Exposure modeling of UV filters in aquatic environments

NASEM Committee Meeting,
May 28th 2021

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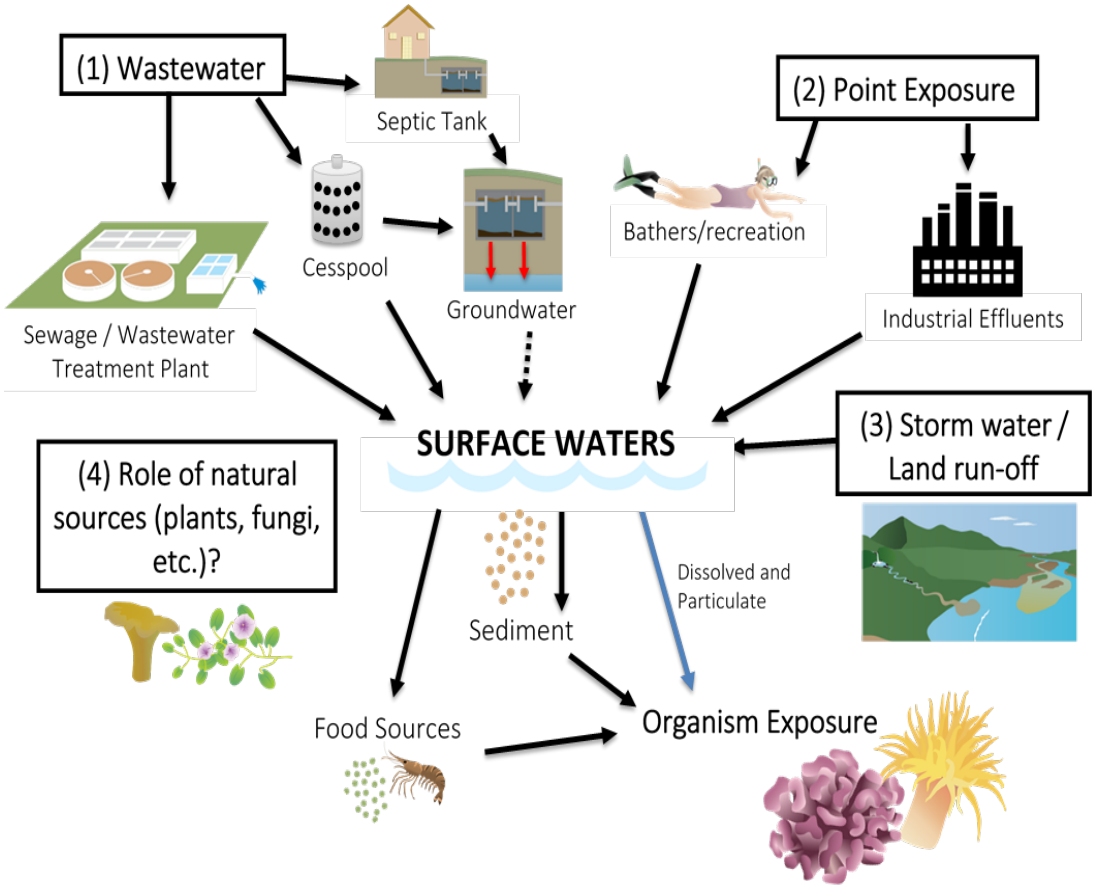
Emissions of UV filters to the aquatic environment



1. Mitchelmore et al. (2021)

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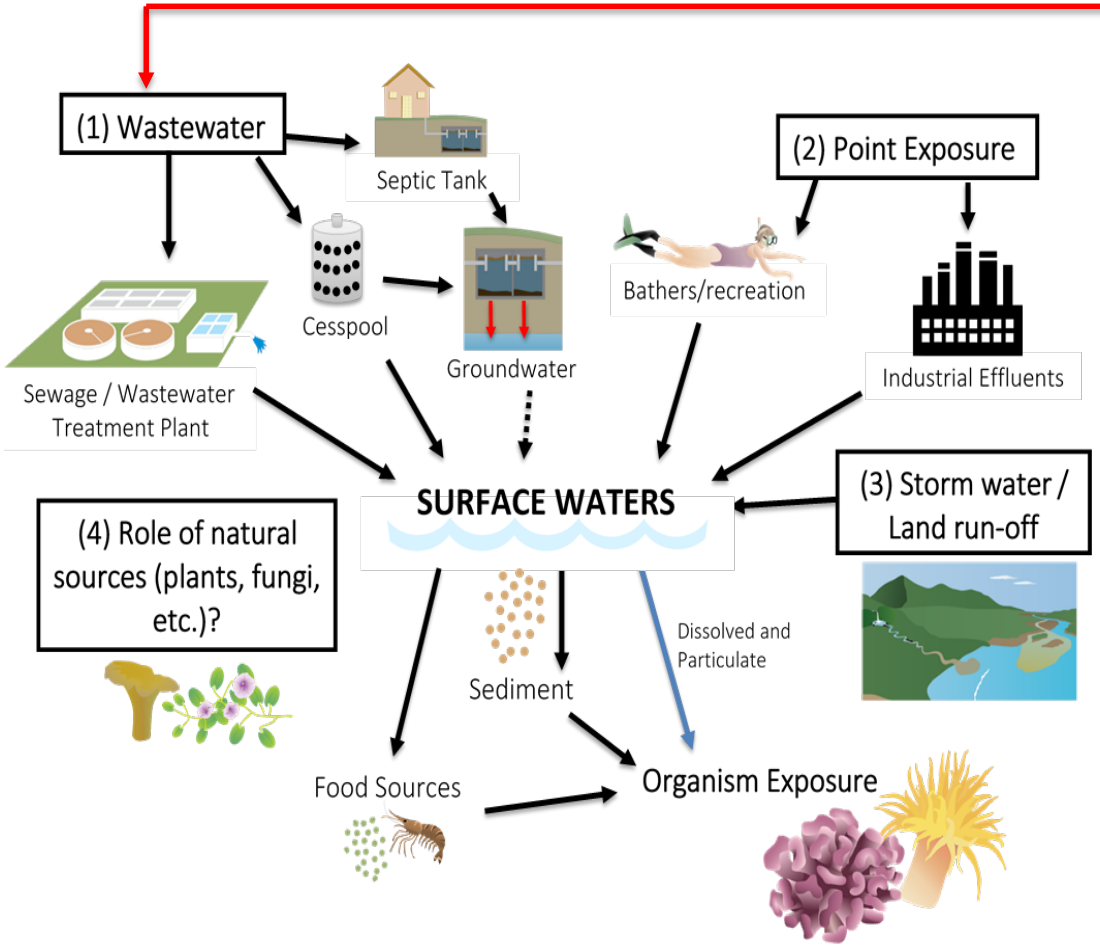
Emissions of UV filters to the aquatic environment



