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Defining Product Intake Fraction to Quantify and Compare Exposure to Consumer Products

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There is a growing consciousness that exposure studies need to better cover near-field exposure associated with products use. To consistently and quantitatively compare human exposure to chemicals in consumer products, we introduce the concept of *product intake fraction,* as the fraction of a chemical within a product that is eventually taken in by the human population. This metric enables consistent comparison of exposures during consumer product use for different product-chemical combinations, exposure duration, exposure routes and pathways and for other life cycle stages. We present example applications of the *product intake fraction* concept, for two chemicals in two personal care products and two chemicals encapsulated in two articles, showing how intakes of these chemicals can primarily occur during product use. We demonstrate the utility of the *product intake fraction* and its application modalities within life cycle assessment and risk assessment contexts. The *product intake fraction* helps to provide a clear interface between the life cycle inventory and impact assessment phases, to identify best suited sentinel products and to calculate overall exposure to chemicals in consumer products, or back-calculate maximum allowable concentrations of substances inside products.

INTRODUCTION

Every consumer product has the potential to expose humans to its chemical content during use and via subsequent environmental emissions. There is a growing consciousness that exposure studies used either in risk assessment (RA) or in life cycle assessment (LCA) need to cover both exposure to far-field[1] environmentally mediated emissions and near-field[1] direct dermal or indoor exposure during product use.[2−5] Studies carried out on specific product-chemical combinations (e.g., phthalates in plastics,[6] flame retardants in household products[7]) and indoor air exposures[8−10] demonstrate that use-stage exposure may exceed environmentally mediated exposures and is therefore essential to consider when assessing exposure to chemicals in products.[11] It has been *qualitatively*

understood for decades that the magnitude of near-field exposures is highly dependent on chemical properties, product characteristics, usage conditions, and user behavior. There is, hence, a need for a *quantitative* and comparative framework characterizing how specific product-chemical combinations differ in their potential for both near-field and environmentally mediated exposures. Several databases have recently become available for a first identification of such product-chemical combinations in terms of chemical occurrence and concentrations in products.[12,13] The availability of these data needs to be complemented by a metric that enables comparison and ranking of the exposure magnitude across a wide range of product-chemical combinations. This metric should be applicable both in RA and LCA contexts to (a) compare orders of magnitude between different chemicals used in a given product and different product usages for a given chemical, (b) identify the key parameters influencing exposure and characterize its dependency on, for example, the product mass used or the exposure duration, (c) identify and compare predominant exposure pathways, (d) compare exposures occurring at different life cycle stages,[14] while consistently differentiating near-field exposure from environmentally mediated exposures, and (e) facilitate the connection between the emission inventory and the impact assessment phase of an LCA.

In this paper, we aim to establish such a consistent comparative framework and metric characterizing how specific products differ in their chemical exposure potential. We provide a common basis to compare exposures to chemicals found in consumer products by (a) identifying an adequate point of departure, that is the best suited quantitative descriptor of chemical mass as a starting point for a product-oriented exposure assessment, (b) defining a new comparative exposure metric, the *product intake fraction* (PiF), that is the chemical mass within a product eventually taken in by humans, (c) providing quantitative examples and demonstrating how PiF integrates into overall exposure frameworks, and (d) discussing the utility and limitations of PiF and its applicability for comparing exposures in LCA and RA contexts.

POINTS OF DEPARTURE FOR COMPARING EXPOSURES TO CHEMICALS IN PRODUCTS

Production volumes are available for various chemicals and have been proposed as a point of departure to determine product exposure.[11] Nazaroff et al.[15] defined the *intake to production*

