Constructing Exposure Workflows for Emerging Contaminants

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Scientific Workflow Overview

- Multi-route, multi-pathway
- One case presented: 1,4-dioxane
- Update of CHEM modules
  - RPGen
  - Product Use Scheduler
  - Source-to-Dose

Demonstrating an Exposure Scientific Workflow

- Series of data manipulation & computational steps
- Tailored to a specific type of decision to be made
- Domain-specific data types & tools for the exposure scientist
- In our case, directed at emerging chemicals
  - Starting with chemicals that can inform a future PFAS workflows
  - Others, as they arise
- High-interest chemical/product combinations
  - Links to alternatives assessments & sustainable chemistry

Methodology – 1. *Select case studies* for product-chemical combinations

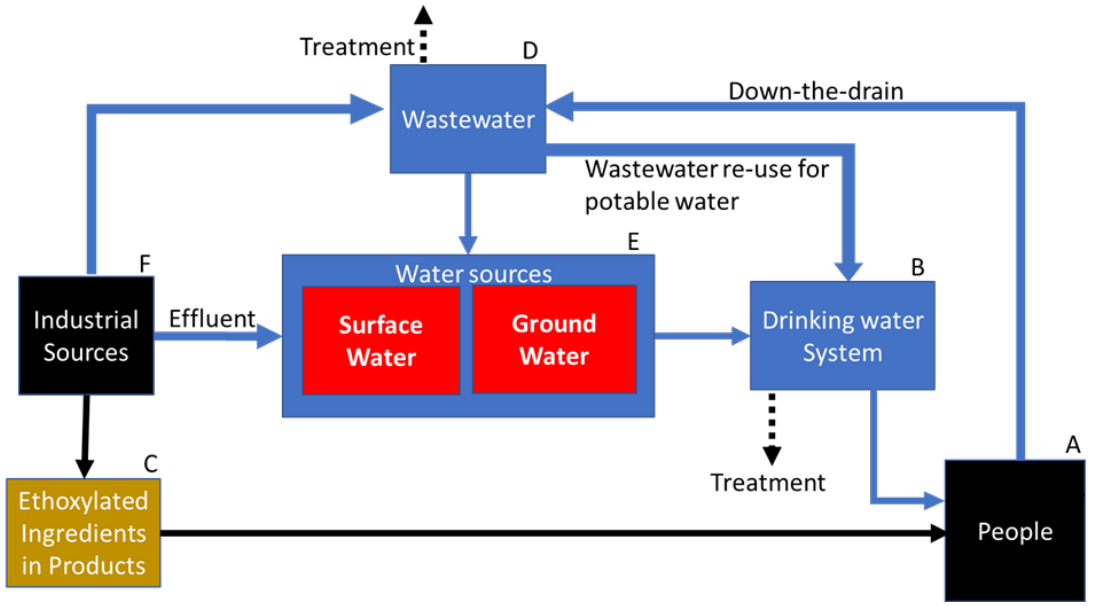
- Examples demonstrate the scope of exposure issues related to chemical/product manufacture and use that are of current interest to decision makers and for which a range of data may be available.
- Fusion of LCA and RA, combing product focused and receptor focused approaches.
- Fusion of data-driven methods and mechanistic modeling required.
  - 1,4-dioxane exposure associated use of contaminated personal care and cleaning products
  - Flame retardants in consumer electronics
  - PFOA in carpet

Methodology – 2. *Problem Formulation*

- Identify the decision context and state the question(s) that need to be addressed
- Map chemical pathway from manufacture to use to disposal and to people along the way
- Identify sources, release and transfer in environmental media, exposure media, and exposure routes.

Methodology – 3. *Conceptual Workflow Development*

- Describe required information on important exposure pathways, extant occurrence data, and product information for the chemicals in exposure media; as well as other model inputs from literature and other databases
- Identify human exposure modeling algorithms for important processes to estimate exposures



