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

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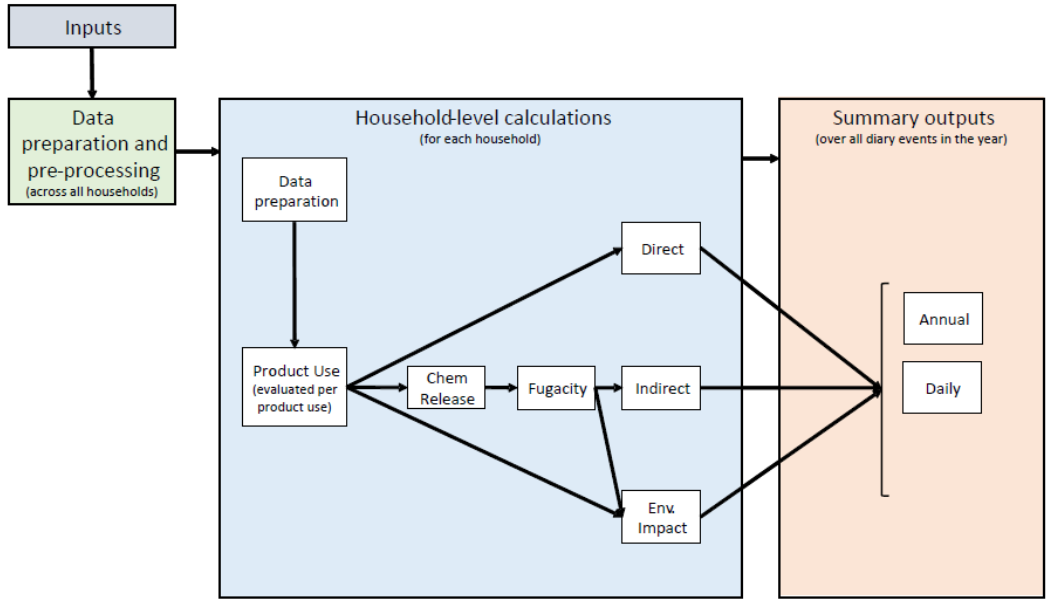
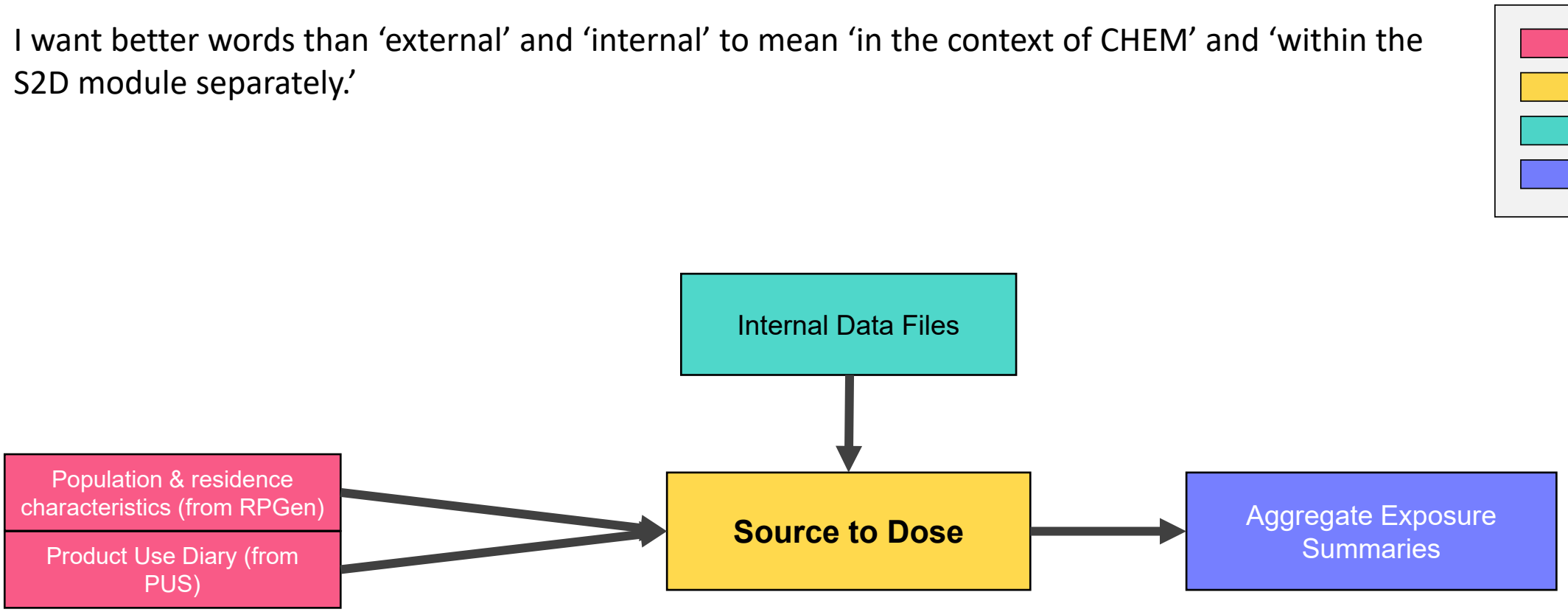
Outline

- 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)

