# A novel model to characterize source contributions of chemical contamination of surface water sources used as drinking water: a case study with 1,4-dioxan

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# *"From Exposure to Human Health: New Developments and Challenges in a Changing Environment"*

*Climate change impacts can drastically affect the quantity and quality of water*

-https://www.unicef.org/stories/water-and-climate-change-10-things-you-should-know

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**Emerging Contaminants and Federal Facility Contaminants of Concern**

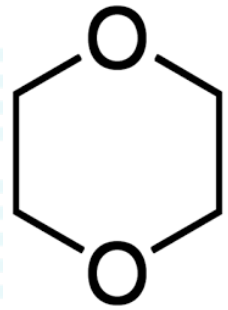
1,2,3-Trichloropropane (TCP)
1,4-Dioxane
2,4,6-Trinitrotoluene (TNT)
Dinitrotoluene (DNT)
Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX)
Nanomaterials
N-Nitroso-dimethylamine (NDMA)
Perchlorate
Perfluorooctane sulfonic acid (PFOS), Perfluorooctanoic acid (PFOA) and other Per- and polyfluoroalkyl substances (PFAS)
Polybrominated biphenyls (PBBs)
Polybrominated diphenyl ethers (PBDEs)
Tungsten

https://www.epa.gov/fedfac/emerging-contaminants-and-federal-facility-contaminants-concern

# Unregulated Contaminant Monitoring Rule (UCMR)

- Established under SDWA Amendments, 1996
- Monitors priority unregulated contaminants in drinking water every five years
- Monitors all large public water systems (PWS) serving over 10,000 people
- Collects representative sample of smaller PWS

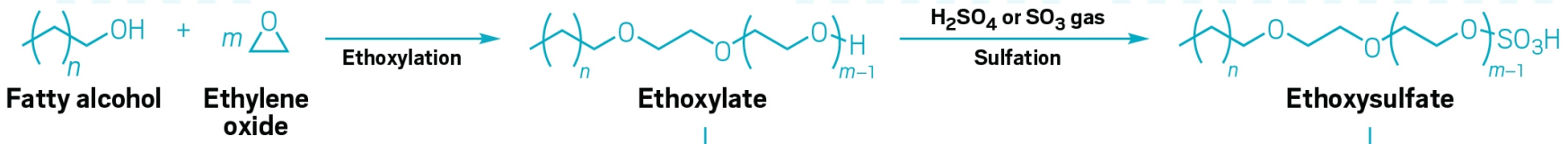
# 1,4- Dioxane: What's the Problem



- Industrial solvent/reagent
- Unintended byproduct in some consumer products
- Persistent, Mobile and Toxic - resistant to biodegradation
- EPA: Likely Carcinogen in Humans
- One of "1st 10" TSCA Chemicals
  - Some occupational risks
  - Non-occupational pathways not fully explored
    - Water Contamination
    - Unintended byproducts

# Ethoxylated fatty alcohols: cheap and effective cleaners

(1)

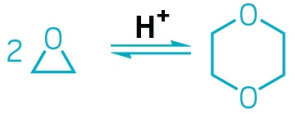


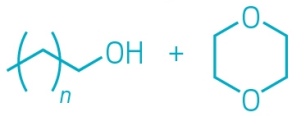

Fatty alcohol | Ethylene oxide | Ethoxylate | Ethoxysulfate

Ring closing forms 1,4-dioxane as a by-product.
$SO_3$ promotes this side reaction.

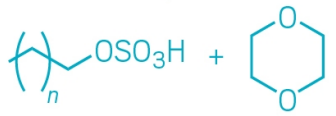
(2)

Ethylene oxide can also dimerize to form 1,4-dioxane.



