



# Source to Dose: A Component in the Combined Human Exposure Model (CHEM)

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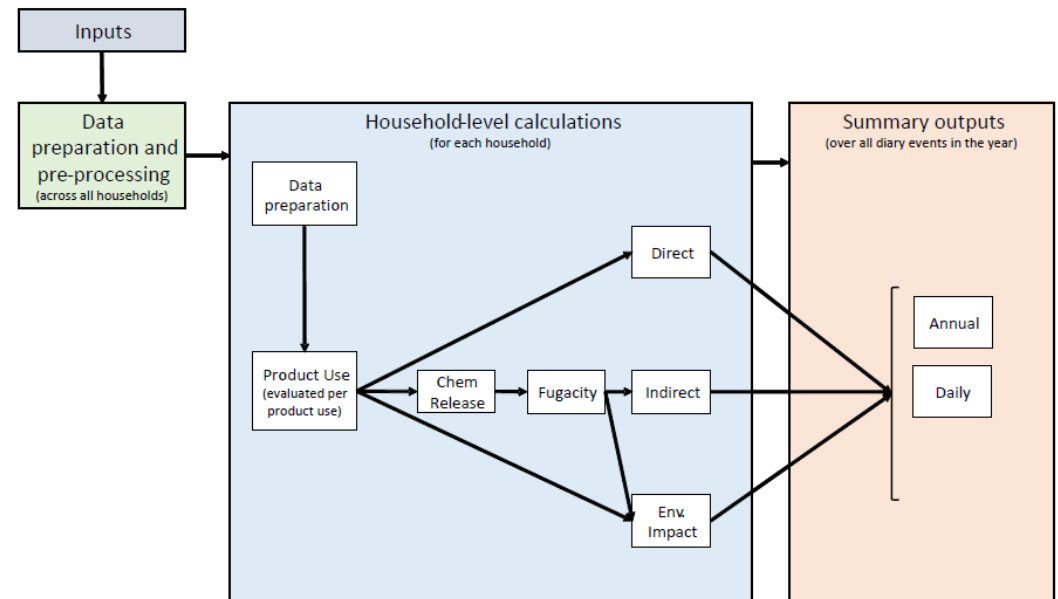
<sup>2</sup>Oak Ridge Institutes for Science and Education, Oak Ridge, TN

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Multisector Engagement for Addressing Emerging Environmental Exposures

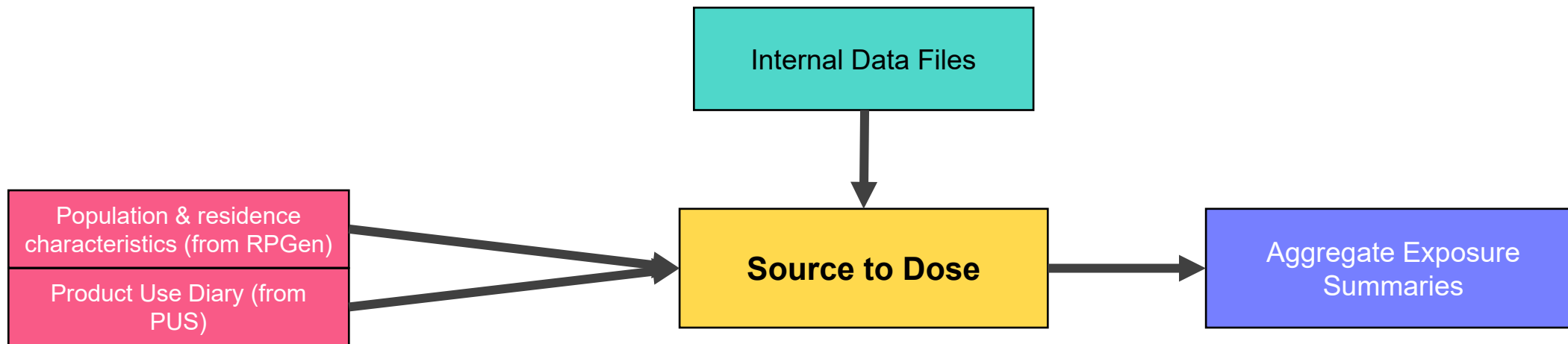
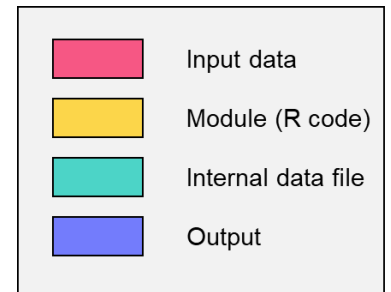
## Outline

- Overview of S2D
  - How S2D fits into CHEM
    - Recap of previous two module outputs
  - Internal Data
  - S2D Flow
    - Direct Exposures
    - Fugacity
    - Indirect Exposures
  - Aggregate Exposure Summaries
- Case Study
  - Brief Recap
  - Results
    - Exposure Probability
    - Exposure Magnitude Distribution
  - Discussion



## Overview of S2D Flow (External)

I want better words than 'external' and 'internal' to mean 'in the context of CHEM' and 'within the S2D module separately.'