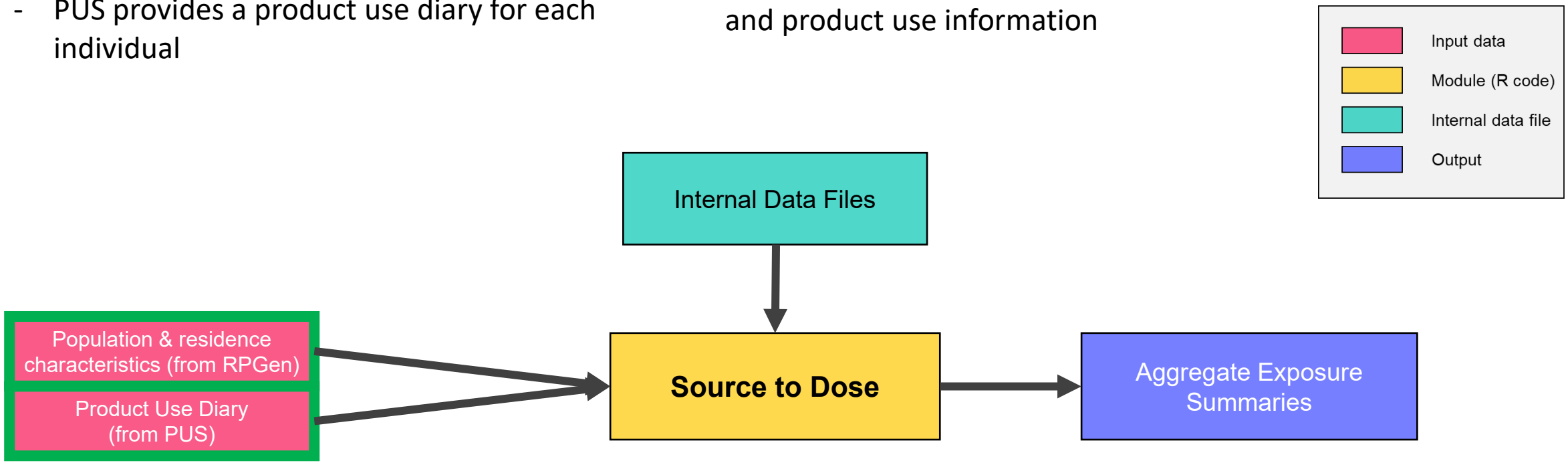
I want better words than ‘external’ and ‘internal’ to mean ‘in the context of CHEM’ and ‘within the S2D module separately.’



Required Inputs

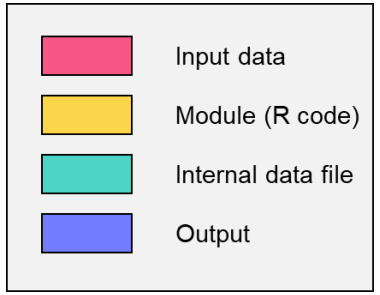
- RPGen provides a file with required physical and residential parameters for each simulated individual that will modeled
- PUS provides a product use diary for each individual

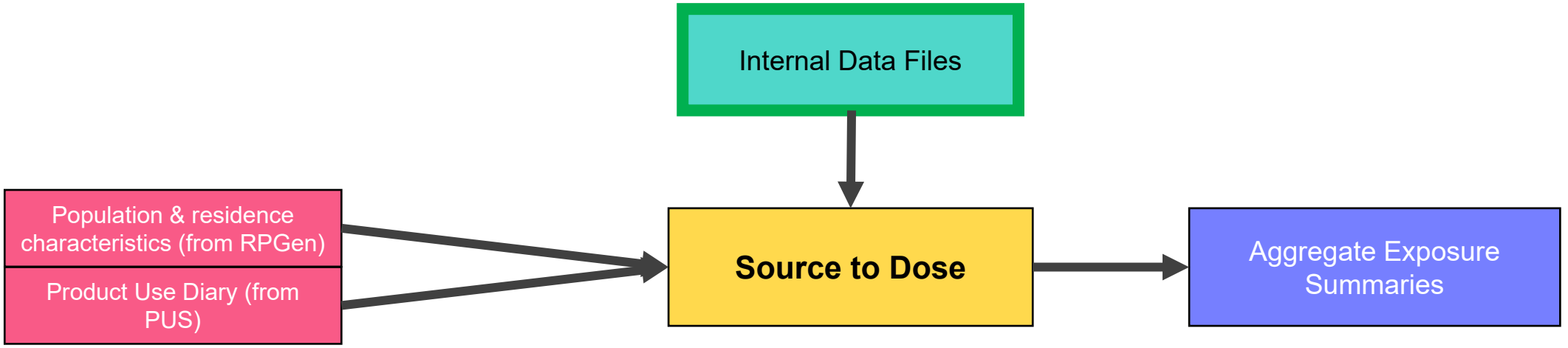
- While S2D was designed to work with RPGen and PUS, it can function alone if provided with analogous residential and product use information



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 it's properties and products it is found in to the proper file





