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Method to incorporate green chemistry principles in early-stage product design for sustainability: case studies with personal care products†

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Applying green chemistry principles in raw material selection for down-the-drain products is a powerful tool to improve product sustainability. We developed a method to support sustainability-minded design, or eco-innovation, implemented as a spreadsheet tool, for assessing the potential environmental impact of down-the-drain personal care products at the early design stage. End-of-life ecological risk assessment (ERA) is traditionally used for down-the-drain products. Life cycle assessments (LCAs) include a broader range of impacts but require supply chain data not available at the early design stage. We used all feasible ERA and LCA measurement scales for environmental concerns as "potential impact indicators" (PI-indicators). PI-indicators from ERA include bioconcentration in fish and Predicted No Effect Concentrations (PNECs) in water, sediment, and/or soil, depending on the environmental fate of ingredients in the product. PI-indicators from LCA include phosphorus content (eutrophication potential), photochemical ozone (smog) formation potential, mineral resource depletion, and direct emissions of greenhouse gases or ozone depleters. Emerging regulatory concerns included are persistence, subsurface migration potential, and partial degradation of polymers. PI-indicators are aggregated using weighting factors to yield a rank between 1 (best) and 10 (worst) for each ingredient and translated to a product rank using a weighted average. The tool allows end users to change PI-indicators as science and priorities change. The method is demonstrated for 10 shampoo and 9 facial makeup products illustrating differentiation among formulas to promote sustainability at the early product design stage.

1. Introduction

Ecological innovation, or *eco-innovation*, is the development of new processes or products with explicit attention to sustainability, one aspect of which is reducing environmental impact.[1] Increasingly, companies are adopting eco-innovation practices in response to pressure from governments, customers, competitors, and internal interests and to achieve cost savings or other competitive advantages.[1,2] To facilitate environmentally-focused eco-innovation, product designers need assessment tools to rapidly compare prospective products' environmental performance. Green chemistry principles[3] are useful to guide the design of such sustainability tools. Specifically, chemical mixtures used in PCPs can be selected to be safer (*i.e.*, avoiding toxicity) and degradable, and higher efficacy products can be selected to prevent waste.

Ecological risk assessment (ERA) and life cycle assessment (LCA) are two widely used environmental assessment techniques available to support eco-innovation underpinned by green chemistry principles. These are generalized techniques that must be implemented differently for each type of product evaluated, depending on use and disposal patterns. Products where the disposition after use is predominantly to wastewater (down-the-drain, or DtD), and hence aquatic environmental exposure is anticipated, include pharmaceuticals, household cleaners, and formulated personal care products (PCPs). Formulated PCPs include cosmetics and related products regulated in some jurisdictions as drugs (*e.g.*, sunscreens, anti-dandruff shampoos), because they contain one or more active ingredients. PCPs are designed for immediate rinse-off (*e.g.*, shampoo) or for disposal through a combination of wiping and washing (*e.g.*, facial make-up) and thus have a full or partial DtD disposition.

ERAs and hazard profiles focusing on the protection of aquatic species and wildlife at the product's end-of-life are commonly used to assess the environmental impact of PCPs.[4,5] Studies addressing PCPs' environmental safety have focused predominantly on fragrance compounds and active ingredients (*e.g.*, DEET, triclosan, oxybenzone),[6–8] but some companies have made proactive efforts to understand end-of-

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life impacts for the entire range of ingredients with a goal of "greener" product design.[9–11] While ERAs are typically used to make regulatory decisions, some governments recently used end-of-life ecological hazards as the basis for restricting the use of PCP ingredients, including cyclic siloxanes, oxybenzone, octinoxate, and plastic microbeads.[12–14] These hazard-based decisions resulted in a need for companies to rapidly reformulate products or cease sales in affected markets.

LCA is an internationally standardized method (ISO 14040) for evaluating a product's environmental impacts. This method is used to support sustainable management efforts and is valuable for identifying a wider range of potential environmental impacts.[15] Although LCAs are resource-intensive, since much of the data required are not in the public domain, there is regulatory pressure to use LCAs more frequently for PCPs. For example, Golsteijn *et al.* performed an LCA for a model shampoo product[16] using Product Environmental Footprint Category Rules (PEFCR) proposed by the European Commission[17] and showed that, while end-of-life ecological impacts are indeed important as expected, other impacts including energy use for ingredient manufacturing and consumer use (*i.e.*, showering) were also important.

Ideally, comprehensive data from both ERA and LCA methods would be considered during product design to help companies understand and minimize the potential for future adverse environmental impacts. However, a major challenge is that thousands of ingredients are used in PCPs, spanning a wide range of chemistries (*i.e.*, organics, inorganics, organometallics, polymers, natural oils, extracts, and exudates along with derivatives and mixtures of these) often lacking crucial life cycle data to estimate the full range of impacts. Also, supply chains are often not selected in the early stages of product design, so assessments at this stage must rely on intrinsic chemical properties and foreseeable product use only. With these limitations in mind, we developed a new environmental assessment tool to support eco-innovation in the early design stage of DtD products, demonstrated here for PCPs, that incorporates all practicable environmental impact indicators commonly used in ERA and LCA.

The tool is implemented as a semi-automated spreadsheet that gathers and processes environmental impact data for ingredients used in formulated products and aggregates the data into a single rank value between 1 (best) and 10 (worst) for each. The tool's output is derived from 10 environmental impact indicators commonly used in ERA and LCA which are readily available at the early design stage. The tool integrates scientific data with organizational priorities (*via* weighting and aggregation decisions) to support eco-innovation by informing design teams of potential future environmental and concomitant business risks.

