Estimating Longitudinal Aggregate Exposure
The Third Module of CHEM: Source to Dose

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Overview of CHEM

The Combined Human Exposure Model (CHEM) is a series of three modules designed to estimate aggregate exposure from consumer products. A brief explanation of the first two is presented below:

- RPGen (Residential Population Generator) creates a simulated population and assigns relevant parameters, both physical such as age and BSA, and household specific, such as appliance presence and house size. This allows the model to account for both indirect exposures due to others in the house as well as statistical correlations between product use and other factors, such as car maintenance products being used more by people with multiple cars.

- PUS (Product Use Scheduler) uses an existing data base of activity diaries, which provide simple activities such as working and sleeping, and assigns various products to the appropriate time frames. This allows the next model to estimate exposure on an hourly timestep over the course of a year.

S2D (Source to Dose) uses the outputs of the previous two diaries to determine the aggregate exposure for one simulated person per household over the course of a year. This is done by examining the various exposure pathways for each product used. While it was originally designed to only account for consumer products, further updates have added in simple algorithms for calculating exposure from both food and articles.

Performing these runs for a large population provides a distribution of expected exposures that can not only be used to estimate real life exposure for a similar population, but also reveal the most common pathways and can even be used to determine the kinds of traits and behaviors that correlate with the highest individual exposures.

Case Study: Rent vs Own

To demonstrate the effectiveness of S2D (and CHEM as a whole) in calculating exposures for different subpopulations, we looked at yearly exposures of 5 different chemicals to 1000 individuals. We then split the population into those who rent vs those who own their residences. To better understand the differences, we did one final run that looked only at the exposures resulting from pucs that renters would not use, such as lawn fertilizer.

Probability of exposure (Figure 1)
- For Toulene(3), we observe a large difference in probability between renters and owners. The large exposure probability in the owners specific pucs run suggests that many owners are only exposed through these owner specific pucs
- For Naphthalene(5), similar probabilities suggests that the owners exposed through owner specific pucs were also typically exposed through at least one other puc

Exposure (Figure 2)
- For Toulene, large exposure through owner specific pucs drive up the exposure distribution for owners relative to renters
- For Naphthalene, the low chance of exposure means the owner specific pucs do not move the mean by much, but the owner distribution does have a larger upper bound than the renter one, due in part to the additive exposures of individuals who are exposed though both general use pucs and owner specific ones
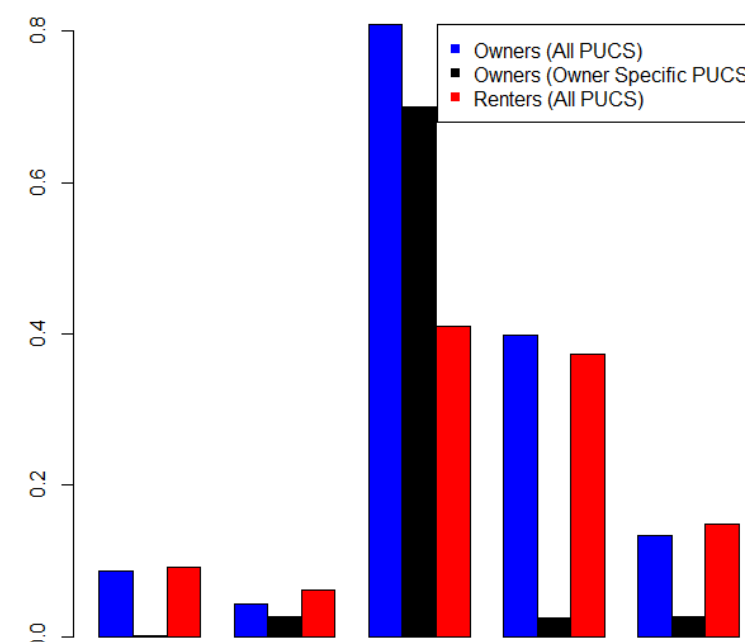

