Screening of Global Chemical Inventories for Substances with Arctic Accumulation Potential

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Introduction

A recent assessment of chemicals of emerging Arctic concern reviewed monitoring data for 16 groups of substances detected over the past 10 to 15 years in Arctic ecosystems [1]. The assessment demonstrated that over 100 individual fluorinated, chlorinated, brominated compounds, as well as current use pesticides, polycyclic aromatics, and siloxanes were detectable in arctic environmental media. Given the wide range of known substances detected, a logical question is whether there are additional chemicals widely used in commerce in Europe, North America, and East Asia with potential to be transported to the Arctic. Over the past 10 years, a number of studies have addressed the question of how many of the thousands of chemicals in commerce in Europe and North America may be persistent (P) and bioaccumulative (B). Also some of the same studies have considered whether chemicals in commerce might meet the Stockholm Convention criteria (i.e. P, B and long range transport potential (LRT)) for classification as persistent organic pollutants (POPs). These studies have generally been carried out by estimating environmentally relevant physical-chemical properties using Quantitative Structure Property Relationship (QSPR) models for tens of thousands of individual compounds with known molecular structures, in publicly available chemical inventories, and then screening the lists to identify those with predicted P, B and/or LRT values that exceed various regulatory guidelines. A combined total of about 150,000 substances listed on the European Inventory of Existing Chemical Substances (EINECS); the European List of Notified Chemical Substances (ELINCS); the US Toxic Substances Control Act Inventory Update Rule (TSCA-IUR); the Canadian Domestic Substances List (DSL); and the European Chemicals Agency (ECHA) list of pre-registered substances under REACH, have been included in recent studies (Table 1). To be listed on the TSCA, EINECS, ELINCS or REACH inventories, these substances must be produced or imported in quantities of over 1 t/y (Europe) or 4.5 to 11.6 t/y (USA). The criteria used for screening varied with each study but generally followed Stockholm Convention, US EPA and/or REACH guidance.

Materials and methods

For the present study we combined the lists of chemicals identified by the studies listed in Table 1. All studies provided lists of chemicals with their chemical abstract registry numbers (CAS RNs) and, in most cases, the common names. The chemical inventories for Europe, China and Japan were downloaded from the respective websites (see list at http://chemsafetypro.com/chemical_inventories.html). A list from Howard and Muir [2] representing the combined TSCA-IUR and the DSL was used for the US/Canada inventory.

Results and discussion

From 1.3 to 3.1% of chemicals that were screened in the studies listed in Table 1 were P and B under REACH criteria and 0.1–1.8% were P, B and had LRT potential by Stockholm Convention criteria according to the study authors. However, to our knowledge no previous study had combined all of the substances into one list. After removing duplicate CAS RNs, we extracted 3743 P and B substances (Table 1). Selecting for chemicals also having atmospheric LRT potential yielded about 1200 substances. This latter value is less precise because not all studies specifically screened for LRT. It should be noted that the substances included in the studies are limited mainly to neutral organic chemicals for which existing QSPR models for predicting P and B are most applicable, and therefore most organometallics, and all inorganics, salts, polymers and surfactants were omitted. The 3743 substances can be roughly categorized into eight classes; brominated (8%), chlorinated (26%), fluorinated (15%) organic compounds, organophosphate esters (1%), siloxanes (1%), musks (0.2%), polycyclic aromatics (0.4%), and a broad class of non-halogenated organics (46%) (Figure 1). The substances include some already regulated chemicals such as polybrominated diphenyl ethers because they were on older lists, for example, the TSCA-IUR and the REACH pre-registration list.

The 3743 CAS RNs were then compared to the chemical inventory lists for Europe, China, Japan and US/Canada. We found 606 of the 3743 substances were also on the REACH inventory and had therefore been subject to recent evaluation and registration, while 814 were in the combined TSCA-IUR and DSL (US/Canada) inventory (Figure 2). The list of 3743 substances was also used to examine P and B substances on the Chinese Inventory of Existing Chemical Substances (IECSC; 42,300 substances with CAS numbers) and Japanese Inventory of existing and new chemical substances (ENCS; 49,400 substances). We found 695 substances on the IECSC and 503 on the ENCS. The number of P and B substances identified represented 1.5 to 3.5% of the organic chemicals on the 4 inventory lists, ie after subtracting metals, alloys, salts and polymers from the total

Table 1. Recent screening studies of chemicals in commerce in Europe and North America for persistence, bioaccumulation and long range transport characteristics. ND: not determined.