Table 1. Comparison of Points of Departure and Metrics to Characterize Exposure to Chemicals

point of departure	metric name	metric[b]	main assessment purpose and limitations
(a) total chemical production volume[15]	intake to production ratio	(mass taken in)/ (mass produced)	chemical delivery efficiency, difficult to characterize multiple product usages with widely differing exposure pathways
(b) chemical mass emitted to environment[16]	intake fraction (iF)	(mass taken in)/ (mass emitted)	population-scale intakes due to environmental emissions, limited to emission-based exposures
(c) chemical mass within product[a]	product intake fraction (PiF)	(mass taken in)/ (mass in product)	comparison of consumer intake of chemicals in products during use with population intake resulting from product disposal, does not cover pre-use product life cycle stages (raw material extraction, manufacturing)

[a]This study. [b]"Mass taken in" is the same descriptor of "chemical mass taken in" in each of these metrics, but may correspond to different quantities depending on the considered point of departure.

ratio as an economy-wide quantitative indicator to assess the extent to which manufactured chemical production results in human exposure (Table 1a). While this metric is useful, it does not facilitate estimates of intake directly related to product use as production volumes do not easily allow differentiation between chemicals used as intermediary reactants in manufacturing from those used within objects and formulations. Additionally, the fractions of production volume used in each product type and population using these products are necessary to assess the intake to production ratio and are difficult to determine.

At the other end of the spectrum, chemical *emissions* can also constitute the point of departure for assessing exposure. Emissions are usually well-defined for exposure to substances released during the upstream production stages of a product life cycle (material extraction, chemical manufacturing, and product formulation) and related population-scale intakes are generally quantified by multiplying media-specific emissions by their respective *intake fractions*. Bennett et al.[16] defined the *intake fraction* (iF) as the cumulated mass of a substance eventually taken in by a population divided by the mass emitted to the environment (Table 1b). This concept marked a shift in exposure assessment by introducing a consistent and transparent metric to assess intakes from environmental emissions. Recently, the iF concept has been extended to assess inhalation exposure to various substances emitted within indoor household[2,8,9] and workplace environments,[17,18] and for assessing ingestion exposure to pesticides via food consumption.[19−21]

There are, however, difficulties and inconsistencies when applying the emission-based iF to evaluate exposure to products, as some studies normalize human intake to the overall mass of product applied,[2] while others normalize to the chemical mass volatilized and emitted from the product into the indoor environment.[22,23] This inconsistency becomes problematic when studying chemicals that may lead to both dermal and inhalation exposures, such as fragrances in cosmetics or flame retardants in furniture. The resulting inhalation related iF for such scenarios is not directly comparable to the iF taken in via the skin, which should be normalized to the mass of product applied, not emitted. Therefore, the emission-based iF must be adapted to a consistent metric applicable for comparing exposures to chemicals in products.

During product use and disposal stages (Figure 1, orange boxes), chemicals in products are taken in via several use-stage
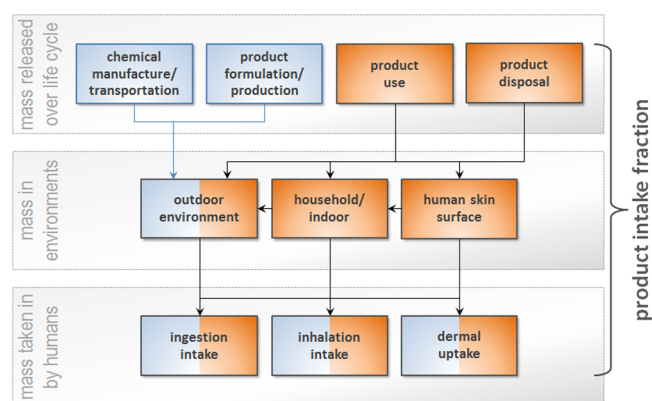

Figure 1. Exposure pathways for chemicals in products. Exposure to chemicals in products during product use and subsequent stages are shown in orange and exposure during upstream production stages in blue. Percentage orange or blue does not reflect actual percentage of exposure.

pathways depending on the product application mode and chemical properties, for example via direct dermal contact or indoor inhalation. Chemicals can also be taken in via subsequent environmentally mediated pathways associated with waste treatment and product disposal.