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

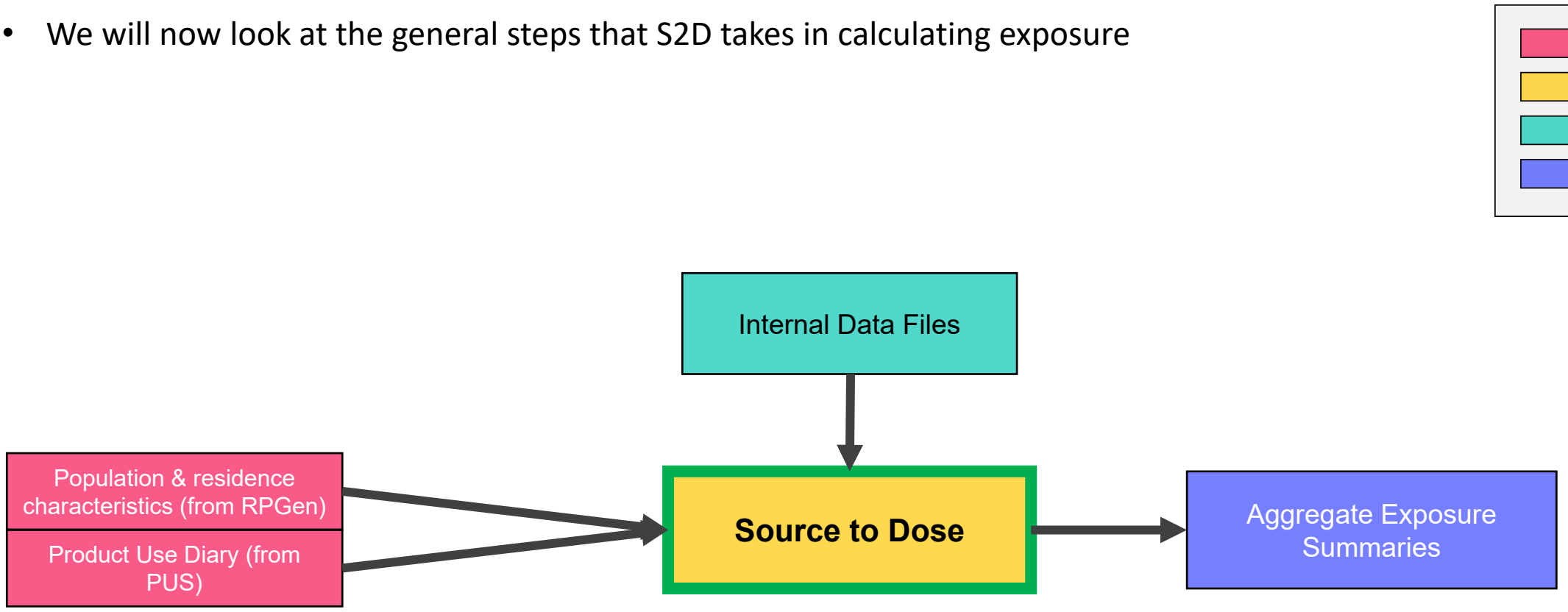
PUC Product Codes:
Three letter codes for each PUC category used to group PUCs

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)

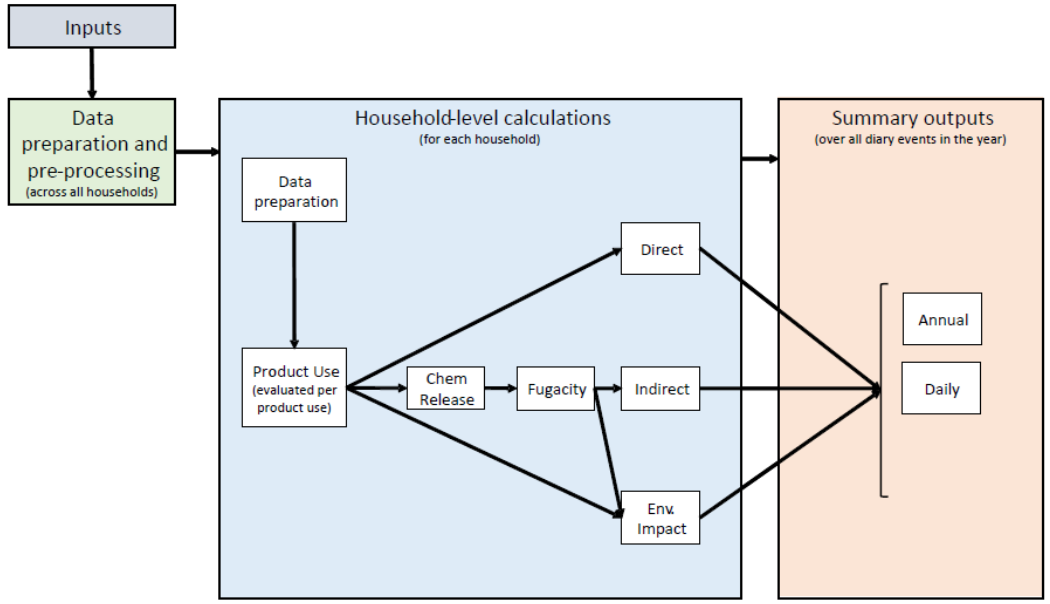
- We will now look at the general steps that S2D takes in calculating exposure



S2D Internal Workflow (Overview)

