Published in final edited form as:
J Expo Sci Environ Epidemiol. 2020 January ; 30(1): 171–183. doi:10.1038/s41370-019-0187-5.

ESTABLISHING A SYSTEM OF CONSUMER PRODUCT USE CATEGORIES TO SUPPORT RAPID MODELING OF HUMAN EXPOSURE

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Abstract

Consumer product categorizations for use in predicting human chemical exposure provide a bridge between product composition data and consumer product use pattern information. Furthermore, the categories reflect other factors relevant to developing consumer product exposure scenarios, such as microenvironment of use (e.g., indoors or outdoors), method of application/form of release (e.g., spray versus liquid), release to various media, removal processes (e.g., rinse-off or wipe-off), and route-specific exposure factors (dermal surface areas of application, fraction of release in respirable form). While challenging, developing harmonized product categories can generalize the factors described above allowing for rapid parameterization of route-specific exposure scenario algorithms for new chemical/product applications and efficient utilization of new data on product use or composition. This can be accomplished via mapping product categories to likewise categorized release and use patterns or exposure factors. Here, hierarchical product use categories (PUCs) for consumer products that provide such mappings are presented and crosswalked with other internationally harmonized product categories for consumer exposure assessment. The PUCs were defined by applying use and exposure scenario information to the products in EPA's Chemical and Products Database (CPDat). This paper demonstrates how these PUCs are being used to rapidly parameterize algorithms for scenario-specific use, fate, and exposure in a probabilistic aggregate model of human exposure to chemicals used in consumer products. The PUCs provide a generic representation of consumer products for use in exposure assessment and

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CODE AVAILABILITY

All code for the CHEM model is available at https://github.com/HumanExposure

ETHICS DECLARATIONS

Conflict of interest

The authors declare that they have no conflict of interest.

DISCLAIMER

The views expressed in this article are those of the author(s) and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

provide an efficient framework for flexible and rapid data reporting and consumer exposure model parameterization.

Keywords

human exposure modeling; consumer products; ExpoCast; SHEDS-HT; HEM; exposure assessment

INTRODUCTION

Risk-based evaluations of chemicals in consumer products require information on human exposures to complement hazard information [1, 2]. Exposure estimates are required for the development of risk metrics for use in assessments related to chemical prioritization, life-cycle impact evaluation, chemical alternatives identification, and chemical and product safety evaluation. Models for exposure assessments can be of different tiers, or levels of refinement, depending on purpose [3,4]. For example, a World Health Organization framework [4] defines four tiers of exposure assessments, including semi-quantitative approaches (Tier 0), generic exposure equations using conservative point value parameter estimates (Tier 1), refined models that include a better definition of the exposure scenario (Tier 2), and probabilistic models that require distributions of parameters as input (Tier 3). In all these assessments, challenges can arise in efficiently evaluating and employing existing data and tools for estimating exposures for a novel application (e.g., a new chemical, product, use, or population); it can be difficult to reconcile multiple models and datasets containing large numbers of parameters and equations. These challenges are especially evident when developing and parameterizing quantitative Tier 3 models that simulate the movement of chemicals along the source-to-dose continuum from product source to receptor of interest.

Development of efficient and reproducible mechanistic exposure model applications is facilitated by the development of consumer product categories suited specifically to exposure estimation. Categories are particularly important for aggregate exposure assessments, wherein exposures to a chemical from a variety of sources or exposure scenarios are considered. A product category represents a generalization of a group of individual products and is how model input data and model results are sorted, summarized, and reported. Appropriate categorization can provide a bridge between different types of required model inputs (e.g., product use data and composition information) and algorithms describing exposure scenarios (e.g., release and use patterns, indoor fate and transport, or intakes via dermal, inhalation, or ingestion routes). Defining the categories and these associated linkages a priori provides a framework for rapidly developing and refining exposure models for specific purposes. That is, a new model application would no longer require a lengthy de novo parameterization effort, as they could build upon the pre-defined linkages among categories, parameter values, and model algorithms.

Consumer product categorization schemes and associated consumer product definitions are used in different ways by organizations to fit their purpose. These differences can create obstacles when comparing and analyzing information on chemicals used in products and the

associated exposures. Historically, certain schemes have been designed to support the tracking and management of production, sales, or trade of products. These schemes include the international Universal Product Code system [5] and the Eurostat Prodcom list [6]. Other schemes were formulated to support chemical data reporting required by regulations in different countries. The European Chemicals Agency (ECHA) provides a scheme in the form of "use descriptors" that are used by chemical registrants for reporting purposes [7]. Similarly, the United States Environmental Protection Agency (EPA) Chemical Data Reporting Rule establishes a scheme in the form of a series of consumer product categories used for reporting purposes [8]. Another scheme was developed for the Household Products Database (HPDB), a repository of product chemical data gleaned from Material Safety Data Sheets (MSDS) maintained by the National Library of Medicine. Finally, several schemes have been used to organize products for use in estimating exposures. Goldsmith et al. [9] categorized a retailer-based MSDS database for use in exposure-based screening by simply collecting the retail product categories (RPCs) associated with each product. These RPCs were previously harmonized with the hierarchal categories of the HPDB to apply both sets of the MSDS data to the parameterization of a high-throughput (HT) mechanistic exposure model for use in chemical prioritization [10]. Recently, the Organization for Economic Cooperation and Development (OECD) led the development of a new harmonized set of chemical function, product, and article categories specifically for use in exposure assessment [11].

According to the OECD definitions, consumer products are consumable liquids, aerosols, semi-solids, or solids that are used a given number of times before they are depleted. Consumer product exposures are elevated during and immediately following use and diminish afterwards. Product use is more likely to include direct contact and/or close proximity of the product and the user. Articles are defined as products or building materials composed of solids, polymers, foams, metals, woods, which are always present within indoor environments for the duration of their useful life, which may be on the order of years. Migration of additive chemicals out of articles can result in exposure through ingestion of dust particles, inhalation, mouthing of the article surface, or skin contact.