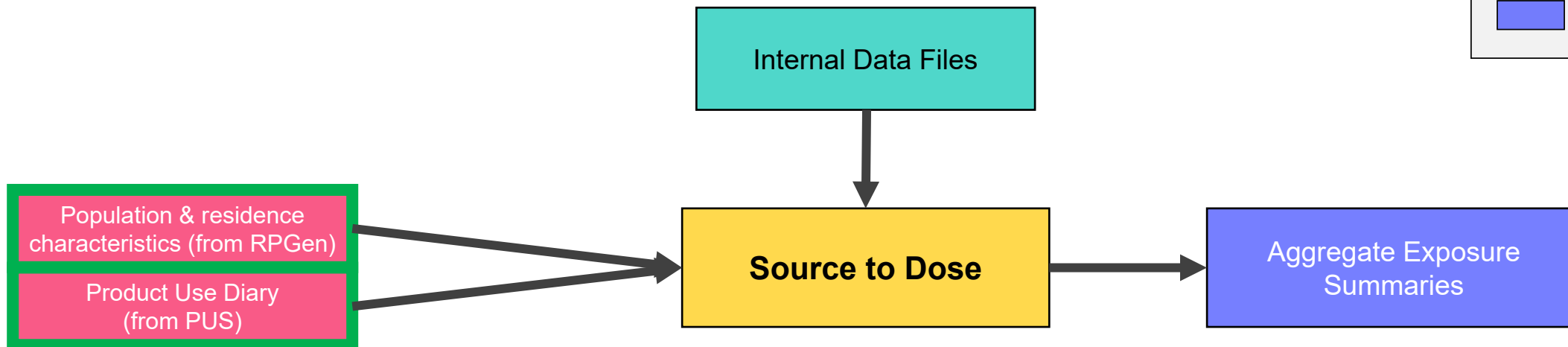
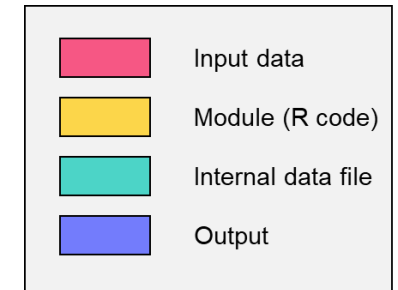


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## Required Inputs

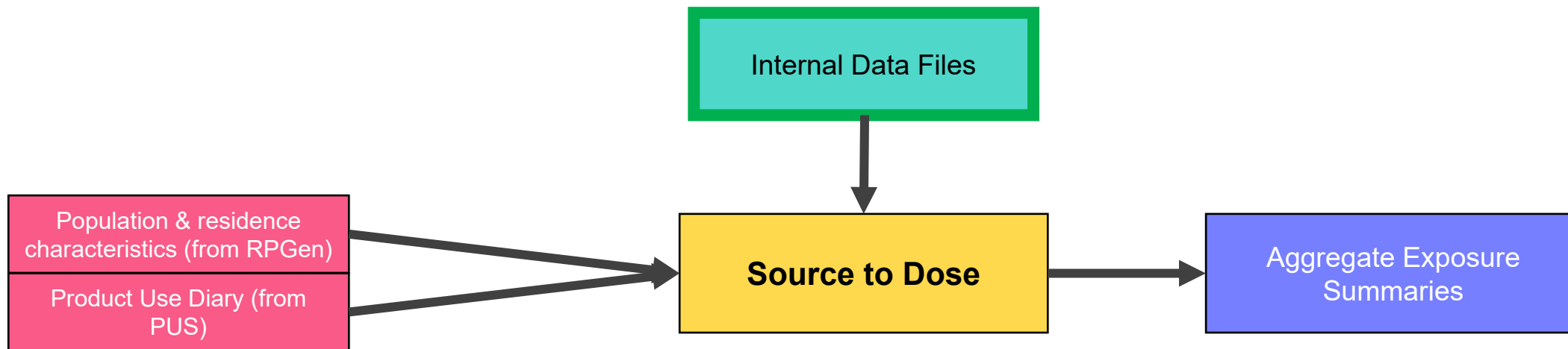
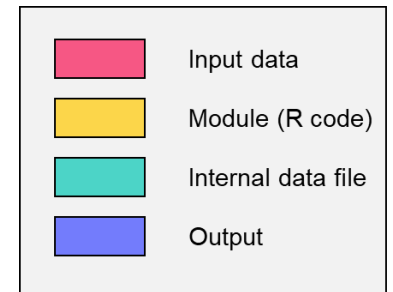
- RGen provides a file with required physical and residential parameters for each simulated individual that will be modeled
- PUS provides a product use diary for each individual
- While S2D was designed to work with RGen and PUS, it can function alone if provided with analogous residential and product use information



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## Internal Data Files

- Next, we will look at the 14 data files that are included in S2D.
- Each of these come in a default form, but can be altered to fit the needs of the user
  - For example, a chemical can be added to the default list of chemicals by adding its properties and products it is found in to the proper file



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## Internal Data Files

### **Basal Vent:**

Information for estimating basal vent

### **Chemical Properties:**

List of properties for each chemical that are relevant in calculating fugacity and exposure

