence, even if they do not exceed the threshold-based criteria for P, B, und LRT. The Convention states that lack of full scientific certainty should not prevent a candidate substance from proceeding in the evaluation or listing.

Additional evidence can be provided especially by environmental measurements or monitoring data. This is especially important for substances accumulating in terrestrial organisms, which might not be captured by our approach, because we evaluated only aquatic bioconcentration and bioaccumulation in the initial screening. In these cases, monitoring data are needed in order to demonstrate the environmental relevance of a proposed POP candidate.

The second group of substances that is not covered by our approach are newly developed substances that are not yet included in the databases that form the starting point of our screening exercise. The regulatory and assessment schemes for new substances are covered by the REACH regulation for industrial chemicals, and by the Regulation on Plant Protection Products and the Biocide Directive (see section 2.3).

Last but not least, it has to be noted that there is no direct or even automatic procedure that leads from the finding that the properties of a chemical exceed the Annex D criteria to regulation of that chemical. Also non-scientific factors (i.e. political, technical and economic factors) can influence which chemicals are proposed for evaluation under the Convention and are eventually regulated under the Convention. As the example of SCCPs, which are generally recognized as POP-like substances, shows, the missing consensus on the adverse effect of the substance can hamper the assessment process of the POPRC and preclude regulation of a chemical that may well have POP properties.

12 Annexes

12.1 Information required for the different Phases and Steps

Table 21 Summary of the most important Information required for the different Phases and Steps of the strategy

Required information	Sources of information	Description and comments	Link / reference
Selection of chemical databases			
CAS number and the SMILES code	CAS Number	CAS – A Division of the American Chemical Society. CAS Registry and CAS Registry Numbers	http://www.cas.org/expertise/cascontent/35 registry/regsys.html
	SMILES CODE	SMILES – A Simplified Chemical Language, Daylight Chemical 37 Information Systems, Inc., 120 Vantis – Suite 550 – Aliso Viejo, CA 38 92656.	http://www.daylight.com/dayhtml/doc/theory/index.pdf
	SMILECAS database included in the EPI Suite software (Estimation Programs Interface Suite for MS Windows, v4.10)	Available at the webpage of the United States Environmental Protection Agency	http://www.epa.gov/opptintr-/exposure/pubs/episuite.htm
	EINECS	European Commission database provided by the JRC Institute for Health and Consumer Protection	http://ihcp.jrc.ec.europa.eu/our_labs/computational_toxicology/information-sources/ec_inventory
Physicochemical property data	PHYSPROP	SRC Physical and Chemical property database	http://www.srcinc.com/what-we-do/product.aspx?id=133
Screening Phase of the selected basic set of chemicals			
Estimation tools	EPI Suite screening-level tool	Estimation Programs Interface Suite for MS Windows, v4.10 is available at the US EPA webpage	http://www.epa.gov/opptintr/exposure/pubs/episuite.htm
	OECD Pov and LRTP Tool		http://www.oecd.org/chemicalsafety/assessmentofchemicals/oecdpovandlrtpscreeningtool.htm
Check of HPVC, High Production Volume Chemicals			
High production volume chemicals	OECD HPV list	A list of chemicals which are produced at levels greater than 1000 tons per year in at least one member country/region	http://www.oecd.org/dataoecd/55/38/33883530.pdf
	ESIS HPVCs list	Chemicals placed on the EU market in volumes exceeding 1000 tonnes per year per producer or importer.	http://esis.jrc.ec.europa.eu/index.php?PGM=hpv
	HPVIS of the US EPA	Organic non-Polymer chemicals with production or import volume greater than 1 Million pounds (450 t) into the USA.	http://www.epa.gov/chemrtk/hpvis/index.html
REACH registration status	ECHA	Registered substances	http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances

