Developing a Conceptual Scientific Workflow to Estimate Chemical Exposures

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Addressing Information Gaps

- Holistic evaluation of chemical impacts requires integration of disparate data streams, modeling of interactions among physical and biological systems, and consideration of tradeoffs associated with management decisions.
- Deploys and evaluates a variety of models that use available data with other mechanistic information to understand how chemicals in products move through the natural and built environment.
- Knowledge grows and gaps close with each new problem. Incrementally advances quality and relevance of data and models.
- Problems of increasing complexity can be addressed, enabling greater insights.
- More nimble modeling methodologies are required to assess important chemical exposure scenarios and pathways across the chemical/product life cycle, especially for emerging chemicals and chemical-product combinations.
- Provides an exposure link between evidence-based risk assessments and life cycle analyses, e.g., alternatives assessment.

Source: https://www.sciencedirect.com/topics/earth-and-planetary-sciences/life-cycle-analysis

What is a Scientific Workflow?

- A scientific workflow executes a series of data handling and computational steps to provide outputs that support decision-making.
- For chemical exposure assessments, scientific workflows are useful tools for efficient and transparent analyses, especially for considering impacts in complex systems.

Exposure Scientific Workflow

Research Question: A targeted question that has a solution which will better characterize a chemical, set of chemicals, pathway, or product.

↓ Scoping of existing literature, data gaps, and/or a screening model will inform the problem formulation from a question.

Problem Formulation: Identifies relevant sources, release and transfer, movement between sources, media, environmental reservoirs and receptors via routes.

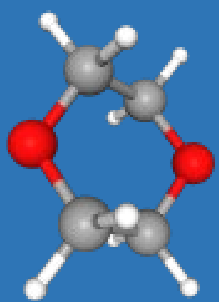
↓ Evaluation of model availability, data availability and richness, existing results, and policy implications

Conceptual Workflow: Series of computational steps in exposure estimation process, including data sources, models, and analysis. About getting the 'best' estimate possible across tier, throughput, data paucity, model dynamics and validation criteria.

- To demonstrate this approach, we begin with relatively data-rich chemicals as test cases to drive conceptual workflow development including ethoxylated solvents, flame retardant and PFAS.
- The goal is to advance the workflows for efficient evaluation of a variety of chemicals and a range of decision contexts.

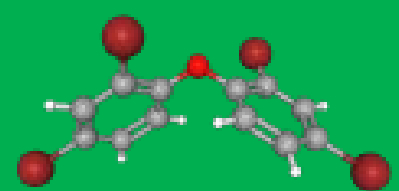
Case 1

1-4 Dioxane



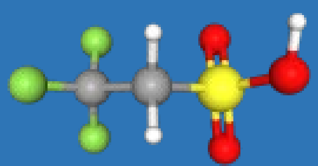
Case 2

PBDE



Case 3

PFAS



Images adapted from PubChem

Sources: National Center for Biotechnology Information (2022). PubChem Compound Summary for CID 31275, Dioxane. Retrieved August 26, 2022 from https://pubchem.ncbi.nlm.nih.gov/compound/Dioxane.