Important pathway for freshwater

Washing off products down-the-drain

1. Mitchelmore et al. (2021)

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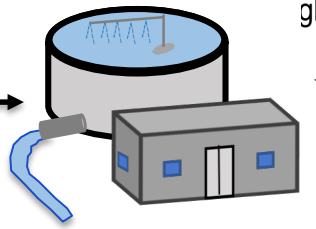
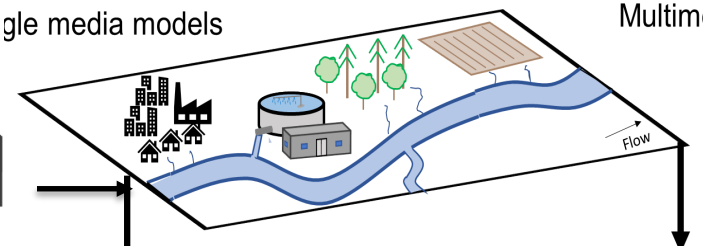
Down-the-drain emissions: UV filters

1. Ingredients used in cosmetic, personal care and over-the-counter drug products (sunscreens)

2. Sunscreen use is not necessarily all associated with aquatic recreation
   - Released down-the-drain through cleansing, bathing, and laundering of clothes

Commonly modeled exposure scenario for consumer chemicals





Emission → Down-the-drain → WWTP removal → Release to freshwater

Previous talk
Dr. Iain Davies (PCPC)

WWTP = wastewater treatment plant

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Down-the-drain exposure assessment: Tiered approach