2 Methods

2.1 Assessment method selection process

We identified quantitative indicators useful for assessing adverse anthropogenic environmental impacts, or potential impact indicators (PI-indicators) available at the early design stage by reviewing the scientific literature and regulatory models. Only methods, models, and data available in the public domain were selected to allow transparency and portability of results. Sources of assessment methods consulted for use include ecolabeling programs (*e.g.*, US EPA Safer Choice, EU Flower, Nordic Swan), regulatory guidance (*e.g.*, US Toxic Substances Control Act; EU REACH, Canada Chemicals Management Plan, UN Globally Harmonized System of Classification and Labeling of Chemicals), LCA models (*e.g.*, USETox, TRACI, ReCiPe), and similar methods reported in the literature.[10,11] PI-indicators that require data from ingredient suppliers were eliminated from consideration, as suppliers are often not determined at the early design stage.

Golsteijn *et al.* identified the most substantial life cycle impacts of a model shampoo product.[16] Important impacts included energy use for heating water during a shower, impacts associated with surfactant feedstock selection and processing by the supplier, and ecological effects after use. Only the latter can be addressed at the early design stage. Manufacturers have redesigned similar products to reduce use-phase impacts, such as laundry detergents redesigned for cold water use.[18] However, this type of design change is not possible for shampoos. Based on this finding by Golsteijn *et al.*,[16] ecotoxicity was developed in the most sophisticated way among the PI-indicators.

The aim of the tool was also to help "future-proof" new products against the need for urgent reformulation under anticipated future regulatory pressure. We reviewed emerging scientific and regulatory concepts about potential environmental impacts of DtD substances. Sources included governmental position papers, peer-reviewed literature, and recent scientific conference proceedings.[19,20] Based on this review, we included persistence as an independent PI-indicator, subsurface migration potential for persistent substances, and for polymers, potential impacts from partial degradation products in addition to those from the parent compounds (see section 3.1).

The tool was deployed in a high throughput design, with automated data collection and calculation for organic mono-constituent substances and individual components of mixtures using Microsoft's Excel 365 and Visual Basic for Applications 7.1. Two additional versions were created with changes to accommodate polymers and inorganic substances, which have properties requiring adaptations to the "base-case" algorithm (see section 2.2) developed for organic substances.

2.2 Data selection process for formulas and ingredients

The compositions of representative PCPs were obtained from Avon Products International and from suggested formulas published by ingredient manufacturers available on the UL Prospector internet database. One shampoo formula was published as a model for testing PEFCR guidelines.[16] Using the combined list of 104 ingredients from 10 shampoos and 9 facial makeup products, we identified distinct substance classes that must undergo different environmental assessment processes. The most common ingredient type was nonpolymer organic substances supplied either as a single constituent or as a mixture with other structurally related compounds (*e.g.*, differing by chain length). This substance class was targeted for initial method development and compromises our "base-case" algorithm. Further details about implementation of the base-case are included in ESI.†

3 Theory

The base-case ranking process for organic substances is shown in Fig. 1, where color coding is used to indicate assessment paths completed for all substances (white boxes) *versus* those triggered only for substances with specific characteristics (shaded boxes). The final outcomes are: Predicted No Effect Concentration (PNEC) values and a final rank value for each PCP ingredient substance. The PI-indicators also yield subrank values (SRVs) for ecotoxicity, bioaccumulation, persistence, and for the group of all other PI-indicators combined (described as "Rare Impact Indicators" in Fig. 1). These can be presented, optionally, for users to understand the source of concern if the final rank is not optimal.

3.1 Inclusion of impacts and weighting factors

PI-indicators selected for inclusion in the tool are listed in Table S1† and include: (1) ecological toxicity during end-of-life exposures, (2) bioconcentration factor in fish as an indicator of potential bioaccumulation, wildlife exposure, and secondary poisoning effects during end-of life, (3) soil mobility of persistent, water soluble substances to protect groundwater, (4) the potential for ground level photochemical ozone (smog) formation, (5) the potential for eutrophication, (6) direct greenhouse gas emissions from PCP end use, (7) direct emission of stratospheric ozone-depleting substances from PCP end use, (8) depletion of scarce mineral resources, (9) persistence as an independent PI-indicator because (a) it is a prerequisite for all other impacts, (b) it is a surrogate for unanticipated impacts not foreseen based on current knowledge, and (c) regulators have begun to use persistence as the sole basis for restricting the use of certain substances in commerce,[21,22] (10) other impacts not otherwise included, where end users can include new or unique concerns not already captured. We chose to present a single numeric rank between 1 (best) and 10 (worst) as the output for ease of integration into the product design process. For design teams needing more detailed information, SRVs (also ranging from 1 to 10) are available.

Impact categories 1 and 2 (ecotoxicity and bioaccumulation potential) are both focused on ecological effects at the end-of life. These are the most common environmental impacts addressed in regulations for DtD products and were identified as an important life cycle impact for shampoo.[16] In recognition of this and consistent with green chemistry principle 4,[3] the categories representing the potential for end-of-life ecological effects were weighted 50% in the ingredient final rank (30% weight for aquatic, soil, and sediment toxicity; 20% for bioaccumulation potential). Impact category 9, persistence, was assigned a weight of 30% toward the final rank, because of its importance as a precursor to all potential impacts and because of the difficulty in mitigating adverse impacts of persistent substances after their emission, consistent with green chemistry principle 10.[3]