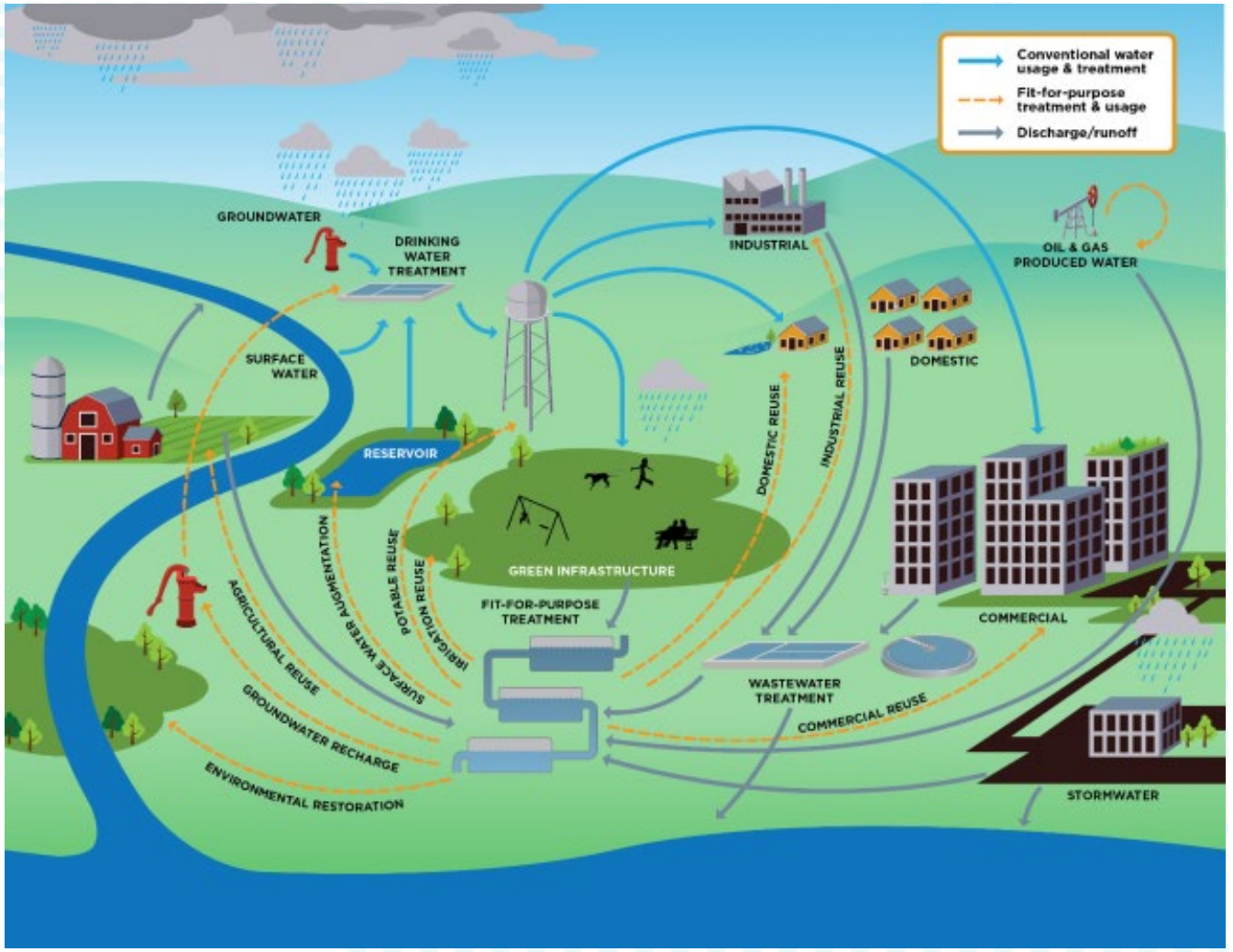




1,4-dioxane

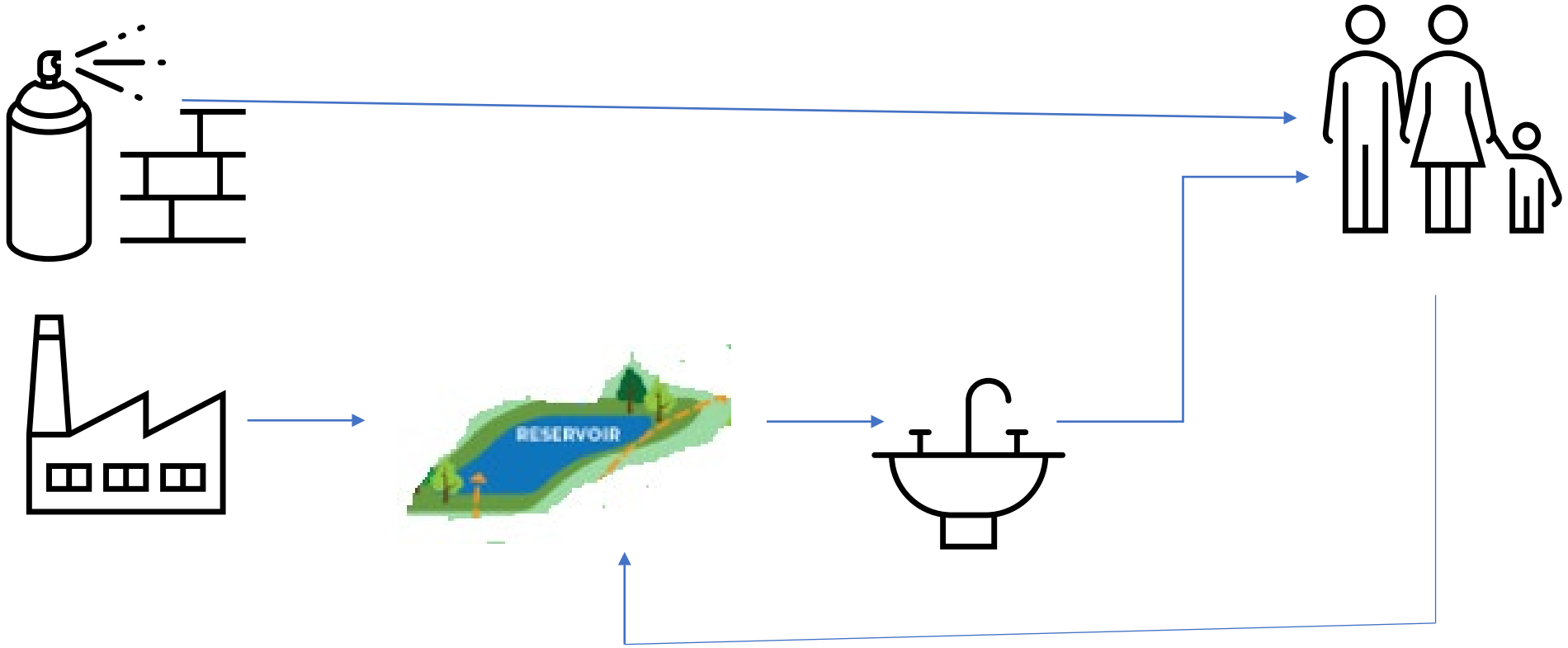



*m* = 1–12
*n* = 12–18

https://cen.acs.org/business/consumer-products/companies-getting-14-dioxane-home/98/i11