### **Fugacity:**

Chemical independent variables required to calculate fugacity

### **Skin surface areas:**

Identifies which body areas are exposed during the use of each PUC

### **Compositions:**

Chemical formulations, including weight fractions, for each PUC

### **PUC MET:**

Mean values of METS associated with each PUC and associated CHAD activity code

### **PUC Product Codes:**

Three letter codes for each PUC category used to group PUCs

### **PUC skin/wipe/rinse:**

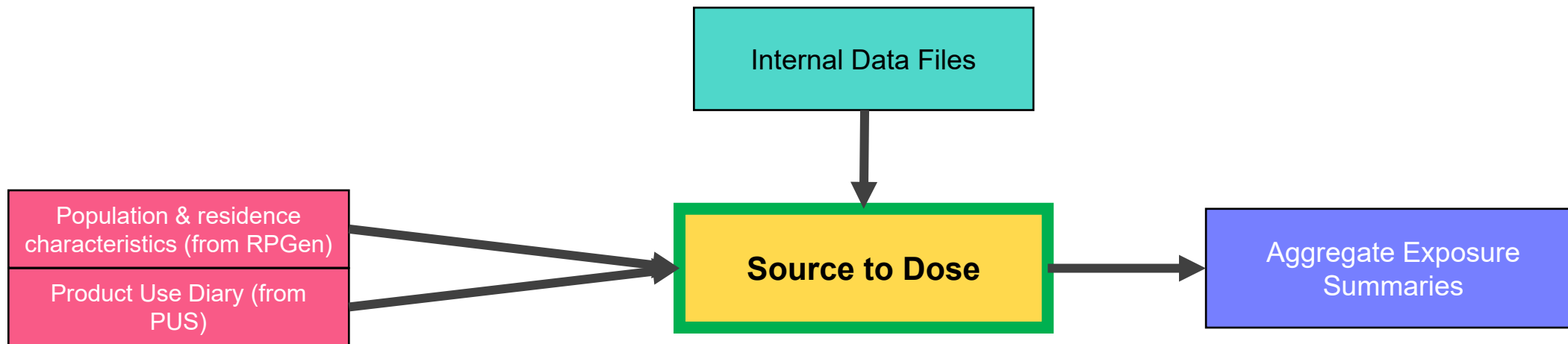
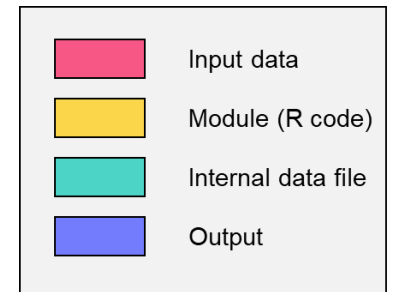
Fraction of the PUC that ends up on the hands vs body and how they are affected by rinsing and wiping

### **Compartment Fractions:**

Fraction of chemical that partitions into each exposure route compartment for each PUC category

## S2D Flow (Internal)

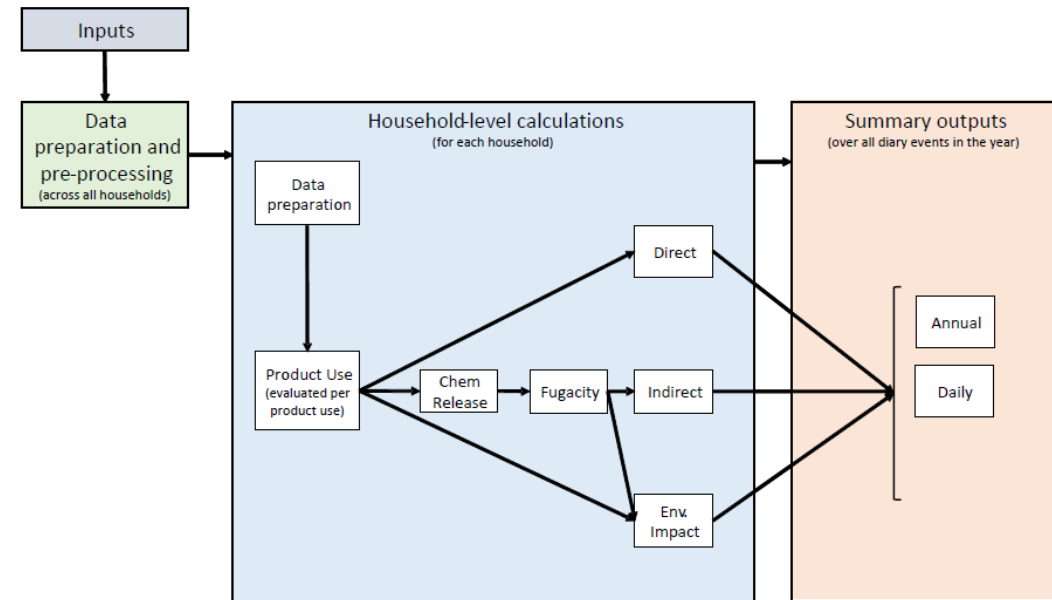
- We will now look at the general steps that S2D takes in calculating exposure



## S2D Internal Workflow (Overview)

Next few slides will talk about the important sections of S2D in detail.