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

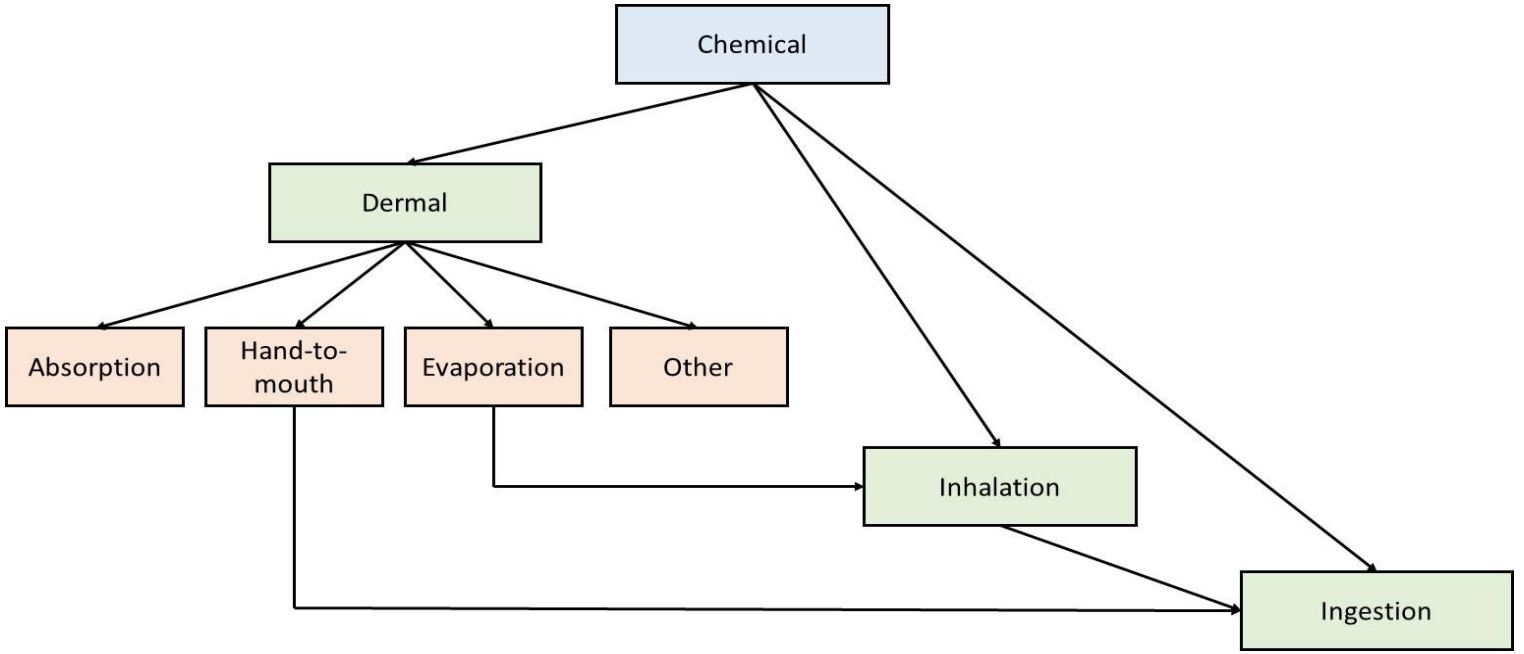
Intend to update the diagram and highlight relevant section as I go



S2D Internal Workflow (Direct)

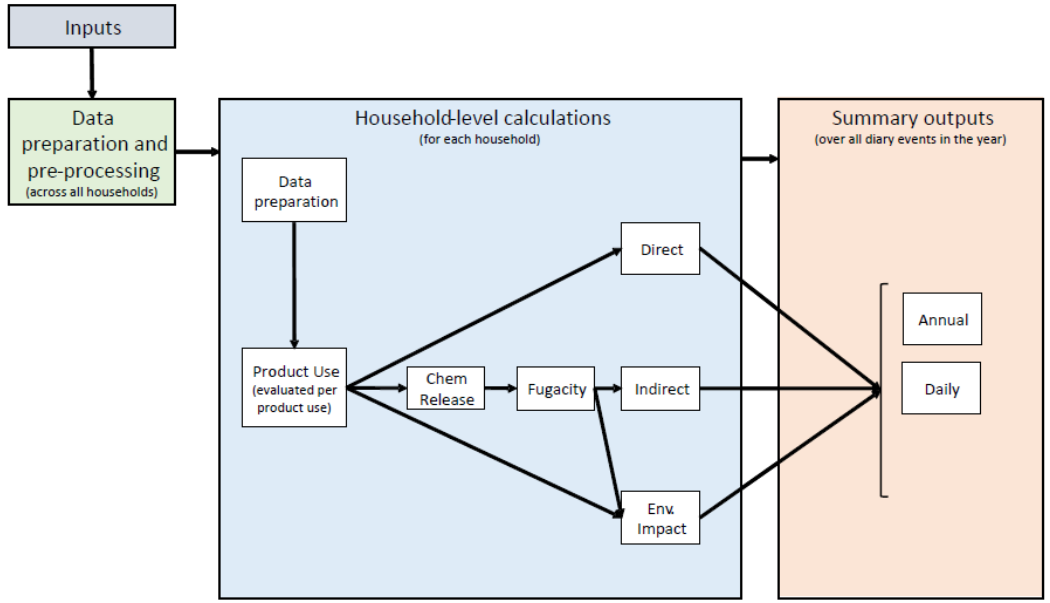
- Determines exposure resulting from direct product use
- Soap on hands is direct; soap that gets on a surface and is later contacted is indirect
- 3 Direct Routes
  - Dermal
  - Ingestion
  - Inhalation

