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The Role of Product Use Scheduler for Estimating Exposure to Methyl, Ethyl, Propyl, and Butyl Parabenzoic Acid (Parabens) within the Combined Human Exposure Model

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DRAFT 2
3962/P653

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Abstract

Paraben exposure assessments must estimate and predict doses received by persons with typical exposures and highly-exposed individuals. Exposures from product use can be significant sources of exposure for these chemicals, especially methyl, ethyl, propyl, and butyl parabenzoic acid, which are used as preservatives in a wide range of consumer products including paints, dyes, arts & toys, and sealers. Because use varies across individuals and paraben levels vary in different consumer products, the general population doses vary widely. To simulate aggregate exposure to the four parabens, we input biomonitoring data into the Combined Human Exposure Model (CHEM) and compared estimates of interindividual variation in these aggregate exposures. Implementing the Product Use Scheduler (PUS) in CHEM allows researchers to assess the differences in Product Use Categories (PUCs), demonstrating the relationship between sentinel and aggregate exposures for each paraben. PUS is the CHEM module that estimates exposure from consumer products. The module accepts a spreadsheet which represents a US population and returns 364-day diaries of product use depending on the characteristics of individuals, households, and co-inhabitants. Output passed to Source-to-Dose (S2D) in CHEM, which estimates down-the-drain release and exposure. This approach provides an opportunity evaluate the applicability of a simulation model in complex product-use longitudinal exposure scenarios

Methods

Based on the chemical prevalence in products, the PUS can provide observations of low or high incidence of exposure. The information provided by the PUS is critical to generating aggregate exposure data using the CHEM model. PUS is employed in this case to determine the prevalence of the four parabens in a home. The total dosage per day in mg/kg for the four parabens was calculated using the full CHEM model. The model contains uncertainty due to a different distributions of varied product usage for these chemicals. . If products containing a paraben have above average market distribution, they would have a greater influence the distribution of doses than if they were rarely used. To account for this, two model runs were generated: one assuming both paraben and non-paraben containing products were utilized and the other assuming that only items containing

Features

Clusters

Some products are often used together (e.g., toothpaste, shower gel, conditioner). These are paired in PUS to create realistic diaries.

Seasonality

In the 364-day diary, children are home from school in summer, impacting the use patterns.

Communal

Some products pertain to the entire household. For example, a spray cleaner, if used, will benefit the entire household, and only one individual partakes in this activity per household.

Ever/Never

Some products are influenced by the characteristics of the household. For example, lawn care product uses are scheduled only if the home as a lawn. Conversely, if the household does not have a lawn, it is assumed that the individuals never use lawn care products.