https://www.epa.gov/waterreuse/basic-information-about-water-reuse#basics

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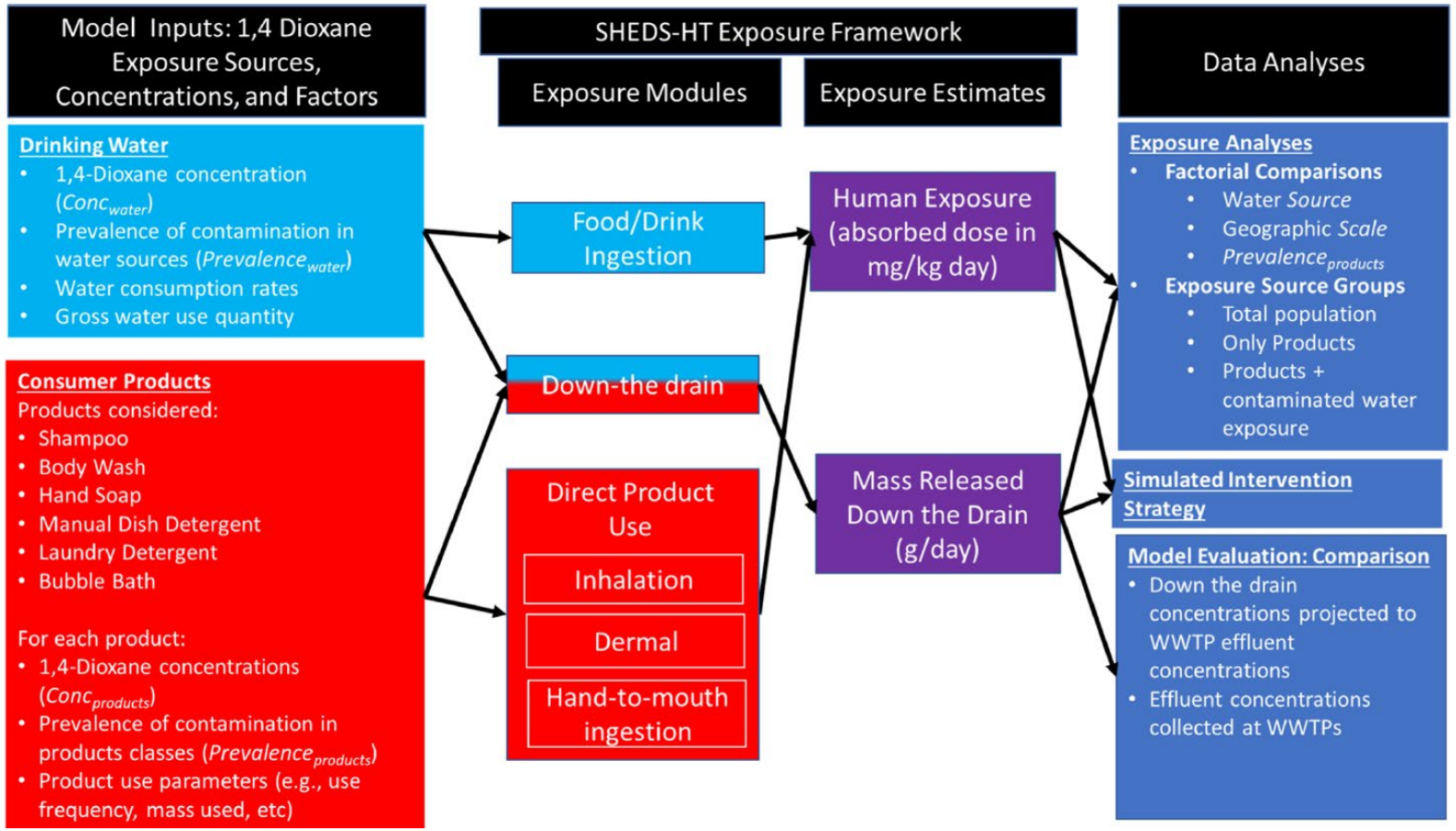
# 1,4- Dioxane Scientific Modeling Workflow