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



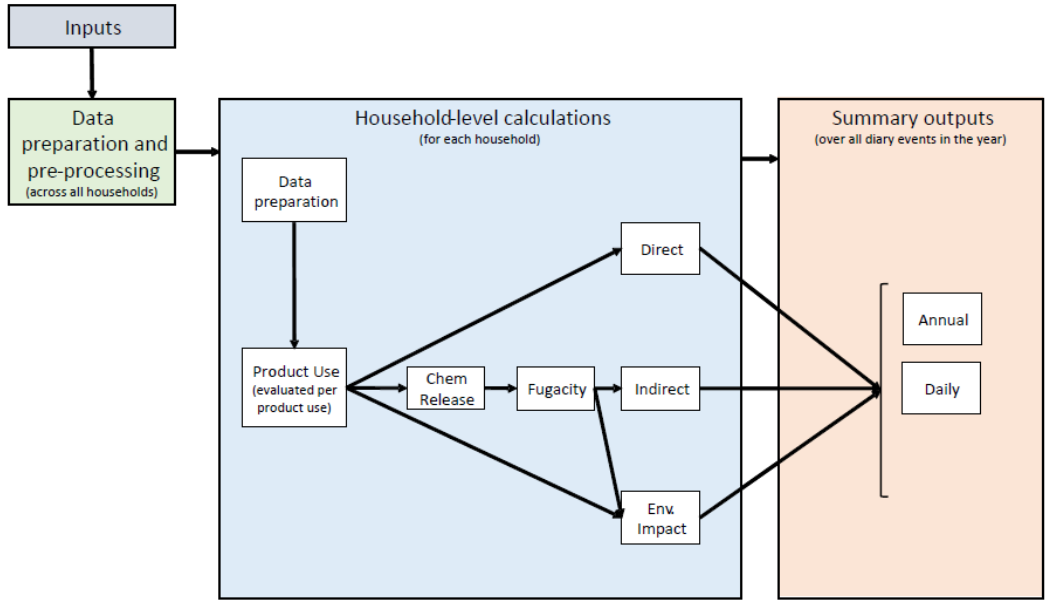
S2D Internal Workflow (Fugacity)

- 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

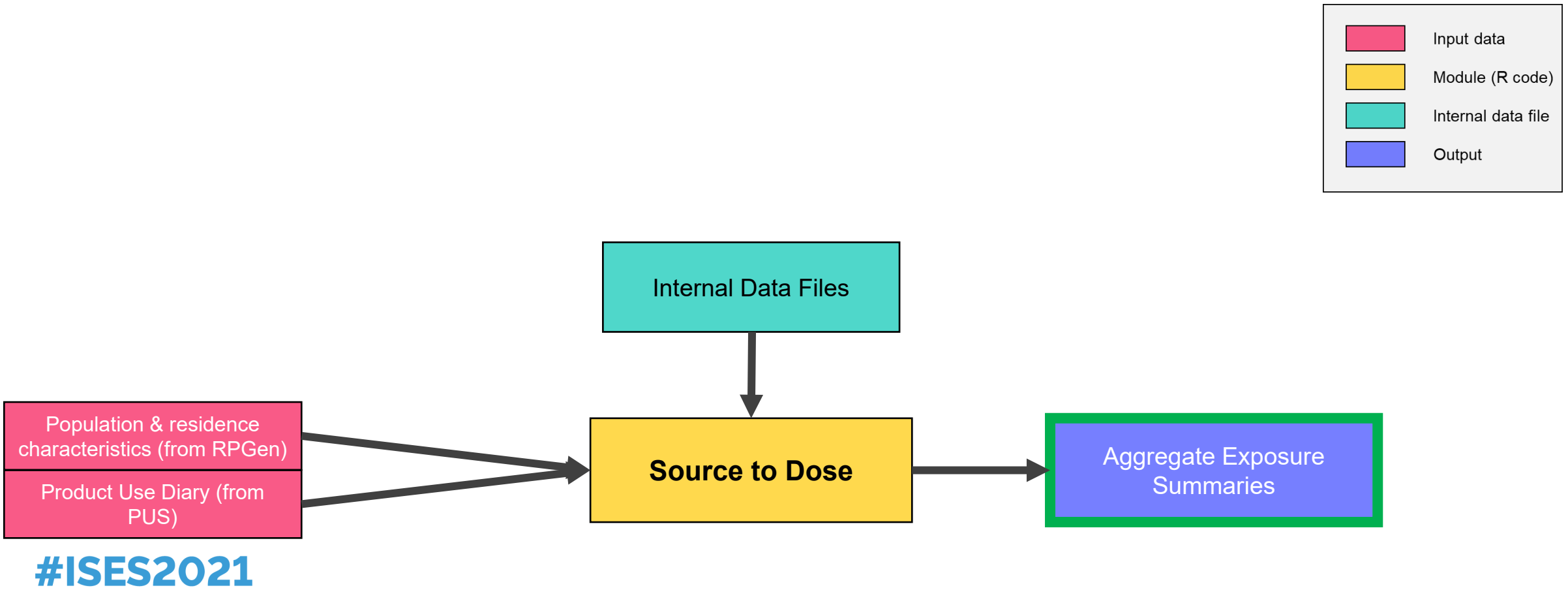


S2D Internal Workflow (Indirect)