Additionally, the ***chemical mass in the product*** is a more appropriate point of departure than emissions or production volume to perform product-related exposure assessments. It is a stable, measurable quantity and only accounts for the fraction of the production volume that reaches the consumer and will eventually be disposed of with the product (Table 1c). It can also represent the quantity applied, for example for cosmetics and pesticides.

■ DEFINING PRODUCT INTAKE FRACTION

To quantify all the chemical intakes associated with the product use-stage and subsequent exposure pathways, we adapt the emission-based iF and define a new product-based metric termed product-chemical intake fraction, shortened here as the product intake fraction. PiF is defined as the chemical mass within a product eventually taken in by humans via all possible exposure pathways per unit of chemical mass within that product ($m_{c,p}$, $kg_{in\ product}$) at the end of the manufacturing process, that is, starting at exposure time $t = 0$ (Table 1c):

$$PiF_{c,p,x} = \frac{\text{cumulative mass of chemical } c \text{ in product } p \text{ taken in by population via exposure pathway } x}{\text{initial mass of chemical } c \text{ in product } p} = \frac{\int_0^\infty \partial I_{c,p,x}(t)/\partial t \ dt[kg_{intake}]}{m_{c,p}[kg_{in\ product}]}$$

(1)

By default, PiF refers to a long-term, time-integrated exposure pathway-specific mass of a chemical in product

taken in ($I_{c,p,x}$, kg_{intake}); it includes the entire exposed population and must be calculated for all relevant exposure

Table 2. Examples of Product Intake Fractions and Related Intakes Determined for Sodium Lauryl Ether Sulfate (SLES, CAS-RN 9004-82-4) and D-limonene (CAS-RN 138-86-3) in Two Personal Care Products, As Well As Diisononyl Phthalate (DINP, CAS-RN 28553-12-0) and Phenol (CAS-RN 108-95-2) in Two Consumer Articles, for Different Amounts Applied, Exposure Durations and Dominant Exposure Pathways

chemical	product-use scenario	amount of product used; % chemical content	exposure duration	dominant exposure pathway	PiF^{use} $kg_{intake}/kg_{in\ product}$	$PiF^{disposal}$ $kg_{intake}/kg_{in\ product}$	chemical intake mg_{intake}
			Chemicals in Personal Care Products[a]				
SLES	shampoo average use	5.05 $g_{product}$; 20%	0.065 h	ingestion and dermal[a]	4.5×10^{-4}	1.3×10^{-4}	0.6
	body lotion average use	8.7 $g_{product}$; 20%	12 h	dermal	0.96	5.6×10^{-6}	1700
	body lotion high-end use	27.9 $g_{product}$; 20%	12 h	dermal	0.62	4.8×10^{-5}	3400
D-limonene	shampoo average use	5.05 $g_{product}$; 0.5%	0.065 h	dermal	0.19	1.2×10^{-5}	4.8
	body lotion average use	8.7 $g_{product}$; 0.5%	12 h	dermal	0.19	1.2×10^{-5}	8.2
	body lotion high-end use	27.9 $g_{product}$; 0.5%	12 h	dermal	0.19	1.2×10^{-5}	26.5
			Chemicals Encapsulated in Articles				
DINP	[b]pacifier low-end use	1.5 $g_{pacifier}$; 40%	45 h[b]	mouthing	0.009	1×10^{-5}	5.4
	pacifier high-end use	1.5 $g_{pacifier}$; 40%	450 h[b]	ingestion	0.09	1×10^{-5}	54
DINP	1 m^2 flooring thick 5 mm	7500 $g_{flooring}$; 20%	15 a	inhalation[c]	5.8×10^{-8}	1×10^{-5}	0.05
	1 m^2 flooring thin 1.5 mm	2250 $g_{flooring}$; 20%	15 a	inhalation	1.9×10^{-7}	1×10^{-5}	0.05
Phenol	1 m^2 flooring thin 1.5 mm	2250 $g_{flooring}$; 0.013%	10 d	inhalation	1.1×10^{-3}	$<1 \times 10^{-10}$	320
			100 d	inhalation	3.5×10^{-3}	$<1 \times 10^{-10}$	1030
			15 a	inhalation	4.9×10^{-3}	$<1 \times 10^{-10}$	1470

