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Reducing the environmental risks of formulated personal care products using an end-of-life scoring and ranking system for ingredients: Method and case studies

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ABSTRACT

Personal care products (PCPs) are used globally wherever there is human activity, and are typically emitted to the environment in wastewater under normal use. Regulators and scientists have thus begun focusing on PCPs as a potential water quality concern. PCP manufacturers are increasingly motivated to leverage available data on potential exposure and hazards to the natural environment to guide sustainable decision making and minimize the potential for products to cause adverse environmental effects. We describe a novel algorithm to: select data on environmental exposure and hazard potential relevant to PCP ingredients after use, evaluate and interpret those data, and translate the information to a single numeric score usable by non-specialists to incorporate environmental protection goals into PCP sustainability decision making. The algorithm has been implemented as the Global Aquatic Ingredient Assessment (GAIA) database tool, incorporating information on environmental persistence, bioaccumulation potential, aquatic toxicity of the parent compound and degradants, excess toxicity from ecological endocrine disruption effects, and the potential for producing photochemical smog. GAIA quantifies environmental hazard potential using an algorithm allowing it to be used as a risk surrogate for PCP product use. GAIA data are also used in environmental risk assessments with product-specific exposure data as a final check during product reformulation or as a post hoc measure of progress toward corporate sustainability goals. Scoring results are demonstrated for eight representative substances: benzophenone-4, ethylene diamine tetraacetate salts, ethylhexylglycerin, menthol, methyl salicylate, musk xylene, phenoxyethanol, and zinc oxide. Case studies show how GAIA scores, used as a front-line decision tool, led to environmental risk reductions in two cases: a newly developed surfactant and a reformulated cleansing product.

1. Introduction

Consumers express interest in selecting products that are safer for the environment (Whan, 2010). "Personal care products" (PCPs) is emerging as a category of chemicals detected in water and identified by the scientific community for further study to better understand potential environmental impacts (Rudd et al., 2014). Regulatory efforts have been underway to establish environmental risk assessment procedures specific to this class of products (Health Canada, 2010). Formulated PCPs are mixtures that comprise a chemically diverse class, including neutral organic compounds, salts, metals, acids, bases, and substances of unknown or variable composition, complex reaction products and biological materials (UVCBs) such as botanical extracts and some polymers. Data for environmental fate and effects are most readily available for distinct organic and inorganic substances, which are the ingredients addressed here. Most formulated PCPs share a similar mode of exposure in the environment, because they are designed to be used on skin, hair, or in the mouth, and are washed off during use or over time, entering domestic wastewater regionally or globally. Because of the chemical diversity in the class, potential environmental hazards vary widely. As a result, it is a challenge to make environmental safety data available in a simple and consistent manner that is accessible to PCP formulators to select components that are more environmentally benign. We developed an

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algorithm, implemented as Global Aquatic Ingredient Assessment (GAIA), to collect, aggregate, and communicate environmental safety information for PCP ingredients and products to formulators in a form that is scientifically sound and sufficiently unambiguous, so that no expertise in environmental science is necessary to understand and use the result. The data aggregated to develop a GAIA score, along with environmental exposure data, are also used to quantify risk reductions that cascade from initial hazard-based decision guidance.

Chemical risk ranking and scoring systems have been developed for other purposes (e.g., Hansen et al., 1999; Russom et al., 2003; Swanson et al., 1997), and whole-systems approaches that include environmental assessment as one dimension have been developed, integrating other data (e.g., economic, social), aimed for broader decision-making (e.g., Iacovidou et al., 2017a, 2017b, 2017b; Millward-Hopkins et al., 2018). The algorithm described here differs from previous ranking and scoring schemes because it was developed specifically for evaluating ingredients in PCPs, so human safety hazards could be excluded, as those attributes are rigorously evaluated separately due to the nature of the products; and it can be used as a hazard-based proxy for potential incremental risks, because of similarities in ingredients' end uses and hence exposure. Additionally, scores are based on a consistent data set for each substance, and range between zero and one hundred, allowing relatively fine distinctions among substances. Finally, the algorithm includes penalties for uncertainty when models are used to fill data gaps.

Here, we present the algorithm as it has been implemented in an electronic database for one organization's global formulator network. While most parameters in the model were selected based on benchmarking against currently accepted science principles from worldwide regulatory and product labeling schemes, some parameters were implemented specifically to meet the end-user organization's unique goals. We explain the basis for parameter selection here, so this process can be readily adapted for other end users and scenarios.