References[1]	**Databases/lists used**	**Total Chemicals initially screened**	**Final list for which parameters estimated**	**Number[2] P & B**	**P & B & LRT**
[2]	TSCA IUR, DSL	22,263	22,263	**610**	**105**
[3]	EINECS, pesticides, pharmaceuticals	107,337	64,721	**1986**	**1171**
[4]	EINECS, ELINCS & SMILECAS[3]	127,281	94,483	**1202**	**ND**
[5]	REACH pre-registration	118,285	48,782	**829**	**125**
[6]	EINECS & SMILECAS[3]	122,000	93,144	**ND**	**510**
[7]	Reassess results of above studies	4412	3567	**1313**	**ND**
		Total (duplicates removed)		**3743**	**~1200**

[1] Howard & Muir [2], Rorije et al. [3], Strempel et al. [4], Öberg & Iqbal [5], Scheringer et al. [6], Gramatica et al. [7]

[2]ND = not determined. [3]SMILECAS database in the US EPA EPISuite program

inventory. Altogether about 21% of the substances identified as P and B on the Chinese and Japanese inventories (190 of 878 CAS RNs after removing duplicates) were unique, ie not in the combined European and US/Canada list of P and B substances. The proportions of brominated, chlorinated, fluorinated, and other classes of potential P and B chemicals on the four inventories were nevertheless similar (Figure 2).

This screening level assessment illustrates that it would be worthwhile to take a global approach to identification of potential P, B and LRT substances. Indeed, more than 50% of global chemical production and sales occur in East Asian countries (China (including Taiwan), Japan, and South Korea) [8]. However, while the approach of screening chemical inventories may be useful as a first step to identifying chemicals with P, B and LRT characteristics, there are other factors to consider when developing priorities for future research and monitoring. Perhaps most important is identification of transformation products, as well as byproducts and impurities, of chemicals in commerce that have P and B potential. Some major Arctic contaminants, such as the perfluoroalkyl acids and perfluoroalkyl sulfonates, are atmospheric or microbial transformation products of fluorinated substances which may not have Arctic accumulation potential until they undergo degradation. Polar transformation products which are very persistent, such as perfluoroalkyl acids, may undergo ocean transport to the Arctic. Ocean LRT is not routinely assessed.

The lists of P and B substances would be particularly useful for non-target and effects directed analysis involving high resolution mass spectrometry analysis of extracts of environmental media. However, the decision on which chemicals to include in monitoring programs and/or analytical screening studies is still very challenging given limited information on uses and physical-chemical properties, as well as lack of analytical standards with which to validate methods.

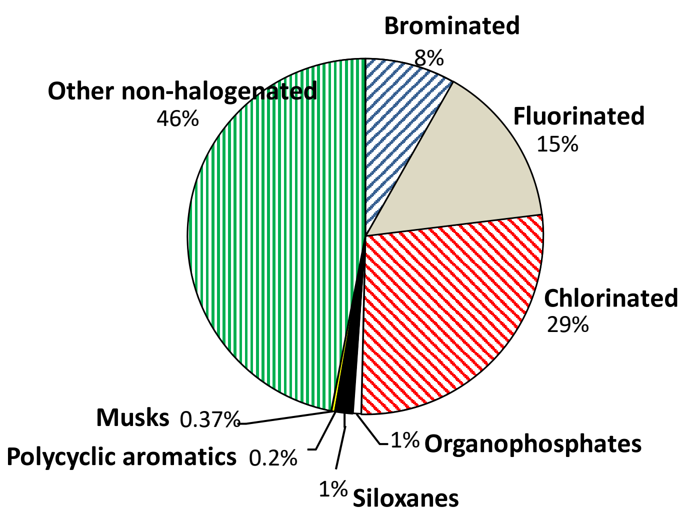

Figure 1. Broad classes of the 3743 Priority Chemicals from the six P and B screening studies listed in Table 1

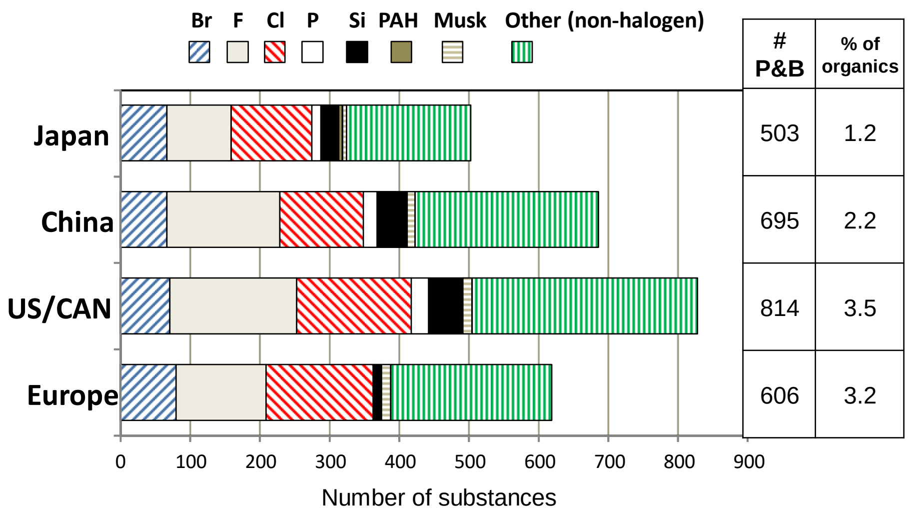

Figure 2. Classes of potential P and B chemicals in the 4 major inventories and % of total organics estimated to be present on those inventories

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