[a]For shampoo, calculated using the model from Ernstoff et al.[24] with application to head and hands surface area of 1598 cm^2, dilution factor of 6 and skin permeation coefficient from Ten Berge.[31] Body lotion calculation adapted from Ernstoff et al.,[24] with application to body area of 17 000 cm^2, dilution factor of 1. [b]PiF is calculated by multiplying the measured leaching rate of DINP out of plastic ((1×10^{-5} g/cm^2/h),[32−34] the mouthing contact area (10 cm^2)[35] and the contact duration over pacifier lifetime (0.6 and 6 h/d[35] for 75 days yielding 45 and 450 h, for low-end and high-end use, respectively). At the end of its use lifetime, the pacifier is disposed of in a landfill assuming 70%[36] leaching of the disposed DINP, multiplied by the population-scale USEtox[26] outdoor air intake fraction. [c]Flooring DINP and phenol releases calculated using Deng et al.,[28] respectively using diffusion coefficients of 1.33×10^{-14} and 1.2×10^{-13} m^2/s as well as material-air partition coefficients of 1.9×10^{12} and 1.2×10^5. Releases are combined with the indoor air intake fraction of 0.0049 calculated from Wenger et al.[7] for a ventilation rate of 0.7 h^{-1} and a volume of 85 m^3/person, without indoor degradation. Abrasion and exposure from dust are not considered in this calculated PiF. At the end of its use lifetime, the pacifier is disposed of in a landfill assuming 70%[36] leaching of the disposed DINP. Phenol is nearly entirely volatilized after 15 years.

pathways. It encompasses exposures associated with the use-stage over the usable product lifetime and with waste treatment during or after product disposal.

■ CALCULATION EXAMPLES AND INTEGRATION INTO EXPOSURE FRAMEWORKS

Similar to the intake fraction, PiF does not replace an exposure assessment, but PiF enables us to characterize and compare the results of exposure assessments across a wide variety of product-chemical combinations, implying that either empirical data or near- and far-field exposure models are needed. Table 2 presents specific examples of PiFs calculated for two chemicals in two personal care products (PCPs: shampoo and body lotion), and two chemicals encapsulated in two articles (pacifier, flooring).

For chemicals in PCPs, PiF due to product use (PiF^{use}, $kg_{intake}/kg_{in\ PCP}$) can be calculated using a dermal exposure model[24] as a function of the chemical-specific skin permeation coefficient, the applied product layer thickness and exposure duration. This model takes into account dermal aqueous and gaseous uptake

and inhalation exposure after volatilization. We adapted calculations originally applied to hair shampoo[24] to body lotion, a commonly used leave-on product. For the surfactant sodium laurel ether sulfate (SLES, CAS-RN 9004-82-4), the PiFs in Table 2 vary substantially depending on exposure duration and product type from 6×10^{-4} to 0.96. In contrast, PiF is nearly constant for D-limonene (CAS-RN 138-86-3), since it is volatilized (81%) and transferred dermally (19%) within minutes. To include the contribution of product disposal, we estimated the PiF due to product waste disposal and treatment ($PiF^{disposal}$, $kg_{intake}/kg_{in\ PCP}$) assuming that the fraction of chemical not absorbed dermally nor volatilized was washed down the drain, transferred to a wastewater treatment plant (WWTP), and emitted to freshwater and soil from application of biosolids,[25] from which *environmentally mediated (emission-based) intake fractions* were estimated with USEtox.[26] For D-limonene, the resulting $PiF^{disposal}$ of 10^{-5} is dominated by drinking water ingestion and is close to 4 orders of magnitude lower than the PiF^{use} of 0.19. To evaluate the applied dermal exposure model, Csiszar et al.[27] compared the PiF-based

cumulative intake for several PCPs to biomarker data and found good agreement for parabens between modeled calculations and biomarker data.

