Environmental exposure and risk assessment for formulated consumer products

INTRODUCTION
Instructors

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What we will cover

• MODULE 1: Introduction to risk assessment
• MODULE 2: Assessment of aquatic environmental exposure for ingredients in formulated consumer products
• MODULE 3: Approaches to aquatic environmental exposure modeling
• MODULE 4: Modeling aquatic environmental exposure using iSTREEM
• MODULE 5: Case studies
What we will emphasize...

• Tiered exposure assessment
• Aquatic environmental exposure assessment
• Aquatic environmental exposure modeling
  • Use and application of the iSTREEM model
  • Case studies using iSTREEM
We will not emphasize...

• Hazard assessment or hazard characterization
• Exposure assessment for other environmental “compartments” (air, soil, sediment)
• Assessment of exposure to chemicals in “articles” (e.g., furniture, toys, building materials,...)
Resources

• Slide decks for each module
• Consumer Product Ingredient Safety
• Articles
  - HESI Risk21: Roadmap and Matrix (Embry et al., 2014)
  - ScenAT (Hodges et al., 2012)
  - iSTREEM (Kapo et al., 2016)
  - HydroROUT (Grill et al., 2016)
What we hope you will get out of the course

• The basics of risk assessment
• An understanding of environmental exposure assessment for formulated consumer products
• The ability to conduct simple analyses
• A knowledge of some resources and the ability to find others
Agenda

• Introduction 1:00 – 1:15 pm
• Introduction to risk assessment 1:15 – 1:45 pm
• Assessment of aquatic environmental exposure for ingredients in formulated consumer products 1:45 – 2:15 pm
• Approaches to aquatic environmental exposure modeling 2:15 – 3:15 pm

BREAK 3:15 – 3:45 pm

• Modeling aquatic environmental exposure 3:45 – 4:20 pm
• Case studies 4:20 – 4:45 pm
• Q & A 4:45 – 5:00 pm
Environmental exposure and risk assessment for formulated consumer products

MODULE 1:
Introduction to Risk Assessment
Overview

• What is risk assessment?
• Elements of risk assessment
• Other considerations in risk assessment
  • Intake vs. Dose
  • Variability/Uncertainty
  • Tiering
What is Risk Assessment?

A process to aid decision-making on sites and situations

- What chemicals are present, and of concern?
- What are safe levels of these chemicals?
- What effects are associated with these chemicals?
- How are people or critters exposed to these chemicals? (HHRA vs. ERA)
- How likely are negative health effects on this site?
- Or associated with this situation?
Understanding Risk

Risk is the probability of an adverse outcome

Quantitative vs. qualitative
Risk Assessment should be quantitative!

What is Risk Assessment?

Five elements (simplest form):
1) Data collection
2) Hazard assessment
3) Dose-response assessment
4) Exposure assessment
5) Risk characterization
What is Risk Assessment?

Five elements (simplest form):

1) Data collection

2) Hazard assessment

3) Dose-response assessment

4) Exposure assessment

5) Risk characterization

These were the “Four Steps of Risk Assessment”
What is Risk Assessment?

Five elements (simplest form):

1) Data collection
2) Hazard assessment
3) Dose-response assessment
4) Exposure assessment
5) Risk characterization

These are often considered “toxicity assessment” or “hazard assessment”
• Scoping
• Problem formulation
• Making it fit for purpose
• Inform decision-making
• Community engagement
Problem Formulation

• Priority Setting: What chemicals are of greatest concern?
  o What is the hazard of concern?
  o What is the source of the hazard?

• How does exposure occur?
  • Pathways
  • Routes of exposure

• What data is required to draw a conclusion?
  • Predetermination of data needs (precision)

• What data is already available?
New Paradigms

• Fit-for-purpose
  o Conservation of resources (far too many needs vs. availability of resources)

• Scoping
  o Previously incorporated into exposure and hazard/toxicity assessment

• Problem Formulation
  o More specific approach to data needs
Step by Step Risk Assessment

1) Data collection

2) Hazard assessment

3) Dose-response assessment

4) Exposure assessment

5) Risk characterization
Data Collection

What media are we interested in?

- Ambient air, workspace air, vehicle exhaust, particulates, surface water, groundwater, drinking water, wastewater, sediment, soil, process sludge, dust, food, etc.

Iterative process: you’ll start off with a base set of data, then as you go through the RA, you’ll figure out new info you need – so you’ll do more sampling.

- What data will give you what you need to make a decision about exposure or toxicity?
Step by Step Risk Assessment

1) Data collection

2) Hazard assessment

3) Dose-response assessment

4) Exposure assessment

5) Risk characterization
Hazard Assessment

Hazard: a condition that may pose human/ecological health problems under certain circumstances

- Toxicity assessment (what adverse outcomes might be caused by exposure to a chemical)

Risk is the probability of a hazard causing an adverse outcome

Thus: HAZARD AND RISK ARE NOT EQUIVALENT
Hazard Assessment/Scoping

Chemicals of Potential Concern: COPCs

Environmental contaminants:
• PAHs, PCDD/Fs, PCBs, heavy metals, BTEX, pesticides, solvents

Consumer product ingredients:
• Dyes, fragrances, solvents, surfactants, emollients, antimicrobials
Hazard Assessment

• Ultimate question: Does the chemical have the potential to cause adverse ecological effects?

• Answer:

  1) Look at existing data (acute and chronic testing; fish, invertebrates, algae, etc.)

