Emerging Contaminants xxx (2017) 1–10

Contents lists available at ScienceDirect

Emerging Contaminants

journal homepage: http://www.keaipublishing.com/en/journals/emerging-contaminants/

# Screening-level exposure-based prioritization to identify potential POPs, vPvBs and planetary boundary threats among Arctic contaminants

Efstathios Reppas-Chrysovitsinos, Anna Sobek, Matthew MacLeod*

*Department of Environmental Science and Analytical Chemistry (ACES), Stockholm University, SE-10691 Stockholm, Sweden*

ARTICLE INFO

*Article history:*
Received 26 April 2017
Received in revised form
5 June 2017
Accepted 26 June 2017
Available online xxx

*Keywords:*
Arctic contaminants
AMAP
Stockholm Convention
REACH
Planetary boundary threats

ABSTRACT

A report that reviews Arctic contaminants that are not currently regulated as persistent organic pollutants (POPs) under international treaties was recently published by the Arctic Monitoring and Assessment Programme (AMAP). We evaluated 464 individual chemicals mentioned in the AMAP report according to hazard profiles for POPs, very persistent and very bioaccumulative (vPvB) chemicals, and two novel and distinct hazard profiles we derived from the planetary boundary threat framework. The two planetary boundary threat profiles assign high priority to chemicals that will be mobile and poorly reversible environmental contaminants. Utilizing persistence as a proxy for poor reversibility, we defined two exposure-based hazard profiles; airborne persistent contaminants (APCs) and waterborne persistent contaminants (WPCs) that are potential planetary boundary threats. We used *in silico* estimates of physicochemical properties and multimedia models to calculate hazard metrics for persistence, bioaccumulation and long-range transport potential, then we synthesized this information into four exposure-based hazard scores of the potential of each AMAP chemical to fit each of the POP, vPvB, APC and WPC exposure-based hazard profiles. As an alternative to adopting a "bright line" score that represented cause for concern, we scored the AMAP chemicals by benchmarking against a reference set of 148 known and relatively well-studied contaminants and expressed their exposure-based hazard scores as percentile ranks against the scores of the reference set chemicals. Our results show that scores in the four exposure-based hazard profiles provide complementary information about the potential environmental exposure-based hazards of the AMAP chemicals. Our POP, vPvB, APC and WPC exposure-based hazard scores identify high priority chemicals for further study from among the AMAP contaminants.



## 1. Introduction

There is growing scientific interest in identifying environmental contaminants of concern among industrial chemicals used in commerce [1,2]. The increasing interest reflects flourishing global chemical production and past experience with chemicals that were used and released to the environment for decades before they were regulated because they posed an unacceptable hazard to the environment and/or human health [3]. Lack of data and poor data quality, especially for new chemicals, is a significant challenge for studies that aim to screen industrial chemicals to identify chemicals of concern. Other challenges include defining hazard metrics that reflect potential impacts of chemicals, and developing methodological approaches, and tools to assess the various hazards.

The Arctic environment has long been a focus of interest for the discovery and early identification of chemicals of concern [4,5]. Chemicals present in the Arctic at levels high enough to be detected and quantified satisfy at least one of the following conditions: i) they possess physicochemical properties that favor their transport from areas of use and emission to the Arctic, ii) they are produced in sufficiently high volumes that their mass distribution covers the hemispheric scale, iii) they are produced locally in the Arctic (e.g., natural or biogenic compounds), and/or iv) they are used and emitted in the Arctic (e.g., chemicals in pharmaceutical and personal care products used by the local population, and chemicals

* Corresponding author.
*E-mail address:* matthew.macleod@aces.su.se (M. MacLeod).
Peer review under responsibility of KeAi Communications Co., Ltd.

http://dx.doi.org/10.1016/j.emcon.2017.06.001

that escape from building materials and consumer products). A report that reviews the occurrence in the Arctic of chemicals that are not currently regulated as POPs was recently published by the Arctic Monitoring and Assessment Programme (AMAP) [6]. The AMAP report describes the detection in the Arctic of per- and polyfluoroalkyl substances, halogenated and organophosphate flame retardants, plasticizers, phthalates, chlorinated paraffins, siloxanes, pharmaceuticals and personal care products, polychlorinated napthalenes, current use pesticides, organotins, polycyclic aromatic hydrocarbons and halogenated natural products for the period 2009–2014 in 15 peer-reviewed chapters. The AMAP report refers to these chemicals as "chemicals of emerging concern" because their production, use and emissions are often increasing and they have been detected in air, water, biota and humans in the Arctic, even though many have been in commerce for several years. Some chemicals that became regulated as POPs after 2009 such as polychlorinated naphthalenes, endosulfan and hexabromocyclododecane- and for which new studies on Arctic occurrence appeared since 2010- are also included in the AMAP report as follow-up chapters for monitoring purposes. In this paper we describe a screening-level prioritization of these Arctic contaminants according to a range of exposure-based hazard metrics.