2. Materials and methods

2.1. Algorithm design

We translated environmental fate and effects data to a numeric score by developing scoring scales with specific aims of (1) distinguishing among good/better/best alternatives, (2) identifying poor performers, for possible restriction from use in future products, (3) assessing only endpoints for which data exist for large numbers of PCP substances, as the algorithm is intended to be used to score the large number (>1000) of ingredients used in PCPs, and (4) using widely accepted science to evaluate environmental safety.

We considered many endpoints typical of life cycle assessment (e.g., energy use, water use, packaging qualities, use of non-renewable feedstocks) that were not selected for inclusion, because they are currently too difficult to quantify for large numbers of substances, or because they differ over time and among suppliers. The algorithm uses intrinsic properties of ingredients, to be time- and manufacturer-invariant. We calculate a Base Score accounting for persistence, bioaccumulation and toxicity (PBT) properties, with an added system of penalties applied to the Base Score to account for "other environmental concerns" because: (1) Data and models for P, B, and T properties exist for a large number of PCP substances, so it is possible to make a quantitative estimate of these characteristics for all scored substances, allowing direct comparison, and (2) we could incorporate knowledge about any additional, potential hazards that apply only to certain classes of PCP substances, to encourage formulators to choose ingredients lacking these additional hazards, when all else is equal. We defined several classes of "other environmental concerns," which are each incorporated into the score as a penalty to the Base Score. These penalties can be adjusted readily to reflect evolving scientific opinion and end user risk valuation preferences. The assumption is that PBT properties are of interest for every chemical, and no score is possible without data on these properties; and with the penalty system, emerging concerns, applicable for only a subset of substances, can be incorporated as well.

2.2. Scoring algorithm

The Base Score is a single number between zero and 100 that integrates a substance's characteristics of environmental persistence in water, soil, sediments, and/or air, its potential to bioaccumulate in food chains, and its direct toxicity to aquatic organisms (i.e., PBT characteristics). A higher score corresponds to more favorable environmental safety characteristics. Scores are reduced for uncertainty (e.g., when *in silico* models are used to fill gaps in the empirical data).

Expected environmental persistence (expressed as a P-score) is evaluated as shown in Fig. 1. If empirical data indicate the substance is readily biodegradable (e.g., OECD test guideline 301 result), the substance's P-score is 100 and the P-evaluation ends. Substances that meet the criteria to be labeled "readily biodegradable" are presumed to completely mineralize rapidly in wastewater treatment plants and/or the environment (OECD, 2006). If insufficient empirical data are available to determine whether the substance is "readily biodegradable," the BIOWIN model (e.g., Tunkel et al., 2000) is used. If the model predicts "readily biodegradable," the P-score is 95, reflecting a five-point uncertainty penalty. .

When a substance is not readily biodegradable, the half-life in each environmental medium of concern is determined (i.e., water, sediment, soil, air), and used as the basis for the P-score using medium-specific scoring scales described in Section 2.3. The EPISuite Fugacity Model (Mackay et al., 1996) is used, with default settings, except 100% of the emission is assigned to water (i.e., zero atmospheric and soil emissions), reflecting the predominant environmental exposure pathway for PCPs. Media of concern are defined as those in which ≥5% of the emissions are predicted to partition, as done for categorizing chemicals under the Canadian Environmental Protection Act (Environment Canada, 2006). Empirical data for half-life in each medium of concern are used preferentially, but are rarely available. When empirical degradation data are lacking, the half-life(s) calculated in the EPISuite Fugacity Model are used. The longest relevant medium-specific half-life is used for persistence scoring.

Bioaccumulation potential (expressed as a B-score) is evaluated as shown in Fig. 1. If the molecular weight is ≥1000, the likelihood of bioaccumulation is low, because the substance is too large to cross biological membranes (i.e., it is not bioavailable) (e.g., Nordic Ecolabelling, 2012), and the B-score assigned is 100. For all other molecules, the empirical bioconcentration factor (BCF) in fish determines the B-score using the scoring scale described in Section 2.3. When multiple reliable empirical results are available, the highest BCF value is used. When empirical data are not available, the BCFBAF model (Meylan et al., 1999) result is used. When modeling is used for the basis of the score, the B-Score is reduced by a five-point uncertainty penalty. If the substance is readily biodegradable, the B-score is assumed to be 100 (i.e., bioaccumulation is not a concern), because degradation is expected to occur before bioaccumulation onset begins, except in the case of "pseudo-persistence." This is when long-term exposure to biodegradable substances occurs immediately downstream of a continuous untreated wastewater emission, so bioaccumulation cannot be ruled