  2) Perform new studies
Hazard Assessment (Human)

• Carcinogenic
  o Cancer: lung, liver, nasal, leukemia, bladder, breast

• Non-carcinogenic
  o Neurological
  o Immunological
  o Sensitization/irritation

• Can cause both: Cr(VI) – lung cancer, septum perforation; styrene (many others)

• Threshold vs. non-threshold mode of action
Step by Step Risk Assessment

1) Data collection

2) Hazard assessment

3) Dose-response assessment

4) Exposure assessment

5) Risk characterization
Dose-Response Assessment

- Toxicity: a dose level produces an effect
  - Cancer vs. non-cancer health effects

- What doses are safe, if any?

- Information from animal testing

- Establishment of criteria values
  - Pre-existing safety values
    - EPA, ATSDR, ACGIH, state DNR/EPA/DOH, etc.
Dose-Response Assessment

Effect (weight loss)

Dose (mg/kg)

LOAEL

NOAEL
Dose-Response Assessment

- Criteria values in risk assessment
  - RfD: Reference dose (oral) [endpoint-specific]
  - RfC: Reference concentration (inhalation)
  - CSF: Cancer slope factor
  - ESL: Effect screening levels: soil, water, fish
  - PNEC: Predicted no-effect concentration
Step by Step Risk Assessment

1) Data collection
2) Hazard assessment
3) Dose-response assessment
4) Exposure assessment
5) Risk characterization
Exposure Assessment

• Exposure: how do “receptors” come into contact with the potential hazards?

• Routes of exposure
  o Inhalation
  o Oral (ingestion)
  o Dermal (skin contact)
Exposure Pathways

Figure 6-2. Site Conceptual Model—Exposure Pathway Schematic

Exposure Assessment

- Exposure scenarios
  - What are the specific conditions of exposure?

- Routes: Inhalation, oral, dermal

- Frequency: How often do people/critters come into contact with the COPCs?

- Duration: How long are people/critters exposed?

- Magnitude: To what doses are they exposed?
Exposure Assessment
(Freshwater Environment)

\[
\text{PEC} = \frac{Q \times Cf \times (1-R)}{365 \times WW \times POP \times DF}
\]

PEC:  Predicted environmental concentration, surface water (mg/L)
Q:    Use rate (kg/year)
Cf:   Conversion factor (10^{-6} kg/mg)
R:    Removal rate (unitless)
WW:   Per capita wastewater generation rate (gallons per cap. per day)
POP:  Population served
DF:   Dilution factor (dimensionless)
Intake vs. Dose

• Intake: the quantity/mass of a COPC that enters the organism
  o “Administered dose”
  o “Applied dose”

• Absorbed dose: the quantity/mass of a COPC that is actually absorbed by the organism
  o Bioavailability
  o Gut/skin/eye/lung absorption

• Realized dose?
Step by Step Risk Assessment

1) Data collection

2) Hazard assessment

3) Dose-response assessment

4) Exposure assessment

5) Risk characterization
Risk Characterization

• Risk: The probability of adverse outcomes

\[
\frac{\text{Exposure concentration}}{\text{Safety level}} = \text{Risk ratio}
\]

• Aka Hazard Quotient (may be protective but no necessarily predictive)
• Sites: How do we achieve a safe level of a COPC?
  ○ Remediation: excavation, treatment in situ
  ○ No-action alternatives: natural attenuation, cap in place, etc.
Variability vs. Uncertainty

Uncertainty: Things we don’t know; lack of perfect knowledge.

Variability: “Real and identifiable differences between individuals in a population.”

Obviously, there is overlap between these two concepts – and uncertainty analysis almost always includes dealing with variability.
Tiered Risk Assessment

Tier 3 Advanced PRA
2-D MCA
Probabilistic Sensitivity Analysis
(Microexposure Modeling, Bayesian Statistics, Geostatistics)

Tier 2 PRA
1-D MCA
Probabilistic Sensitivity Analysis

Tier 1 Point Estimate Risk Assessment
Point Estimate Sensitivity Analysis

Problem Formulation/Scoping/Work Planning/Data Collection

Complete RI/FS Process

Increasing Complexity/Resource Requirements
Characterization of Variability and/or Uncertainty
Tiered Approach to Assessment

- Tiered process maximizes efficiency
- Achieve a desired and realistic level of protection with progressively less uncertainty

Adapted from K. Woodburn, Dow Performance Silicones
Summary

• Fundamental steps of traditional risk assessment:
  o Exposure assessment
  o Toxicity assessment (hazard, dose-response)
  o Risk characterization

• Renewed focus on scoping and problem formulation via EPA and RISK21 frameworks
Environmental exposure and risk assessment for formulated consumer products

MODULE 2:
Assessment of aquatic environmental exposure for ingredients in formulated consumer products
Overview

• Environmental exposure assessment framework
• Tier exposure assessment approaches
• Calculating the PEC (load ÷ dilution)
• Elements influencing PEC calculation
ACI Consumer Product Environmental Exposure Assessment Framework

• Assumptions
  – Products are nationally distributed
  – Products are very evenly distributed
  – Product use is attributed to households (as opposed to businesses)

• Variability in distribution can be addressed
ACI Consumer Product Environmental Exposure Assessment Framework

• Majority of releases occur as disposal “down-the-drain” following consumer use
• Waste from homes is piped to a WWTP or treated by a septic system
• The greatest environmental risk is to biota in freshwater streams receiving WWTP effluent
  — Generally lower dilution than lake/ocean releases
  — Biota may not be able to migrate from exposure
Environmental Fate of Consumer Product Ingredients