The differences between products and articles necessitate distinctive approaches for estimating consumer exposure [12]. This paper focuses on consumer products and expands and refines earlier harmonized schema to develop a hierarchical set of consumer product categories appropriate for use in high- and mid-throughput, population-based, mechanistic exposure models. This scheme consists of (1) a hierarchical set of categories for consumer products referred to as Product Use Categories or PUCs; and (2) a set of attributes tagged to individual products. This system (hereafter referred to as the PUC system) is appropriate for use in models of combined exposures to one or more consumer products. It addresses a variety of design criteria required to capture generalized product use patterns and exposure processes while remaining consistent with the OECD scheme. A case-study example of how the PUC system is being used to organize and integrate exposure data and algorithms in the development of a new mid-throughput Combined Human Exposure Model (CHEM) [13] is presented. The PUC system forms the basis for efficient organization of consumer product data and exposure information in terms of products and chemicals-within-products, allowing for rapid model parameterization for new chemicals.

METHODS

The starting point for the PUC system was the categories developed by Isaacs et al. for use in the High-Throughput Stochastic Human Exposure and Dose Simulation (SHEDS-HT) model. Those categories were based on a harmonization of two previous category sets associated with collated product MSDS sheets. In SHEDS-HT the categories were linked to literature-based product use (i.e., “habits and practices”) data and composition data from the collected MSDS sources. The categories themselves, however, were not necessarily optimized for use in mechanistic human exposure modeling.

The criteria that define the PUCs and provide the basis for assigning products to a specific category are described below. All models require a simplification of reality appropriate for the model’s intended use [14]. The categories developed here embody a reasonable representation of consumer products in commerce for use in exposure assessments, including screening and prioritization or higher-tier assessments. An important issue in developing PUC definitions is determining the optimal level of resolution. Highly aggregated categories may result in poorly refined exposure estimates, while highly differentiated categories would be a burden to parameterize (with many categories having sparse data) and produce poorly generalizable results. The design considerations below develop PUCs that capture differences in potential exposures among consumer products, populations, and chemicals, yet afford enough generalization to reduce burden in parameterization and reporting.

Criterion 1: Consumer Product Use Patterns

The PUC system can be used to define diaries of product use in exposure models. To capture population variability in exposures, PUCs, and attributes should define groups that are resolved enough to allow for characterization of variability in product use patterns, or “habits and practices,” in a population of users. Habits and practices data used by models include following characteristics of product use: the prevalence of users in a population, the amount (mass) in a single application or usage event, the frequency of usage events among product users, and the duration of an usage event [10, 15, 16]. An ideal categorization system should group together products with similar use patterns. Categories need adequate resolution to reflect products designed for population groups (demographic groups or cohorts) and which have different habits and practices data. Examples include children’s products such as sunscreens (which would have different prevalence of use by children than regular sunscreens). Other examples include products used by specific ethnic groups, such as certain health and beauty aids. Further refinement could address social and cultural preferences (e.g., distinct categories for natural products or imported products). Similarly, all the products within a category should have a uniform dependence on any housing characteristics that drive use. This will allow for the dependence of product use on these characteristics when applied at the PUC level to model populations. For example, it is important to distinguish carpet cleaners from hard floor cleaners to avoid the latter being assigned for use in modeled households that have no carpeting.

When grouping products based on habits and practices it is useful to consider the needs that a product satisfies. Recently, there have been efforts to incorporate needs-based behavior

modeling into the realm of human exposure modeling. These “agent-based” models have been used in economics and marketing research to simulate consumer behaviors [17, 18]. These approaches have the potential to simulate patterns of consumer product use over time, incorporating dependence of behavior on factors such as demographics and geography. These models can supplement survey-based habits and practices information, which can be limited due to costs of representative studies. Therefore, products serving personal versus communal needs should be distinguished in the development of PUCs. Products can fulfill multiple needs. These needs can be divided into two categories, primary needs and other benefits. For example, while all shampoos clean hair they may differ in their ability to provide other benefits (provide a specific fragrance, moisturize hair, cost less, etc.) The use of needs to define PUCs and attributes are limited to primary needs.

Criterion 2: Exposure Scenario

An exposure scenario is a general description of the conditions under which the product is used (e.g., where and how) and the migration of chemicals in the product to a human receptor. Specific release and transfer processes form the basis for the development of numerical algorithms for estimating exposures. The numerical algorithms are often tailored to exposure route, the direct pathway by which a chemical enters the body (typically dermal absorption, ingestion, or inhalation). There are a variety of approaches and definitions of exposure scenarios relevant to consumer products [10, 15, 16, 19,20,21]. However, some common aspects often considered when formulating scenarios include the environmental compartment of the release (e.g., air, skin, or surfaces), microenvironment where the release occurs (e.g., indoors or outdoors), and method of application/form of release (e.g., vapor, liquid, or aerosol). The exposure scenario dictates the type of input data needed to calculate route-specific exposures. These input data (collectively, “exposure factors”) include information specific to the product being modeled (e.g., dermal surface areas of product application, fraction of product released as an aerosol); the level of refinement of the data is determined by the complexity of the exposure algorithm. A system of PUCs and attributes were developed that discriminate among product properties relevant to exposure scenarios and their related exposure factors. Examples of attributes include method of application/ form of release of the product (e.g., a spray versus gel hair styling product), location of use (e.g., interior versus exterior paints), and application points (e.g., skin, pet, or garden for different types of insect repellents).

Other Design Criteria

PUCs should be consistent with the consensus OECD internationally harmonized categories for exposure assessment [11]. It is natural that optimal product categories for process-based modeling will be different than these broader categories. However, to ensure that any data collected on product use and formulation to support modeling are of use to regulatory exposure assessors, a straightforward crosswalk should be maintained (with each PUC mapping to a single reporting category). Other crosswalks (to models outside EPA, to categorizations used in marketing data, etc.) can be maintained as well. This allows for flexibility in reporting of product data and allows improved data-sharing across groups.