Required information	Sources of information	Description and comments	Link / reference
		lists of substances identified by industry to be registered by 31 May 2013 (Data as of 15th September 2011)	http://echa.europa.eu/information-on-chemicals/registered-substances/identified-substances-for-registration-in-2013
		List on substances identified but not registered (Data as of 15th September 2011)	http://echa.europa.eu/information-on-chemicals/registered-substances/identified-substances-for-registration-in-2010
		Candidate list for authorization of substances of very high concern	http://echa.europa.eu/chem_data/candidate_list_table_en.asp
Check of toxicity			
Toxicity	ECHA	The ECHA CHEM webpage contains information on 7 529 registered unique substances and contains information from 30 213 dossiers (as of July 2012); the database is steadily growing	http://echa.europa.eu/web/guest/information-on-chemicals/registered-substances
	OECD eChemPortal	OECD eChemPortal can be searched for toxicity and ecotoxicity information. The portal searches chemical information in 24 different databases (status in September 2012) Hosted by the OECD; OECD eChemPortal provides links to the collaborating institutions	http://www.oecd.org/document/9/0,3746,en_2649_49389220_35211849_1_1_1_49389220,00.html (www.echemportal.org)
	JRC Publications Repository	Data of research publications produced by the European Commission's Joint Research Centre	http://publications.jrc.ec.europa.eu/repository/
	Restricted and Priority Substances Database	This database contains 29 lists of substances that are legally or voluntarily restricted or are recommended for restriction due to their hazards. Besides, the lists that were presented and discussed in section 6.2.2, also companies' lists are included	http://www.subsport.eu/listoflists
	EU Endocrine Disruption Database	Information about endocrine disruptors can be found in EU Endocrine Disruption Database (2012)	http://ec.europa.eu/environment/endocrine/strategy/short_en.htm, 2012-04-16
	PAN – pesticides database	Toxicological information is also presented in the PAN – pesticides database and in the footprint database	http://www.pesticideinfo.org/
	PPDB	Pesticide Properties DataBase, University of Hertfordshire	http://sitem.herts.ac.uk/aeru/footprint/en/
	HSDB	Hazardous Substances Data Bank. Comprehensive, peer-reviewed toxicology data for about 5,000 chemicals.	http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB 2012-04-16
	TSCATS	The Toxic Substance Control Act Test Submission Database (TSCATS), the database has nevertheless not been updated since 2004.	http://www.syrres.com/what-we-do/product.aspx?id=136
	ATSDR	Agency for Toxic Substances and Disease Registry TOXICOLOGICAL PROFILE FOR PYRETHRINS AND PYRETHROIDS	http://www.atsdr.cdc.gov/toxprofiles/tp.asp?id=787&tid=153
	NORMAN databases	NORMAN organises the development and maintenance of three web-based databases for collection & evaluation of data / information on emerging substances.	http://www.norman-network.net/index_php.php?module=public/databases/databasex&menu2=public/databases

Required information	Sources of information	Description and comments	Link / reference
			/databases
	OECD Series on Emission Scenario Documents	Guidance Document on Emission Scenario Documents	http://www.oecd.org/officialdocuments/displaydocumentpdf/?cote=env/jm/mono(2000)12&doclanguage=en
Check of Monitoring Data			
Monitoring	ISI Web of Science	ISI Web of Knowledge is an academic citation indexing and search service. Web of Knowledge coverage encompasses the sciences, social sciences, arts and humanities. It has the attribute that multiple databases can be searched simultaneously	http://wokinfo.com/
	OAIster	OAIster is a union catalog of millions of records representing open access resources that was built by harvesting from open access collections worldwide	http://www.oclc.org/oaister/
		A freely-accessible site for searching only OAIster records	http://oaister.worldcat.org/
	PaperFirst (OCLC)	Covers every published congress, symposium, conference, exposition, workshop and meeting received by The British Library Document Supply Centre	http://www.oclc.org/de/de/default.htm
	ProceedingsFirst (OCLC)		http://www.oclc.org/support/documentation/firstsearch/databases/dbdetails/details/proceedings.htm
	PubMed	PubMed comprises more than 22 million citations for biomedical literature from MEDLINE, life science journals, and online books	http://www.ncbi.nlm.nih.gov/pubmed
	Science Citation Index Expanded	Overcome information overload and focus on essential data from over 6,650 of the world's leading scientific and technical journals across 150 disciplines	http://ip-science.thomsonreuters.com/cgi-bin/jrnlst/jloptions.cgi?PC=D
	SciFinder Web		https://scifinder.cas.org
	SpringerLink	A global publishing company which publishes books, e-books and peer-reviewed journals in science, technical and medical (STM) publishing	http://www.springerlink.com/
	Google Scholar	Provides a search of scholarly literature across many disciplines and sources, including theses, books, abstracts and articles	http://scholar.google.de/

12.2 Brainstorming meeting for reflection of the analysis and for the preparation of the strategy development

The brainstorming meeting took place on 3 May 2012 at Öko-Institut, Freiburg with the project team, UBA and the chair of the POPRC, Dr Reiner Arndt. The main topic of this meeting was to clarify requirements, conditions and needs for a proposal of possible POP substances. Important suggestions and questions raised from the brainstorming meeting were:

a. As the POP Protocol lists more substances then the Stockholm Convention, it might provide additional possible POP candidates (see section 6.2.2).

b. Does the SVHC assessment of REACH provide a basis for generating possible POP candidates? Would it be sufficient to assess the LRT of each chemical on the REACH candidate list? Also the Member States that are reviewing a part of the registration dossiers should put some emphasis on the PBT evaluation and on whether the substances even have POP characteristics.

c. Should the sectoral assessment of industrial chemicals, plant protection products and biocides cooperate more closely with regard to the identification of new POPs?

d. Did the authors of the previous screening exercises feed in their results in political and regulatory processes?

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