Municipal Wastewater Treatment Plants

Onsite Treatment

Household Wastewater

Direct Discharge

Biosolids

Effluent

Soils

Surface waters

Ground water

Drinking water
Risk Assessment

• Identification and quantification of the risk
• Resulting from a specific use or occurrence of a chemical or physical agent
• Taking into account possible harmful effects on individuals or populations
• Exposed to the agent in the amount and manner proposed and through all possible routes of exposure
Ecological Risk

• Comparing toxicity information and the amount of the chemical a given organism may be exposed to in the environment is called risk assessment

• A chemical can be toxic at one exposure level, and have little or no effect at another

• Risk is the intersection of exposure and effects

• Environmental exposure may have a geospatial component
Ecological Risk Assessment Framework

- Planning (Risk Assessor/Risk Manager/Interested Parties Dialogue)
- Problem Formulation
  - Analysis
    - Characterization of exposure
    - Characterization of effects
- Risk Characterization
  - Communicating Results to the Risk Manager
  - Risk Management and Communicating Risks to Interested Parties

Tiered Risk Assessment Approach

- Tiered system efficiently allocates resources to assessment efforts of varying complexities and potential risks
- Lower tiers use extremely conservative assumptions used to screen out negligible risks
- When a chemical is not predicted to cause adverse effects on the environment at screening level, the possibility of harming the environment is low
- Higher level tiers incorporate additional information to refine the exposure profile based on more realistic situations
Deterministic Risk Assessment

- Ratio of toxicant exposure concentration to a reference value regarded as corresponding to a threshold of toxicity
- Exposure typically determined from models (monitoring not usually available)
- Toxicity typically determined from laboratory studies for standard test species
- Risk often compared to Level of Concern (LOC) (safety factor, margin of safety, or assessment factor)
U.S. Environmental Protection Agency

• Deterministic risk assessment uses Risk Quotient (RQ)
  \[ RQ = \frac{\text{exposure}}{\text{toxicity}} \]

• Example:
  – Exposure: estimated environmental concentration (EEC) = 10 ug/L
  – Toxicity: LC50 for most sensitive freshwater fish = 11 ug/L
    \( \text{(LC50 = concentration causing 50% mortality of population)} \)
  – For acute risk the level of concern (LOC) = 0.5

\[
RQ = \frac{\text{EEC}}{\text{LC50}}
\]
\[
RQ = \frac{10 \text{ ug/L}}{11 \text{ ug/L}}
\]
\[
RQ = 0.91
\]
Since \( RQ > LOC \), the risk is unacceptable

RQ calculated for acute (e.g., LC50) and chronic (e.g., NOEC) toxicity value for most sensitive species in each taxonomic group (e.g., fish, invertebrates, aquatic plants)
Probabilistic Assessment

• Standard assumptions/scenarios can only account for certain variability and by necessity are designed to be protective

• Probabilistic approaches can be used to help refine our understanding of environmental exposure by characterizing the interaction of important factors and their variability in the environment

• They can be used to refine assumptions in lower-tier assessments

• Probabilistic assessments quantify one or more sources of variability and/or uncertainty
Benefits and Costs

• Probabilistic approaches in risk assessment provide a better understanding of what the real world looks like
• It puts risk into context
• It allows researchers and regulators to focus on areas of greatest concern such as where to conduct monitoring studies or implement mitigation
Tiers for Ecological Exposure Assessment

**Tier 1**
- Conservative assumptions
  - Single national production volume
  - Single WWTP removal rate
  - No dilution
- Tools
  - Simple equations
  - E-FAST

**Tier 2**
- More detailed inputs
  - National/regional use rates
  - Variable WWTP removal rates
  - Stream dilution
- Tools
  - Market forensics
  - SimpleTreat/ASTreat
  - iSTREEM®

**Tier 3**
- Detailed modeling & monitoring
  - Use rates in specific markets
  - Watershed-specific modeling and monitoring
- Tools
  - iSTREEM®
  - Field monitoring data

Approach: Broad evaluation

Approach: Specific, detailed focus
US Environmental Protection Agency
Tiered Process

- **Tier I**: Initial Worst-case Screening
- **Tier II**: Multiple High-exposure Scenarios
- **Tier III**: Spatial/temporal Modeling
- **Tier IV**: Site Specific Analysis

**Actual Concentration Range**

**Exposure Concentration**

**Frequency of Occurrence**

- 90th centile
Exposure Refinement

Cumulative Frequency (%) vs. Concentration (µg/L)

Tier 1
Tier 2
Tier 3
Tier 4
Calculating Environmental Concentrations

• Screening level
  – Spreadsheet
  – Computer model (simple)

• Refined
  – Computer model
  – Incorporates larger range of data
  – Often includes spatial and temporal variability
US FDA Exposure Assessment Guidance
Expected Introduction Concentration (EIC)*

\[
EIC_{aquatic} = \frac{A \cdot D}{B \cdot C} = \frac{\text{Annual production volume}}{\text{Annual WWTP effluent volume}} = \frac{\text{Load}}{\text{Dilution}}
\]

- A = kg/year production volume of the substance
- B = liters per day entering POTWs **
- C = 365 days
- D = \(10^6\) mg/kg (conversion factor)

Assumptions:
- Even distribution of the substance throughout the U.S. per day
- Total consumption/use of the substance (100% released to WWTP)
- No human metabolism nor environmental depletion mechanisms in WWT process

**The total flow of wastewater to POTWs in the United States is 32,345 million gallons per day (1.22 \(\times\) \(10^{11}\) liters per day) for a total population served of 226,302,213. USEPA Clean Watersheds Needs Survey (CWNS) 2008 Report to Congress, Appendix I, Table I-3.

