Developing scientific workflows for exposure assessments: a case study with 1,4-dioxane exposure

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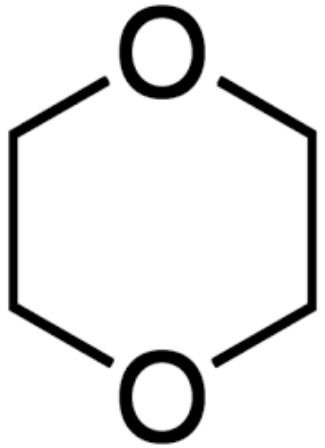
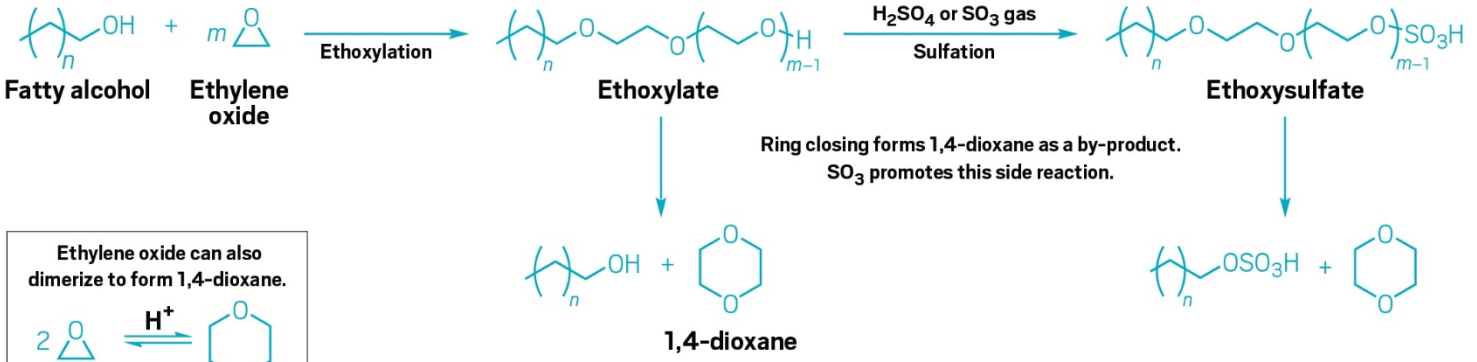
1,4-Dioxane: workflow case study

- Used in industrial applications
  - Solvent
  - Anti-fouling agent
  - Industrial reagent
- Created as un-intentional byproduct in some consumer products due to ethoxylation/sulfation of surfactants
  - Soaps/shampoos
  - Laundry detergent
  - Dish detergent
- Health concerns
  - Probable human carcinogen
  - Acute toxicity
  - Persistent, mobile and Toxic (ECHA)