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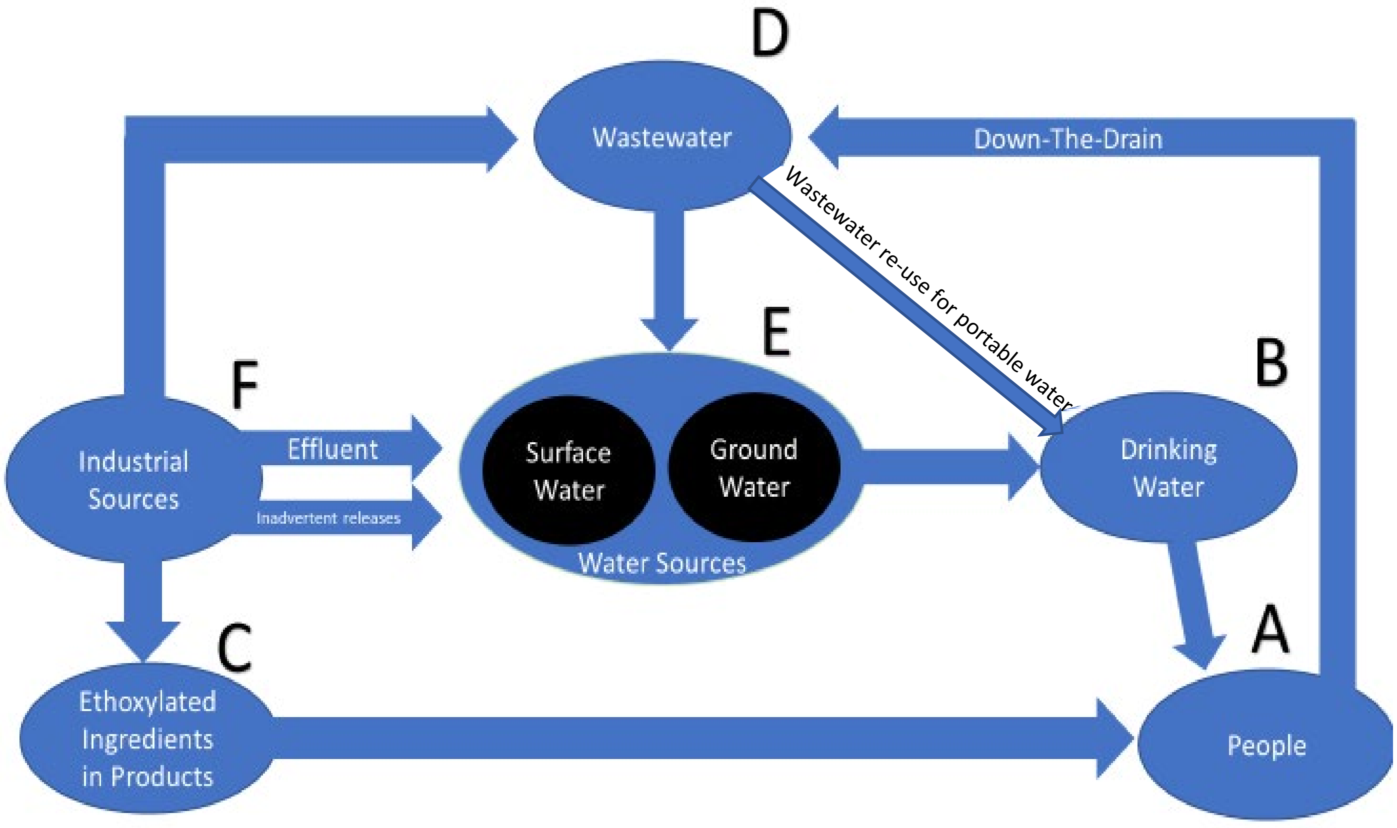
Case 1:
1,4-dioxane Exposure Associated Use of Contaminated Products

- 1,4-Dioxane is a persistent and mobile organic chemical (PMOC), which is highly miscible and mobile in the aquatic environment and is not susceptible to most standard forms of wastewater and drinking water treatment
- Decision makers at both the national and state levels in the US are seeking to understand the relative importance of the contribution of consumer products to 1,4-dioxane contamination of drinking water vs. the contribution from historical industrial pollution
- The EPA (Dawson et al., 2022) recently developed and implemented a scientific workflow to evaluate exposure to 1,4-dioxane in the residential environment, mainly elucidating exposure and the down-the-drain pathway during problem formulation

Example workflow for water & consumer product pathways: 1,4-dioxane



Example workflow: 1,4-dioxane based on SHEDS-HT

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

Exposure Modules

Exposure Estimates

Data Analyses

Drinking Water

- 1,4 Dioxane concentration ($Conc_{water}$)
- Prevalence of contamination in the water sources($Prevalence_{water}$)
- Water consumption rates
- Gross water use quality

Consumer Products

Products considered:

- Shampoo
- Body Wash
- Hand Soap
- Bubble Bath
- Manual Dish Detergent
- Laundry Detergent

For each product:

- 1,4 Dioxane concentration ($Conc_{products}$)
- Prevalence of contamination in the product classes($Prevalence_{products}$)
- Product use parameters (e.g., use, frequency, mass used, etc.)