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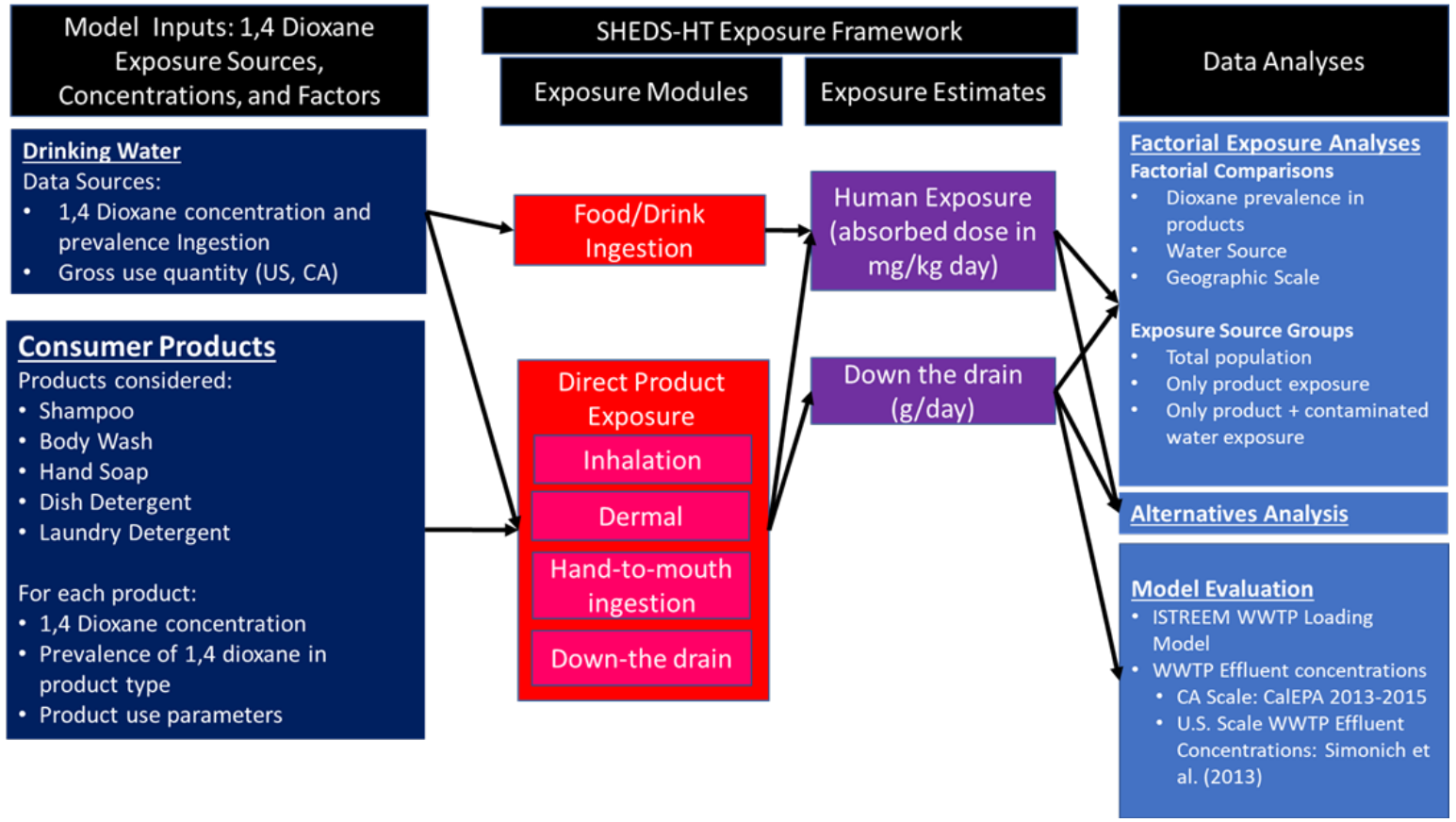
Interim Findings – *Conceptual Workflow Development*

- Conceptual workflow includes the data sources, exposure model, and analysis steps to evaluate exposure scenarios.
- Simulations were run using SHEDS-HT.
- Black arrows demonstrate the flow of information from one step to the next.
- More on this from next presentation.



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Conclusions

- The steps of the workflow can be represented by a visual graph, aiding in both planning, execution, and evaluation.
- Because scientific workflows usually exist as an interrelated collection of analytical scripts (e.g., written in open-source software like R or Python), they facilitate efficient, replicable, and transparently documented results.
- Workflows developed for one decision context may be broadly re-usable beyond the chemicals and exposure scenarios for which they are originally designed.
- This approach will enable decision makers to access data and modeling algorithms required to synthesize information for characterizing human exposure to industrial chemicals.