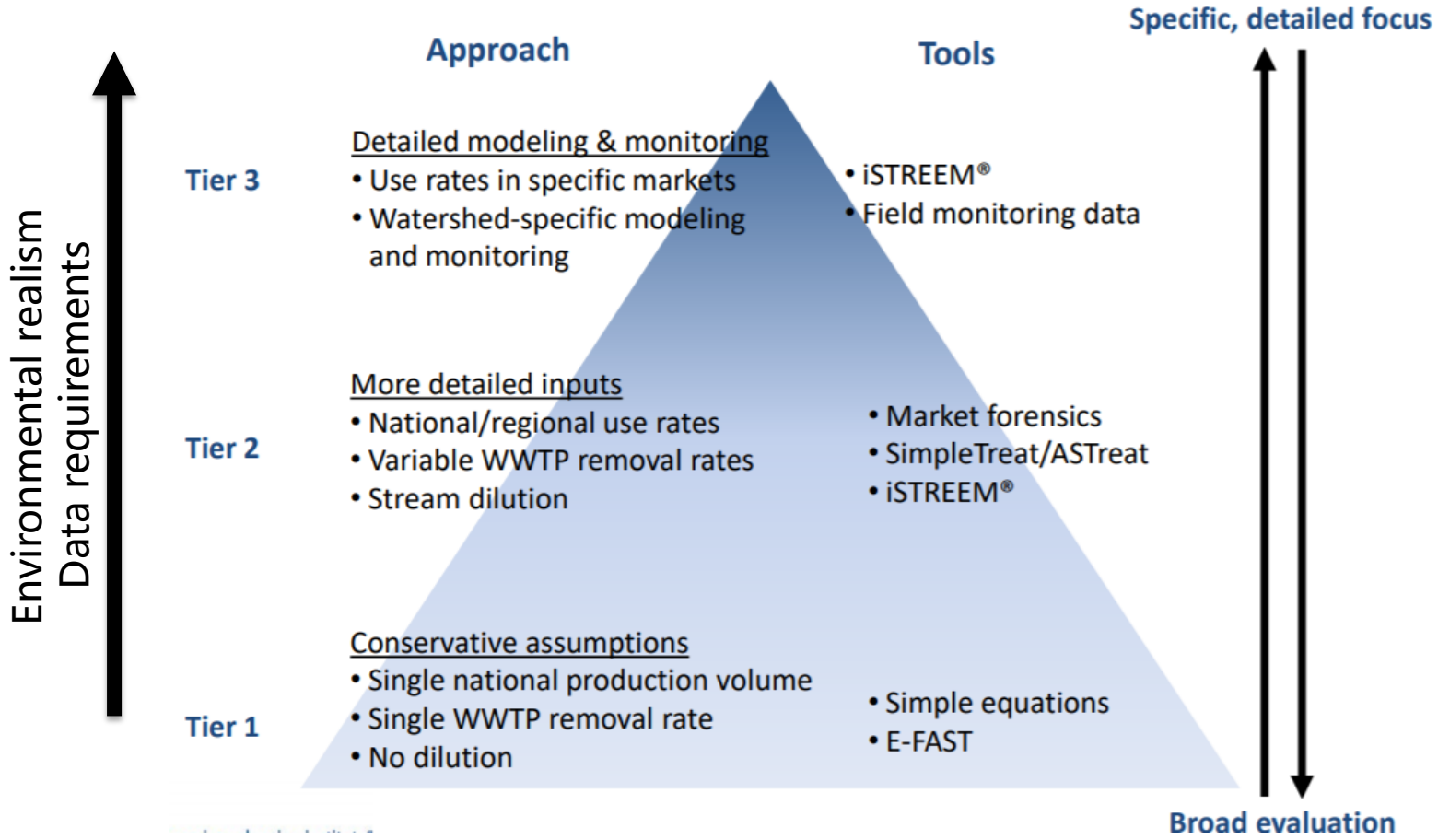


Image source: American Cleaning Institute

Down-the-drain exposure assessment: Tiered approach

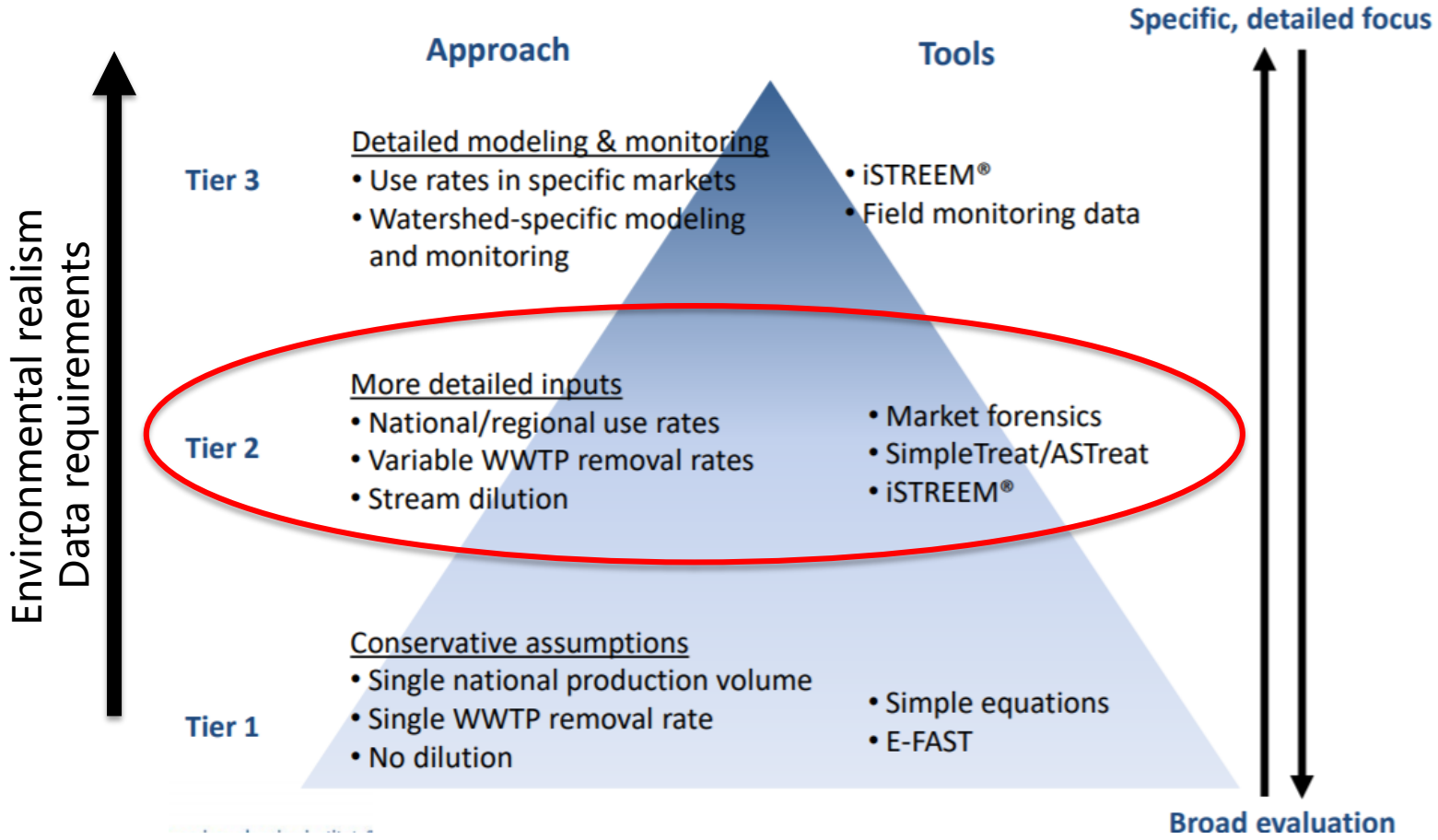
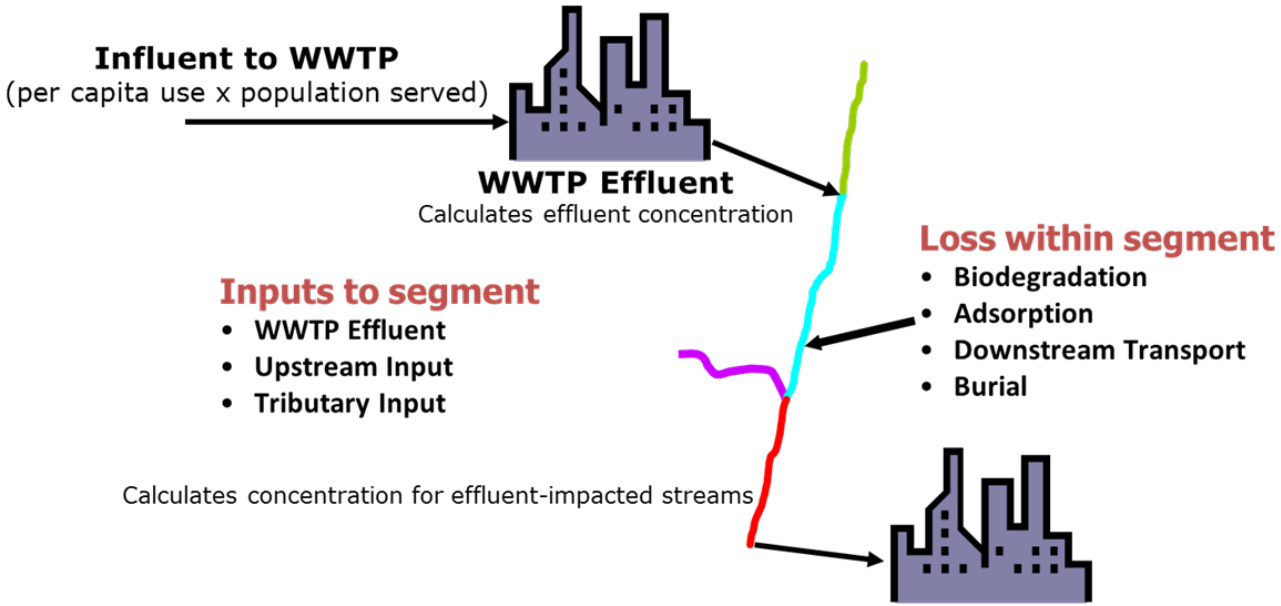
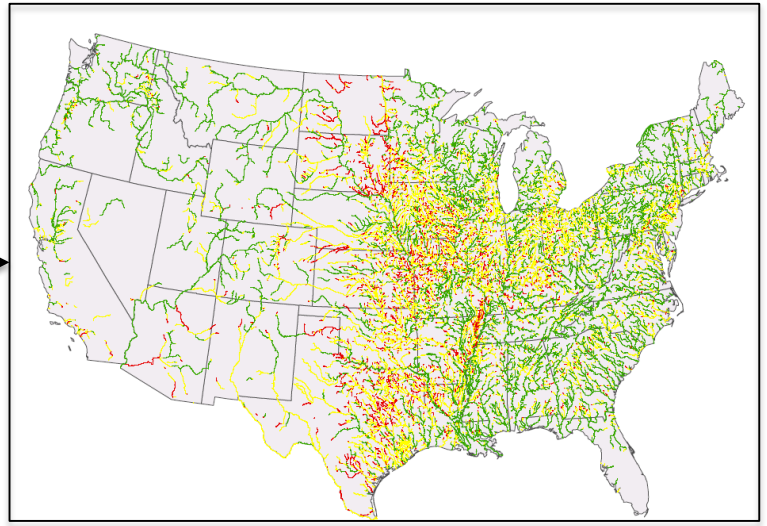


Image source: American Cleaning Institute

Down-the-drain exposure assessment: higher-tier exposure model iSTREEM®



227 876 unique river segments



www.istreem.org

american cleaning institute®
www.cleaninginstitute.org

Parameterizing iSTREEM®:

Compound-specific iSTREEM® parameters

Emission: grams/ per capita / day

Wastewater treatment removal: % removed

In-stream decay rate: k (day^{-1})

Oxybenzone case study

Emission – 0.011 g/c/day

- 100% washed down-the-drain
  - Conservative assumption
  - Could refine with habits and practices data

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Parameterizing iSTREEM®: WWTP Removal

Wastewater treatment removal 86%

- Average of 26 data points from 10 peer-reviewed studies
  - Estimated removals based on monitoring data.
- Simpletreat model predicted 71% removal
- Consistent with physicochemical properties (e.g., Logkow, biodegradable)