For chemicals encapsulated in articles (e.g., toys, furniture, building materials), diisononyl phthalate (DINP, CAS-RN 28553-12-0) in *pacifiers* has sufficient empirical information to provide an example of measurement-based PiF for exposure via mouthing. PiF^{use} ($kg_{intake}/kg_{in\ pacifier}$) is the total mass of DINP that is ingested by the mouthing child during the overall mouthing time divided by the original DINP mass within the pacifier nipple. The ingested mass was estimated based on a measured DINP leaching rate out of plastic[26−28] with the resulting PiF^{use} directly proportional to exposure duration and in the relatively high range of 0.01−0.1. In comparison, the population-scale $PiF^{disposal}$ is close to 10^{-5}, 4 orders of magnitude lower than the PiF^{use} of the individual child using the pacifier.

Chemicals encapsulated in flooring exemplify a less direct exposure pathway. We applied the Deng diffusion model[28] to determine chemical releases from flooring and multiplied these by the indoor intake fraction[7] to determine the PiF for a volatile organic compound (VOC, phenol) and a semivolatile organic compound (SVOC, DINP). The DINP releases from flooring lead to a PiF more than 6 orders of magnitude lower than from the pacifier, as SVOC releases from material are limited by the high material surface−air partitioning coefficient. The low PiF for SVOC volatilization implies for such small releases that abrasion of the material over the flooring lifetime may lead to substantially higher PiF than volatilization and deserves further attention.[29] Compared to SVOCs, fractions volatilized from flooring are much higher for a VOC like phenol, as the VOC PiF approaches or equals the indoor inhalation intake fraction of 4.9×10^{-3}.[7]

PiF Integration into Exposure Frameworks. The corresponding exposure pathway-specific intake, $I_{c,p,x}$ (kg_{intake}), can be calculated in a straightforward manner by multiplying the associated PiF ($kg_{intake}/kg_{in\ product}$) by the mass of product applied, M_p ($kg_{product}$), and the chemical fraction in product, $f_{c,p}$ ($kg_{in\ product}/kg_{product}$): $I_{c,p,x} = PiF_{c,p,x} \times M_p \times f_{c,p}$. Depending on the product-chemical combination, the resulting intake may be directly proportional to the mass of chemical applied (e.g., D-limonene in PCPs, where PiF is fixed for most relevant application scenarios) and independent of exposure duration. PiF and intakes can also be proportional to exposure duration, for example for DINP in pacifiers and flooring, or a more complex function of exposure duration and mass applied with PiF saturation effects in the case of SLES in PCPs.

While the absolute chemical intake cannot be directly compared across various categories of products, PiF provides a directly comparable product usage perspective and population-based measure of the ability of product-chemical combinations to cause large intake doses in users per unit mass of chemical in product.

Identifying Factors of Influence and Plausible PiF Ranges Per Product Class. The examples in Table 2 show that the product-chemical specific PiF helps characterize the influence of the mode of entry in the near- or far-field environments. PiF will vary based on whether a chemical is directly embedded inside a product (e.g., furniture and clothing), released into the air (e.g., sprays and aerosols), applied on surfaces (e.g., cleaning products), or directly applied on the skin or ingested (e.g., cosmetics or food additives). For a given class of product, PiF-based sensitivity studies can identify

the key parameters influencing exposure, be it the chemical properties, the location of use or the exposed population (e.g., density and proximity of room occupants). Throughout the past 15 years of research quantifying intake fractions (iF), ranges have been defined for specific exposure pathways (e.g., food chain ingestion due to emission to freshwater) and related to physicochemical properties (e.g., octanol−water and air−water partition coefficients K_{ow} and K_{aw}), giving practitioners a developed intuition about plausible iF ranges. We anticipate a similarly useful outcome of using PiF in product-related exposure studies. As a first example, Ernstoff et al.[24] investigated several possible chemicals in shampoo and found a generally restricted range of PiF due to use-stage dermal intake from 10^{-4} to 10^{-1}, a much wider range of PiF due to use-stage inhalation from $<10^{-10}$ to 10^{-1}, and a restricted range of total intake due to environmentally mediated PiF around 10^{-4} to 10^{-5} dominated by various ingestion pathways.