The PUCs should be hierarchical, allowing for straightforward aggregation for lower-tier assessments or reporting, or for estimating the contribution of certain types of products to aggregate exposures (e.g., contribution of personal care products versus household cleaners). In addition, a hierarchical classification allows for easier mapping to other categorizations that might have various levels of refinement. The categories should be defined, labeled, and annotated to promote easy expansion (addition of new categories) or refinement (splitting of a single category into two new subcategories).

The PUCs should be no more specific than required, to facilitate categorization of new products. For example, products of the same type having different colors, fragrances, or brands would not require new categories. Since products are assigned to PUCs based on publicly available data, the definitions of PUCs should be based on knowledge easily obtainable from the label of the consumer product.

Role of Formulation in Defining Categories

Composition of products is not proposed as a criterion for PUCs. Composition data are, however, strongly reflected in the categories determined by the two primary criteria. Different product categories that meet different needs will differ in composition. For example, dandruff shampoos are distinguished from other shampoos by the presence of anti-seborrheic agents not present in general shampoo formulations. Different product forms (e.g., liquids versus sprays) that vary in composition are not separated into different categories but are reflected by the attributes assigned to the different products (as described below). Finally, demographics of user populations (e.g., products marketed to children) may affect formulations as well, as products may contain different ingredients (e.g., fewer fragrances or more coloring agents).

Products meeting a common need will also affect product composition in a more general fashion. Products providing a specific function will have ingredients that provide a common set of functions. For example, perfumes all contain solvents that allow the dispersion of the product over a large surface area of skin, the semivolatile fragrances that impart aromas, and the extenders that slow down the evaporation rates of the fragrances. The specific chemicals that provide these functions will vary from product to product, but one or more chemicals will be present that provides each of the function.

Development of PUCs and attributes and assignment to consumer products in EPA's Chemicals and Products Database (CPDat)

The proposed system of PUCs was defined by applying the above criteria to refine the product categories used in EPA's Office of Research and Development's Chemical and Products Database (CPDat) [22], which were the same as those used by SHEDS-HT. CPDat currently contains few article categories as composition data are scarce. As such, PUCs were developed for consumer products only. Products that meet similar needs and have similar exposure scenarios were assigned to a single PUC. The resulting set of PUCs all contained at least one example product. The PUCs were defined in such a way that there was always a direct mapping of PUC to the OECD consumer product category; for example, two-component and single-component adhesives were separated to align with the OECD

categorization. Products were also annotated with attributes, which are product characteristics that can be used to additionally subset the individual products within each PUC. Attributes identify groups of products that have the same product and use patterns, are used in similar locations, involve similar populations of users, and can be addressed by the same exposure scenario. Attributes are different from PUCs in that they may be common to products in multiple PUCs. Attribute types include product form (e.g., aerosol, liquid), microenvironment for which the product is intended to be used (e.g., indoor, outdoor), or demographics of the intended population of users. Potential forms associated with each PUC were obtained via a review of the first 100 product images associated with a Google Images (www.google.com) search of the PUC name. A default form was selected for each PUC based on the most prevalent form (for use in modeling a product when its form is not known).

Case Study Application

The utility of the proposed PUCs is demonstrated here via their application within the Tier 3 mechanistic beta Combined Human Exposure Model (CHEM) [13]. CHEM is a population-based, longitudinal, Monte Carlo model for evaluating residential exposures to chemicals having consumer product sources. CHEM estimates aggregate exposure to various product types via algorithms describing product use, product composition, and chemical absorption via dermal, inhalation, or ingestion routes. The model includes “source-to-dose” exposure scenario algorithms that describe chemical releases to indoor media or compartments, transfers between these compartments during use and disposal, and contact with these compartments by human receptors. Each individual PUC developed here was linked to the corresponding CHEM inputs for these processes, including those describing consumer product use patterns, exposure factors, location of use, and exposure scenario inputs. CHEM was parameterized using this system for glycerol (CASRN 56–81-5) in five PUCs; all weight fraction (WF) data were obtained from the CPDat database. Glycerol was selected as an example chemical as it is present in CPDat in PUCs having a variety of forms, exposure scenarios, and exposure routes. The PUCs considered in this example were hair spray (form attribute = spray), hair conditioner (form attribute = liquid), toothpaste, laundry detergent (form attribute = liquid), and bathroom cleaner (form attribute = liquid). Exposures via various routes and the contribution to exposures and absorbed doses were estimated. Note that these are not all PUCs in which glycerol was present in the CPDat database; this simple example is meant to demonstrate the utility of the PUCs on organizing model input data and results and is not reflective of any true aggregate exposure exposures. A full discussion of the CHEM model and estimation of aggregate exposures for chemicals is beyond the scope of this manuscript.

RESULTS

Product Use Categories in the Chemical and Products Database

In total, 237 PUCs were developed from examination of the 15,043 products in EPA’s Chemicals and Products Database (CPDat). These PUCs are summarized in Table 1; a full listing of the categories including definitions is provided in Supplemental Table 1. As mentioned above, the PUCs cover consumer products (formulations); over-the-counter

pharmaceuticals are not covered as they were not previously included in CPDat. The PUCs follow a three-tiered hierarchy (Level 1–Level 3). The ten Level 1 categories represent high-level product sectors, such as personal care products or vehicle-related products. The 96 Level 2 categories describe unique product families under each of the product sectors. For example, laundry and fabric treatment products are under cleaning/household and make-up is under personal care products. The Level 3 categories are specific product types in a family that fulfill the same need (and thus similar habits and practice data) and have the same exposure scenario. Every combination of Level 1–Level 3 categories is unique, and the combination of Level 1, Level 2, and Level 3 categories together define the 237 PUCs.