Estimated removals: monitoring studies in literature

Predicted removals: SimpleTreat model

Standard test data: OECD TG 303A

Oxybenzone is well removed in wastewater treatment

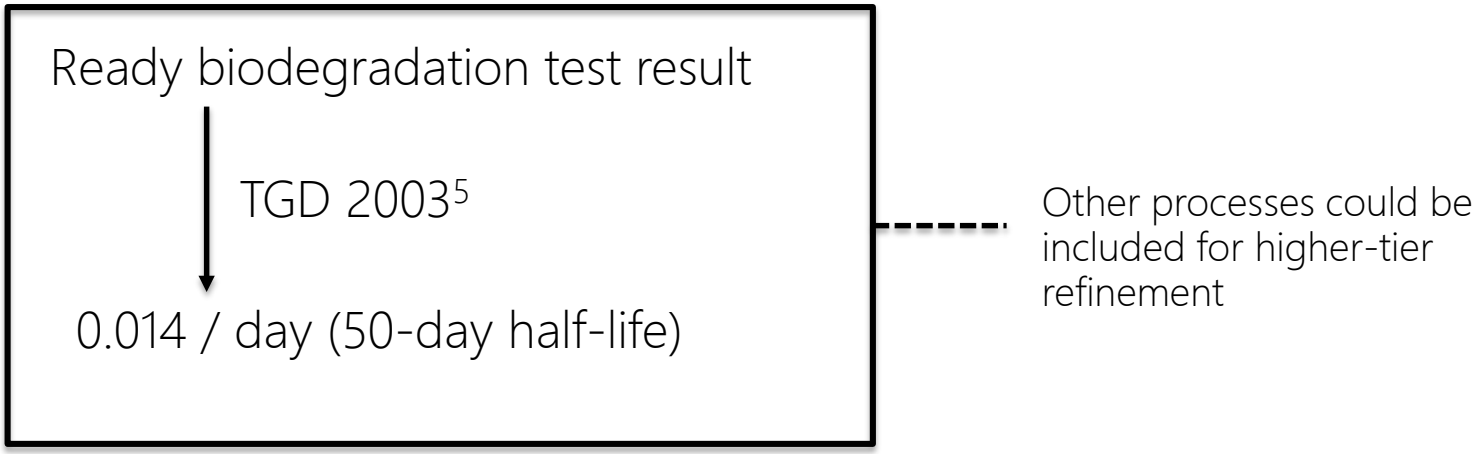
Parameterizing iSTREEM®: In-stream decay

Characterizing in-stream decay:

Ready biodegradability test - biodegradable

Biodegradation appropriate in-stream loss refinement for oxybenzone

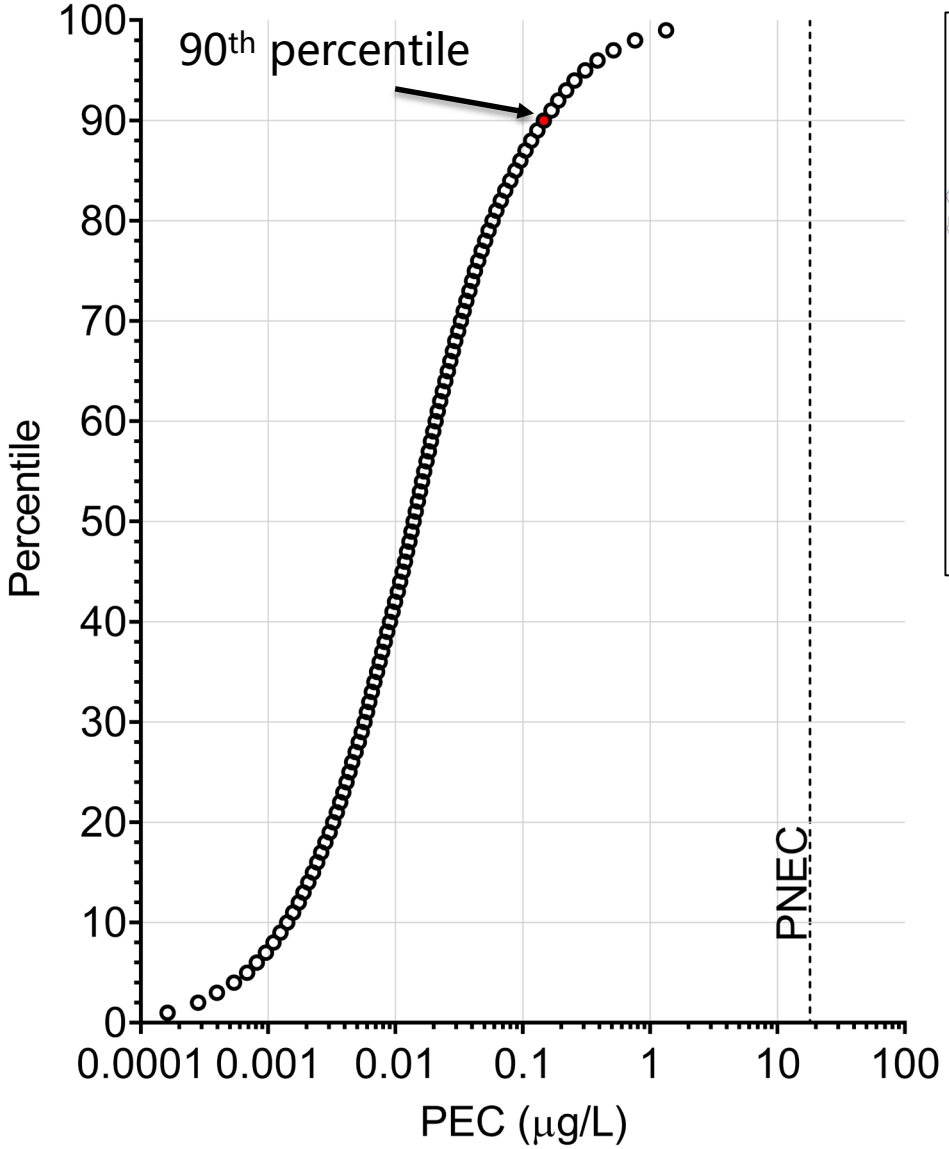
Calculating in-stream decay rate (/day):