Depending on study goals, PiF can also be used to compare exposure pathways and routes. For a given exposure route, PiF can be directly compared or added across various pathways, for example direct dermal application and subsequent dermal gaseous exchange of the volatilized fraction.[30] Since subsequent exposure-responses may differ depending on route of exposure, it is useful to differentiate the PiF for each route.

Complementing Other Metrics. These examples also enable us to understand how the PiF relates and compares to the intake to production ratio and to the intake fraction metrics. Taking sodium lauryl ether sulfate (SLES) and diisononyl phthalate (DINP) as examples: these chemicals have very different physicochemical properties and are used in a wide variety of products, ranging from categories like personal care products (soap, body wash, shampoo) to laundry detergents for SLES and from floorings to electric wires for DINP. For such chemical-product combinations, the PiF can help support decision making on a per-product and per-chemical basis. In contrast, the overall intake to production ratio aggregates intakes over all products such that it is more difficult to disaggregate the individual source contributions for chemicals. To note, the PiF could be applied to calculate product-specific intake to production ratios in the rare instances data are available on the fraction of production volume used in every product type.

The intake fraction concept only applies to exposure pathways involving emissions to environmental compartments and is thereby not suited to estimate intakes occurring following direct application. The role of the PiF is to enable us to consistently combine various iFs (e.g., the inhalation iF for indoor releases from flooring or cosmetics, with the environmental iF from WWTP or landfill releases), with exposures occurring during product use not accounted for by iF, such as direct dermal contact exposures.

We further discuss the utility and applicability of the PiF in the context of LCA as a functional product-oriented approach, and in the context of risk assessment as a receptor-oriented approach.

■ UTILITY AND MODALITY OF APPLYING THE PRODUCT INTAKE FRACTION IN LIFE CYCLE ASSESSMENT AND RISK ASSESSMENT CONTEXTS

Application in a Life Cycle Assessment Context, As a Product-Oriented Approach. To assess human health impacts, LCA first calculates life cycle inventory (LCI) flows usually reflecting resource extractions and environmental

Table 3. Utility of the Product Intake Fraction for Comparing Various Exposure Dimensions

main utility-exposure comparison	key elements	application modalities
comparison of product-chemical combinations	mode of chemical entry into the near-field (e.g., encapsulated, sprayed, applied to surfaces or skin)	definition of plausible PiF ranges per product class
identification of key parameters influencing exposure	roles of product mass applied, exposure duration, chemical properties	contour plots, as a function of product and chemical properties
comparison of exposure routes and pathways	inhalation (near person, indoor, outdoor), ingestion (hand to mouth, drinking, food), dermal (aqueous, gaseous)	by default, inhalation, ingestion, and dermal PiF are kept separate for subsequent combination with toxicity data
comparison of product life cycle stages	use-stage, disposal-stage and upstream life cycle stages	complementary role of PiF and of iF for upstream and downstream impacts
connection point to life cycle inventory analysis results	mass of chemical in product per functional unit × PiF × effect factor	PiF as a product-oriented metric characterizes exposure to in-product chemicals in LCA
identification of best suited sentinel products	representative of a high-end exposure situation	sentinel products are used in large quantities, while maintaining a high PiF
Forward and backward comparisons with ADI and OED	key to define chemical usage and ranges of product chemical content	back-calculate maximum acceptable concentrations of substances inside products.