The remaining seven impacts are observed more rarely among PCP ingredients, and we found that weighting them the same way as ecological effects and persistence unacceptably diminished their influence on the final rank (*i.e.*, the impact of any one would not be mathematically capable of changing the final rank value by a full unit). If we made all 10 categories carry equal weight, each one could influence the rank by one unit. But by doing so, most final product ranks would be clustered between 1 and 3, because few PCP ingredients are impactful in most or all categories. To address this, we created a group for these rarer impact categories that carries 20% of the total weight. The PI-indicators are toggled to "yes" if the concern exceeds a threshold value, or "no" if it does not. These PI-indicators were divided into two groups: (1) emissions with a global reach (*e.g.*, climate change) and (2) emissions potentially affecting local areas susceptible to the impact (*e.g.*, eutrophication). Each "yes" for a local impact (*i.e.*, categories 3–5) decrements the group's SRV by half (*i.e.*, drops from 1 to 5 or from 5 to 10). Each "yes" for a global impact (*i.e.*, categories 6–8), decrements the group's SRV from 1 to 10. Thus, a single localized impact would decrement the final substance rank by one unit, and for a global impact, two units. A potential drawback is that additional "yes" values cannot demote the SRV below 10, which could hypothetically result in losing information (*i.e.*, where potential impacts exist that do not influence the final rank). We found this compromise acceptable, because this situation is exceedingly rare – we did not encounter it among the 104 ingredients evaluated here. These weighting factors are detailed in Table S1.† Conditions that cause each assessment path to be triggered are listed in Table S2† and described in the remainder of section 3.

PI-indicators associated with human health were omitted, as the focus for this model is on environmental impact. Human health safety is addressed separately in mandated product safety assessments for PCPs to ensure that products comply with applicable regulations and ingredients are used at safe levels without posing a health risk to consumers under normal or reasonably foreseeable conditions of use.

3.2 Ecotoxicity implementation

3.2.1 Predicted no effect concentrations. Life cycle assessment models include databases characterizing impacts for large numbers of substances, so we considered using an LCA tool as the basis for this impact category. The PEFCR guidance[17] recommends the USETox life cycle impact assessment approach for assessing freshwater ecotoxicity. Concerns have been raised with this approach for shampoos because of its sensitivity to limited aquatic toxicity data sets,[23,24] and it does not include the potential for effects on sediment and soil organisms. Hence, we chose to rank aquatic toxicity using