Intend to update the diagram and highlight relevant section as I go

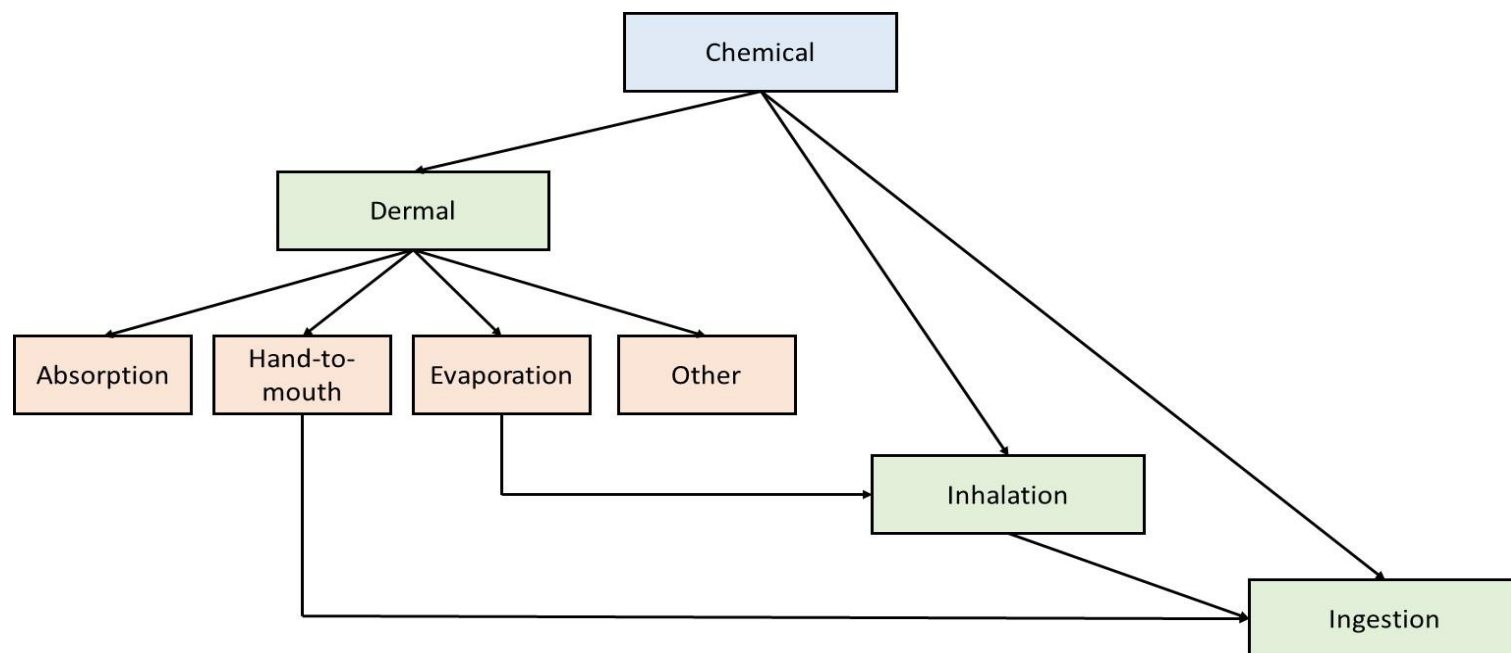




## S2D Internal Workflow (Direct)

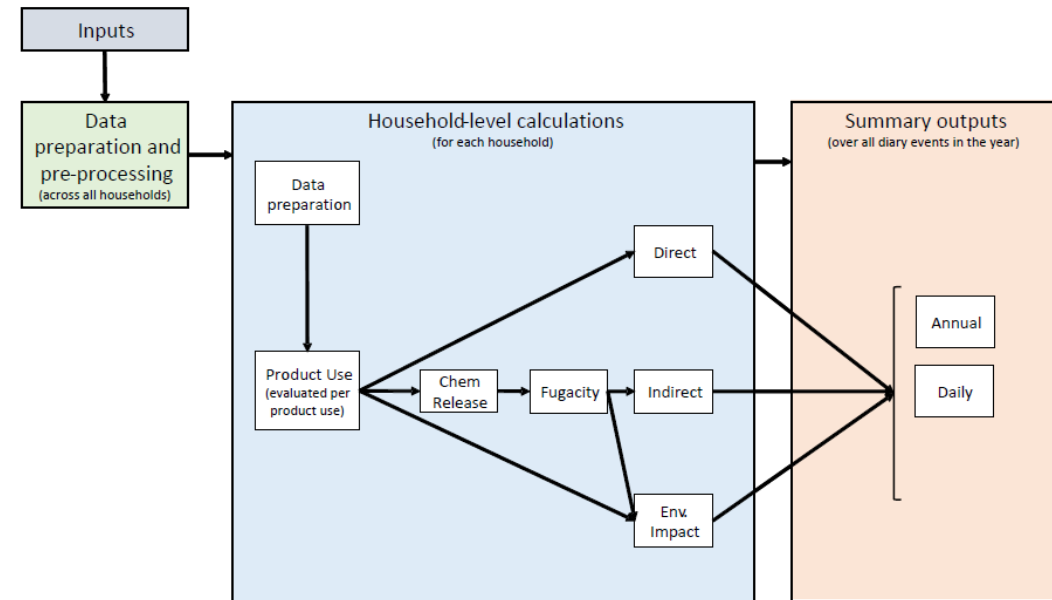
- Determines exposure resulting from direct product use
- Soap on hands is direct; soap that gets on a surface and is later contacted is indirect
- 3 Direct Routes
  - Dermal
  - Ingestion
  - Inhalation

Below is a diagram of the 3 routes and how they can interact ([S2D Tech Manual Citation?](#))