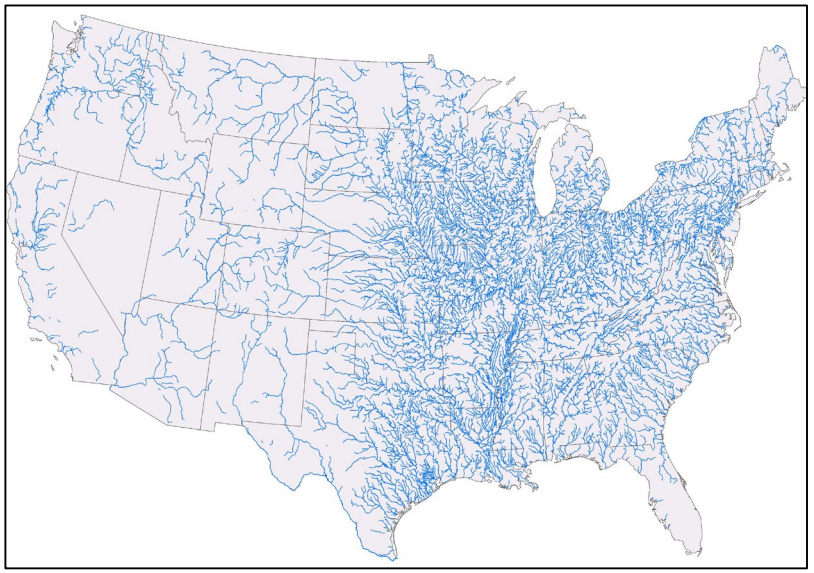


2. 62% degraded in 28 days, didn't meet 10 day window. Manometric respirometry ready biodegradation test, i.e., OECD TG 301F (ECHA 2020).

3. EC JRC (2003)

iSTREEM® exposure results: Oxybenzone





4. Burns et al. (2021). National scale down-the-drain environmental risk assessment of oxybenzone in the United States. *IEAM*. https://doi.org/10.1002/ieam.4430

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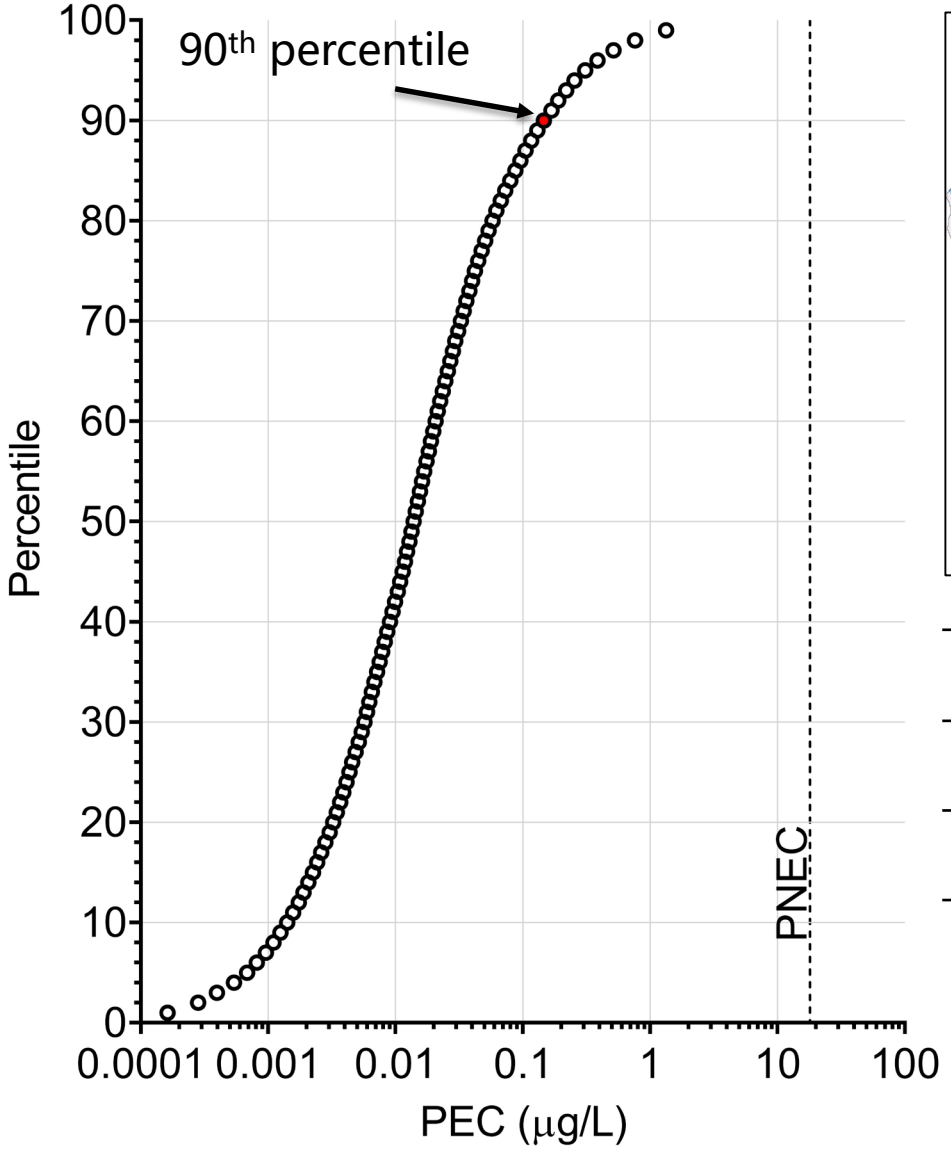
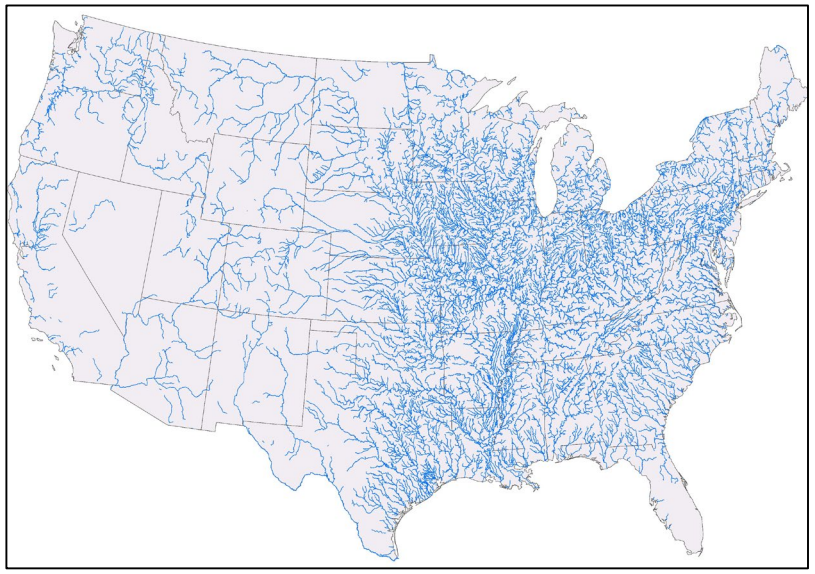
iSTREEM® exposure results: Oxybenzone