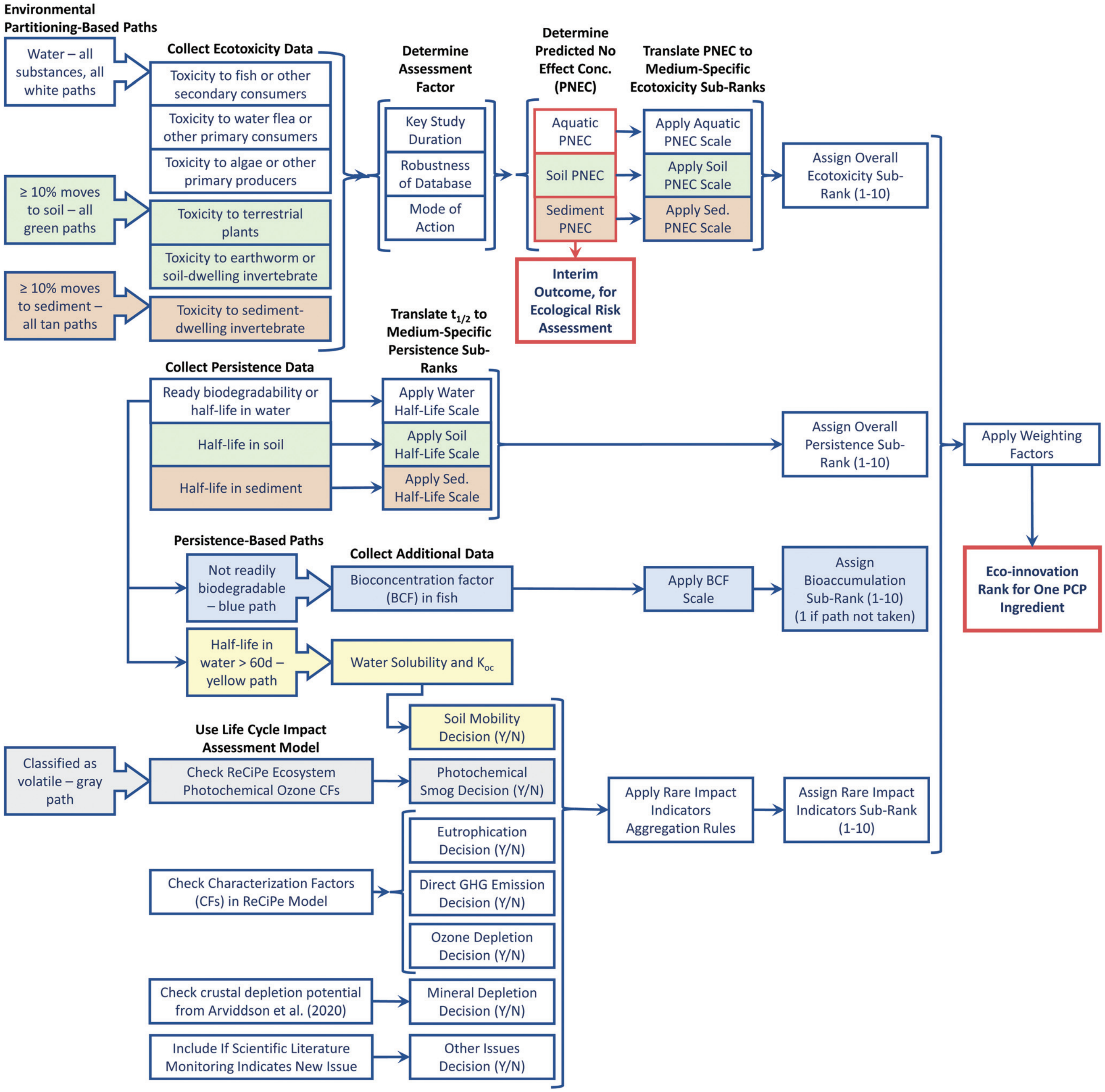

Fig. 1 Overview of the ranking process for the "base-case" – organic small molecules. Red boxes show process outcomes: (1) PNECs in water and if triggered, in sediment and soil, (2) PCP Eco-innovation rank for one substance. Shapes with wide, rightward-facing arrows show triggering step for assessment paths. The color of each shape indicates a distinct assessment path. White: all substances. Green: substances that partition ≥10% to soil *via* biosolids; tan: substances that partition ≥10% to sediment after emission; blue: non-readily biodegradable substances; yellow: substances persistent in water (half-life >60 days); gray: volatile substances (boiling temperature <250 °C).

PNECs derived from a method recently developed at Environment and Climate Change Canada.[25] A benefit of this method is that it results in PNECs that can be directly imported into ERAs, allowing efforts in eco-innovation to be leveraged for other organizational needs. We selected this approach because Okonski *et al.* used a consistent and logical rule set for selecting critical toxicological endpoints and assigning Assessment Factors (AFs), allowing consistent results for different assessors, while using diverse data from any study duration in guideline studies, QSAR models, and read-across data as well as accounting for available knowledge on the substance's mode of action.[25] A simplified version of the method was deployed here to allow high throughput screening, because some aspects of the full method require data that cannot be automated. Details of implementation are given in ESI.†

Ecotoxicity in sediment or soil is only considered when the substance is not readily biodegradable, and modeling indicates ≥10% of the emitted mass would partition to that environmental compartment. Implementation details are provided in ESI.† As a default, the tool calculates PNECs for soil and sediment from the aquatic PNEC using the equilibrium partitioning approach from REACH guidance.[26] Empirical data for toxicity to sediment or soil organisms and an appropriate AF are preferred, if available, and must be manually input. All model parameters used to derive PNECs are detailed in Table S3.†

3.2.2 Potential for bioaccumulation and secondary poisoning. In site-specific ERAs and regulatory environmental hazard assessments, it is customary to consider the potential for substances to bioaccumulate in ecosystems, which can lead to secondary poisoning in predators due to higher exposures than predicted based on direct ingestion or absorption from the environment (*i.e.*, biomagnification). While a bioaccumulation factor (BAF) is preferred for characterizing this endpoint because it accounts for exposure from the environment and food, BAF values are rarely available. Hence, the bioconcentration factor (BCF) in fish is commonly used. Arnot and Gobas developed a QSAR model meant to estimate the potential for biomagnification and secondary poisoning in aquatic ecosystems by accounting for competition between chemical uptake from the environment and metabolism within the organism, deployed in the US EPA BCFBAF model.[27] We used this as the default value for the bioaccumulation PI-indicator, evaluated only for substances that are not readily biodegradable, because it is assumed that exposure is highly mitigated for readily biodegradable substances.[28]

3.3 Persistence

Persistence is not an environmental impact; however, it is used here as a surrogate for exposure and multiple impacts. Regulators recently began using persistence as a rationale to restrict the use of substances, even in the absence of any known hazards.[21,22] Beyond the concern for overt regulation, persistence is also a surrogate for unanticipated adverse environmental effects. Only a narrow range of species and ecosystem interactions are ever studied, so it is inevitable that sensitive species or complex interactions leading to toxicity are sometimes unknown. For example, mass eagle deaths in the Southeastern US were due to complex interactions between pollutant chemicals in water and species from several trophic levels.[29] Because the pollutant initiating this chain reaction is persistent, the impact to eagles will be difficult to halt. To encourage product designers to create PCPs that are less likely to contribute to such complex and unexpected ecosystem perturbations, which may be difficult to reverse, persistence was selected as an independent impact category.

Ready biodegradability is a designation attained by a substance that meets certain thresholds for speed and completeness of biodegradation in a stringent standardized screening test. Guidance from the Organization for Economic Cooperation and Development (OECD) for interpreting these test results indicates that readily biodegradable substances can be assumed to undergo rapid and complete biodegradation in the environment.[28] The QSAR BIOWIN, within EPISuite, predicts the outcome of a ready biodegradability test and is used in the tool as the default to identify substances of no concern for persistence. Non-readily biodegradable substances are evaluated by their half-life in water, and if ≥10% of the substance's emissions partition to sediment or soil, half-life in those compartments is included also as described in ESI and shown in Tables S4 and S6.†

3.4 Rarer impacts

The remaining group of seven potential impacts were considered categorically as either "Yes" for a potential impact that reaches a threshold of concern, as defined in the tool, or "No" if the threshold is not reached. The "Yes" and "No" responses were translated to a rank for this group of indicators as described in section 3.1 and summarized in Table S1.† This simpler implementation was selected because these impacts are more rarely observed, and as such it was not necessary to make finer distinctions among degrees of impact. The modular nature of the tool allows this decision to be changed and ranks automatically recalculated in the future if it is clear there is a need to determine the intensity of these potential impacts with greater granularity.

3.4.1 Soil mobility. The soil mobility PI-indicator identifies persistent, water-soluble substances capable of subsurface migration *via* leaching through soil and potentially contaminating groundwater resources. This concern could apply in regions where septic systems and drinking water wells are common (*e.g.*, the US States of New Hampshire and Maine, where half of all households use septic systems according to the US EPA Septic Systems Overview internet site). Two of the criteria proposed by Neumann and Schliebner[19] were adopted to toggle this indicator to "Yes": (1) water solubility >0.15 mg L^{-1} and (2) organic carbon-water partition coefficient ($\text{Log}\,K_{\text{oc}}$) $< 10\,000$. These criteria capture more substances than the full set of criteria proposed by Neumann and Schliebner (2017) for designating a substance as persistent, mobile, and toxic (PMT), because that designation is reserved for substances of very high concern, eligible for restriction.[19] For eco-innovation efforts, we opted to include persistent and mobile substances without regard to toxicity as a precautionary approach.