In addition to assigning a product to a specific PUC, a set of “attributes” were defined and assigned to each product. Table 2 provides a list of the attributes currently defined for the products in CPDat and examples of the products with which they are associated. Potential and default forms associated with each PUC and the default form for the PUC are given in Supplemental Table 1.

The products in CPDat, and the chemicals they contain, are visualized according to PUC in Fig. 1. The hierarchical nature of the PUCs is represented by the circular structure of the figure, with more refined levels being represented by smaller circles within the more general groups. The size of the circles demonstrates the relative magnitude of the number of products in CPDat assigned to a given Level 1–Level 3 category; Level 2 categories containing >100 products are labeled. In addition, the Level 3 categories are colored by the number of unique chemicals (Chemical Abstract Service Registration Numbers, CASRN) in the PUC. Figure 1 shows that the database contains many personal care products relative to other Level 1 categories, followed by cleaning and household care products. The largest numbers of products are associated with the Level 2 categories hair styling and care, laundry and fabric treatment products, and paint/stains. The largest number of unique chemicals are associated with scented products such as fragrances (e.g., perfumes and colognes), general moisturizers (e.g., hand and body lotions), and air fresheners.

Personal and Communal Needs

The assignment of PUCs as serving personal or communal needs is provided in Supplemental Table 1. Communal status was assigned to products that meet needs related to the residence, yard, pets, and individuals who require care (e.g., infants). Personal status was assigned to products that are used on the person’s own body or are associated with personal hobbies, sports, education, and employment (e.g., working in a home office). These assignments can be used as inputs to models that utilize needs to model product use (such as EPA’s CHEM).

Crosswalks with Other Product Categorizations

A crosswalk between the product use categories and the internationally harmonized OECD product categories [11] is provided in Supplemental Table 2. Not every PUC had a specific OECD categorization match, simply due to the smaller overall scope of the OECD set; OECD defines an “other category”, but PUCs without direct matches were not specifically assigned to that category. This crosswalk allows anyone using the OECD product categories

to easily utilize consumer product data from EPA's databases and models. An additional crosswalk between PUCs and the consumer exposure scenarios within EPA's Consumer Exposure Model (CEM) and other similar consumer exposure models (i.e., CONSEXPO TRA and ECETOC) is provided in Supplemental Table 3. These different exposure models contain different consumer scenarios based on product use categories depending on the specific needs of the organizations who developed the models. For example, CEM is a suite of scenario-specific mechanistic exposure models used by the EPA's Office of Pollution Prevention and Toxics in support of evaluations under the Toxic Substances Control Act [23].

Case Study Application of PUCs: Rapid Prototyping of Exposure Algorithms

A demonstration of how product use categories enable a rapid parameterization or instantiation of exposure model inputs is illustrated in Fig. 2. The figure illustrates the linkage between the PUC system and (1) composition information (2) exposure scenarios (3) exposure factors (4) habits and practices data, and (5) product release data in in EPA's beta Combined Human Exposure Model (CHEM) [13]. The composition inputs for CHEM come directly from the CPDat data for products within each PUC. Each PUC-attribute combination has a set of "active" CHEM exposure scenarios, which may include: direct ingestion of product, direct dermal application of product, inhalation or vapor or aerosol during use, and contact with indoor air or surfaces post-use, i.e., "indirect exposure". These exposure scenarios dictate what equations are active for a given product, and what additional pieces of input information (i.e., exposure factors) are necessary to estimate human exposures and chemical disposals (which are useful as inputs to ecological models). All exposure factors for these scenarios (e.g., dermal areas of application, fraction of product aerosolized) are determined by PUC-attribute combination, as are other inputs describing disposal of product (e.g., rinse-off and wipe-off) after product use (Supplemental Fig. 1). Each PUC or PUC-attribute combination is also linked directly to habits and practices information developed for use in CHEM. That information, along with the personal/communal assignment and initial agent-based model results for limited activities [24] are used to model longitudinal consumer product use in CHEM. Finally, each PUC-attribute combination has a product release type in CHEM (e.g., "spray product applied to surfaces"); the possible product release types are defined in Table 3. These release types determine the compartmental releases fractions, i.e., the initial partitioning of release of product (and chemical) to compartments (indoor/outdoor air, surfaces, skin, etc.) in the residential environment (Supplemental Fig. S1). The assignment of all PUCs to product release type in CHEM is given in Supplemental Table S4, compartmental release fractions for each release type are given in Supplemental Table S5. Note that these releases simply describe the partitioning immediately upon product use and are only a function of PUC and attribute; these releases are upstream from additional model algorithms describing transfer among compartments (which may be PUC, attribute, or chemical property-dependent). Note that for many PUCs, these factors are currently assumed in modeling (and impart uncertainty in model estimates), since empirical emission data may not be available.

CHEM was parameterized using this system for glycerol in five PUCs. Supplemental Table S6 provides the CHEM PUC-specific model inputs for this case-study (including exposure

factors, compartment release fractions, and summary statistics of the CPDat WF data). Table 4 provides mean daily exposure results by PUC for the entire population and direct users (individuals who use a product within the PUC directly). For the entire population, summary statistics are provided for the aggregate exposure case (all PUCs contributing to exposure) and each PUC individually. Exposures are given by route; all reported results are medians (across households) of average daily values. For the entire population, the highest median exposures (in terms of absorbed mass) were for toothpaste via the ingestion route.

The CHEM example demonstrates how the PUCs can be used to summarize and interpret the results of aggregate assessments, e.g., characterization of the contribution of different product types to absorption via various routes and to total exposure. The PUC system allows for improved interpretation of the impact of model inputs on route-specific exposures. For example, in the case-study direct users of hair spray had higher dermal absorptions than direct users of hair conditioners. It was easily determined from examination of the inputs by PUC that this was likely due to (1) higher WFs in hair spray products and (2) differences in removal fractions (conditioner is rinsed off, whereas the fraction of hair spray released to skin is retained).