Food/Drink Ingestion

Down-the-Drain

Direct Product Use:

- ❑ Inhalation
- ❑ Dermal
- ❑ Hand-to-Mouth Ingestion

Human Exposure (absorbed dose in mg/kg/day)

Mass Released Down the Drain (g/day)

Exposure Analyses

- **Factorial Comparisons**
  - Water Sources
  - Geographic Scale
  - $Prevalence_{products}$
- **Exposure Source Groups**
  - Total Population
  - Only Products
  - Products + Contaminated Water Exposure

Simulated Intervention Strategy

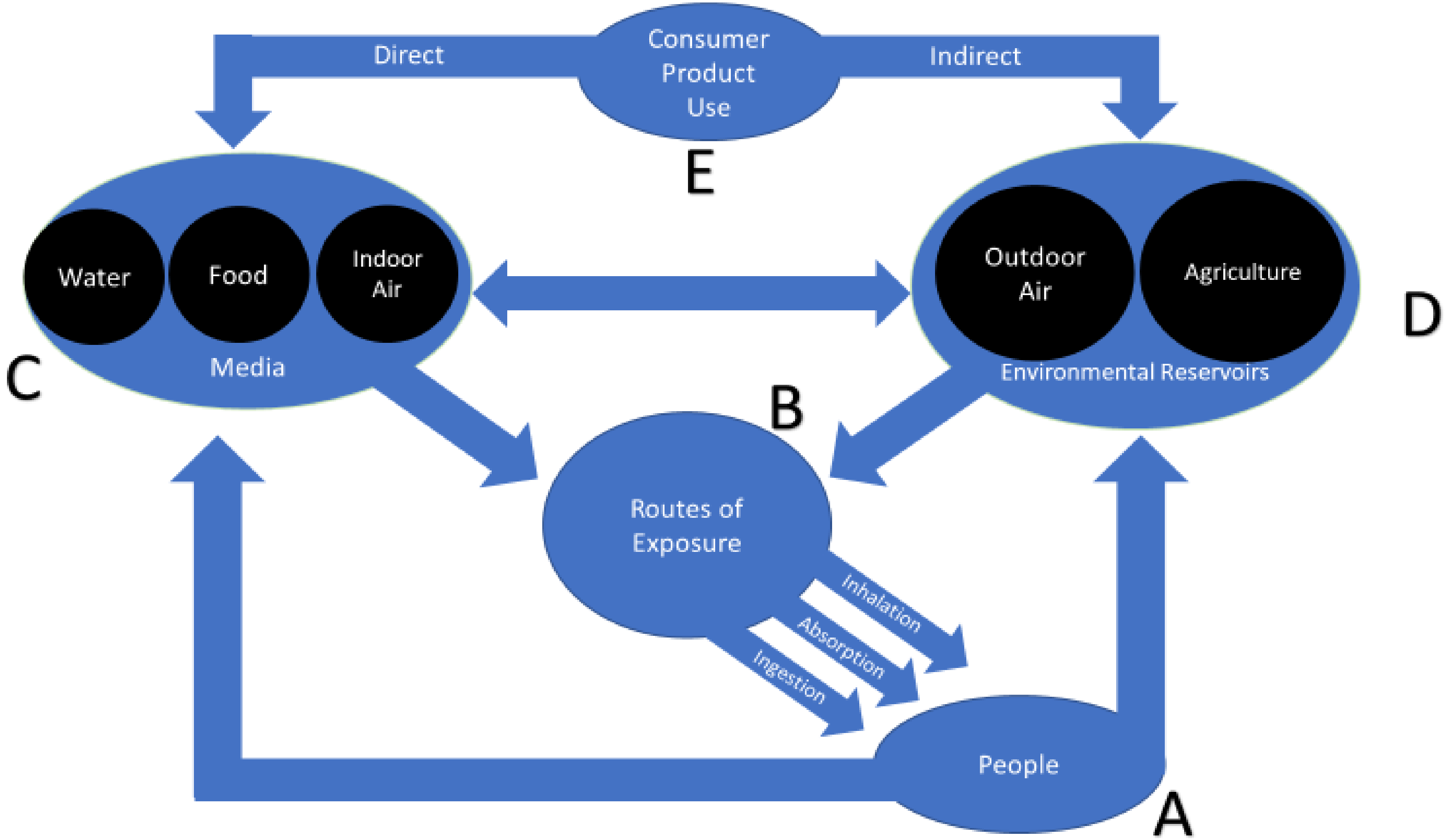
Model Evaluation: Comparison

- Down-the-Drain concentrations projects to WWTP effluent concentrations
- Effluent concentrations collected at WWTPs