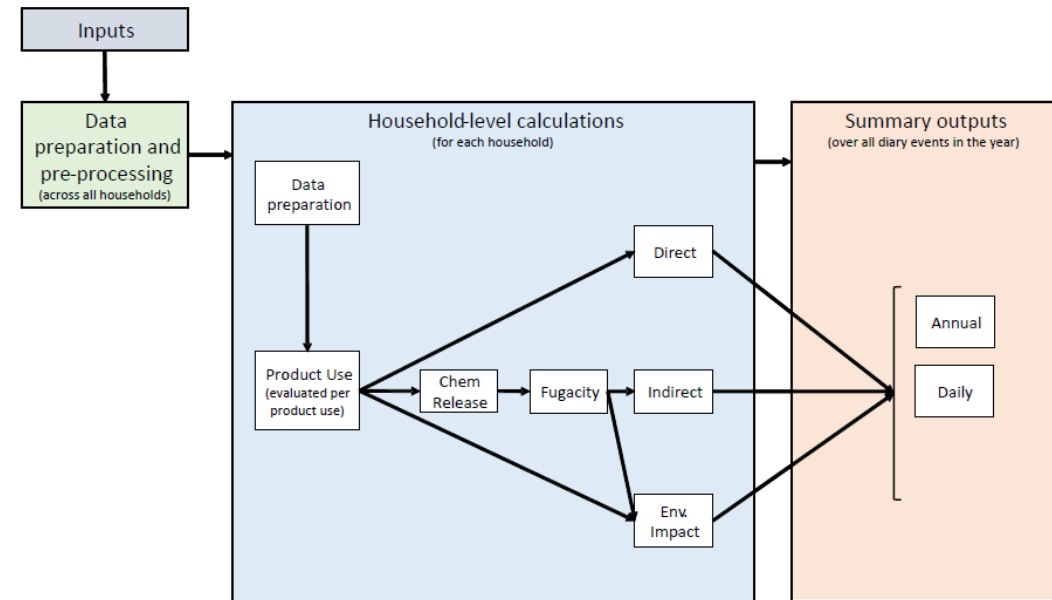
## S2D Internal Workflow (Fugacity)

- Determines how chemical concentrations on surfaces and in air develop over time
- Used to determine both indirect exposure and environmental impact
- Uses full-house averages, since floor plans are not simulated and room of use not determined

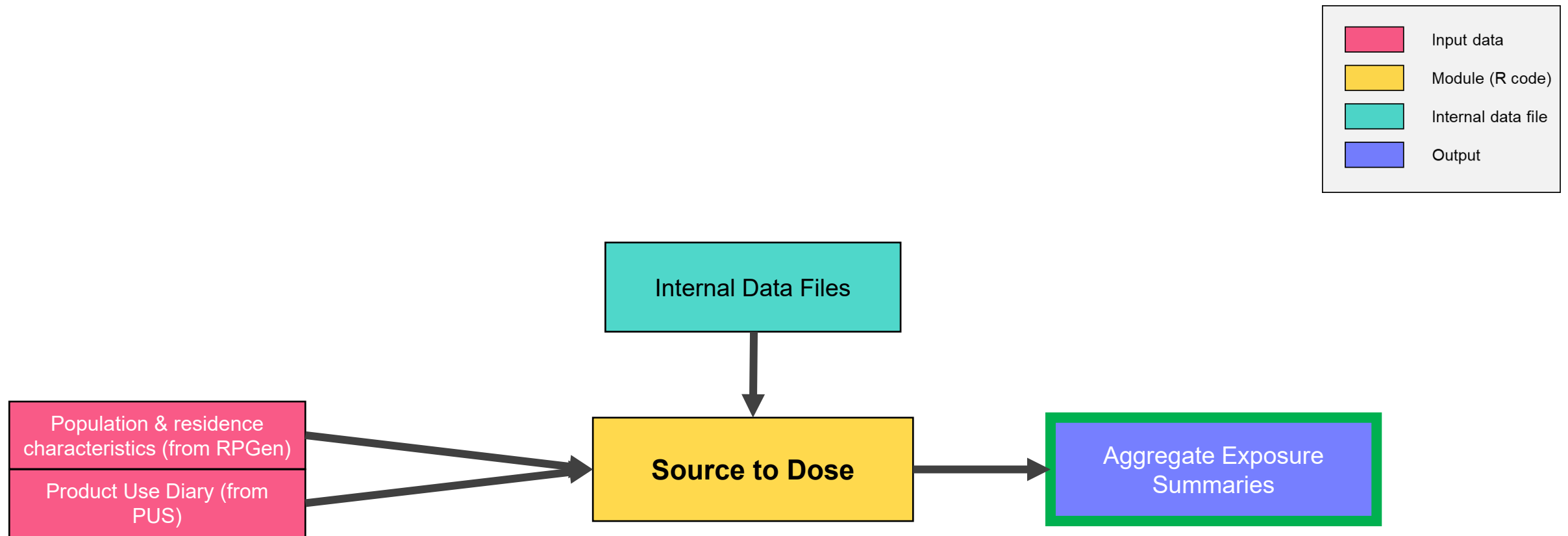


## S2D Internal Workflow (Indirect)

- Indirect exposures occur sometime after product use and involves interacting with chemicals that have been left in the air or on surfaces
- Same 3 routes as direct
- 3 exposure periods:
  - Home awake
  - Home asleep
  - Away from home
- These periods determine which kinds of indirect exposure the individual can experience at a given time



## Aggregate Exposure Summaries



## Aggregate Exposure Summaries

metric	DTXSID3020205	DTXSID7021360
dir.derm.exp (mg/day)	0.0924852732347993	0.189590581947143
dir.inhal.exp (mg/day)	0.000311522600200688	0.0391955262271068
dir.ingest.exp (mg/day)	4.68021797902781e-10	0
ind.derm.exp (mg/day)	2.57124863789732	0.400606960969601
ind.inhal.exp (mg/day)	0.000550991634147559	0.216388260770768
ind.ingest.exp (mg/day)	0.00347716551376642	1.6300736128826e-07
out.sur (mg/day)	0	0
out.air (mg/day)	0.32899164916264	1415.2980986509
drain (mg/day)	2.7108752257348e-05	0
waste (mg/day)	2.59345938689746	19.5197966825207