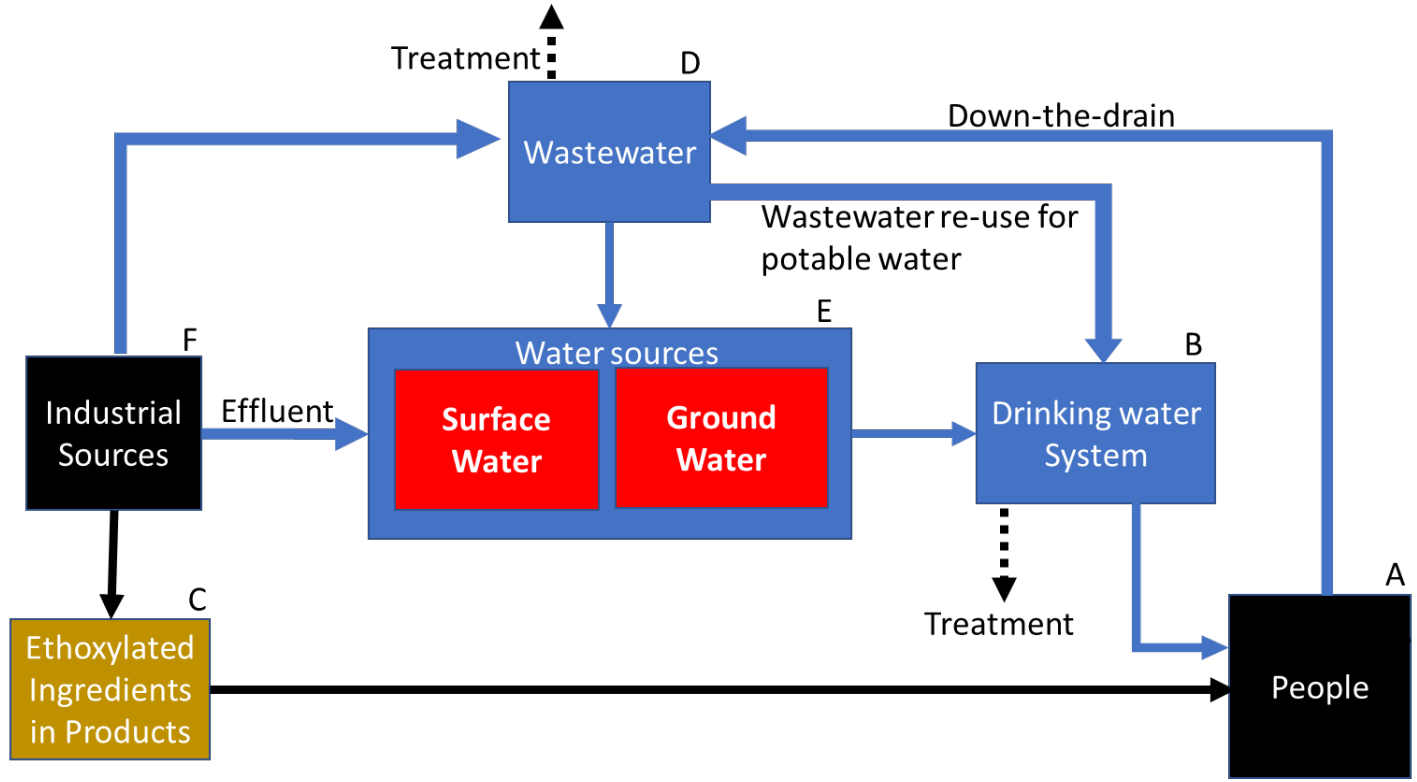




m = 1–12
n = 12–18

Exposure Pathways

- Complex exposure scenario
  - Primary Sources
    - Contaminated drinking water
      - Legacy
      - Industrial release
      - Down-the-drain
    - Direct consumer use of contaminated products
  - Routes: Dermal, inhalation, ingestion

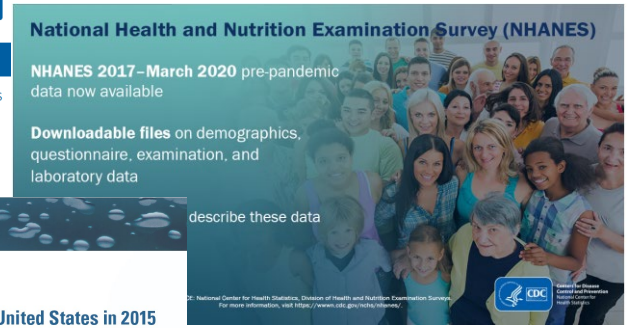


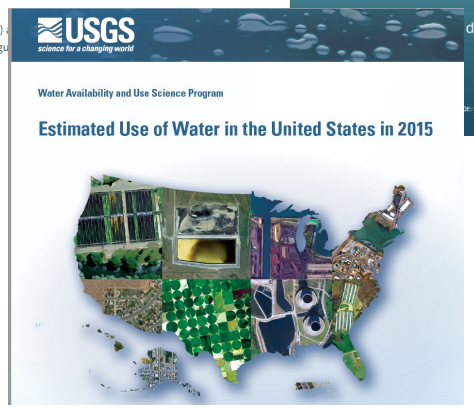
Study Objectives

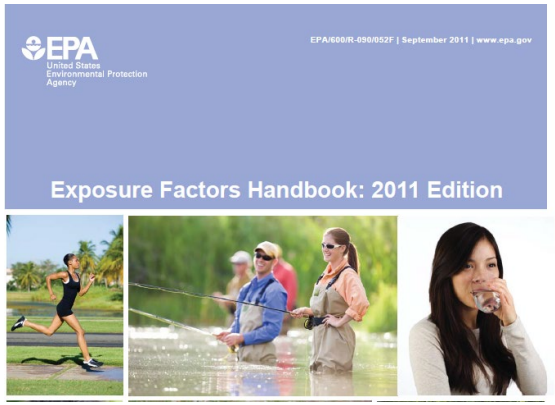
1. **Conduct exposure and down-the-drain (DTD) assessment: water ingestion and product use**
    - SHEDS-HT: Probabilistic, population-level exposure modeling platform
    - Factorial comparison of Human Exposure and DTD
        - Spatial (US or CA)
        - Water Source (Groundwater, Surface water, Mixed sources)
        - $Product_{prevalence}$(High, Low)
    - Subpopulations
        - Total population
        - Products Only
        - Both Products and contaminated water
    - Model Evaluation
        - Convert DTD predictions to predicted wastewater effluent concentrations
        - Compare against empirical wastewater concentrations
2. **Simulate regulatory action**
    1. Simulate 1ppm threshold in consumer products
    2. Compare exposure/DTD between scenarios

Model Parameterization Sources

- Drinking water
  - 1,4-Dioxane concentrations:
    - Monitored as part of UCMR3(2013-2015)
  - Consumption: NHANES
  - General Use: USGS
- Consumer products
  - 1,4-Dioxane concentrations
    - Consumer advocacy groups
    - Primary literature
  - Use and exposure factors
    - Exposure factors handbook
    - Literature-based usage parameters







ISES 2021 VIRTUAL MEETING

Multisector Engagement for Addressing Emerging Environmental Exposures

Assemble Data Inputs

Model Inputs: 1,4 Dioxane Exposure Sources, Concentrations, and Factors

Drinking Water

Data Sources:

- 1,4 Dioxane concentration and prevalence Ingestion
- Gross use quantity (US, CA)

Consumer Products

Products considered:

- Shampoo
- Body Wash
- Hand Soap
- Dish Detergent
- Laundry Detergent

For each product:

- 1,4 Dioxane concentration
- Prevalence of 1,4 dioxane in product type
- Product use parameters

Model simulation and output processing

SHEDS-HT Exposure Framework

Exposure Modules

Exposure Estimates

Food/Drink Ingestion

Direct Product Exposure

- Inhalation
- Dermal
- Hand-to-mouth ingestion
- Down-the drain

Human Exposure (absorbed dose in mg/kg day)