U.S. PEC Percentile (µg/L)				PNEC
25th	50th	75th	90th	(µg/L)
0.004	0.01	0.04	0.15	18

Mid-point of dataset

Risk assessment 'reasonable worst-case'

4. Burns et al. (2021). National scale down-the-drain environmental risk assessment of oxybenzone in the United States. *IEAM*. https://doi.org/10.1002/ieam.4430

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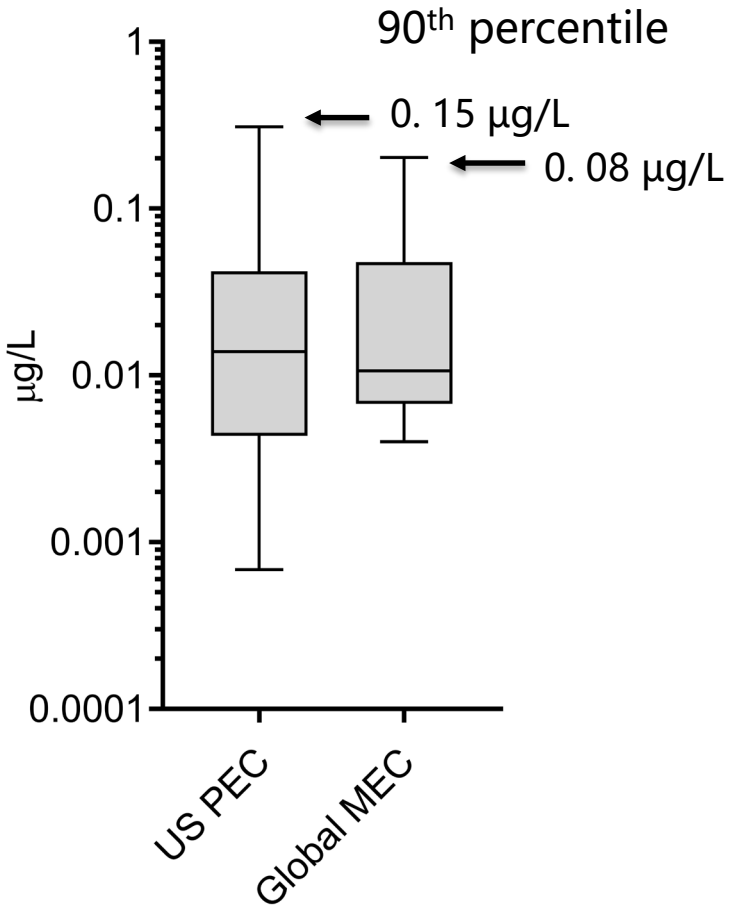
iSTREEM® exposure results: comparison with monitoring data (MEC)



MECs representing modeled exposure scenario

Limited U.S. freshwater data

- Representative of direct discharge

Global monitoring data used comparison in lieu of U.S. data. Predictions are:

- Reasonable and not unrealistic
- Conservative

100% down-the-drain assumption was determined to be protective

Direct discharge exposure scenario : Freshwater monitoring data

Three southwest U.S. rivers[5]

Concentrations below limit of detection (0.05 µg/L)

- Upstream of recreation
- After recreation ceased (e.g. evening or next day)

→ Background concentration

- aligns with iSTREEM® predictions

Estimated 90th percentile measured concentration of 0.68 µg/L **during** recreation