ACI Exposure Assessment Framework
Predicted Environmental Concentration (PEC)

\[
P_E = \frac{Q \times C_f (1 - R)}{365 \times WW \times POP \times DF}
\]

- **Q** = quantity of substance used (kg/year)
- **Cf** = 10⁶; conversion factor (kg to mg)
- **R** = fraction of chemical removed by WWTP
- **WW** = per cap. wastewater generation (L/cap/day)
- **POP** = population served
- **DF** = dilution factor of the receiving water

Load (in effluent) following removal by WWTP
\(\text{DF} = 36,500,000,000\)
\(\text{PEC} = 2.74\text{ mg/L}\)

Dilution by effluent plus the receiving stream

\(\text{PEC} = \frac{Q \times C_f (1 - R)}{365 \times WW \times POP \times DF}\)
User Inputs for PEC calculation

\[ \text{PEC} = \frac{Q \times Cf (1 - R)}{365 \times WW \times \text{POP} \times DF} \]

- Chemical load
- Chemical removal
- Dilution factor
- In-river decay (optional)
How do I determine the load?

• Are you interested in just your product?
  – Use your market volume projection
  – Use national or regional sales data for particular products
  – Derive national or regional use rates

• Are you interested in the entire market?
  – Obtain a market survey for the material
  – Examples of sources: IRI, Euromonitor, Neilsen Scantrack®, Chemical Economics Handbook
  – However, this approach may significantly over estimate the WWTP load where there are uses beyond formulated consumer products \( \rightarrow \) think TiO\(_2\)
Determining Load

• Production volume compared to wastewater load
  – Mass is likely comparable
    • An ingredient in shower gel, shampoo, or laundry detergent
  – Probable difference in mass produced vs. down the drain
    • Titanium dioxide (variable uses as a pigment in paints, sunscreen and food coloring)
    • An ingredient in pet shampoo (depends on whether pet is bathed indoors or outdoors)
    • An ingredient in household hard surface cleaners in which only a portion goes down the drain and a portion is wiped up (and the wipe thrown in the trash)
What is the anthropogenic input from a consumer product?

WWTP load = Population served × Per capita use rate

Use market data to derive the per capita use rate (commonly used as: g / cap / day)
Determining Load via Market Volume

Simple form:

\[
\text{Per Capita Daily Load} = \frac{\text{Production Volume (kg)} \times 1000 \; \text{g/kg}}{\text{Population}} / 365 \; \text{days}
\]

More involved example (insect repellent DEET):

- Total annual use of 9.2 million pounds (4,173,046 kg) for the US (USEPA)
- Population of 311,580,000 (www.census.gov)
- The annual loading was applied over 9-month period to represent the insect control season
- In-use DEET is 10% absorbed and 25% volatilized, therefore 65% is assumed to be left on the skin available for washing off (Aronson et al., 2012)
- Net per-capita load is 0.0318 g / person / day

\[
\text{Load} = \frac{4,173,046 \; \text{kg} \times 1000 \; \text{g/kg}}{311,358,000} / 274 \; \text{days} * 65\% \text{ available}
\]

\[= 0.0318 \; \text{g/cap/day}\]
Calculate Load from Monitoring Studies

• Using influent or effluent monitoring data

• Assumptions about:
  – Population served
  – Per capita water use / influent volume
  – Removal rate (for effluent studies)
  – Representativeness of facility selection
Case Study: Regional Market Survey
Alcohol-based Ingredients

• Numerous alcohol-based surfactants
  – Nonionic
    • Alcohol ethoxylate (AE)
  – Anionic
    • Alcohol sulfates (AS)
    • Alcohol ethoxysulfates (AES)
• Free alcohols
Detailed Field Study of Alcohol-Based Surfactants
Hawksbill Creek Watershed, Luray, VA
IRI Grocery Store Data Markets
National Product Market Information

• Major Formulated Consumer Products (>4,000 products)
  – Liquid Laundry Detergent (177)
  – Powdered Laundry Detergent (90)
  – Hand/Body Hygiene Products (1668)
  – Fabric Softener (148)
  – Hand Dish Detergent (129)
  – Shampoo (1459)
  – Automatic Dish Detergent (66)
  – Deodorant (335)
## Number of Products per Market

<table>
<thead>
<tr>
<th>Product</th>
<th>National</th>
<th>Oklahoma</th>
<th>Portland</th>
<th>Cleveland</th>
<th>Roanoke</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Laundry Detergent</td>
<td>177</td>
<td>72</td>
<td>76</td>
<td>76</td>
<td>67</td>
</tr>
<tr>
<td>Powdered Laundry Detergent</td>
<td>90</td>
<td>51</td>
<td>41</td>
<td>40</td>
<td>36</td>
</tr>
<tr>
<td>Fabric Softener</td>
<td>148</td>
<td>83</td>
<td>69</td>
<td>80</td>
<td>79</td>
</tr>
<tr>
<td>Hand Dish Detergent</td>
<td>129</td>
<td>51</td>
<td>48</td>
<td>53</td>
<td>55</td>
</tr>
<tr>
<td>Automatic Dish Detergent</td>
<td>66</td>
<td>44</td>
<td>36</td>
<td>37</td>
<td>44</td>
</tr>
<tr>
<td>Hand/Body Hygiene Products</td>
<td>1668</td>
<td>608</td>
<td>643</td>
<td>619</td>
<td>629</td>
</tr>
<tr>
<td>Shampoo</td>
<td>1459</td>
<td>639</td>
<td>587</td>
<td>665</td>
<td>662</td>
</tr>
<tr>
<td>Deodorant</td>
<td>335</td>
<td>187</td>
<td>176</td>
<td>185</td>
<td>189</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>4,072</strong></td>
<td><strong>1,735</strong></td>
<td><strong>1,676</strong></td>
<td><strong>1,755</strong></td>
<td><strong>1,761</strong></td>
</tr>
</tbody>
</table>
Distribution of Products in US – 2012
(10.6 billion lb.)