3.4.2 Ground level photochemical ozone (smog). Some volatile substances undergo photochemical reactions to form ozone, which at ground level damages human and wildlife respiratory systems, stomata and wax layers on plants, and materials such as rubber and paint. Some PCPs have been identified as contributing to ground level ozone[30] and are subject to regulation because of it.[31] We evaluate this impact only for volatile PCP ingredients, defined here as having a normal boiling point <250 °C. Any volatile substance with a positive value for either the Photo-Chemical Oxidant Formation Potential: ecosystems in the ReCiPe LCA Characterization Factors (CF) database or the Maximum

Incremental Reactivity level is toggled "Yes" for this impact category.

3.4.3 Eutrophication. In healthy water bodies, nutrient scarcity limits the growth of aquatic plants. Eutrophication occurs when limiting nutrients are emitted to water, promoting overgrowth of algae, blocking the water surface. As the plant material dies, sinks, and decays, the oxygen level in the water body drops and other organisms are negatively impacted. Both inorganic and organic substances containing phosphorus can contribute to eutrophication.[32] We used the freshwater eutrophication CF from ReCiPe – the presence of phosphorus in the substance – to toggle the PI-indicator to "Yes".

3.4.4 Global impacts. The remaining three defined impact categories are global in scope and apply to a limited number of PCP ingredients. The ReCiPe model's CFs for global warming and stratospheric ozone depletion are used to determine whether these categories are a concern. For global warming and ozone depletion, the PI-indicator is "Yes" if the ingredient substance is listed in ReCiPe as directly contributing to either of the impacts.

Mineral resource depletion is commonly evaluated in LCA by considering geological factors as well as socioeconomic and technological factors (*e.g.*, extraction efficiency), but these are subject to dramatic change.[33] The ReCiPe CFs are based on the concept that use of a mineral resource irreversibly diminishes the most easily obtained supply of that resource, leaving future generations to obtain the mineral only through more expensive means (*e.g.* from ores that are less rich). This results in relatively high CF values for some minerals that are abundant in the earth's crust (*e.g.*, silicon), yielding LCA outcomes that some practitioners have rejected as unrealistic, so Arvidsson *et al.* developed a mineral resource indicator, Crustal Scarcity Potentials (CSPs), that attempts to correct this concern,[34] which we adopted as the PI-indicator. The CSPs are normalized to silicon which has an assigned abundance of one, with higher CSP values denoting lower abundance. We selected the CSP for zinc as the threshold at or above which this indicator is toggled to "Yes", but excluded nitrogen, because the atmosphere, not the earth's crust, serves as its primary source.

3.5 Translating indicator values to sub-rank and rank values

The PI-indicator values (*e.g.*, PNECs, half-life values) are translated to SRVs using the mathematical scales in Table S5.† The scales for SRV calculations range from 0 to 9 because our mathematical expressions are simpler when the lowest rank value is zero rather than one. In the final presentation to end users, ranks are incremented by one to achieve a range from 1 to 10. Each equation used to translate a PI-indicator to its SRV was derived to comport with the conclusions in the regulatory and ecolabel literature reviewed (section 2.1) on levels of concern. For example, the bioconcentration factor in fish is translated to an SRV in a log linear model optimized to match these benchmarks: a BCF of 100 yields a SRV of 0 (best) because that BCF exempts persistent substances from being considered as PBT substances;[35] a BCF of 500 (SRV 4) is considered "low level" bioaccumulation;[35] a BCF of 2000 (SRV 7) is considered "bioaccumulative" and 5000 (SRV 9, worst) is "very bioaccumulative" under REACH. These SRVs are suitable to be shared with product designers interested in better understanding the source of any impacts reflected by a poor final rank for a proposed new product. The four SRVs (see Fig. 1) are weighted according to the scheme described in section 3.1 when aggregating to achieve the final rank for an ingredient.

For a finished product, the ingredient ranks are multiplied by their respective fractional weight in the formula and those values are summed. Water generally should be excluded from the formula in this step, because its presence reduces sensitivity of the rank. Also, its inclusion would promote the use of products with a higher water content when they are likely to be less efficacious, so a larger dose is required, and impacts are not necessarily avoided.

Any ingredient comprising less than 5.5% of a product's formula (dry weight basis) is not mathematically capable of influencing the rank, regardless of its SRV. However, it could be problematic to include exceedingly poor-performing ingredients in a formula, even as minor constituents, so it is recommended to use the tool for a second, gatekeeping function. For example, ingredients with a rank above a certain threshold (*e.g.*, 6) would be flagged for additional levels of scientific review and approval before their use would be allowed.

3.6 Inorganics and polymers

Inorganic and polymeric ingredients require alterations from the base-case approach. Slow transformation (inorganics) or degradation (polymers) can potentially lead to persistent or slowly degrading daughter products (called fragments here) in the environment that could potentially pose an environmental risk. We accounted for these by identifying the fragment of highest concern based on scientific consensus in the literature or professional judgment and determining a rank for both the ingredient and the fragment. The final rank is a weighted average of the parent rank (70%) and the fragment rank (30%). The lower weight for the fragment reflects uncertainty in its identity and rate of formation (and hence exposure potential). There are two special cases for inorganics: (1) those that rapidly and fully dissociate in water (*e.g.*, NaOH) are weighted 0% parent/100% fragment, (2) those considered insoluble and hence dissociate very slowly, if at all, are weighted 90% parent/10% fragment. These alternative weighting approaches are meant to reflect the chemical species likely present in the environment.