Down the drain (g/day)

Analysis

Data Analyses

Factorial Exposure Analyses

Factorial Comparisons

- Dioxane prevalence in products
- Water Source
- Geographic Scale

Exposure Source Groups

- Total population
- Only product exposure
- Only product + contaminated water exposure

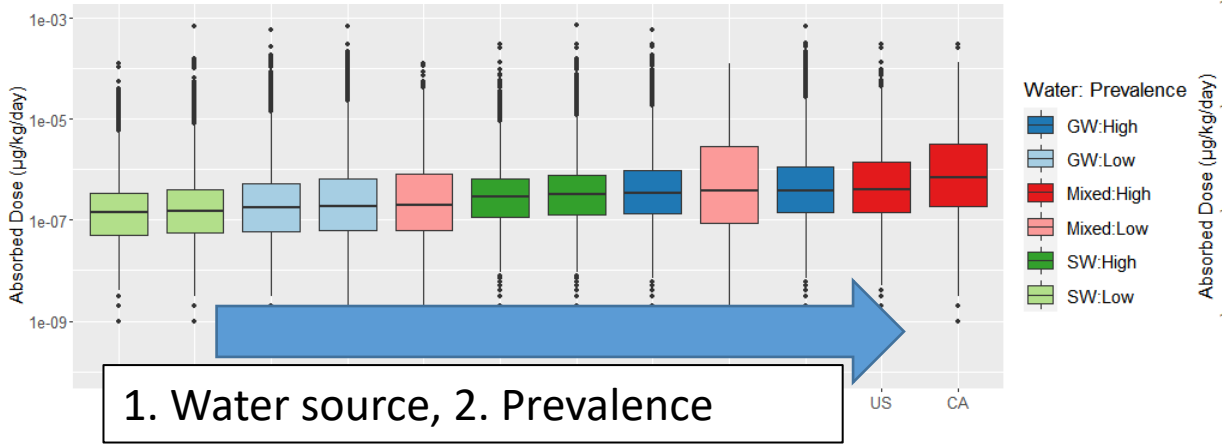
Alternatives Analysis

Model Evaluation

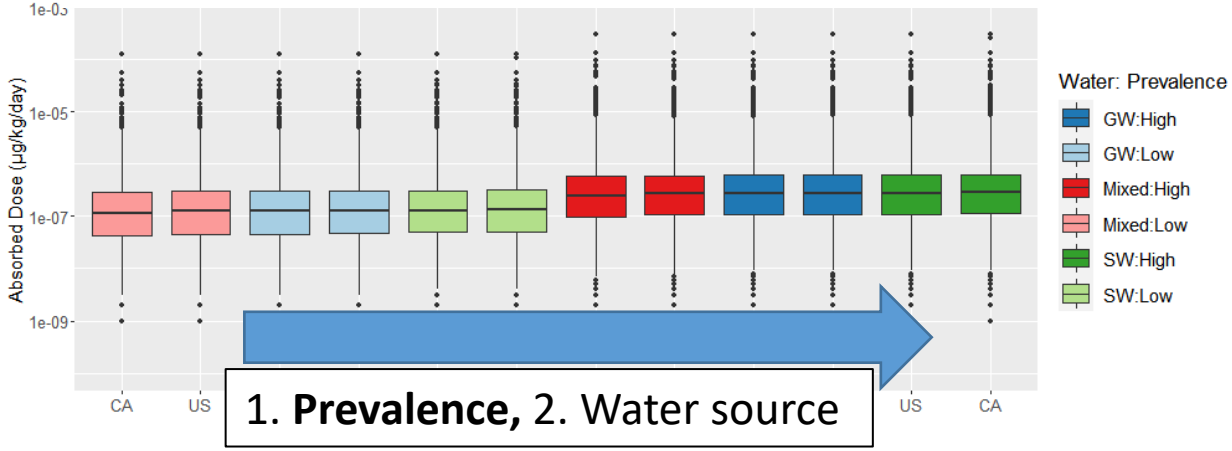
- ISTREEM WWTP Loading Model
- WWTP Effluent concentrations
  - CA Scale: CalEPA 2013-2015
  - U.S. Scale WWTP Effluent Concentrations: Simonich et al. (2013)