Results

Figure 1. Comparison of PUCs and product count per paraben

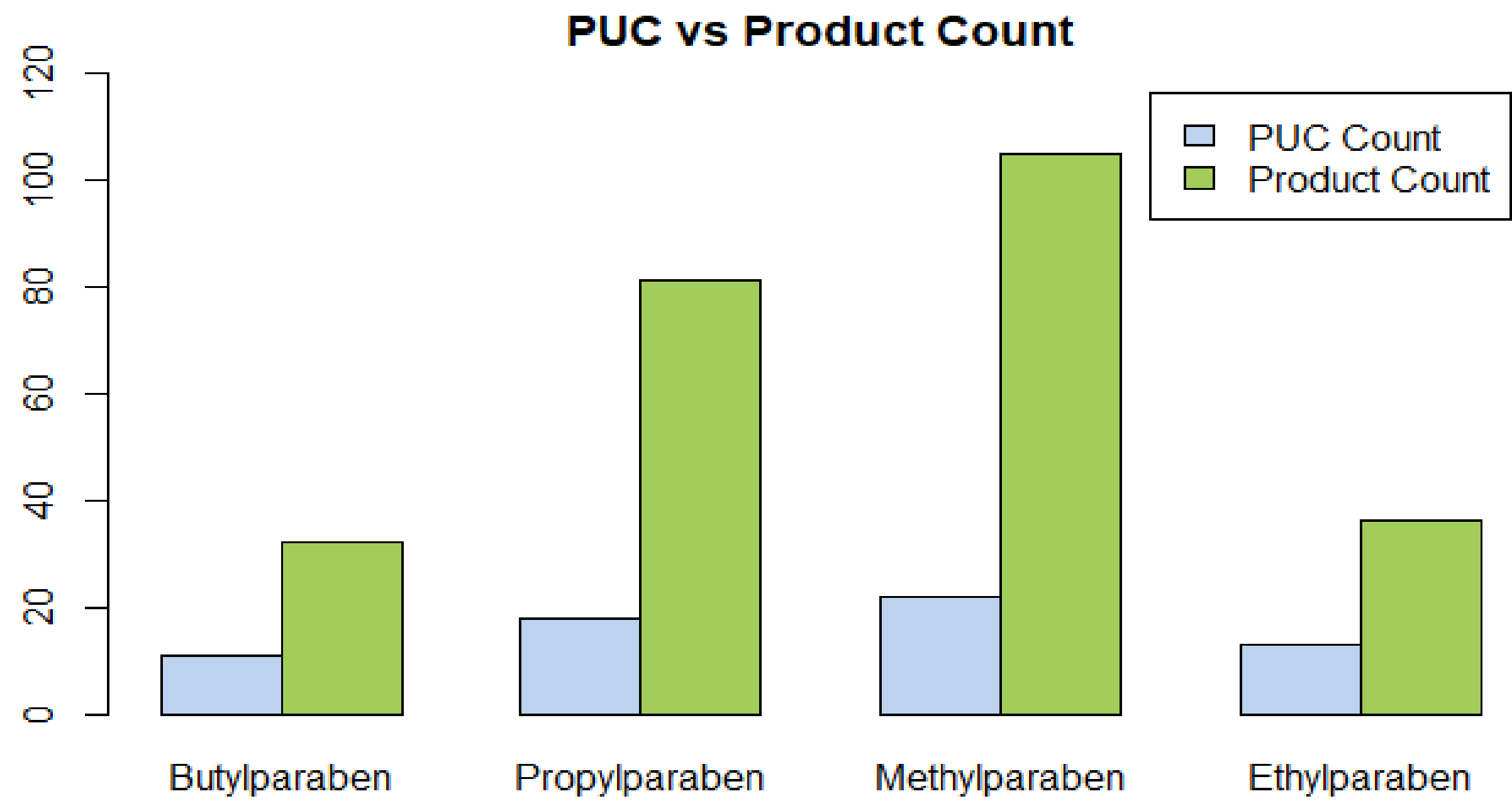
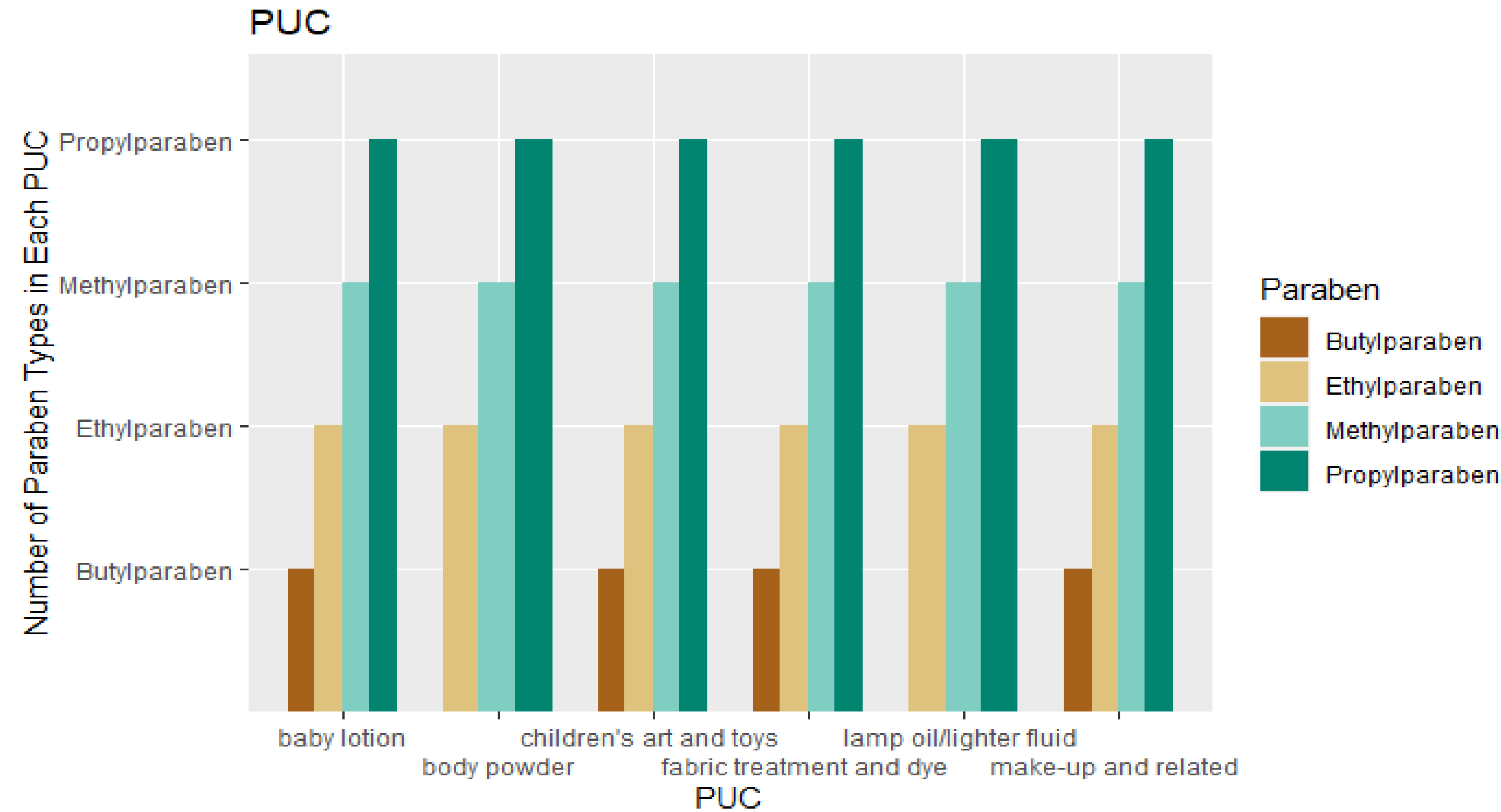