Average daily exposures for 1 individual, and 2 chemicals, in our case study (all PUCs)

## Case Study

Quick slide to remind of the case study

Will have been presented in earlier slides, but a refresher may be useful

More words on slide, less talking, as I assume they will be able to pause if they skipped a previous section

### **Owner Specific PUCS:**

1. Fill in

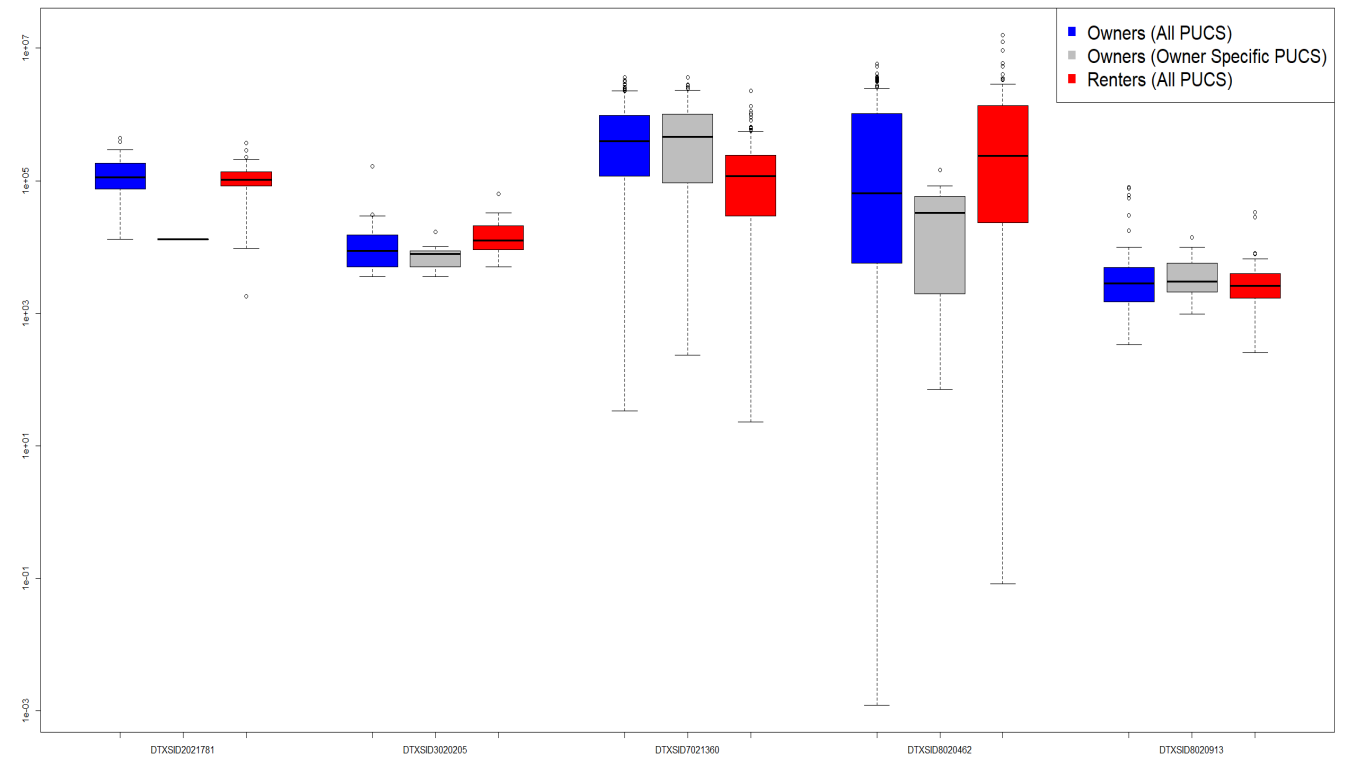
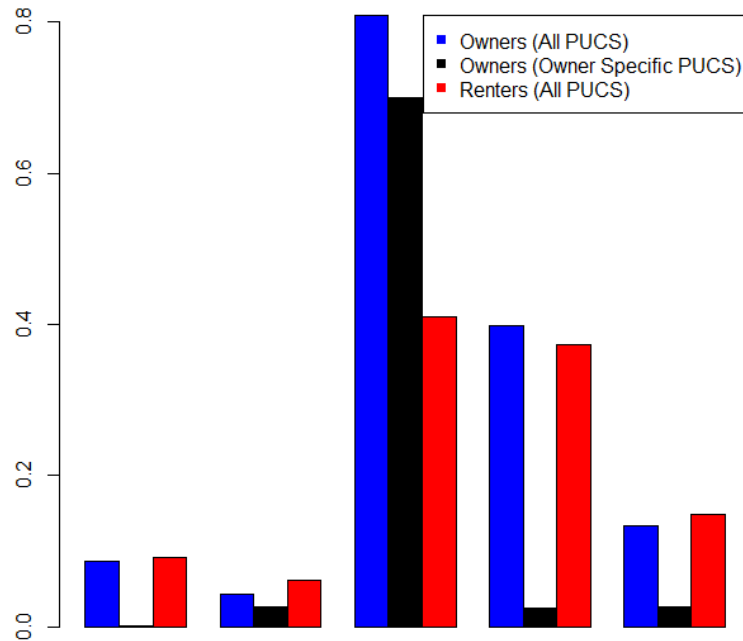
### **Chemicals:**