Results: Population Exposures

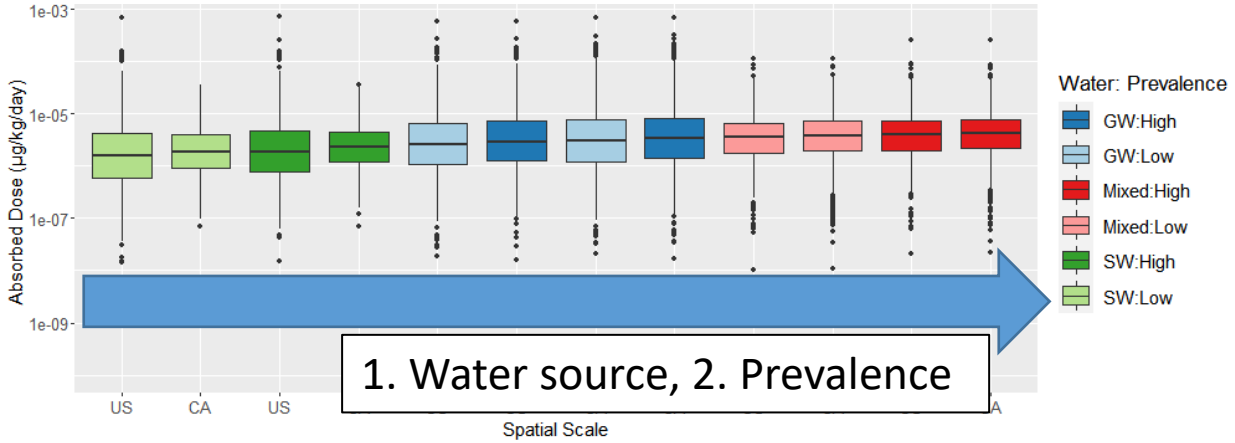
Population: Total



Population: Products-Only

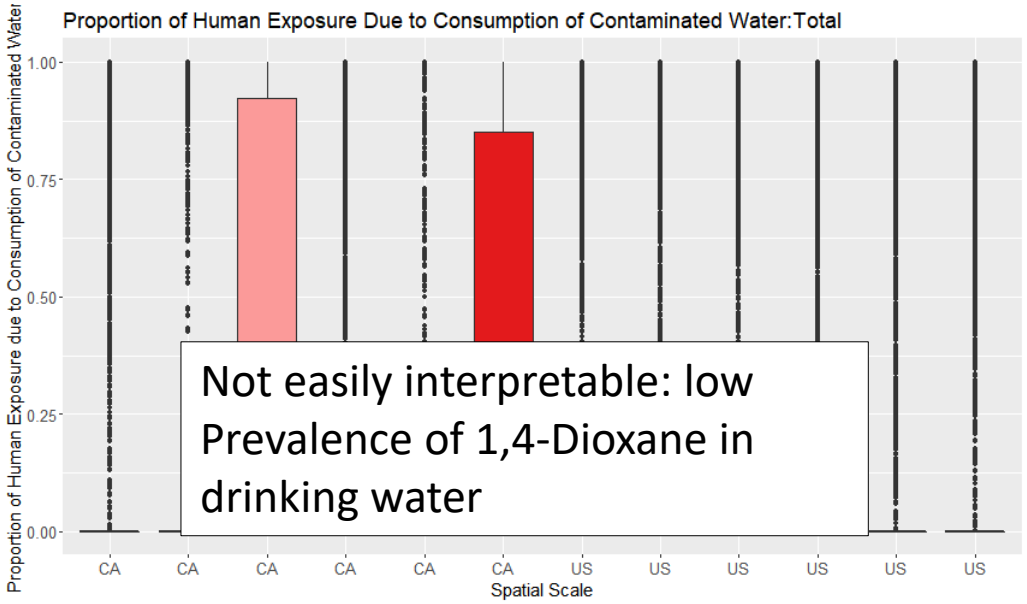


Population: Both Contaminated Water and Products