Predictive models are typically not useful for high molecular weight polymers or metals, so these ranks require the use of hand-curated data. Inorganics and their fragments are generally well studied and understood, but few data for polymers exist in the public domain because current regulatory schemes (*e.g.*, REACH) exempt many polymers from public disclosure of environmental safety data. Hence, a rule set was needed for assigning estimated data, shown in Table S6.†

The concept of persistence as it applies for organic substances is not meaningful for inorganics, because the hazardous moiety is often a metal atom (*e.g.*, Al, Cu, Zn), which is infinitely persistent but also naturally-occurring and in many cases, both an essential nutrient and a potential toxicant. Hence, persistence is not unequivocally a negative attribute for inorganics. Furthermore, considering inorganics as infinitely persistent (a severe penalty under this system) would improperly ignore the fact that they undergo transformations in the environment (*e.g.*, oxidation, precipitation) that alter their bioavailability and potential toxicity. Hence, persistence was considered differently than for organics, described with two approaches that yield the same rank: (1) the persistence category is omitted and the weighting factors for the other impact categories are increased, maintaining their relative weights, or (2) persistence is considered only as important as the known effects, so the rank that would be yielded from the other impact categories alone is substituted as the persistence rank.

3.7 Minimally processed natural ingredients

Another category of ingredients frequently lacking sufficient data to derive a rank is minimally processed natural ingredients. Ingredients in this class are common in PCPs, though many are used at low levels in the product. Examples include lanolin, honey, sesame oil, corn starch, guar and xanthan gums, fruit juices, and ground or powdered plant parts (*e.g.*, oatmeal). These are generally chemically complex, heterogeneous, and variable mixtures. Few have a well-characterized chemical composition. When empirical data were lacking, we assigned a default category rank of three based on data from well-studied chemical components from these mixtures. These data show a general pattern that persistence and bioaccumulation potential are low and aquatic toxicity ranges from very low to relatively potent. Most have no other concerns among the rarer impact categories. This reflects that microbes have evolved the ability to metabolize natural materials, eliminating extreme persistence as a concern; however, plants evolved the ability to produce toxins as a defense against predation, so aquatic toxicity is sometimes a concern.[36] This combination of properties led to a 5th percentile rank of three among natural ingredient components having empirical data to support their rank values.

4 Results and discussion

The results of the ranking system are shown in Table 1 for 10 shampoos and 9 facial makeup products with underlying details explained in ESI and Tables S7, S8.† Shampoos include a less diverse set of ingredients than facial makeup, and shampoo ingredients are dominated by surfactants, most of which yield a rank of 3, driven by low persistence but relatively potent aquatic toxicity. While the ingredient ranks for shampoos range from 1 to 7 (mean 3.1; standard deviation 1.6), the product ranks were all 2 or 3. In contrast, the makeup ingredient ranks ranged from 1 to 9 (mean 3.5; standard deviation 1.8), and the product ranks ranged from 2 to 5. The nine facial makeups include solids and liquids, some of which include ultraviolet protection. The range of ingredients is wider, with many polymers and inorganics represented. The poorest ranking (Light Foundation, rank 5) was dominated by the influence of zinc oxide (rank 7) and cyclopentasiloxane (rank 7), present at over 10.1% and 38.9%, respectively. In contrast, the Concealer Stick (rank 4) contains a more even distribution of relatively poorly-ranked ingredients (ranks 5+) not dominated by any one or two, making eco-innovation-driven design changes more difficult than when one or two individual ingredients could be targeted.

Table 1 Product ranks

Shampoo product	Rank	Facial makeup product	Rank
Children's	3	Foundation stick	3
Revitalizing	2	Concealer stick	4
Men's	3	Creamy stick foundation	3
Men's dandruff	3	Cream-powder foundation	3
Hair & body	3	Liquid foundation	2
Post-treatment	3	Liquid concealer	3
Color protect	3	Powder cream concealer	2
Color correct	3	Thin liquid foundation	4
Bar	3	Light foundation	5
PEFCR model shampoo	3		

Details of product composition and ingredient ranks in Table S7 (shampoo) and Table S8† (facial makeup).

The wide range of values shows that the tool discerns among alternatives based on the 10 environmental risk and sustainability metrics used. Some results yield important, yet counterintuitive information to product designers. For example, many companies market mineral sunscreen products as environmentally friendly, on the basis that they contain titanium dioxide or zinc oxide rather than organic compounds as ultraviolet filters (UVFs). However, the poor rank for zinc oxide (rank 7) reflects that its free ion form, Zn^{2+}, is a relatively potent aquatic toxicant, and can behave as persistent in some environments, and its use can potentially result in incremental depletion of finite global zinc reserves, which identifies this ingredient as a prime target for higher-level assessment to ensure its use remains at environmentally sustainable levels. In contrast, titanium dioxide achieves a rank of 1 because of its lower aquatic toxic potency and its abundance in the earth's crust. (Note that this rank is based on data for non-nanoparticle TiO_2. Testing protocols and aquatic toxicity differ for TiO_2 nanoparticles.[37]) Here the ranking system identifies an area for further study–namely, whether companies shifting away from organic UVFs to minerals due to their perceived superior environmental safety might have unintended deleterious consequences.