Case 2: Flame Retardant Lifecycle Exposure Scenarios

- PBDEs are synthetic compounds that are utilized as additives in several industrial and consumer items to retard fire and flames
- Despite the phase-out of various varieties such as penta-BDE, octa-BDE, and deca-BDE, many consumer products such as computers, furniture, and televisions still contain PBDEs and can be used for many more years due to product life cycle
- This case examines the product use stage of PBDE. It does not include packaging, transportation, and distribution life cycle stages because these segments are not expected to influence the outcome. Most exposure information is available for the use phase

Example workflow: Flame retardant



PDBE Case Proposed Workflow

Model Inputs: PBDE Concentrations, Exposure Sources, Concentrations, and Factors

Consumer Products
- Product considered: computer cases
- EPA Comptox Dashboard and CATALOGIC for PBDE characteristics

For each product:
- PBDE concentration ($Conc_{products}$)
- Prevalence of contamination in the product classes($Prevalence_{products}$)
- Product use parameters (e.g., use, frequency, mass used, etc.)

Probable Models

ICECRM
- ❑ Inhalation
- ❑ Dermal Uptake
- ❑ Nondietary Ingestion

RAIDAR
- ❑ Drinking Water
- ❑ Food
- ❑ Fate and Transport

Analysis

- Combined Human Exposure Estimate (absorbed dose in mg/kg/day)
- Vulnerable Populations
- Sensitivity Analysis of Model Parameters
- Concentration in Environmental Reservoirs

Results

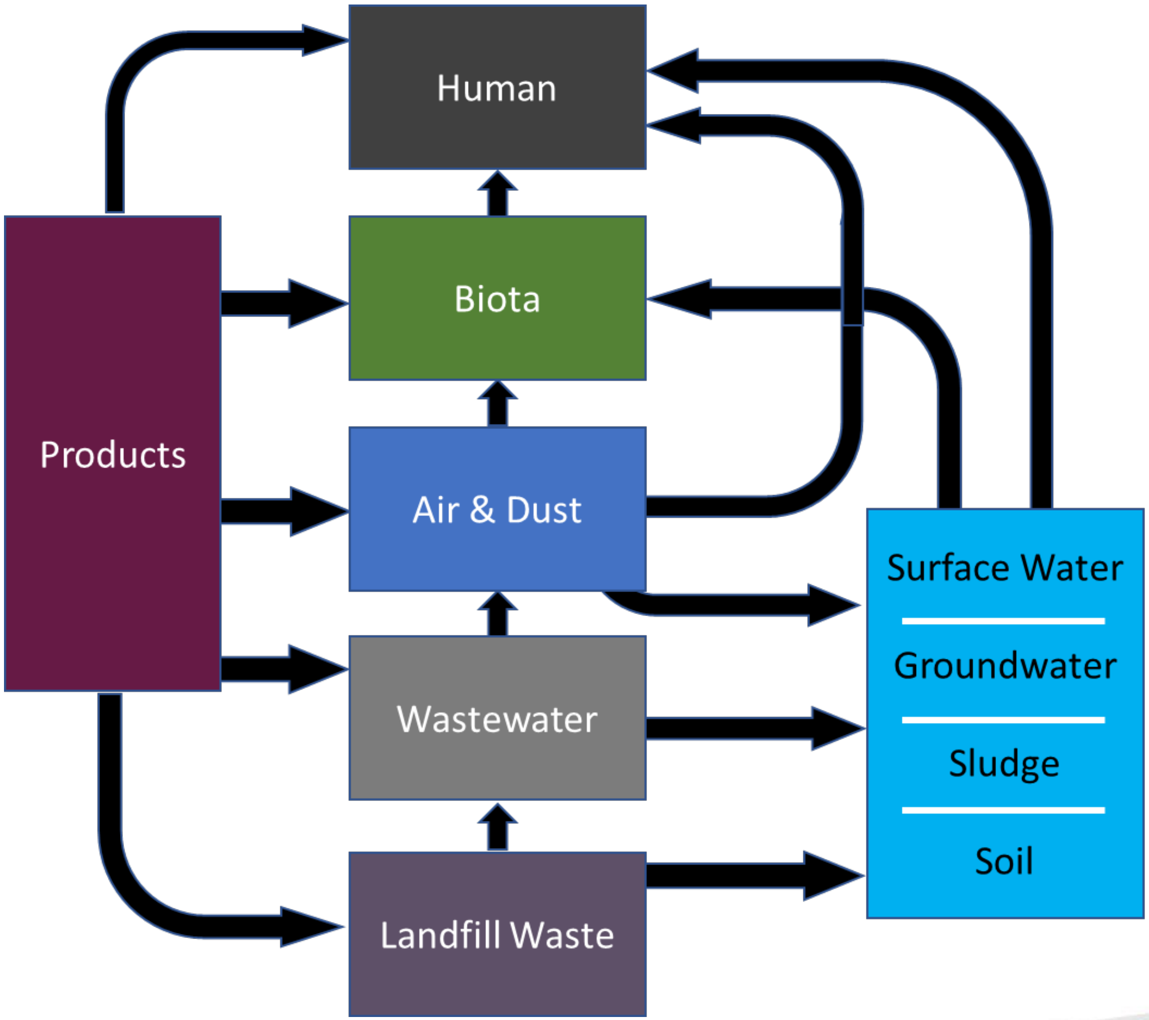
Literature
- **Rauert et al. 2015**
- **Diamond and Kvasnicka,2020**