- 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

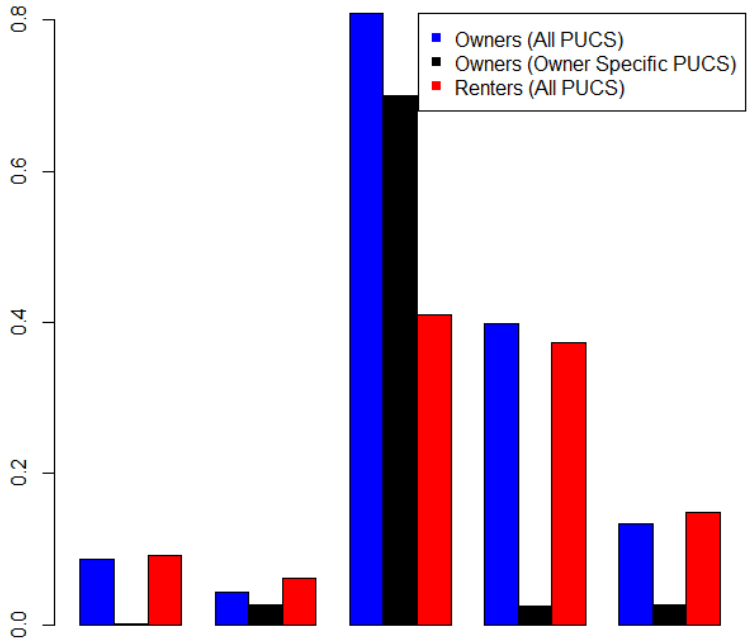
Owner Specific PUCS:

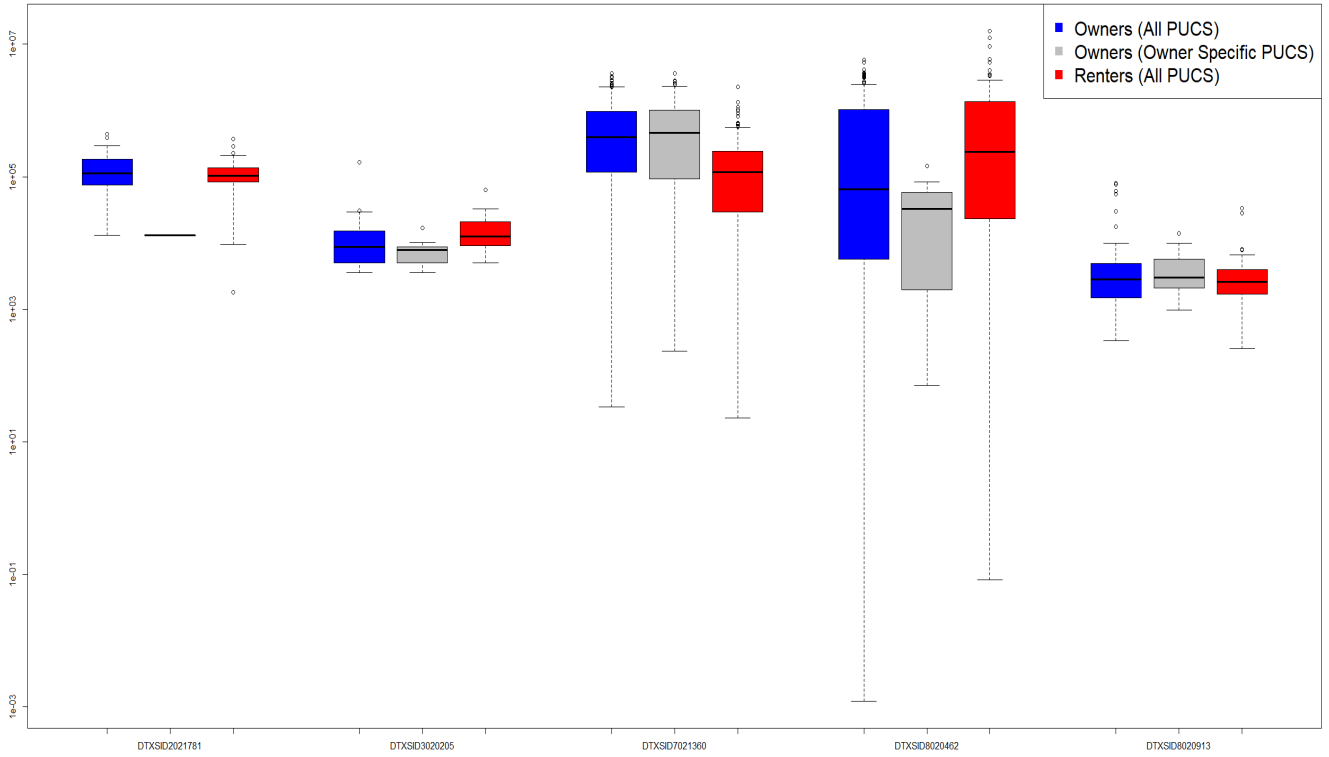
1. Fill in

Chemicals:

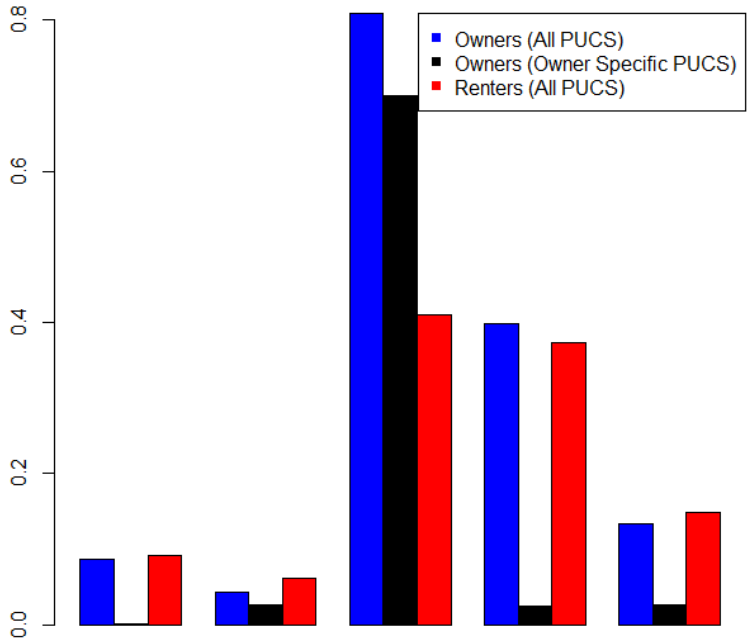
1. Dibutyl phthalate
2. Toluene
3. Benzyl butly phthalate
4. Diethylene glycol
5. Naphthalene