The ingredient ranks are mainly hazard-based, including consideration of exposure only indirectly, through selection of the appropriate environmental compartments to evaluate and in the use of persistence as an independent impact category, partially as a surrogate for exposure potential. The product

Table 2 Efficacy-normalization and screening level aquatic risk calculation

INCI name	Rank	Aquatic PNEC (mg L^{-1})	Note	STP removal[d] (%)	Note	Bar shampoo %	PEFCR model shampoo %
Agar	3	0.02	[a]	90	[e]	15.7	—
Cocamide MEA	3	0.017		96		—	4.7
Cocamidopropyl Betaine	3	0.095		92		—	29.9
Dimethicone	4	100	[b]	90	[e]	—	3.7
Glycerin	1	126		92		14.7	—
Glyceryl caprylate/caprate	3	0.026		92		5.2	—
Glycol distearate	3	0.0001	[c]	>99		—	1.9
Helianthus Annuus seed oil	3	0.02	[a]	90	[e]	5.2	—
Hydrochloric acid	1	100	[b]	90	[e]	—	3.0
Lauryl lactyl lactate	3	0.026		>99		5.2	—
Propylene glycol	2	41		92		—	3.7
Simmondsia Chinensis seed oil	3	0.02	[a]	90	[e]	5.2	—
Sodium C12–18 alkyl sulfate	3	0.86		87		47.6	—
Sodium laureth sulfate	3	0.5		75		—	48.6
Overall product rank						3	3
Efficacy-adjusted rank						2	3
Mass per use excluding water (g)[f]						1.2	2.8
Critical dilution volume (L per use)						1797	1776
Annual critical sales mass (kg) for a population of 100 000						47 337	115 439
Number of annual uses at critical sales mass						4.06×10^7	4.11×10^7

[a] PNEC that would result from a critical benchmark (L/EC50) of 1 mg L^{-1} from a data set of three acute tests representing three trophic levels; used for unprocessed natural ingredients lacking data. [b] 100 mg L^{-1} assigned to benign substances: common ions; non-toxic slowly degrading polymers. [c] 0.0001 mg L^{-1} used when modeling predicts lower value.[42] [d] US EPA EPI Suite STP model removal using BIOWIN biodegradability rates. [e] 90% assigned for natural extracts (due to expected biodegradability) and polymers (due to sorption) when modeling not possible. [f] 10.5 g (wet weight) per use for liquid shampoos;[38] 1.22 g per use for bar shampoo based on authors' informal survey of marketing claims and supporting data.

rank introduces an additional element of exposure by using a mass-weighted average calculation, de-emphasizing the influence of ingredients present at low levels. An additional element of exposure can be added when comparing alternative products head-to-head if those products have a different efficacy. This tool implicitly assumes that efficacy is similar between DtD formulas of a given product type, so the dose used and hence exposure potential, would be similar. To account for differences in exposure due to differences in efficacy in a comparison among rival product designs, the formula ranks can be normalized to an equivalent dose for direct comparison by "crediting" the more efficacious formula for the lower mass of (non-water) ingredients required per use. This is demonstrated in Table 2 for two shampoos by calculating the ranks assuming a single use of each product.

Bar shampoos, which do not require plastic packaging, are increasingly marketed for sustainability also due to their water-free, highly concentrated formulas, but the bar shampoo evaluated here has the same rank as traditional shampoos unless normalized for efficacy. The bar shampoo requires only 1.2 g of dry (non-water) ingredients per use according to product marketing, *versus* 2.8 g for the PEFCR model shampoo.[38] If they were equally efficacious, both would require the same ingredient mass, which for simplicity in the calculation, we assume is 2.8 g. To normalize the two ranks for efficacy (valid only in direct head-to-head comparison), we add water (with a perfect rank of 1) to the calculation for the bar shampoo formula until the new per-use mass is 2.8 g. This results in an improved rank (2) for the bar relative to the PEFCR model shampoo (3) accounting for the lower mass of non-water ingredients required per use for the bar. Most PCPs in a product class are similarly efficacious, but when this is not the case, this method can identify when equally- or poorer-ranked products are superior from an eco-innovation perspective.

The ERA of DtD products is needed in several contexts, including to ensure protection of receiving waters at manufacturing facilities and to support "green" marketing claims. One potential use of the screening-level PNECs obtained in this approach is shown in Table 2. The PNEC values and STP removal projections for two of the products from Table 1 were used to determine the critical dilution volume (CDV) for each ingredient for one use. A similar CDV approach is used in eco-label methods for down-the drain products.[39] The finished product's CDV ($\mathrm{CDV_{prod}}$) represents the amount of water (L mg^{-1}) required to dilute the product after use to a level at which no adverse aquatic effects are expected, and is calculated as:

$$\mathrm{CDV_{prod}} = \sum_{\mathrm{ing}=1}^{i} \frac{m_{\mathrm{ing}_i}(1-\eta_{\mathrm{rem}_i})}{\mathrm{PNEC}_{\mathrm{ing}_i}} \quad (1)$$

where m_{ing} is the mass of ingredient per use, η_{rem} is the modeled STP removal efficiency, $\mathrm{PNEC_{ing}}$ is the ingredient PNEC, and i is the number of non-water ingredients in the formula. The $\mathrm{CDV_{prod}}$ values are conservative (*i.e.*, likely overprotective) because the PNECs developed automatically in the tool are screening-level values that would undergo refinement *via* inclusion of a wider database (and concomitant lower AF) if risk could not be ruled out.