Results: Proportion of exposure due to contaminated drinking water

Population: Total



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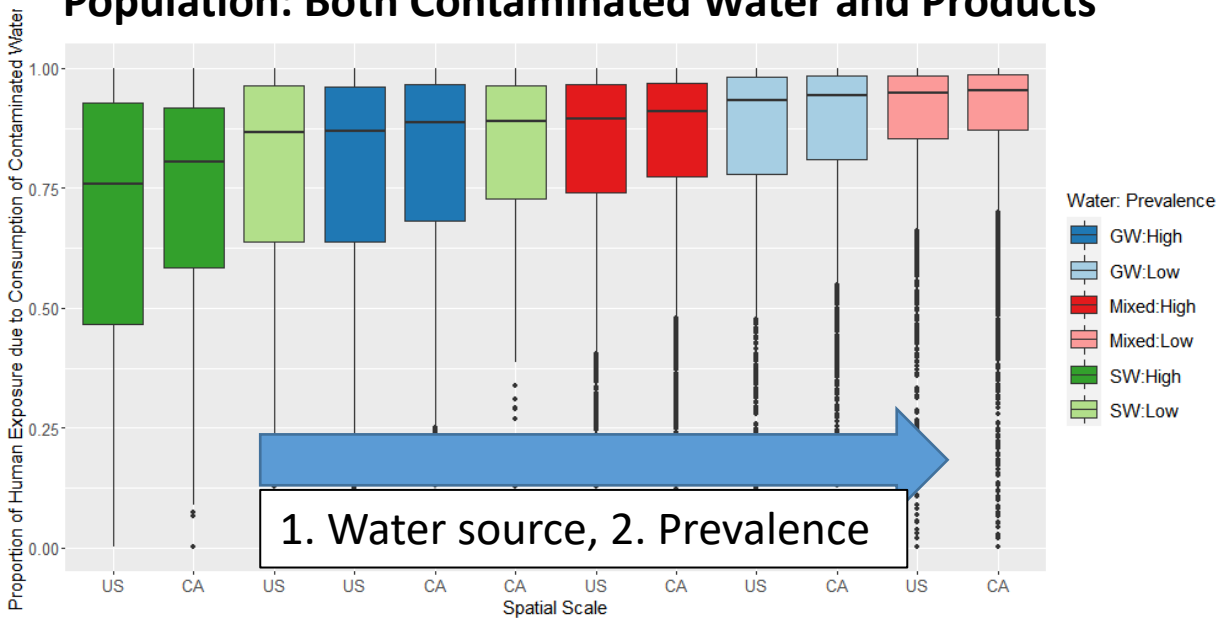
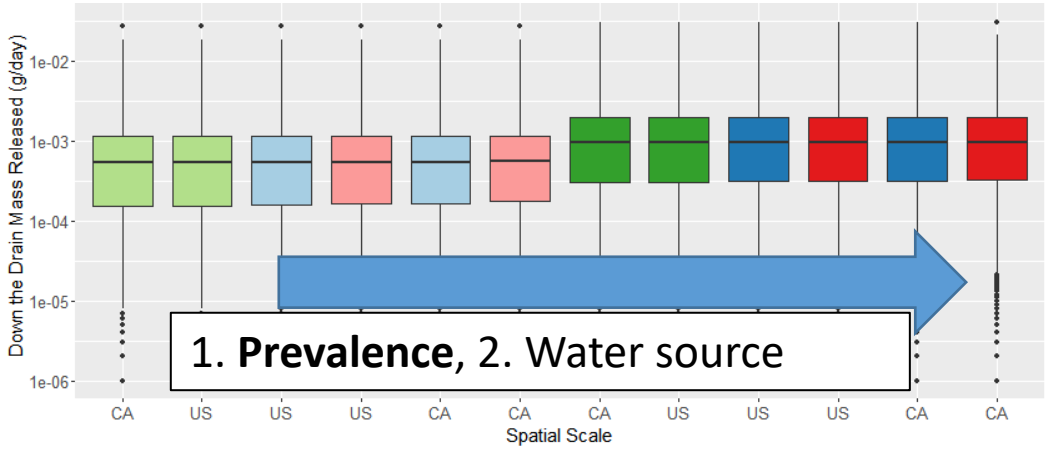
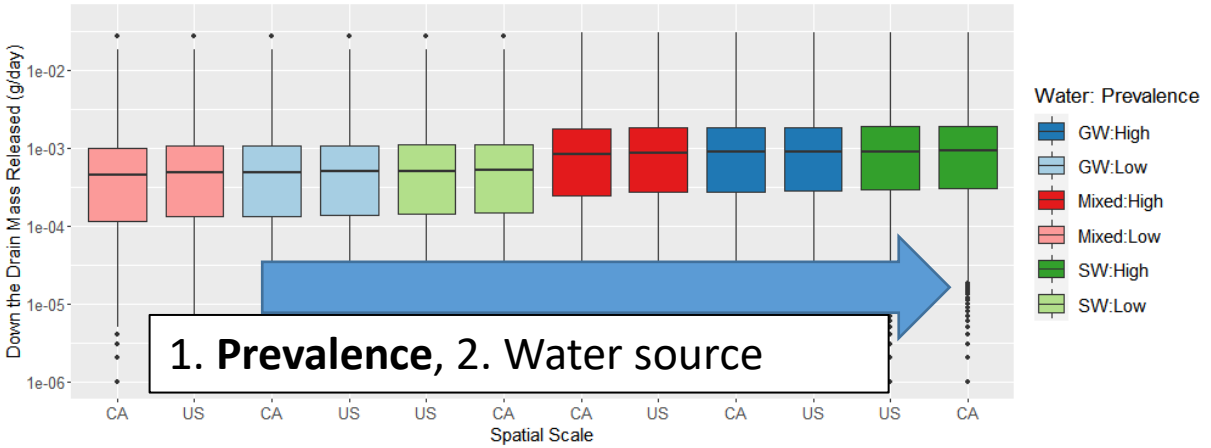