DISCUSSION

The 2017 report by the National Academy of Sciences (NAS) “Using 21st Century Science to Improve Risk-Related Evaluations” identified the need to expand substantially efforts to obtain and organize information on chemical quantities in, and rates of release from consumer products and materials [2]. The PUC system presented here is useful for meaningful organization of chemical-product data. The system provides a means to subset, sort, and report product composition information and to link to consumer exposure scenarios and information on habits and practices.

Recently, EPA’s Office of Research and Development has implemented new web-based tools for reporting of chemical data, including product data via the Computational Toxicology (CompTox) Chemicals Dashboard [25]. The PUC system provides a natural way of organizing product data within the dashboard for exploration or download by users and will be used to organize products in future public releases of CPDat. It also includes standardized tools to manage and curate different sources of chemical-product data such as MSDS information, ingredient lists, and analytical measurements, thereby ensuring timely incorporation of new product data into CPDat and the Dashboard. The proposed system of PUCs is not intended to be a final or permanent solution for organizing consumer products as the system will likely evolve concomitantly with data and models. Currently implemented EPA data curation tools allow for the assignment of new products to PUCs individually, or in batches via name-based rules (e.g., assignment of all products containing the words “toothpaste” to the corresponding PUC). The use of text-based machine-learning classifiers for the assignment of PUCS to large groups of products has also been explored. These classifier methods can provide an initial PUC assignment that can be used for some applications. The implementation of a formal data curation workflow that also assigns an indicator of the level of curation for each product PUC assignment is anticipated. Future data management tools may feature the flexibility to refine, split, or aggregate PUCs and

their associated products. New PUCs will be added as new sources of data are obtained and pushed into the database. However, the need to have version-control for PUCs, attributes, and their associated products is recognized, and features will be implemented in the tools to do so. Each version of PUCs can be linked to downstream exposure model results, allowing for benchmarking of exposure predictions associated with a defined set of input data, improving both transparency and sustainability of modeling efforts.

The PUCs defined here aid in the identification and prioritization of gaps in exposure information for consumer products. For example, summarizing available habits and practices data for each PUC allows for comparing the depth and breadth of use pattern data in relation to the number of available products, allowing identification of categories where better data are most needed. Similarly, summarization by PUC allows identification of product types for which limited product composition or emission data are available, guiding new efforts to collect publicly available information or measured data.

The scenarios and equations of CHEM are not the only algorithms that can be linked to these PUCs. Indeed, a harmonized framework is planned where other equations and scenarios from existing consumer exposure models can be used to estimate exposures and can be linked to these PUCs, thereby comprising a modular library of fully parameterized algorithms that can be rapidly implemented for model comparison. Model estimates (e.g., average daily doses or average daily concentrations) and exposure descriptors (e.g., central tendency, high-end) can be compared within the PUCs. In the future, building upon this generalization, the goal is to create a suite of pre-populated exposure model results for “generic” chemicals-within PUCs, where a generic chemical is simply one having a fixed set (or ranges) of physical chemical properties. Generic chemicals could be defined via Latin hypercube sampling of the physicochemical property space of chemicals in CPDat associated with a PUC. For example, if a consumer exposure model takes as input vapor pressures, water solubilities, and octanol water partition coefficients (e.g., for estimating indoor fate and transport and dermal absorption), we could develop a set of model predictions spanning reasonable ranges of these parameters for a PUC (e.g., surface cleaners). Such results could form a resource for rapid read-across of exposure results for new chemicals in the PUC.

Potential users of the PUC system should be aware of the limitations of the PUC definitions and how they may impact the results of any assessment. For example, we have assigned a default form attribute for each PUC, for use as an assumption when product form is not available. However, in bespoke exposure assessments form would likely be known and would potentially impact parameterization decisions or algorithm selection. In such applications the PUCs and any a priori linkages to model parameters or algorithms can provide a starting point for customization rather than a final template. By their nature, aggregation of products into categories will result in potential overestimation or underestimation of actual product exposure (as is the case with any model system). In the future, modeling exercises that compare the results of more refined exposure assessments with those based on PUCs can quantify these impacts. Finally, the PUCs developed here were based on products available in the U.S. market. Applications to other global markets would likely require expansion of the categories to reflect additional product types, and the

PUCs would need to be linked to market-specific habits and practices information and any market-specific chemical ingredient data. However, the PUC framework could be expanded for such customization in a straightforward manner.

In the future, the list of PUCs will be extended beyond formulated products to include other types of products such as articles (durable goods such as clothing and furniture), pharmaceuticals, or food or product packaging. Accordingly, when these products are incorporated into models such as CHEM, linkages between their PUCs and required model inputs and algorithms will be generated. As the PUC system matures, we plan to version different implementations of the PUC system according to FAIR (Findable, Accessible, Interoperable, Reusable) principles via the CompTox Chemicals Dashboard [25], which seeks to employ FAIR standards [26].