- Liquid Laundry Detergent
- Powdered Laundry Detergent
- Fabric Softener
- Hand Dish Detergent
- Automatic Dish Detergent
- Hand/Body Hygiene Products
- Shampoo
- Deodorant
Product Information – Roanoke Market
(10/5/2008 - 3/22/2009)

• Categories (>1,000 products)
  – Liquid Laundry Detergent (58)
  – Powdered Laundry Detergent (27)
  – Fabric Softener (38)
  – Hand Dish Detergent (53)
  – Automatic Dish Detergent (33)
  – Liquid Hand Soap (77)
  – Shampoo (474)
  – Deodorant (157)
Leading Brands + Private Label

From 1,000 products, 82.5% of the market volume is captured in 23 branded products (including flankers) and 5 private label product areas.

## Alcohols Use in Roanoke Market

<table>
<thead>
<tr>
<th>Product</th>
<th>Market Volume (Units)</th>
<th>Unit Size</th>
<th>B Grams per unit</th>
<th>C Mean Alcohols Content* (%)</th>
<th>A ∙ B ∙ C Mass Alcohols (grams)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid Laundry Detergent</td>
<td>14,574,437</td>
<td>16 oz. eq</td>
<td>453.6</td>
<td>15.0%</td>
<td>991,644,662</td>
</tr>
<tr>
<td>Powdered Laundry Detergent</td>
<td>3,276,490</td>
<td>16 oz. eq</td>
<td>453.6</td>
<td>3.0%</td>
<td>44,586,469</td>
</tr>
<tr>
<td>Hand Dish Detergent</td>
<td>3,301,954</td>
<td>16 oz. eq</td>
<td>453.6</td>
<td>25.0%</td>
<td>374,441,636</td>
</tr>
<tr>
<td>Liquid Hand Soap</td>
<td>729,995</td>
<td>16 oz. eq</td>
<td>453.6</td>
<td>10.0%</td>
<td>33,112,577</td>
</tr>
<tr>
<td>Shampoo</td>
<td>763,948</td>
<td>16 oz. eq</td>
<td>453.6</td>
<td>30.0%</td>
<td>103,958,089</td>
</tr>
<tr>
<td>Deodorant</td>
<td>718,723</td>
<td>75 grams</td>
<td>75</td>
<td>17.5%</td>
<td>9,433,234</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>1,557,176,667</strong></td>
<td></td>
<td></td>
<td></td>
<td><strong>1,557,176,667</strong></td>
</tr>
</tbody>
</table>

Per Capita Contribution in Roanoke Market

• Total consumer products: 10,327 metric tons
  – Total alcohols in products sold: 1,557,176,667 g
• Survey period: 24 weeks (168 days)
• Population: 2,291,845
• Per capita use products: 26.82 g/cap/day
  – Per capita alcohol contribution: 4.0 g/cap/day
Geographic Product Use Comparison

<table>
<thead>
<tr>
<th>Market Region</th>
<th>Per capita use rate (g per capita per day)</th>
<th>% of national average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Entire United States</td>
<td>47.6</td>
<td></td>
</tr>
<tr>
<td>Cleveland market</td>
<td>20.0</td>
<td>42.0%</td>
</tr>
<tr>
<td>Oklahoma (entire state)</td>
<td>24.6</td>
<td>51.7%</td>
</tr>
<tr>
<td>Portland market</td>
<td>12.6</td>
<td>26.5%</td>
</tr>
<tr>
<td><strong>Roanoke market</strong></td>
<td><strong>26.8</strong></td>
<td><strong>56.3%</strong></td>
</tr>
</tbody>
</table>

• There is regional variability in product use
US Median Household Income

Market % of National
- Roanoke – 79.1%
- Oklahoma – 85.6%
- Cleveland – 94.4%
- Portland – 102.4%

Median household income in 2009 by county


The data provided are indirect estimates produced by statistical model-based methods using sample survey, decennial census, and administrative data sources. The estimates contain error stemming from model error, sampling error, and nonsampling error.
Tier 2 Loading Estimation

• Analysis of market data is a cheap/easy way to quantify potential environmental exposure

• Analysis of market data can provide additional insights regarding variability of use:
  – Regional distribution
  – Seasonality
    • Sunscreen
    • Bug repellant
How do I determine removal rate?

• Laboratory testing (e.g., OECD, EPA guideline)
  – Readily biodegradable
  – Inherently biodegradable
• Bench scale studies
• Influent / effluent studies
• Estimation based on phys/chemical properties
  – Models such as SimpleTreat, ASTREAT
• Will be different depending on treatment type
Wastewater Treatment Type - Trends

Figure ES-2. Population served by POTWs nationwide for select years between 1940 and 2008 and projected (if all needs are met), organized by wastewater treatment type.
Source: U.S. Public Health Service and EPA Clean Watersheds Needs Surveys
How do I determine dilution?

• Conservative assumptions (no dilution)
• Use of public data sets
  – Link facility flow with river flow
    • E.g., EPA CWNS and USGS RF1 / NHD or gaging data
  – Information from discharge permits
• Many existing tools have dilution factors built-in
How do I determine decay?