Measured Concentrations
- GLNPO Water & Fish data
- Venier et al 2016
- IADN

Case 3: PFAS treatment use on converted textiles or leathers

- PFASs become part of a nearly closed cycle that leads to chronic human and environmental exposures
- Due to their hydrophobic and oil-resistant qualities, various types of PFAS treatments have been employed in many consumer products including converted textiles or leathers that are widely utilized in the home and a for a variety of professional applications
- Converted textiles and leather may contribute to widespread PFAS exposure and pollution and are currently the focus of assessment to identify alternatives

Example workflow: Aggregate exposures via textiles & leather treatment



Textile/leather Treatment Case Proposed Workflow

Model Inputs: Chemical Concentrations, Exposure Sources, Concentrations, and Factors

Chemical Properties and Concentration

- Human health assessment using IRIS
- Chemical characteristics and profile from ATDSR
- Review TSCA

Consumer Products

Products considered:

- Converted textiles
- Leathers

For each product:

- PFAS concentration ($Conc_{products}$)
- Prevalence of contamination in the product classes($Prevalence_{products}$)
- Product use parameters:
  - TRI
  - PFAS in converted textile and leathers literature
  - EPA Comptox
  - Assumptions

Probable Models

SHEDS-HT

- ❑ Inhalation
- ❑ Ingestion of dust
- ❑ Drinking water ingestion

Analysis

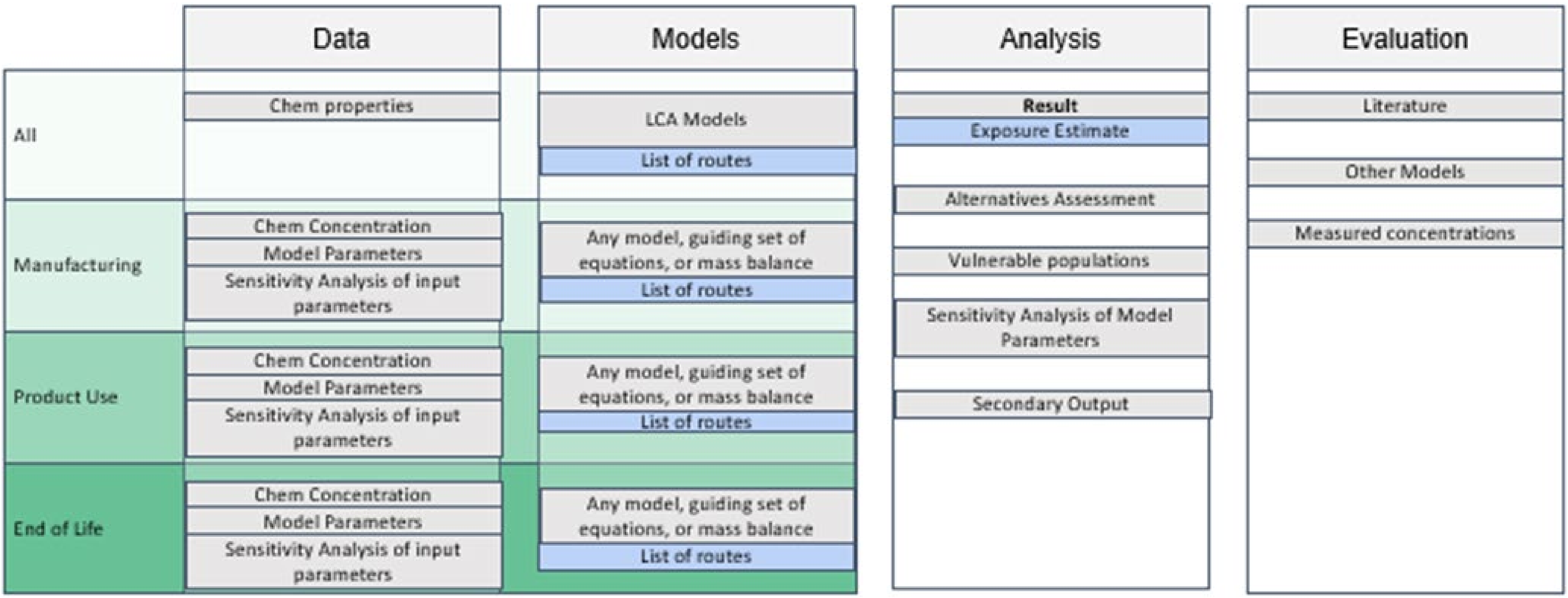
- Exposure Estimate (absorbed dose in ng/kg/day)
- Vulnerable Populations
- Sensitivity Analysis of Model Parameters
- Alternatives Assesment