CONCLUSIONS

Exposure assessments for consumer products are required to support multiple tiers of risk-based chemical evaluations, including prioritization frameworks, life-cycle impact assessments, chemical risk assessments, and product safety assessments. Grouping of products via efficient and meaningful categorization schemes plays a key role in effective exposure assessments. Categories provide a means to effectively provide linkages among chemical constituents and formulations, habits and practices information, and exposure algorithms. A set of flexible, expandable, and intuitive consumer product use categories was developed for linking product and chemical information in human exposure models and databases. The resulting PUCs allow rapid parameterization of models for new chemical-product combinations as new data or research applications arise. An initial case example for the PUCs (CHEM) demonstrated their utility in organizing model inputs; the PUCs will be versatile enough to support both mid-throughput and high-throughput models. The PUCs provide a generalizable, extensible approach for organizing, representing, and populating model input information and exposure model results.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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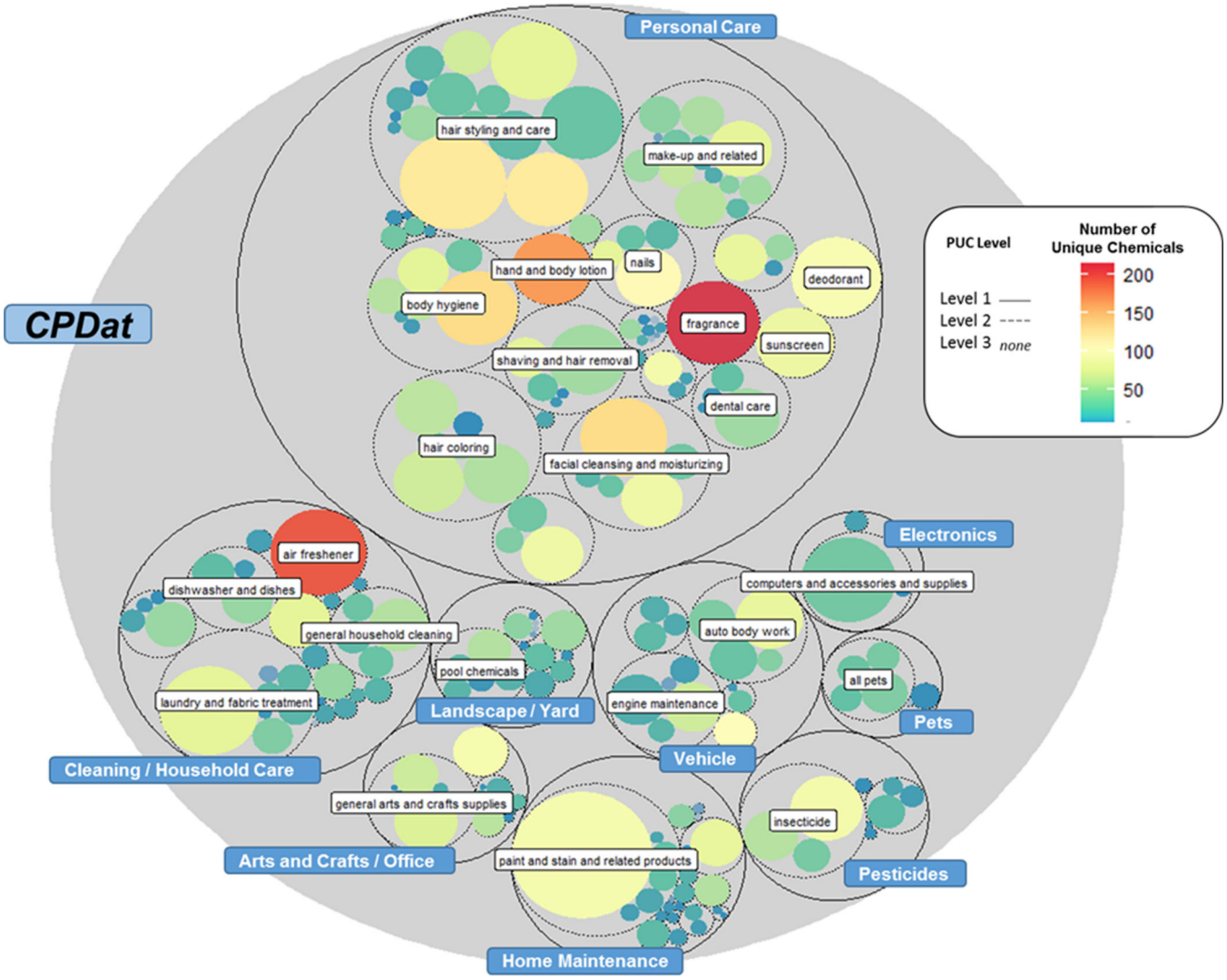

Figure 1.

Products and chemicals in EPA's Chemical and Products Database (CPDat) in terms of product use categories (PUCs). The circles represent the different levels of categories, which make-up a PUC; the size of the circles is scaled by the number of products in the PUC. Level 2 PUCs having at least 100 products in the database are labeled