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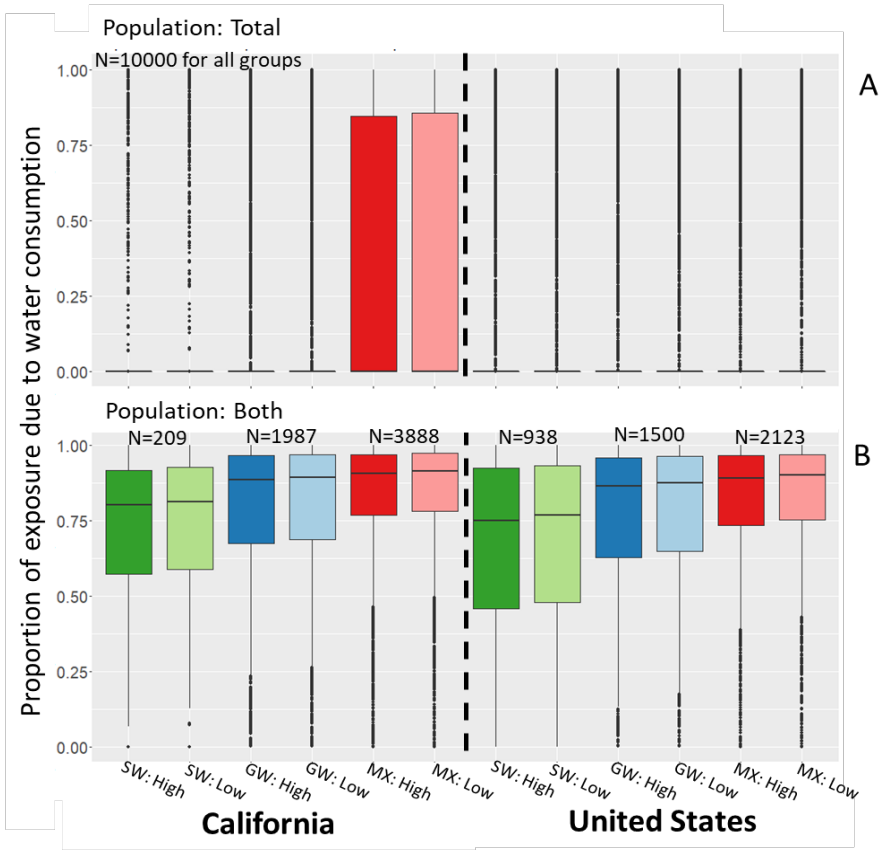
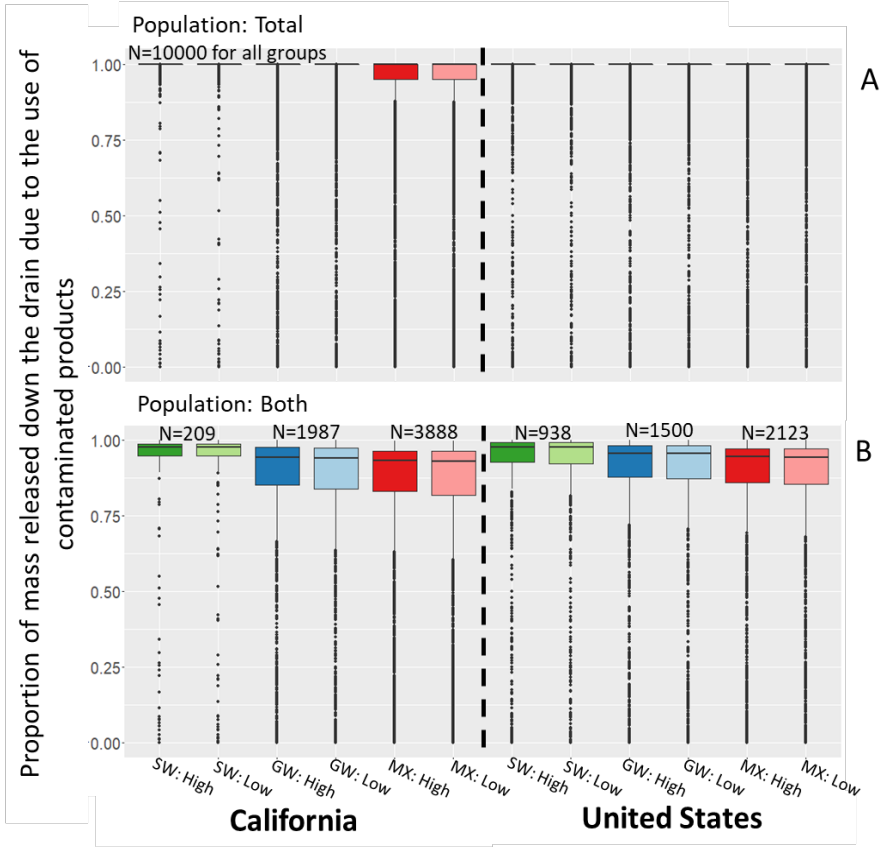
# Results