emissions per a defined unit of product function, the "functional unit" (FU). For example, in the case of flooring the functional unit may be 1 m^2 of standardized performance flooring used over 15 years, as a basis to compare different flooring materials. Though being product focused, most LCA studies have paradoxically neglected chemical intake during the product use-stage and primarily focused on exposure to chemicals emitted into environmental media (air, soil, water, etc.) during product manufacturing and disposal.[26,37−41] To facilitate and extend LCA practices with an improved focus on chemical exposure during product use, in addition to the chemical emissions to the environment during raw material extraction and manufacturing stages, we suggest reporting an additional required LCI flow, that is, *the mass of chemical in product per functional unit* (e.g., 2.25 kg$_{flooring}$/m^2 × 0.013% = 0.029 kg$_{phenol\ in\ flooring}$/m^2 according to Table 2). This LCI flow constitutes an intuitive point of departure to determine product-related exposures. It can directly be multiplied by the PiF yielding the exposure to a chemical in a product per functional unit. Like iF, PiF is compatible with the traditional LCIA (life cycle impact assessment) framework and can be multiplied by effect factors relating potential human health impacts to chemical exposure (e.g., in incidence risk/kg$_{intake}$) to determine characterization factors, i.e. human health impacts per mass of a chemical within a product (e.g., in incidence risk/kg$_{in\ product}$) used per FU. In this way, PiF facilitates a fair and consistent comparison of exposures to chemicals within or across a variety of products.

PiF also Enables Comparison between Different Life Cycle Stages. The use-stage PiF is directly comparable to the environmentally mediated PiF due to product disposal as both are calculated per unit chemical mass in product. Results for the various product-chemical combinations in Table 2 suggest that environmentally mediated exposures due to disposal are often orders of magnitude lower than the near-field use-stage exposures, but these exposures may also be of similar magnitude for bioaccumulative substances when the use-stage PiF is relatively low, for example SLES in shampoo.[24] The comparison between life cycle stages could be extended to chemical emissions associated with upstream processes, for example, raw material extraction and product manufacturing, once LCI flows are combined with LCIA characterization, relating exposures and impacts across all life cycle stages to the same product FU.

Application in a Risk Assessment Context, As a Receptor-Oriented Approach. In RA, once a given chemical−product combination has been identified, for example, using one of the recently available chemical-product databases,[12,13] exposure is characterized by assessing the daily chemical intake by the product user. To estimate daily exposures of consumers to chemicals in PCPs, we multiply PiF^{use} by the mass of PCP applied per person per day, the fraction of the chemical in the product, and normalize to the user's body weight, yielding for example a daily SLES intake of 1.7 g$_{SLES\ intake}$/70 kg$_{BW}$ = 24 mg/kg$_{BW}$/d for an average body lotion application (Table 2). Such doses can be compared to reference doses (RfD, mg/kg$_{BW}$/d), acceptable daily intakes (ADI, mg/kg$_{BW}$/d), or to the minimum oral equivalency doses (OED, mg/kg$_{BW}$/d) as back-calculated from the U.S. Environmental Protection Agency's (EPA) ToxCast minimum bioactivity concentrations, AC$_{50}$.[42] Taking flooring as another example for chemicals encapsulated in articles, the average flooring area per person can be used to relate the product to the user's exposure dose, but the relationship between product and exposed users is less direct to establish for such products. By default, the overall PiF has been defined as the intake integrated over the entire population. However, in a receptor-oriented approach like RA, it is necessary to differentiate the fractions taken in by various individuals; for example in the case of a PCP, the user is directly exposed, household members may be exposed through indoor air, and the general population is exposed via the fraction of chemicals washed out, transferred to wastewater treatment and subsequently emitted to the outdoor environment.

The average proportion between PiF^{use} and PiF^{disposal} remains valid when considering the aggregate cumulative exposure from an individual receptor perspective. The PiF^{disposal} associated with a single use is a sum of very small individual exposures distributed over the entire population, N_{pop}. When considering the PiF disposal for aggregate cumulative exposure from an individual receptor perspective ($PiF^{disposal}_{individual\ cumulated}$) and assuming the entire population uses this same product, this small individual exposure is remultiplied by the entire population ($PiF^{disposal}_{individual\ cumulated} = N_{pop} \cdot PiF^{disposal}/N_{pop} = PiF^{disposal}$) and on average each individual therefore receives the PiF^{disposal} in addition to their own PiF^{use}.