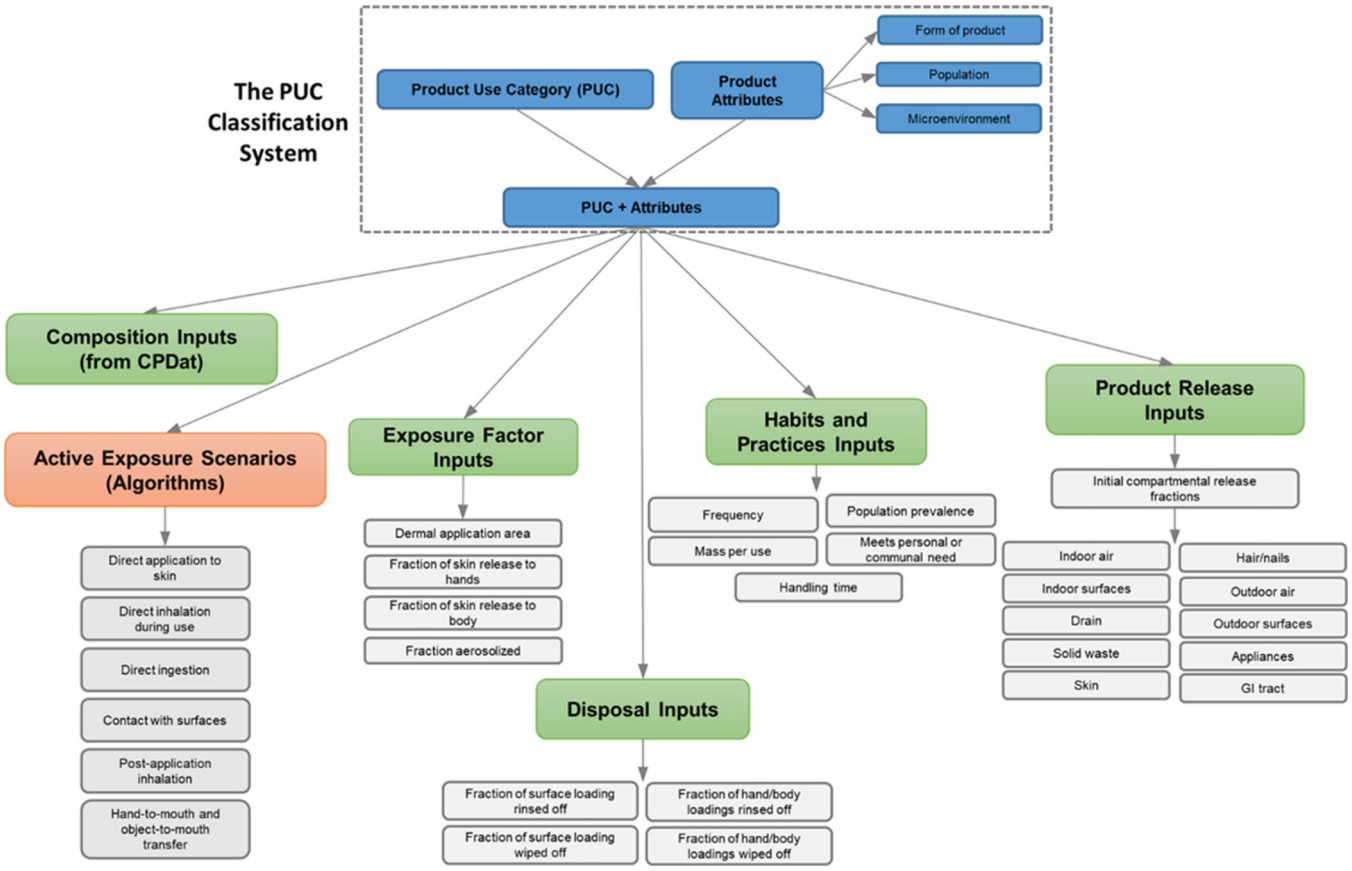

Figure 2.

Linkages between product use categories (PUCs) and the beta Combined Human Exposure Model (CHEM) inputs and algorithms. Knowledge of the PUC and attributes for a product allows CHEM to automatically populate the CHEM inputs for habits and practices, exposure scenario, product release, and exposure factor variables, allowing for rapid prototyping of exposure model runs for new chemicals

Table 1.

A full listing of all Level 1–Level 3 categories is provided in Supplemental Table 1

Level 1 Categories	Level 2 Categories	Number of Level 3 Categories
Arts and crafts/office supplies	Body paint, children's art and toys, fabric treatment and dye, fogger, general arts and crafts supplies, home office, pottery making	17
Cleaning products and household care	Air freshener, bathroom, carpet and floor, dishwasher and dishes, drain products, fireplace, general household cleaning, hand cleaner, heavy duty cleaner, houseplant care, lamp oil/lighter fluid, laundry and fabric treatment, lime remover, metal-specific, oven, shoes, upholstery specific, wood specific	35
Electronics/small appliances	Computers and accessories/supplies, electronics cleaner	3
Home maintenance	Adhesives and adhesive removers, caulk/sealant, concrete, corrosion protection, degreaser, finish, insulation, lock deicer, lubricant, paint/stain and related products, patch and repair, plumbing, refrigerant, roof, septic system, surface sealers, tiling, welding	32
Landscape/yard	Cleaner, grill/camping fuel, herbicide, lawn fertilizer, lawnmower, plants and garden, pool chemicals, surface deicer	16
Personal care	Acne treatment, bite relief, body adhesive, body care set, body hygiene, body oil, body powder, child-specific, dental care, deodorant, eye care and contacts, facial cleansing and moisturizing, foot care, fragrance, general moisturizing, glitter, hair coloring, hair styling and care, liniment, make-up and related, nails, self-tanner, sexual wellness, shaving and hair removal, specialized bath products, sunscreen	96
Pesticides	Animal repellent, fungicide, insect repellent, insecticide, rodenticide	6
Pet care	All pets, cats, fish	6
Sports equipment	Bicycling, fishing, gun cleaner, skiing	4
Vehicle	Auto body work, boat care and maintenance, car interior, car surface treatment, engine maintenance	19

Table 2.

Attributes are characteristics of individual products that may be common over multiple product use categories (PUCs) and can be used to subset or tag products within a PUC for reporting or assignment of properties. Additional attributes may be defined as new products are added to EPA's product database or as PUCs are further refined

Attribute type	Attribute	Definition
Form	Aerosol	Product is sold in a pressurized container containing one or more propellants. The spray produced may consist of smaller droplets than the sprays created by pump sprayers and may be more inhalable.
Form	Cartridge	Product is a liquid or powder product enclosed in a cartridge for use in computer printers.
Form	Foam	Product is mixed with air or other gas during application or use.
Form	Foam spray	Product is formed into a foam during use as a result of its being sprayed.
Form	Gas	Gas products such as fuels for camping equipment.
Form	Gel	Product is a viscous liquid that is too thick to easily pour from a bottle. The material consists of a single phase where all components are dissolved in a single solvent.
Form	Hose spray	Product is a designed to be used in a hose-end sprayer.
Form	Hot melt	Product is intended to be used in a device that melts the product as part of the product application process.
Form	Impregnated sheets	Product is a fiber sheet impregnated with a solid (e.g., dryer sheets)
Form	Liquid	Product is readily poured from a container but may be applied using a brush or other device.
Form	Paste	Product is a viscous liquid or semisolid that is too viscous to easily pour from a bottle. The material consists of multiple phases (oil, aqueous, solids) that has been mechanically mixed.
Form	Pods	Product consists of an oil, liquid, gel, powder or paste that is contained in a flexible plastic container. The container is designed to dissolve in water and release its contents. May be any shape.
Form	Powder	Product is free-flowing and composed of small grains of solid product.
Form	Pump spray	Product is released as a spray by means of a hand powered device, consisting of a pump and a nozzle, that produces a stream or spray of droplets.
Form	Solid	Product has a fixed shape.
Form	Trap	Product is an adhesive designed for trapping insects or rodents
Form	Two-component	Product is sold as two components that are mixed prior to use.
Form	Wipes	Product consists of a textile pad impregnated with an oil, liquid, gel, or paste.
Microenvironment	Exterior	Product is identified by labeling for exterior use (e.g., paints and primers).
Microenvironment	Interior	Product is identified by labeling for interior use (e.g., paints and primers).
Population	Child	Product is identified by label as marketed to children (e.g., sunscreens).