1. Dibutyl phthalate
2. Toluene
3. Benzyl butly phthalate
4. Diethylene glycol
5. Naphthalene

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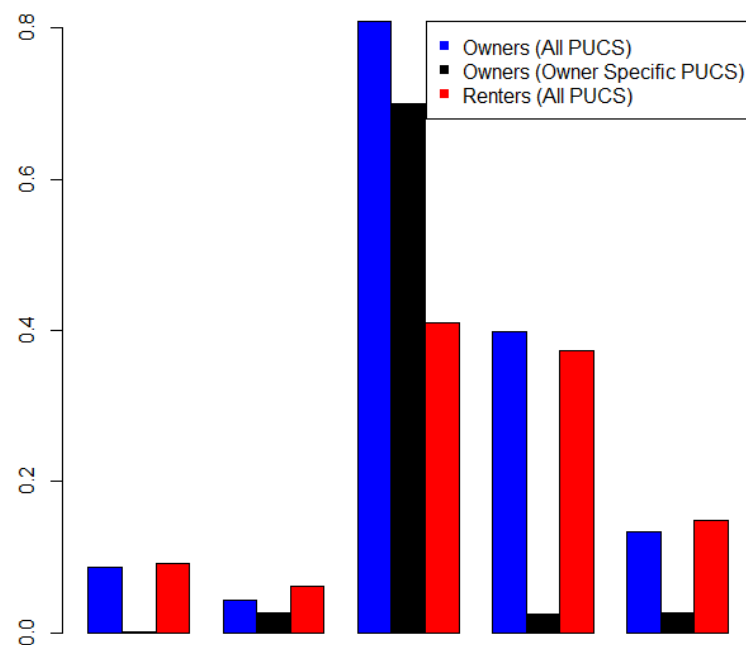
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## Case Study Results Overview



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## Case Study Prevalence

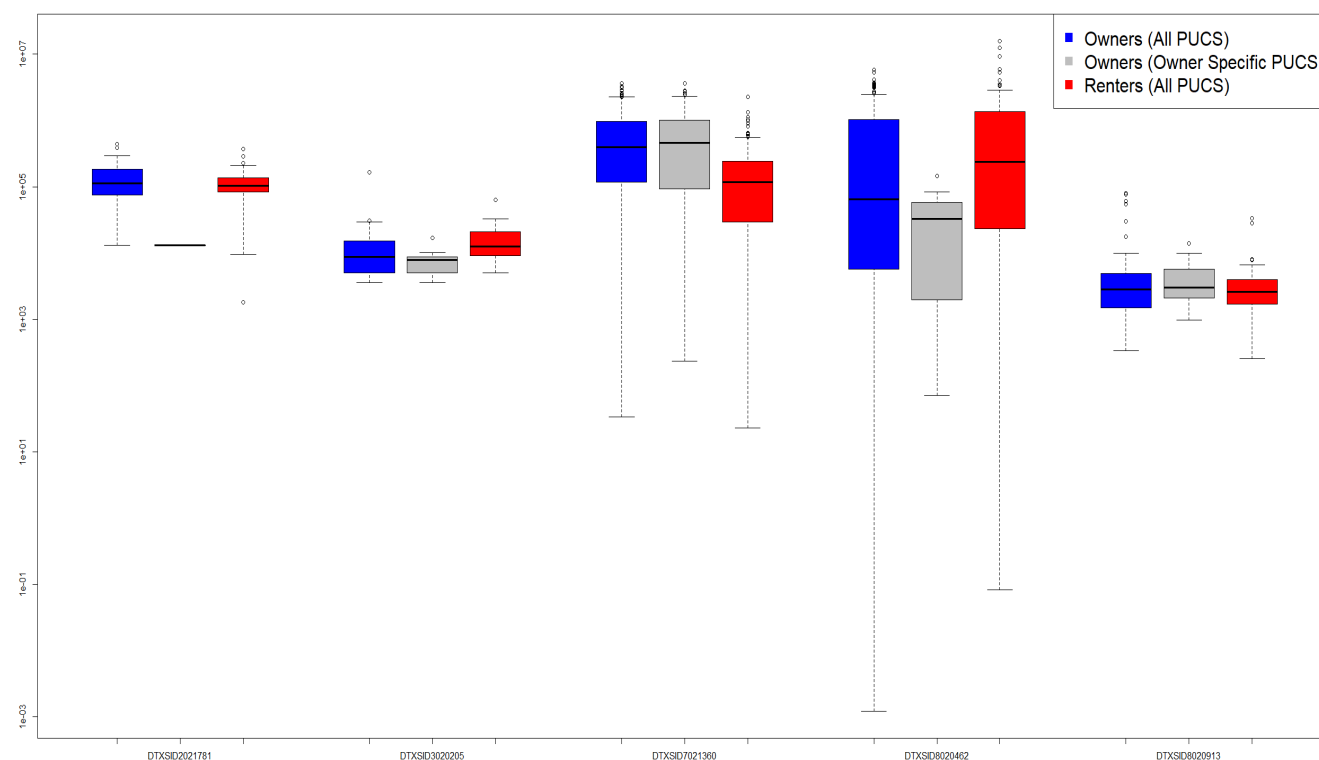


- For Toulene(3), we observe a large difference in probability between renters and owners. The large exposure probability in the owners specific pucs run suggests that many owners are only exposed through these owner specific pucs
- For Naphthalene(5), similar probabilities suggests that the owners exposed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