In cases where the exact chemical content is unknown, a range of plausible concentrations may be provided based on the function of the chemical inside a product using databases like the European Commission's CosIng database, in conjunction with typical functional ranges from Frame formulations.[43] Thus, there is a high need to establish typical functional ranges and to

compose a list of appropriate sentinel products for various use classes,[44] such as PCPs or cleaning agents. For an initial exposure risk screening of a given product class, the comparative capabilities of the PiF will support the identification of best suitable sentinel products,[44] which are representative of a high-end exposure situation. Sentinel products can be identified as products which are used in large quantities while maintaining a high PiF. For example, for PCPs body lotion is suggested as a sentinel product due to long exposure durations and large quantities used.

In the absence of reliable concentration data, PiF may also be used to back-calculate a *maximum acceptable fraction of a chemical within a product*, $f_{c,\,p\,max}$, from the RfD, ADI, or from the minimum OED, such that $f_{c,p\,max} = RfD_c \times BW/(PiF_{c,p} \times M_p)$ where BW is body weight (kg_{BW}) and M_p is the daily mass of product applied ($kg_{product}/d$). This maximum acceptable fraction can then be compared to plausible ranges of chemical concentrations in products. Applying this equation to D-limonene for high-end body lotion users (reference dose of 5.5 $mg/kg_{BW}/d$),[45] the back-calculated maximum concentration in body lotion amounts to 3.3%, which is larger than the 0.5% indicated in Table 2, but still close to current maximum concentrations reported for D-limonene in a product ingredient database (0.1−2.5%).[12]

Table 3 summarizes the main utility of the PiF metric indicating its key application modalities in different contexts.

■ FINAL DISCUSSION AND OUTLOOK

The product intake fraction is an important step in consistently analyzing consumer and population-scale exposure to chemicals in products. It uses the quantity of chemical inside a product as a point of departure, a readily measured or estimated parameter based on product composition. The presented examples illustrate how the PiF can be used for comparing chemical exposures in LCA and in RA contexts, to either determine intakes or to back-calculate maximum acceptable chemical content in products. Determining PiF will be a key element in characterizing and comparing consumer product exposure and making LCA fully suited for comparing the impacts of products on human health and for studying chemical substitution. Exposure estimates made in this manner also constitute important data which are complementary to high-throughput toxicology risk screening, such as the ToxCast data from the U.S. EPA.[46] The PiF metric is especially well adapted for comparing direct or near-field applications, while allowing for a consistent usage of the intake fraction in case of environmentally mediated exposures.

When estimating PiF it is important to transparently provide assumptions and methods which are applicable to the product in question. For example, determining whether steady-state (e.g., SVOC releases from flooring or furniture)[47] or dynamic modeling (e.g., pulse application of cosmetics) is best applicable.

The PiF depends on the reliability of the input data and near- and far-field models. Hence, there is a need for both *more reliable exposure data and improved modeling of consumer product exposure pathways*. Models are becoming increasingly available for indoor air environments and dermal application of cosmetics.[8,48] Specific data and models need to be provided or refined to quantify the PiF for a larger number of product-chemical combinations, for example for chemicals embedded in products like clothing and furniture, and for products used in enclosed environments like washing machines and dishwashers.

Further empirical data and research are especially needed to better understand poorly characterized exposure pathways, for example, material abrasion, food contact of packaging, and gaseous exchange between air and skin.[49] For these challenging purposes, it is key to intensify knowledge sharing between industry, academia, and government agencies, building on the increasing amount of data made available via public disclosure of ingredients and product use assumptions. In this context, PiF as a comparative metric will help focusing data collection efforts on the most important parameters and product-chemical combinations.

Obtaining reliable data on plausible ranges in *chemical content* will be crucial and is under development for categories, such as PCPs and detergents, but will require substantial effort for the wider variety of products presently in use. For these, the use of the PiF to back-calculate maximum chemical content may be a very useful alternative to calculating exposure doses.

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Notes
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