Results

Model Evaluation: Comparison

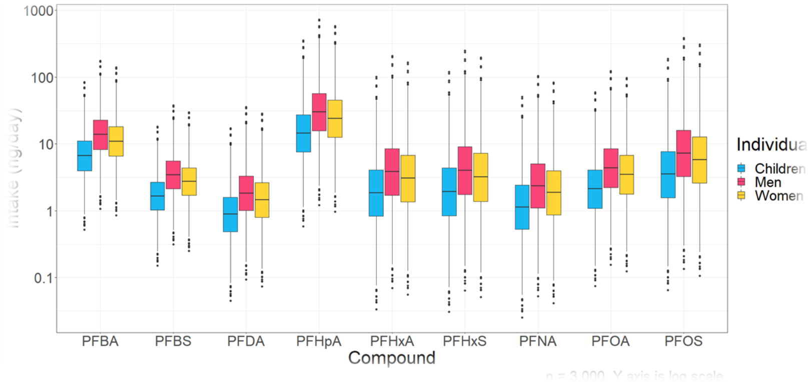
- Compare exposure estimate with Combined Human Exposure Model (CHEM)

Proposed Workflow Template

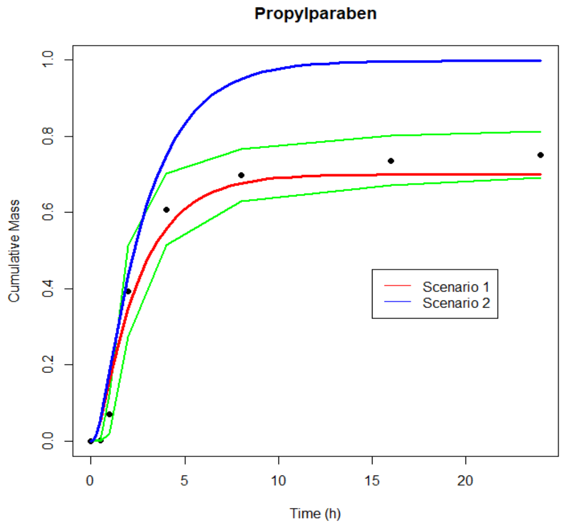


Enhancements to Conceptual Workflow Currently Being Developed

- Lorber-Egeghy-East Method R Package



- Dermal Exposure



- Combined Human Exposure Modules

Summary

- Scientific workflows provide a way to integrate data from various knowledgebases, apply algorithms, and identify gaps in data needed to conduct aggregate exposures.
- Such gaps include the need for reliable dermal models, paucity of data for PFAS and other emerging contaminants
- Uncertainties exist in human activities, representative exposure scenarios, and product use parameters.
- To address these gaps, EPA has built a conceptual exposure scientific workflow that is being populated by improved tools and data.
- References are available upon request at vallero.daniel@epa.gov.