## Case Study Exposure

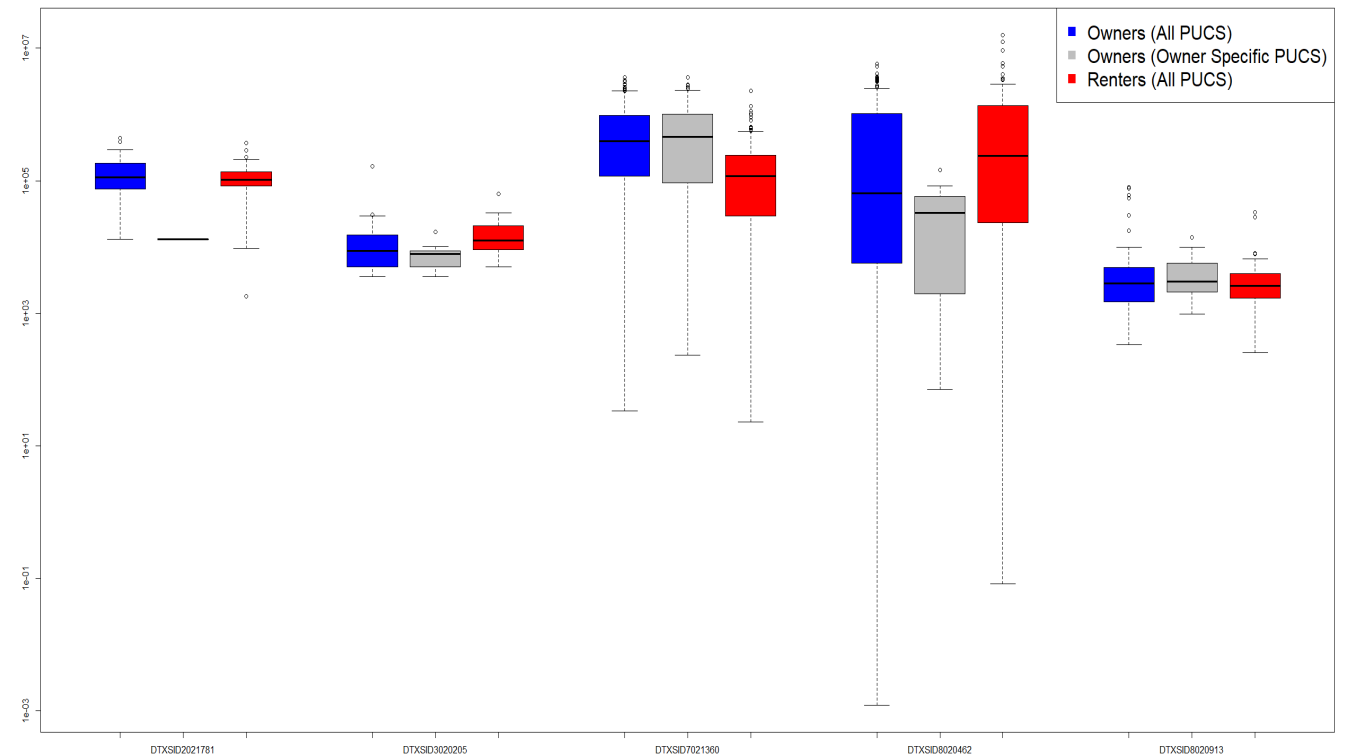
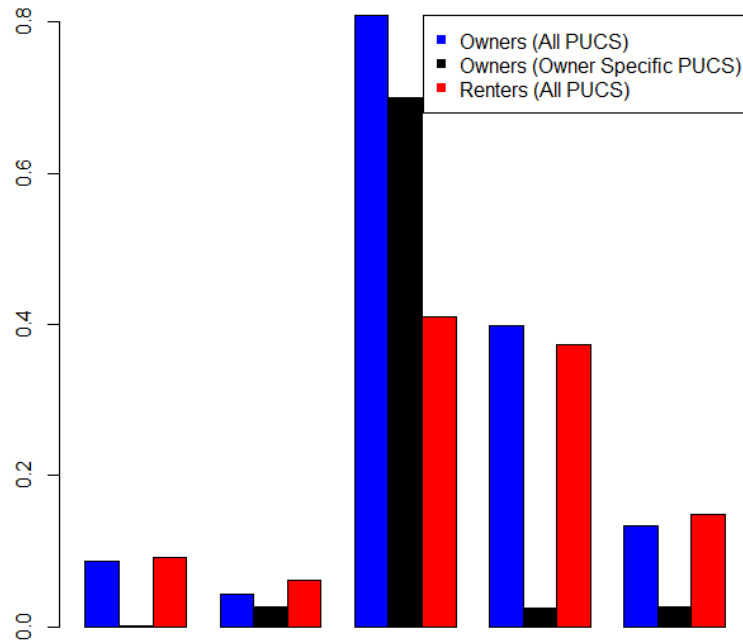
- For Toulene, large exposure through owner specific pucs drive up the exposure distribution for owners relative to renters
- For Naphthalene, the low chance of exposure means the owner specific pucs do not move the mean by much, but the owner distribution does have a larger upper bound than the renter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



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## Case Study Results Discussion



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## Case Study Conclusions

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