Case Study Results Overview





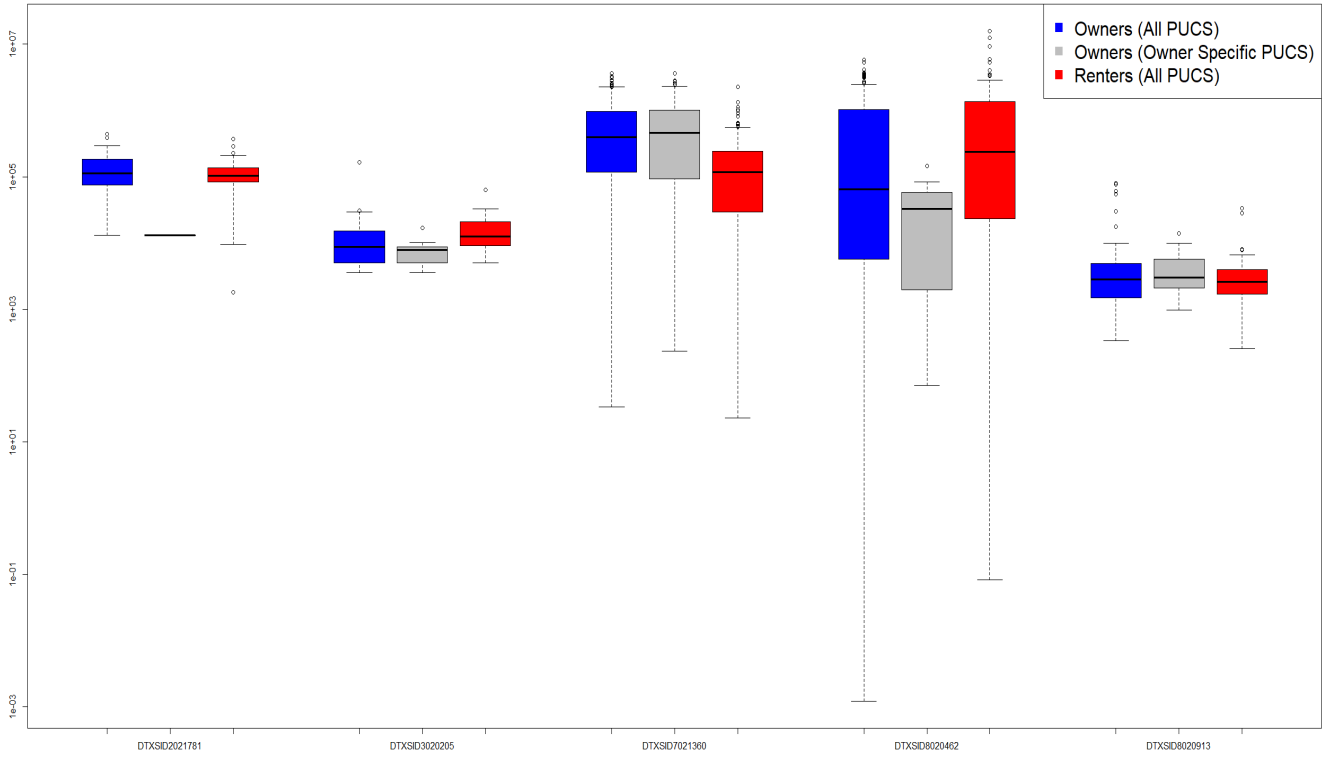
Case Study Prevalence



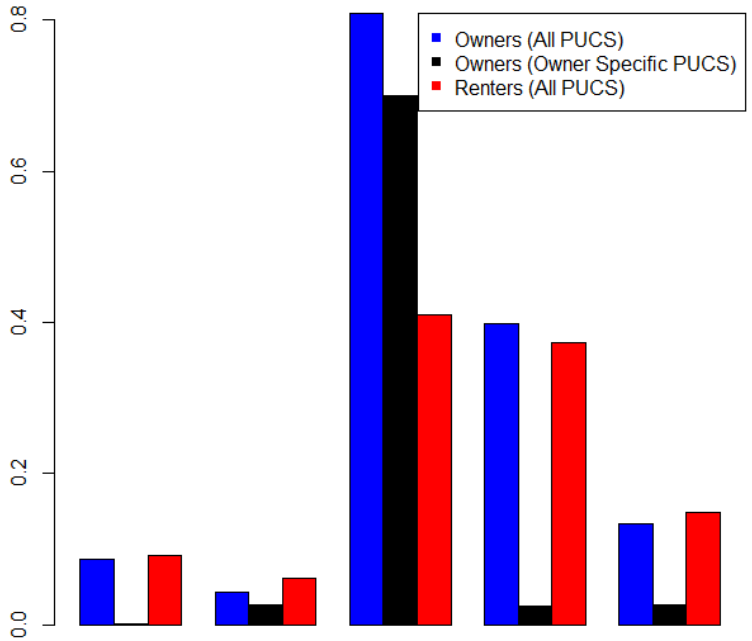
- For Toulene(3), we observe a large difference in probability between renters and owners. The large exposure probability in the owners specific pucs run suggests that many owners are only exposed through these owner specific pucs
- For Naphthalene(5), similar probabilities suggests that the owners exposed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

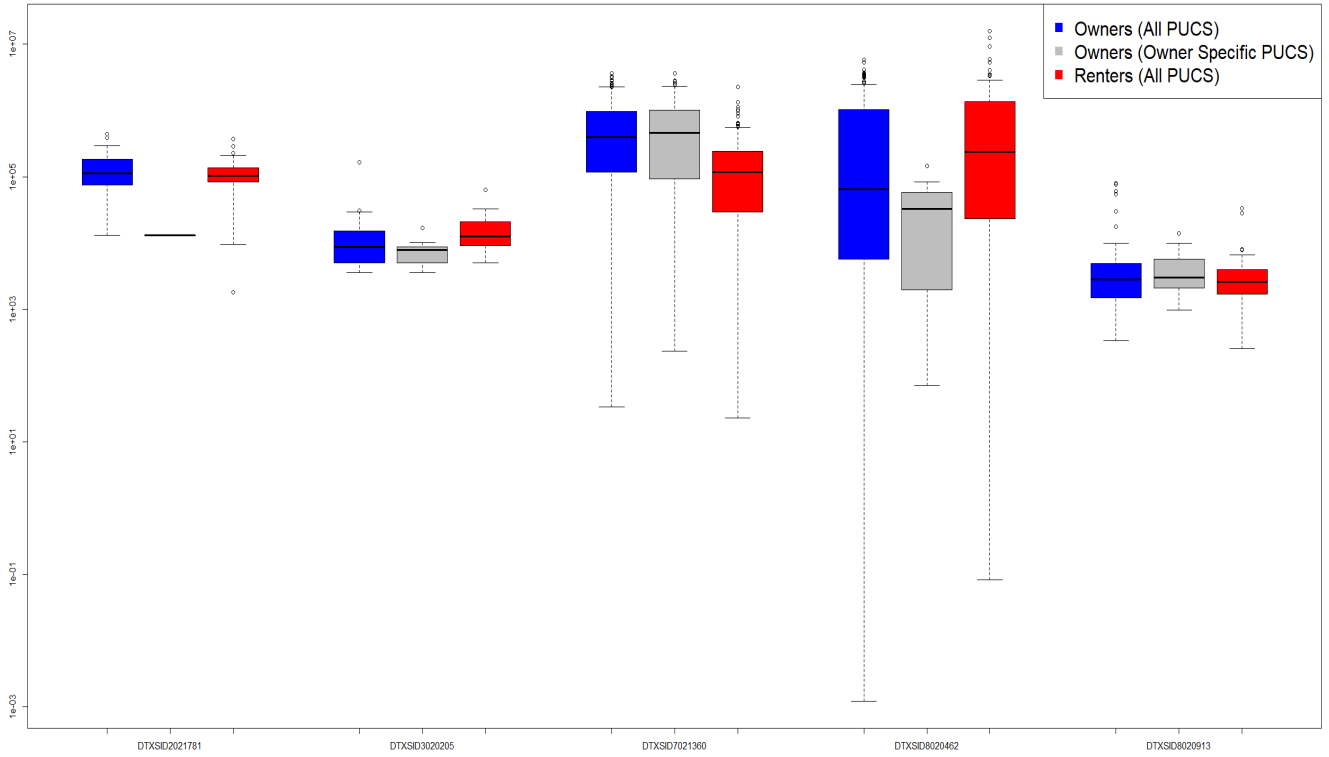
Case Study Exposure

- 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



Case Study Results Discussion





Case Study Conclusions