Results: Mass released down-the-drain by population

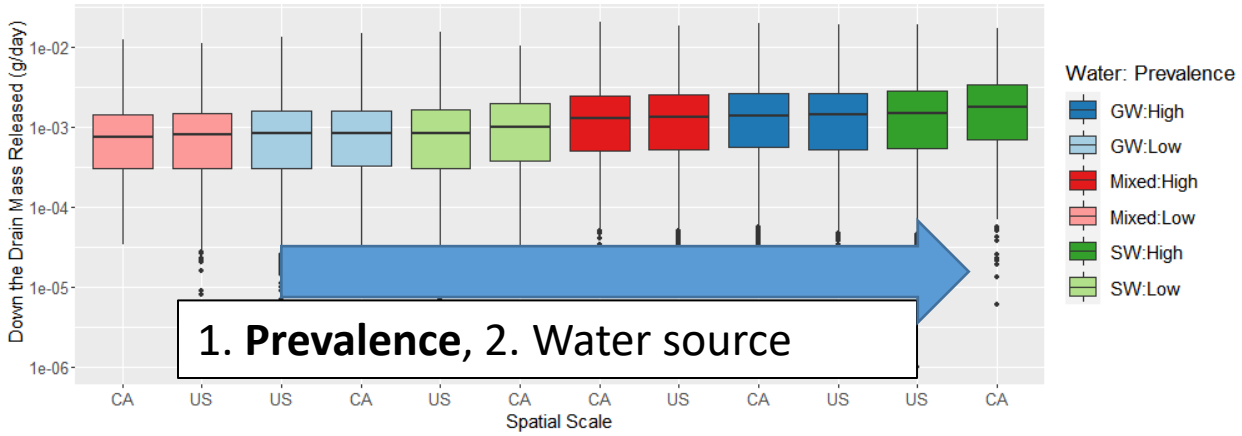
Population: Total



Population: Products-Only

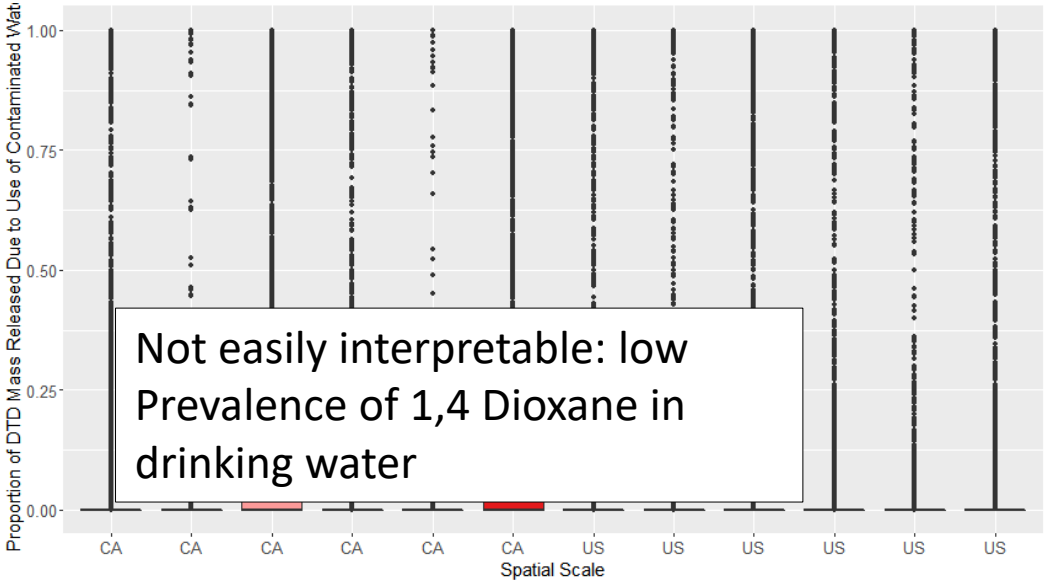


Population: Both Contaminated Water & Products

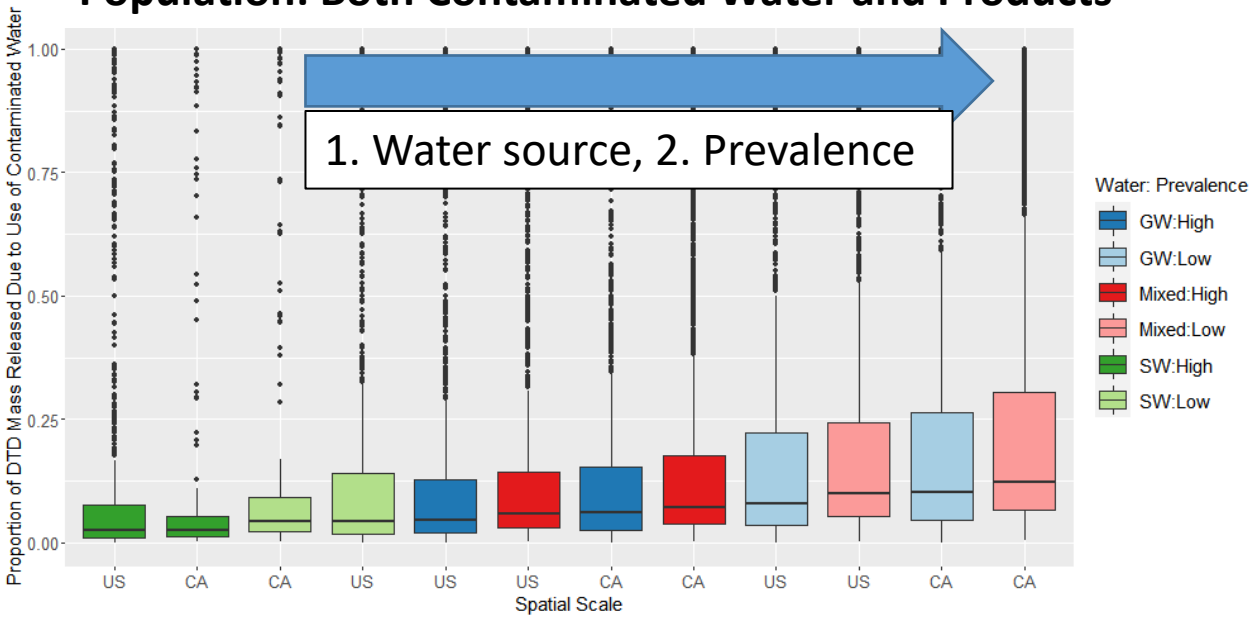


Results: DTD Source Attribution

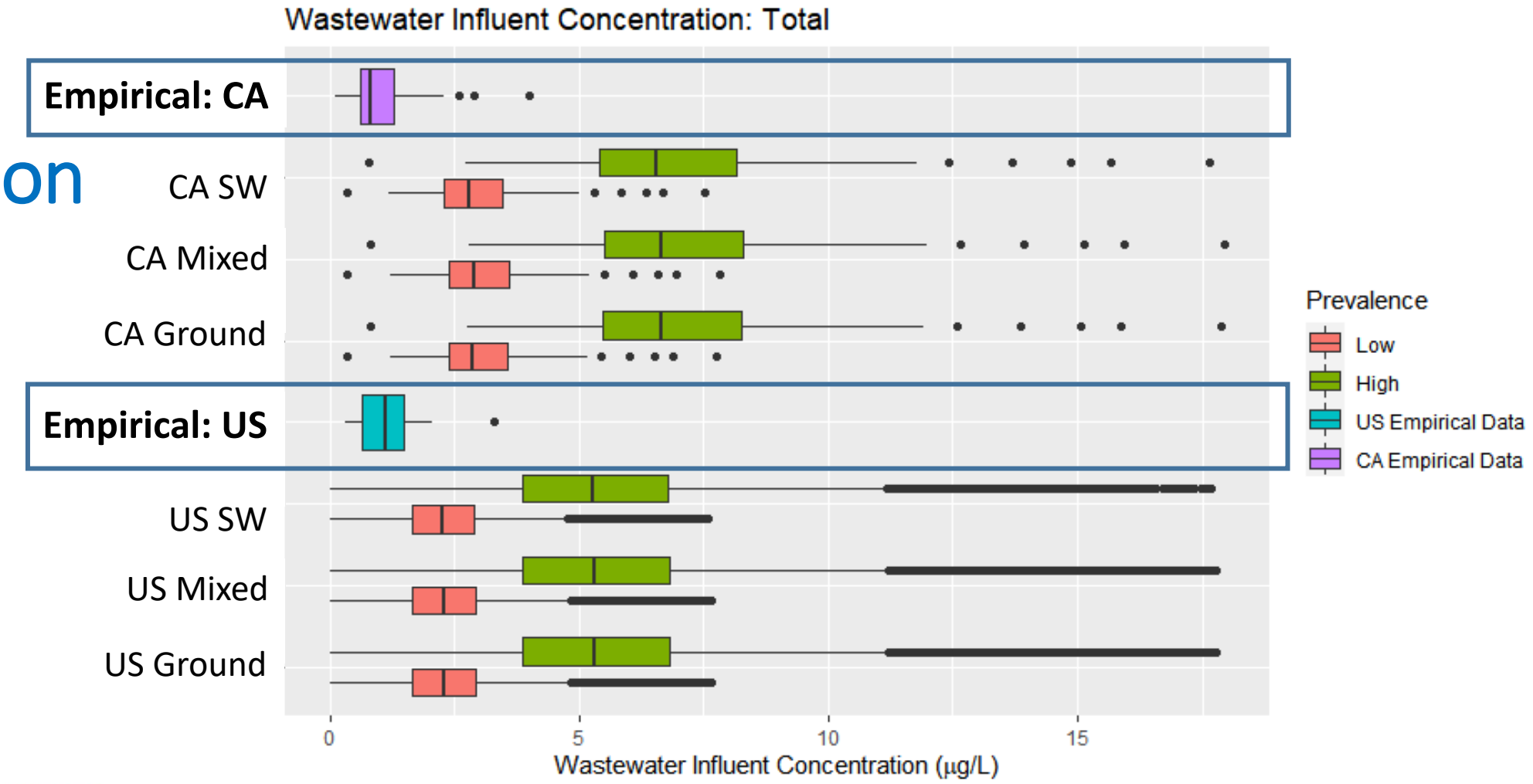
Population: Total



Population: Both Contaminated Water and Products



Model Evaluation



Simulated 1 ppm threshold

Human Exposure (mg/kg/day)

Water	Subpopulation	No Action: Mean	No Action: SD	1 ug/L Threshold: Mean	1 ug/L Threshold: SD	Proportion Reduction of mean exposure	t-statistic	p-value
Ground	Total	2.420E-06	1.229E-05	1.758E-06	1.122E-05	0.274	-45.277	
Mixed		2.825E-06	6.638E-06	2.162E-06	4.451E-06	0.235	-31.849	
Surface		8.528E-07	4.987E-06	1.901E-07	1.029E-06	0.777	-70.883	
Ground	Products-Only	7.380E-07	4.452E-06	1.166E-07	4.455E-07	0.842	-66.709	<0.001
Mixed		7.205E-07	4.952E-06	1.113E-07	4.545E-07	0.846	-57.448	
Surface		7.872E-07	4.961E-06	1.241E-07	5.812E-07	0.842	-73.919	