Figure 2. Common paraben product use categories



References

1. Dionisio, K., Hong, T, Levasseur, J. Arun, V. (2018, September). *Product Use Scheduler Module Technical Manual*. EPA. https://github.com/HumanExposure/HEM-Documentation/blob/master/ProdUseSched_TechMan_2018Sept11.pdf
2. Price, P., Issacs, K. (2020). Prediction and Evaluation of Aggregate Exposure to Parabens from the Use of Consumer Products.
3. Calafat, Antonia M., et al. (2010)."Urinary concentrations of four parabens in the US population: NHANES 2005–2006." EHP 118.5: 679-685.

Table 1. Estimated dosage per day for select percentiles of parabens

Chem Prediction of Doses(mg/kg/day) for Select Percentiles				
Percentile	Methylparaben	Ethylparaben	Propylparaben	Butylparaben
50th	0.0034	0.0000	0.0086	0.0000
75th	0.0135	0.0005	0.0677	0.0002
90th	0.0326	0.0025	0.2468	0.0017
95th	0.0527	0.0092	0.4237	0.0039

Discussion

Observations from the Simulations

- Parabens are distinctive from many other PUS chemicals in that they do not differentiate between homeowners and renters.
- Propylparaben and methylparaben have a high prevalence of consumer usage as per PUS. Both parabens have a reasonably higher utilization rate than their counterparts, ethylparaben and butylparaben.
- Product Count: 105 (methyl) and 81 (propyl)
- PUC Count: 22 (methyl) and 18 (propyl)
- As a result of this finding, CHEM model runs based on just these two simulations show promise.
- As seen in Figure 2, butylparaben has the lowest rate of incidence and is absent from certain major product use categories. This might indicate a lower risk from product use.
- The CHEM dosage estimations seen in Table 1 also corroborate the butylparaben findings, indicating a reduced risk of aggregate exposure compared to methylparaben and propylparaben.
- CHEM's simulation-based estimations revealed significant inter-individual dosage variability, with the 95th percentile receiving one to three orders of magnitude more does than the median. When solely paraben-containing products were used in the model run, the findings were one to four orders of magnitude greater than when mixed composition products were included. Thus, simulation models may be used to determine the maximum portions of aggregate exposure distributions for some parabens.
- When compared to NHANES biomonitoring of the metabolites of four parabens in urine samples collected in 2005 and 2006 (Calafat et al., 2010), an overestimation of propylparaben is implied, possibly due to a small market share of the product.

Model Improvements Needed

Small market distribution of products can lead to overestimation. A question to be asked of each chemical in CHEM is whether the chemical present in products and use categories for this modelling is sufficiently effective and worthwhile. To provide the most accurate outcomes , more research and updating of data inputs are anticipated. Improved data formatting and simplicity of use would help to enhance the utility and widen the use of this model. In addition, the repetitive and related PUCs should be condensed even further to increase relevance, precision and accuracy.



Although this work was reviewed by EPA and approved for presentation, it may not necessarily reflect official Agency policy.