- Laboratory testing (e.g., OECD, EPA guideline)
- Bench scale studies
- Field-based studies
- Estimation based on phys/chemical properties

Example:
- DEET in the stream and river system is assumed to decline at a rate of 0.0234 day-1 based on an OECD 301D study. This value is an intermediate among several results that have been reported (Weeks et al., 2012; Aronson et al., 2012).
Summary

• The framework for exposure assessment of consumer product ingredients is simple but provides versatility in scope and application
• Using a tiered approach permits conservative or refined assessment
• The refined approach to estimation of predicted environmental concentration (PEC) will require a number of assessment parameters to be determined
Exposure and risk assessment for formulated consumer products

MODULE 3:
Approaches to aquatic environmental exposure modeling
Many approaches to modeling aquatic exposure to down-the-drain chemicals

- **Screening-level**
  - E-FAST (US)
  - EUSES (EU)

- **Higher tier**
  - CRAM* (Canada)
  - HydroROUT CFM* (St. Lawrence R.)
  - GREAT-ER (Europe)
  - STREAM-EU (Europe)
  - ScenAT* (World)
  - PhATE™* (US)
  - iSTREEM® (US + Ontario)

*Not publically available
E-FAST 2014 Down-the-Drain Model

E-FAST (2014)
Exposure and Fate Assessment Screening Tool

Select a Chemical ID and modify its physical-chemical and fate properties before continuing to any module.
E-FAST DtD – Define Chemical
E-FAST DtD – Select Module

E-FAST (2014)
Exposure and Fate Assessment Screening Tool

Select from one of the three modules below:

- General Population and Ecological Exposure From Industrial Releases
- Down The Drain
- Consumer Exposure Pathway

Exposed Population
- Adult
- Youth (age 16-20)
- Youth (age 11-15)
- Child (age 6-10)
- Small Child (age 3-5)
- Infant (age 1-2)
- Infant (age < 1)

Select Document Report Format
- Click here to select WordPerfect V. 5.1 and up.
- Microsoft Word

Chemical ID: tmpcas

Return to EFAST(2014) Main Page
E-FAST DtD – Specify Production Volume

Disposal Model

Chemical ID: kmpcas

Production Volume: 1.45E+04 kg/year
Exposure Duration: 30.00 years

PDM Option
- Run PDM (SIC Code Analysis)
- Do NOT run PDM (SIC Code Analysis)

Run the Disposal Model
Aquatic Exposure Estimates
Output Report File

<table>
<thead>
<tr>
<th>WWT REMOVAL (%)</th>
<th>PRODUCTION VOLUME (kg/yr)</th>
<th>HOUSEHOLD RELEASE DAYS</th>
<th>PRETREATMENT RELEASE (g/person/day)</th>
<th>POST-TREATMENT RELEASE (g/person/day)</th>
<th>BODY WEIGHT (kg)</th>
<th>BCF (L/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>90.00</td>
<td>1.45E+04</td>
<td>365.00</td>
<td>1.37E-04</td>
<td>1.37E-05</td>
<td>80.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<snip – removed drinking water and fish ingestion tables>

### 50th Percentile Aquatic Exposure Estimates - Surface Water

<table>
<thead>
<tr>
<th>DESCRIPTOR</th>
<th>Harmonic Mean</th>
<th>3Q5</th>
<th>7Q10</th>
<th>1Q10</th>
</tr>
</thead>
<tbody>
<tr>
<td>STREAM DILUTION FACTOR</td>
<td>134.85</td>
<td>39.66</td>
<td>24.22</td>
<td>20.08</td>
</tr>
<tr>
<td>CONCENTRATION (µg/L)</td>
<td>2.61E-04</td>
<td>8.88E-04</td>
<td>1.45E-03</td>
<td>1.75E-03</td>
</tr>
</tbody>
</table>

### 10th Percentile Aquatic Exposure Estimates - Surface Water

<table>
<thead>
<tr>
<th>DESCRIPTOR</th>
<th>Harmonic Mean</th>
<th>3Q5</th>
<th>7Q10</th>
<th>1Q10</th>
</tr>
</thead>
<tbody>
<tr>
<td>STREAM DILUTION FACTOR</td>
<td>7.95</td>
<td>1.80</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>CONCENTRATION (µg/L)</td>
<td>4.43E-03</td>
<td>1.96E-02</td>
<td>3.52E-02</td>
<td>3.52E-02</td>
</tr>
</tbody>
</table>
Surface Water Exposure – which flow / dilution factor?

<table>
<thead>
<tr>
<th>Descriptor</th>
<th>Use</th>
<th>50(^{th})-percentile Stream Dilution Factor</th>
<th>10(^{th})-percentile Stream Dilution Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>7Q10 (lowest 7-day flow over 10 years)</td>
<td>Potential chronic aquatic life impacts</td>
<td>24.22</td>
<td>1.00</td>
</tr>
<tr>
<td>1Q10 (lowest 1-day flow over 10 years)</td>
<td>Potential acute aquatic life impacts</td>
<td>20.08</td>
<td>1.00</td>
</tr>
<tr>
<td>30Q5 (lowest 30-day flow over 5 years)</td>
<td>Acute human exposure via drinking water</td>
<td>39.66</td>
<td>1.80</td>
</tr>
<tr>
<td>Harmonic Mean Flow</td>
<td>Chronic human exposure via drinking water and fish ingestion</td>
<td>134.85</td>
<td>7.95</td>
</tr>
</tbody>
</table>
E-FAST Surface Water Exposure Estimates

• PEC = \[\frac{Q \times Cf \times (1-R)}{365 \times WW \times POP \times DF}\]  
  \[\text{Load}\]  
  \[\text{Dilution}\]