Direct discharge leads to short-term concentration pulses

Not representative of the long-term down-the-drain modeled scenario

5. Rand et al. (2020)

Direct discharge exposure scenario : Marine monitoring data

U.S. Virgin Islands – Trunk Bay

Maximum concentration of 6.1 µg/L measured

- Observed concentrations exponentially decrease with distance from shore

France – Marseille, Prophète Beach

BP-3 detected in bathing zone during recreation

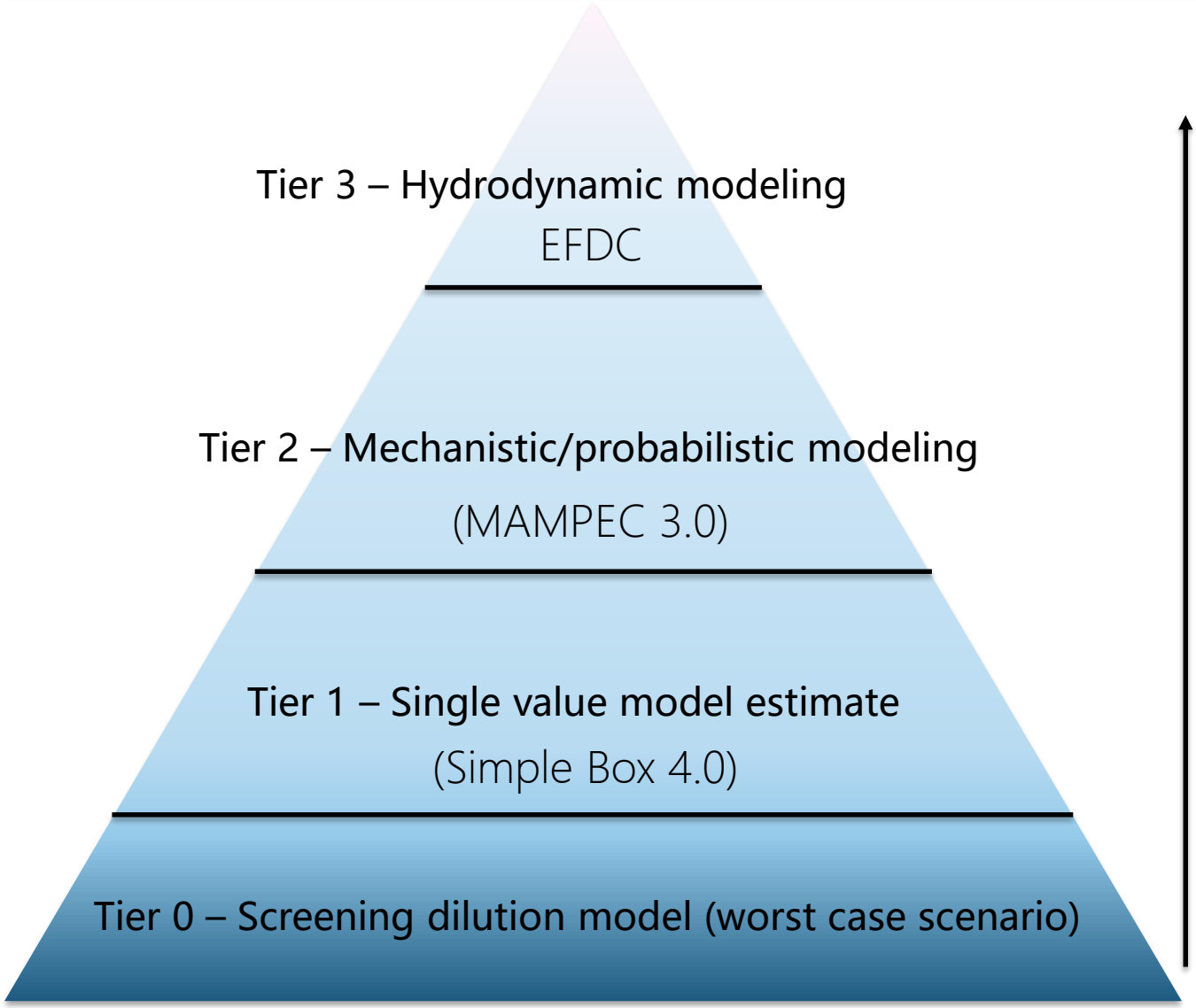
- Not detected prior to or next morning after recreation
- Not detected beyond bathing zone

Direct discharge leads to short-term concentration pulses

Modeling of direct discharge scenario needed for marine environment

6. Bargar et al. 2015
7. Labille et al. 2020

Marine exposure modeling: Direct discharge



Environmental realism
Data demand
Expert knowledge

8. Maples-Reynolds et al. (2021)

Conclusions

Two main exposure scenarios to consider when modeling:

Down-the-drain

- Emissions from both daily use and sunscreen
- Data indicate UV filters are moderately to well removed in wastewater treatment
- Model predictions are realistic yet conservative[4,9]

PCPC ESC published method for predicting down-the-drain exposure in U.S. freshwater and conducting ERA for BP-3[4]

Work is on-going for assessment of remaining UV filters

Direct recreational release

- Refine assumptions (e.g., fraction washed-off)
- Temporal pulses
- Localized

Marine exposure modelling framework developed

Work is on-going to develop marine exposure assessment

4. Burns et al. (2021)
9. Kapo et al. (2016)

References

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Thank you!

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