Ground	Both Contaminated Water & Products	9.201E-06	2.495E-05	8.372E-06	2.404E-05	0.090	-5.525	
Mixed		6.132E-06	7.541E-06	5.385E-06	5.798E-06	0.122	-8.101	
Surface		3.910E-06	5.239E-06	3.267E-06	5.016E-06	0.164	-2.909	0.002

Down the Drain mass released (g/day)

Water	Subpopulation	No Action: Mean	No Action: SD	1 ug/L Threshold: Mean	1 ug/L Threshold: SD	Proportion Reduction of mean DTD mass released	t-statistic	p-value
Ground	Total	1.483E-03	1.884E-03	2.410E-04	2.867E-04	0.837	-57.980	
Mixed		1.492E-03	1.866E-03	2.501E-04	2.314E-04	0.832	-59.096	
Surface		1.456E-03	1.858E-03	2.135E-04	2.177E-04	0.853	-56.579	
Ground	Products-Only	1.356E-03	1.768E-03	1.983E-04	2.012E-04	0.854	-51.133	
Mixed		1.275E-03	1.717E-03	1.881E-04	1.936E-04	0.852	-43.679	<0.001
Surface		1.435E-03	1.828E-03	2.097E-04	2.135E-04	0.854	-55.843	
Ground	Both Contaminated Water & Products	1.995E-03	2.223E-03	4.135E-04	4.617E-04	0.793	-37.193	
Mixed		1.833E-03	2.032E-03	3.476E-04	2.514E-04	0.810	-59.101	
Surface		2.434E-03	2.768E-03	3.881E-04	3.184E-04	0.841	-12.027	