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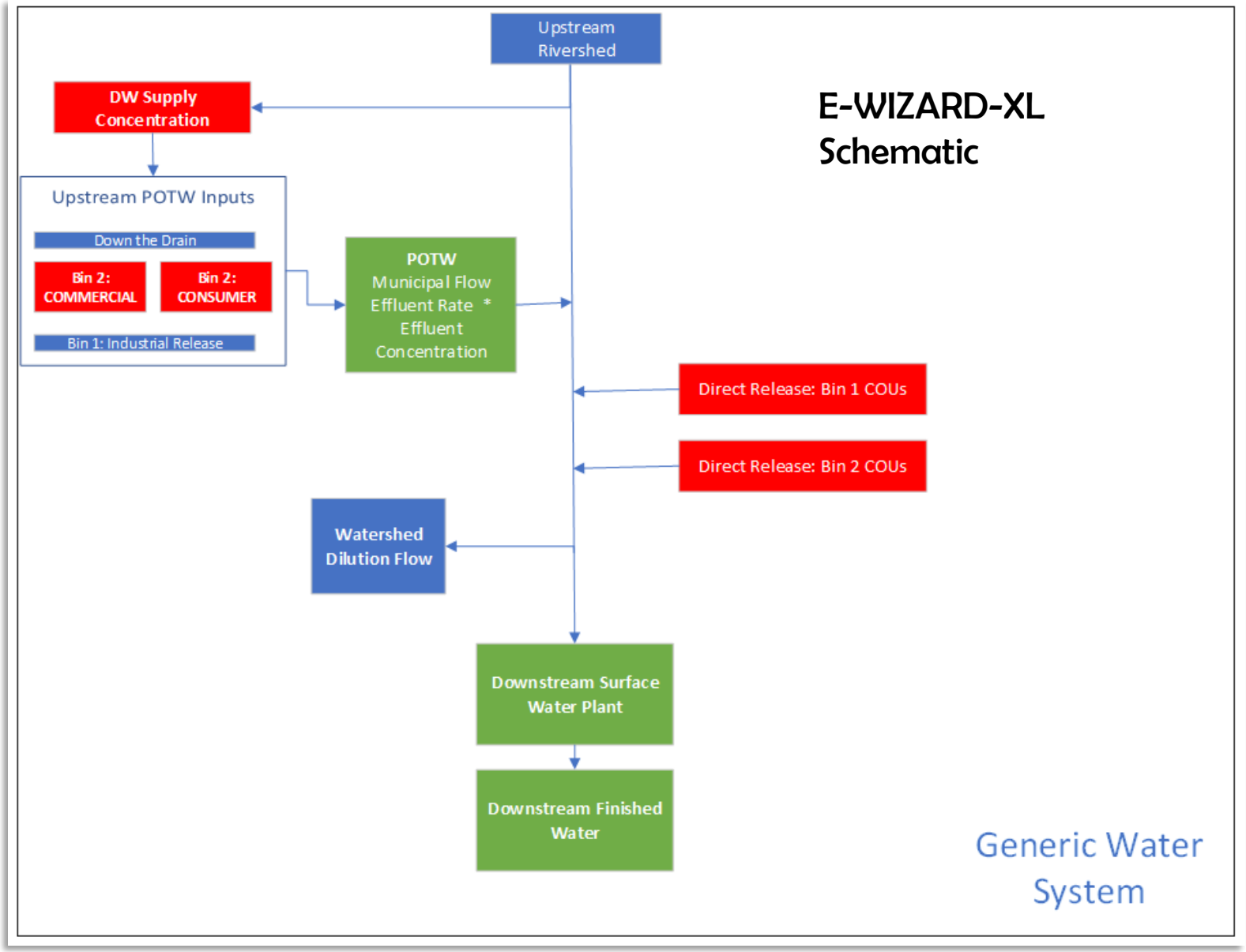
# Takeaways

- Human Exposure: Driven by water consumption when water is contaminated (Both population)
- Mass released down the drain: Driven by the use of consumer products, regardless of water contamination status
- Regulatory approaches aimed at reducing product concentrations may have the largest impact for populations primarily exposed via product use
- Important limitations:
  - Ultimate sources of water contamination and impacts of MRDTD on drinking water concentrations not ascertained here
  - The list of product classes included in assessment was not exhaustive; i.e., model estimates may be underestimates
  - Exposure estimates likely not reflective of areas with high drinking water concentrations

E-Wizard-XL program estimates chemical concentration of surface water in a portion of a watershed from down the drain and industrial releases.