The inverse of CDV_{prod} is a pseudo-PNEC for the product and can be used to evaluate risk in near-downstream waters at an STP by adopting a generic exposure scenario and assuming additive effects to determine the tolerable mass of product that can be sold in a region if no other emissions were present. (Evaluating incremental risk considering other emissions is beyond the scope of this illustration.) The European Medicines Agency ERA Guideline assesses exposure for DtD drug products with a formula that simplifies to:

$$C_{\text{water}} = m_{\text{prod}}/2000 \quad (2)$$

where C_{water} is the concentration of the product components in water downstream from an STP, m_{prod} is the daily mass of product used per person in a model city, and 2000 is the volume of dilution water per person (200 L × 10, dilution factor). When C_{water} is equal to the pseudo-PNEC (*i.e.*, 1/CDV_{prod}), the risk ratio is one, and solving for m_{prod} × regional population yields the mass of the product that can be used in a region with an expectation of no adverse aquatic effects, and above which a more refined ERA is warranted because risk cannot be excluded. For example, in Table 2, sodium C12–18 alkyl sulfate would theoretically require 84.9 L of dilution water per use to maintain its level below the PNEC at the STP outfall after mixing (47.6% in the bar formula × 1.2 g bar/use × (1–0.87) × 10^3 mg g^{-1}/0.86 mg L^{-1}). The CDV calculated for each ingredient is summed to obtain the product CDV values of 1.54 L and 0.63 L for the bar and PEFCR shampoos, respectively. The inverses of these values are the pseudo-PNECs, which are substituted as C_{water} into eqn (2), and assuming a model population of 100 000, this yields the sales mass tolerable for each product in that population (2000 L d^{-1}/1.54 L mg^{-1} × 10^{-6} kg mg^{-1} × 10^5 people × 365 d year^{-1}). In Table 2, the illustrative screening-level values for product sales with no foreseen aquatic risk in a city of 100 000 is about 47 000 kg for the bar shampoo and 115 000 kg for the PEFCR shampoo. However, because of the bar shampoo's greater reported efficacy, these sales represent a similar number of annual uses (about 41 million). This approach can be extrapolated to any size region where uniform use rates are a reasonable assumption. This type of evaluation can be used to compare a slate of alternative product designs when sales projections are not yet available or for projecting when future sales of a product might reach a level of concern.

In USETox and other LCA-type paradigms, the Effect Factor (EF) (a measure of hazard) is multiplied by a fate factor meant to diminish the influence of the EF if the substance is not persistent. In doing so, these approaches acknowledge that risk is a joint function of hazard and exposure. Here, we treat persistence as an independent hazard, partially as a proxy for exposure. This is similar to hazard-based regulatory approaches, like PBT assessment under REACH, where consideration of risk is implicit *via* criteria that require joint persistence, bioaccumulation, and toxicity (or severe persistence and bioaccumulation) characteristics to qualify as a concern. Here, a similar effect is reached. To illustrate: a hypothetical substance that is completely benign but highly persistent or one that is readily biodegradable but potently toxic would each have a rank of 4 in this method, but a hypothetical PBT substance (according to REACH criteria) would have a rank of 8 in this method. Because this method includes a wider range of PI-indicators than P, B, and T, a rank of 8 can also occur due to other combinations of potential impacts. A poor rank does not indicate that safe use is not possible, but that deeper evaluation is warranted to determine the limits of safe use. Substances with a rank of 6 or higher have moderate to severe hazard characteristics in more than one category and warrant further assessment.

This method represents a significant improvement on the state of the art by systematically including many potential impacts from both ERA and LCA methods, and by using PNEC values that are sufficiently comprehensive for use in screening-level ERAs with no modification. One limitation is that the method was not designed to rigorously evaluate environmental exposure. Another limitation is that effects are assumed to be additive – a common regulatory assumption when data are lacking to indicate synergistic or antagonistic interactions, which can result in under- or overestimation of effects, respectively. Also, there is sometimes wide variation among substances in the uncertainty of the data underlying PI-indicators. This is only addressed for the ecotoxicity category, because PNEC values depend on the robustness of the database. We anticipate that further use of the method followed by higher level assessments for some products will reveal the importance of neglecting variation in uncertainty.

5 Conclusion

The PCP eco-innovation ranking method is applicable for all DtD products, can be implemented modularly with impact categories and weighting factors easily altered to fit evolving sustainability goals, and is unique in combining ERA and LCA approaches together to support early stages of product design. The system cannot include certain useful sustainability indicators, including energy, land use, and water impacts because these are unknown at the earliest design stages, but it includes all common indicators that can be evaluated before supply chains are established. Unlike previously published systems,[9–11] this one is built to derive PNECs that can feed directly into the ERA process, and be used in higher-tier, quantitative risk evaluations. Further, this tool can help companies measure and achieve internally- and externally-reported sustainability objectives. UN Sustainable Development Goals include a target to manage chemicals throughout their life cycle and "significantly reduce their release… in order to minimize their adverse impacts" (Target 12.4).[40] The tool also aligns with the Carbon Disclosure Project's Water Security

Questions (*e.g.* W3.3) and Global Reporting Initiative Disclosures (*e.g.* Section 303-1a).[41] The use of this method is expected to result in the development of PCPs with improved environmental sustainability characteristics and lower risk of regulatory scrutiny for potential environmental impacts, which would benefit both businesses using the tool and the public.

Abbreviations

CF	Characterization factor
CDV	Critical dilution volume
CSP	Crustal scarcity potential
DtD	Down-the drain
EF	Effect factor
PCPs	Personal care products
PI-Indicator	Potential impact indicator
PEFCR	Product environmental footprint category rules
STP	Sewage treatment plant
SRV	Sub-rank value

Author contributions

Jennifer K. Saxe: conceptualization, methodology, software, data curation, writing-original draft. Lisa Hoffman: conceptualization, data curation, writing – review & editing. Ramez Labib: conceptualization, writing – review & editing, funding acquisition.

Conflicts of interest

There is no conflict of interest to declare.

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