Hazard metrics for chemicals are important tools in regulatory classification schemes that include the Stockholm Convention [7] on persistent organic pollutants (POPs), which prioritizes chemicals that are persistent (P), bioaccumulative (B), toxic (T), and have potential for long-range transport (LRT), and the European chemicals regulation REACH [8], which prioritizes chemicals that combine P, B and T, and also those that are very persistent and very bioaccumulative (vPvB). Persistence (P), bioaccumulation potential (B) and long-range transport potential (LRT) are exposure-based chemical hazard criteria that can be assessed with the help of multimedia models [9]. These criteria are independent of the quantity of chemical used or emitted [10] and can thus be employed in hazard-based scoring and ranking assessments. In the absence of information about emission rate and toxicity, chemicals with high exposure hazard should be given priority for more detailed hazard and risk assessment studies.

Recently, a set of chemical profiles that are not encompassed by existing regulatory schemes were defined to identify chemical pollutants that pose a potential planetary boundary threat [11]. The planetary boundary conceptual framework delimits a "safe operating space for humanity" that exists within a set of quantitative boundaries [12,13]. Five of the planetary boundaries that were originally proposed (ozone depletion, climate change, ocean acidification, nitrogen-phosphorous cycles and chemical pollution) are governed by chemical agents. Other, currently unknown, chemical pollution planetary boundaries may exist [11,14,15]. For a chemical agent to be a planetary boundary threat, the chemical must cause, amplify and/or accelerate a poorly reversible, unknown disruptive effect on an Earth system process and the effect must remain undiscovered until it is of planetary scale. Seven chemical profiles that fit planetary boundary threat scenarios for chemical pollution have been identified [14].

Two of the profiles for chemicals to be planetary boundary threats depend heavily on the nature of environmental exposure to the chemicals. Chemicals fit the first of these two profiles if they cause poorly reversible contamination combined with volatility such that they are distributed through the atmosphere and reach globally homogeneous distribution too rapidly to avoid a planetary scale effect even if the effect is first discovered at a local or regional scale. Chemicals fit the second profile if they cause poorly reversible contamination and are water-soluble such that they are distributed in the oceans and trigger an effect that is only manifested at the global scale, or they trigger an effect that occurs with a time delay that corresponds approximately to the time required for global distribution such that the effect manifests nearly simultaneously at local, regional and planetary scales. These two profiles are fulfilled, respectively, by airborne persistent contaminants (APCs) and waterborne persistent contaminants (WPCs). Chemicals can be assessed as APCs and WPCs with the aid of multimedia models that calculate metrics of persistence (P) and potential for long-range transport (LRT).

The exposure-based hazard profiles for POPs and vPvB chemicals do not fully coincide with each other, and also do not fully coincide with the profiles of planetary boundary threats [11,14]. Therefore, it is not advisable to combine all the different profiles into one generic exposure-based hazard profile. We hypothesize that among the chemicals detected in the Arctic and included in the AMAP report there are different sets of chemicals of concern according to hazard profiles defined by POP, vPvB and the APC and WPC planetary boundary threat profiles. We further hypothesize that the report includes chemicals of relatively low exposure-based hazard concern according to all four profiles that are present in the Arctic due to local production/consumption patterns.

Our aims in this study are i) to propose exposure-based hazard profiles for planetary boundary threats from airborne persistent contaminants (APCs) and waterborne persistent contaminants (WPCs) that can function complementarily to the POP and vPvB profiles, ii) to develop a ranking method to prioritize chemicals that fit each of these exposure-based hazard profiles based on benchmarking against relatively well-known environmental contaminants, and iii) to use our hazard profiles and ranking method to prioritize chemicals in the AMAP dataset that should be assigned high priority for further study.

## 2. Materials and methods

### 2.1. Compilation of the AMAP chemical property database

We compiled a database of physicochemical properties for the 631 chemicals that appear in a draft version of the AMAP report. Our database includes the following information on each chemical:

1) SMILES code obtained using ChemSpiPy [16] and PubChemPy [17] to access the Chemspider [18] and Pubchem [19] online databases, respectively and curated using the OpenBabel [20] software.
2) Molecular weight, vapor pressure and subcooled liquid vapor pressure, the logarithms of octanol-air, octanol-water and air-water partition ratios (log $K_{OA}$, log $K_{OW}$ and log $K_{AW}$, respectively), the logarithm of the bioaccumulation factor (log *BAF*), water solubility, and the half-lives in air, water, soil and sediment estimated by EPI Suite [21] from SMILES.
3) Acid and base dissociation constants (p$K_a$ and p$K_b$) estimated from SMILES by the ACD Labs/Percepta PhysChem Profiler [22].

For the purposes of this study, we removed all organometallic compounds and any compound that is likely to be ionized within an environmentally relevant pH range (i.e. compounds with estimated p$K_a$ lower than 5 or p$K_b$ greater than 8) from the AMAP database. Organometallics were removed because they fall outside the applicability domain of EPI Suite. Ionized chemicals were removed because of uncertainties associated with their partitioning properties and bioaccumulation potential, leading to unquantifiable uncertainty propagation from EPI Suite to our selected multimedia model (the OECD Tool, see below) and to the synthesis of the screening information in the prioritization scheme. A total of 464 chemicals that are cited in the AMAP report remained in the database after the removal of these compounds. The chemical