Summary and Discussion

- Small effects of factorial conditions; most variance due to population variability
  - Monte Carlo selection

- Human exposure primarily influenced by water source
  - SW < GW < Mix; how is this possible?
    - Mix could be made up of GW and SW sources with higher concentration than included either GW or SW-specific sources
  - Drinking water pathway via oral route
    - 2020 EPA Risk Evaluation: Oral vs Dermal

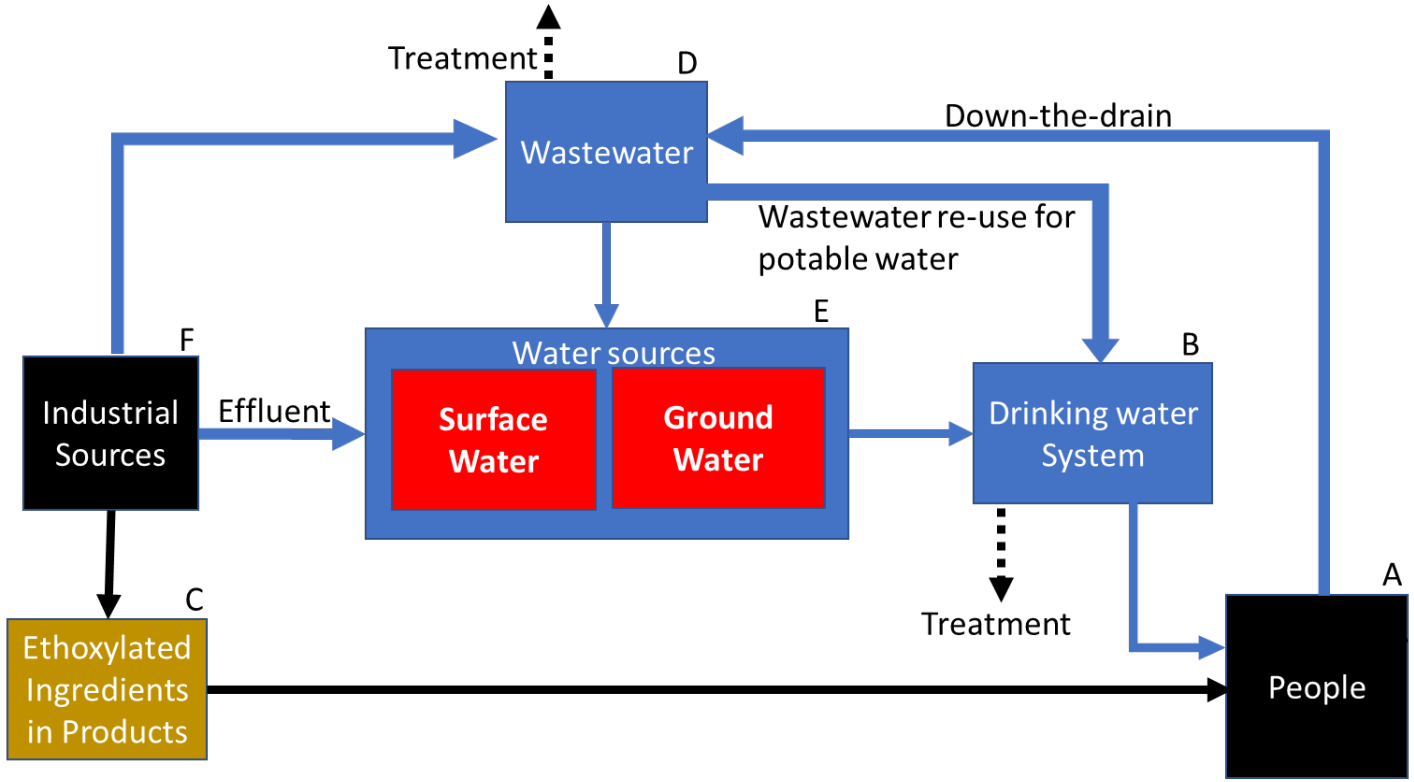
- DTD primarily influenced by $Prevalence_{products}$:High vs Low

- Subpopulation important consideration for source attribution
  - Low $Prevalence_{water}$ of Total population obfuscates role of water source in both human exposure and DTD mass released.

- 1 ppm product concentration threshold regulatory action
  - Variable exposure reduction
  - Broadly reduced DTD mass released across all factorial groups

Workflow limitations and future applications

- How do exposure sources influence drinking water concentrations?
- Workflow **cannot** parse influence of exposure sources on finished drinking water
  - SHEDS-HT uses static inputs (A-D) to produce a snapshot
  - Depend on location, watershed, and water system
    - Water source **(E)**
    - Proportion of treated water re-use **(E)**
    - Industrial inputs **(F)**
- Potential solution: mass-balance modeling framework
  - Existing platforms
    - ISTREEM
    - E-FAST
  - SHEDS-HT provides critical link
  - Exposure different scenarios



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- QUESTIONS?