Table 3.

Product Release Types in the beta Human Exposure Model (HEM). A complete mapping of PUCs to release types is given in Supplemental Table 3.

Product Release Type	Code	Example Level 3 PUC – Attribute Combination
Aerosols for application to body surfaces	ABS	Face cream/moisturizer (aerosol)
Aerosols for application to indoor air	AIA	Air freshener (aerosol)
Aerosols for application to indoor surfaces	AIS	Primer (aerosol)
Aerosols for application to non-dermal body (hair/nails)	AHN	Hair color—temporary (aerosol)
Aerosols for application to outdoor air	AOA	(No current products in CPDat)
Aerosols for application to outdoor surfaces	AOS	(No current products in CPDat)
Dusts or powders for application to body surfaces	DBS	Body powder (powder)
Dusts or powders for application to indoor surfaces	DIS	Carpet deodorizer (powder)
Dusts or powders for application to non-dermal body (hair/nails)	DHN	Dry shampoo (powder)
Dusts or powders for application to nose, mouth, or lips	DGI	(No current PUCs in CPDat)
Dusts or powders for application to outdoor surfaces	DOS	Garden fertilizer
Dusts or powders for application within appliances	DAP	Automatic dishwashing detergent (powder)
Liquids, lotions, or gels for application to body surfaces	LBS	Body wash
Liquids, lotions, pods, or gels for application to drains	LDR	Drain treatments
Liquids, lotions, or gels for application to indoor surfaces	LIS	Floor cleaner (liquid)
Liquids, lotions, or gels for application to indoor surfaces with hands	LSH	Finger paint
Liquids, lotions, or gels for application to non-dermal body (hair/nails)	LHN	Hair color—permanent
Liquids, lotions, or gels for application to nose, mouth, or lips	LGI	Toothpaste
Liquids, lotions, or gels for application to outdoor surfaces	LOS	Paint (exterior)
Liquids, lotions, or gels for application within appliances	LAP	Laundry detergent (liquid)
Pods for application within appliances	PAP	Automatic dishwashing detergent (pods)
Solid formulations	SOL	Bar soap
Soluble products added to bath water	BAT	Bath salts
Sprays (pump) for application to body surfaces	SBS	Body oil spray
Sprays (pump) for application to indoor air	SIA	Air freshener (pump spray)
Sprays (pump) for application to non-dermal body (hair/nails)	SHN	Hair styling (pump spray)
Sprays (pump) for application to nose, mouth, or lips	SGI	Mouthwash (pump spray)
Sprays (pump or hose) for application to outdoor air	SOA	(No current PUCs in CPDat)
Sprays (pump or hose) for application to outdoor surfaces	SOS	Body repair (pump spray)
Sprays (pump) for application to indoor surfaces	SIS	Surface cleaner (pump spray)
Traps - interior (pesticides)	TRI	Insecticide (interior, trap)
Traps - exterior (pesticides)	TRE	Insecticide (exterior, trap)

Table 4.

Product Release Types in the beta Human Exposure Model (HEM). A complete mapping of PUCs to release types is given in Supplemental Table 3.

UC	Number of households	Total mass used by household annually (mg)	Average daily direct dermal absorption (mg)	Average daily direct ingestion absorption (mg)	Average daily direct inhalation absorption (mg)	Fraction absorption via dermal route	Fraction absorption via ingestion route	Fraction absorption via inhalation route	Average daily release to solid waste (mg)	Average daily release to drain (mg)	Fraction of total absorption
All (aggregate)	1000	1,392,380	1.638	1.3e+00	1.2e-04	0.65	0.3521	2.5e-04	38.3	2934.13	NA
Hair spray	760	70,069	0.000	0.0e+00	0.0e+00	0.98	0.0219	6.5e-04	1.9	0.95	5.5e-01
Hair Conditioner	954	103,281	0.027	6.9e-05	1.9e-06	0.99	0.0075	8.1e-05	2.8	28.09	4.4e-03
Toothpaste	1000	312,519	0.831	1.3e+00	5.2e-05	0.39	0.6105	2.5e-05	8.6	832.98	5.6e-01
Bathroom cleaner	394	104,474	0.000	0.0e+00	0.0e+00	0.95	0.0465	2.0e-03	2.9	281.28	3.7e-02
Laundry detergent	647	1,397,568	0.000	0.0e+00	0.0e+00	0.92	0.0728	3.1e-03	38.4	3800.69	4.3e-06
	Number of direct users										
Hair spray—direct users	367		7.79	0.00934	7.00E-04	0.99	0.0065	2.80E-04	2.1	1	0.783
Hair conditioner —direct users	678		0.079	0.00025	5.40E-06	1	0.0041	7.80E-05	2.9	29	0.012
Toothpaste —direct users	1000		0.831	1.28249	5.20E-05	0.39	0.6105	2.50E-05	8.6	833	0.559
Bathroom cleaner—direct users	150		0.052	0.00022	2.20E-04	0.97	0.0306	2.50E-03	3.1	306	0.045
Laundry detergent—direct users	254		0.027	0.00299	2.80E-06	0.9	0.0997	9.50E-05	37.2	3686	0.006