• If DF = 1, then

\[EIC_{\text{aquatic}} = \frac{\text{Annual production volume}}{\text{Annual WWTP effluent volume}} = \frac{\text{Load}}{\text{Dilution}}\]

*EPA \rightarrow 1.13 \times 10^{11} \text{ Liters per day for 290,800,000 people} = 388 \text{ L/cap/day}

FDA \rightarrow 1.22 \times 10^{11} \text{ Liters per day for 226,302,213 people} = 539 \text{ L/cap/day}
E-FAST Probabilistic Dilution Model (PDM)

- Chemical ID: tmpcas
- Production Volume: 1.45E+04 kg/year
- Exposure Duration: 30.00 years
- PDM Option:
  - Run PDM (SIC Code Analysis)
  - Do NOT run PDM (SIC Code Analysis)
- Concentration of Concern:
  - Run #1: 0.00145 ug/L
  - Run #2: 0.00175 ug/L
  - Run #3: 0.005 ug/L
- Run the Disposal Model
E-FAST PDM Output

Disposal Results

- Production Volume: $1.45 \times 10^4$ kg/year
- WWT Removal: 90.00% 
- Release days: 365.00 days
- Bioconcentration Factor: 0.00 L/kg

Exposed Population: Adult

- Pretreatment release: $1.37 \times 10^{-4}$ g/person/day
- Post-treatment release: $1.37 \times 10^{-5}$ g/person/day

PDM Disposal Exposure Estimates

- Concentration of concern (ug/L):
  - High-end scenario: $1.45 \times 10^{-3}$
  - Average case scenario: $1.75 \times 10^{-3}$
  - Low-end scenario: $5.00 \times 10^{-3}$

- Number of days concentration of concern exceeded (days):
  - High-end scenario: 62.15 days
  - Average case scenario: 56.35 days
  - Low-end scenario: 30.34 days

- % of year concentration of concern exceeded (%):
  - High-end scenario: 17.03%
  - Average case scenario: 15.44%
  - Low-end scenario: 8.31%
E-FAST Surface Water Exposure Estimates

• Screening level
• E-FAST uses a very conservative approach
  – Assumes no stream dilution for ecological exposure (10th percentile dilution distribution)
  – Considers only mixing zone concentration (no downstream attenuation)
  – However, does not consider potential upstream sources of chemical
  – Variable dilution employed in PDM
European Union screening level exposure

• Specific legislation lays out requirements for down-the-drain environmental risk assessments in Europe
  – General chemicals: REACH
  – Biocides: Biocidal Products Regulation (BPR)
  – Human pharmaceuticals
  – Plant Protection Products

• Emissions calculated according to Emission Scenario Documents

• Calculations implemented in EUSES software

Special thanks to Paul Mason (SC Johnson) for use of these slides
Exposure Assessment

- Exposure can be calculated at local, regional and continental scale
Standard Local Environment

Wastewater Treatment Plant

- Wastewater
- Air
  - Volatilization
  - Sludge Application
- Agricultural Soil
  - Deposition
- Groundwater
- Surface Water
- Sediment
  - Leaching
  - Dilution

Predicted Environmental Concentration (PEC) calculated for each compartment
Standard Local Environment

- 10000 Inhabitants in wastewater catchment
- 4000 Houses
- 200 Litres of wastewater per person/day

Wastewater Treatment Plant
Standard Local Environment

- Influent volume 2,000,000 L/day
- Fate in WWTP estimated using SimpleTreat model (unless measured data are available)
- Assumed 100% connectivity at local scale
Standard Local Environment

\[ PEC_{\text{surface water}}: \]
- Dilution by a factor of 10 in surface water
- River with flow \(1.8 \times 10^6 \text{m}^3/\text{d}\)

\[ PEC_{\text{sediment}}: \]
- Instantaneous partitioning onto suspended sediment (15 mg/L, 10% OC)
- Freshly deposited
- No mixing with bulk sediment
- No temporal aspect (continuous emission)

Marine \( PEC_{\text{surface water}} \) & \( PEC_{\text{sediment}} \):
- Further dilution by factor of 10
Estimating Emissions

• Emission Scenario Documents (ESDs)
  – Key emission pathways/exposed compartments
  – Methodology for quantifying emissions
  – ESDs covering 19 product types including domestic products

Emission Estimation

Two key pieces of information

• The potential for environmental release
  – Emission fractions defined by ESDs

• The quantity of substance used
  – Consumption approach: quantity used per person per day
  – Tonnage approach: EU tonnage allocated to region / local level, fraction going down the drain, emission days, incorporates safety factors
Tonnage Approach

Default approach for general chemicals under REACH

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Input/Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relevant tonnage of substance in EU for this application (tonnes/yr)</td>
<td>TONNAGE</td>
<td>Applicant</td>
</tr>
<tr>
<td>Fraction for the region (wide dispersive uses)</td>
<td>$F_{\text{prodregion}}$</td>
<td>0.1</td>
</tr>
<tr>
<td>Fraction of the main source STP</td>
<td>$F_{\text{mainsource}}$</td>
<td>0.002</td>
</tr>
<tr>
<td>Fraction released to wastewater</td>
<td>$F_{\text{water}}$</td>
<td>ESD</td>
</tr>
<tr>
<td>Number of emission days for life cycle (worst case proposed)</td>
<td>$T_{\text{emission}}$</td>
<td>Applicant</td>
</tr>
</tbody>
</table>