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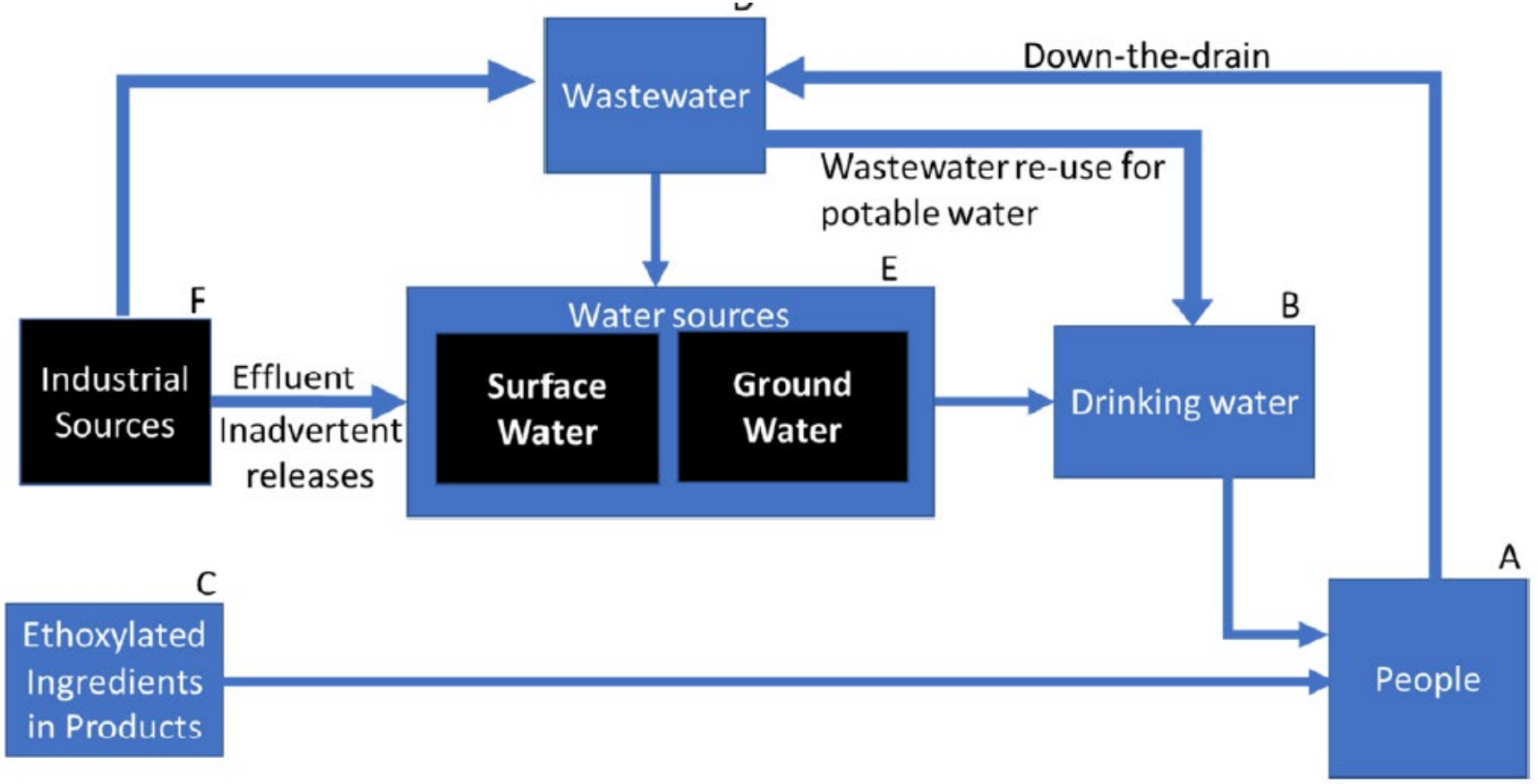
# Thank you!

# Questions?

# Exposure Scenario for 1,4- Dioxane

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