Figure 1: Fraction of simulated individuals with non-zero exposure to each chemical. Groupings include owners and renters simulated with all pucs available (blue and red respectively), and owners simulated with only owner specific pucs available (black).
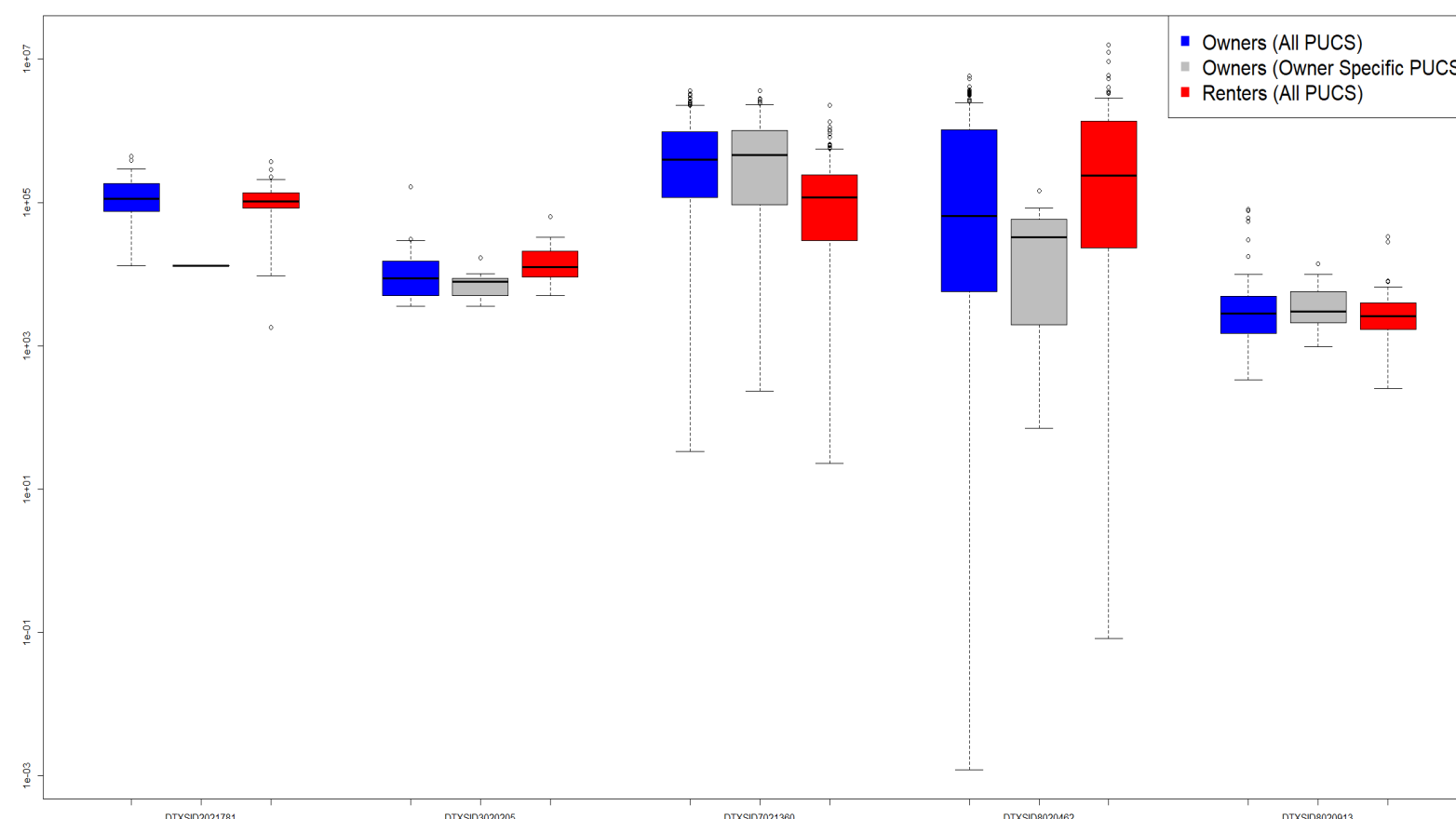

Figure 2: Exposure distributions (mg/year) for each chemical and subgroup. Groupings include owners and renters simulated with all pucs available (blue and red respectively), and owners simulated with only owner specific pucs available (grey).

Source to Dose Overview

- Products are categorized into product use categories (PUCs) based on how and when the product is applied
    - These categories determine the fraction of the component chemicals that are used in calculating exposure through each route
    - For example, products like shampoo will be applied to the skin and mostly affect the dermal route, whereas products like air fresheners will have a larger affect on inhalation
- Chemical composition is determined using a set of formulations for the given PUC
    - Instead of using a specific product, a representative formulation is selected from a list of 100 possible formulations
    - This list is created by randomly sampling from the distribution of compositions for all products in the specific PUC
    - In other words, instead of modeling the simulated person using one specific brand of shampoo, that person is modeled as using a shampoo with chemical composition that is determined based on the compositions of all shampoos
- For each exposure event, the amount of chemical that is absorbed through each route is calculated
    - The results of these calculations are aggregated over one year of activity
    - This process repeats for each simulated individual

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