Relevant tonnage in the region for this application (tonnes/yr):

$$TONNAGE_{\text{REG}} = TONNAGE \times F_{\text{prodregion}}$$

Local emission rate to wastewater (kg/d):

$$E_{\text{local\,water}} = TONNAGE_{\text{REG}} \times 10^3 \times F_{\text{mainsource}} \times F_{\text{water}}/T_{\text{emission}}$$
Tonnage-based Concepts

- \( F_{\text{prod\ region}} = \frac{\text{Population of Region}}{\text{Population of EU}} = \frac{20,000,000}{500,000,000} \times 2.5 = 0.1 \)

Tonnage-based Concepts

- Default fraction of the main local source \( (F_{\text{mainsource}}) \)

\[
F_{\text{mainsource}} = \frac{\text{Population connected to STP}}{\text{Population of region}} \times \text{SF} = \frac{10,000}{20,000,000} \times 4 = 0.002
\]

Higher Tier Models

– CRAM* (Canada)
– HydroROUT CFM* (St. Lawrence River Basin only)
– GREAT-ER (Europe)
– STREAM-EU (Europe)
– ScenAT (World)
– PhATE* (US)
– iSTREEM (US and Ontario)
– LF2000-WQX (UK)
– GWAVA (World)
– SESAME (China)

* Indicates model is not publicly available
Environment Canada
Consumer Release Aquatic Model (CRAM)

- Excel spreadsheet w/deterministic and probabilistic modes
- Probabilistic model estimates exposure using Monte Carlo simulation and:
  - Distribution information
    - Per person water discharge
    - Wastewater system treatment levels
    - Receiving water body type
    - Receiving water body flows (dilution factor, DF)
  - And deterministic parameters
    - Per capita consumption of consumer products
- PEC derived from effluent concentration & DF
  - Flowing water bodies DF capped at 10; static bodies DF = 10
HydroROUT Contaminant Fate Model

- Ontario, Quebec, and St. Lawrence River Basin (incl. NY and VT)
- Utilized HydroSHEDS hydrology (500m pixel), 11,426 reaches and 894 lakes
- Model includes individual locations, facility flow and population-served for 1198 WWTP facilities;
- User specifies an annual per capita consumption and fraction metabolized
- Includes treatment levels (none, primary, lagoon, sec/tert) provided for each individual facility; user specifies removal % per treatment level.
- Includes mean and low flow (Q90 approximated as lowest avg monthly flow over 30 years) based on surface runoff from WaterGAP
- User specifies first-order in-stream loss (k)
- No probabilistic component (corroboration activity used 500 MC runs)
- User structure and output format are unknown, model is proprietary


GREAT-ER

- 16 representative European watersheds
- Uses model-specific river network segments
- Model includes individual facility locations, and sizes.
- Probability density function of treatment removal % (range specified by user), as well as removal in sewer
- User specifies a per-capita use rate for one or more watersheds
- Probability density function of flow values
- User specifies first-order in-stream loss (k)
- Uses Monte-Carlo simulations for probabilistic approach
- Both stand alone and web-based tool
- Publicly available


STREAM-EU

- Application of model to Danube River Basin (2857 km), but could cover other areas in Europe
- Emissions by subcatchment – including soil (sludge) to surface water
- Does not include individual facilities, but uses % of population served by WWTP combined with population in subcatchments, using a constant emission per person
- Includes treatment level (three types) – primary, secondary/tertiary, none. % removal determined by effluent study.
- Danube catchment modeled with 4 approaches based on: population, wastewater, GDP, or a combination.
- Model can address up to 11 compartments and four phases
- Model is part of SOLUTIONS project


ScenAT

- Global coverage (88 countries)
- Processes at administrative unit level (e.g., county, province)
- Includes population and affordability class (per capita GDP)
- User specifies water use (urban and rural), ingredient volume, and inclusion (%) for products. Allocates chemical load based on socio-economic parameters
- User specifies a single WWTP treatment removal (%)
- Single flow scenario (mean annual)
- No in-stream loss (k) other than user can specify removal (%) for impact zone
- No probabilistic component
- Stand alone tool with output in Excel and mapping format
- Model is proprietary – Unilever


PhATE™

- 11 representative U.S. watersheds
- USEPA RF1 river network segments
- Model includes individual locations, facility flow and population-served for 1302 WWTP facilities; user specifies an annual national production volume for a chemical (kg/yr)
- Includes treatment level (five types) provided for each individual facility; user specifies removal % per treatment level.
- Includes mean and low (7Q10) flow scenarios
- User specifies first-order in-stream loss (k)
- No probabilistic component
- Stand alone tool with output in MS Access format
- Model is proprietary – PhARMA organization

iSTREEM®

- US national coverage + southern Ontario, several refined catchments
- USEPA RF1 river network segments
- Model includes individual locations, facility flow and population-served for >10,000 WWTP facilities; user specifies a national or market region-specific chemical loading factor (g/cap/day)
- Model includes treatment process (for six types) provided for each individual facility; user specifies removal (%) per treatment type.
- Includes mean and low (7Q10) flow scenarios
- User specifies first-order in-stream loss (k)
- No probabilistic component
- Web-based tool with output in database (*.dbf), ESRI geodatabase and web map interface
- Model is publicly available (www.iSTREEM.org)


iSTREEM® Model

• iSTREEM®
  – Allows for site-specific dilution factors (mean and low flow conditions)
  – Reports effluent, mixing zone, and downstream concentrations (including in-stream decay)
  – Accounts for upstream sources
Model History

• Origins tracing back to the 1980s and the algorithms used in USEPA’s Water Use Improvement and Impairment model (WUI2)
• The core of the model (ROUT) was developed by The Procter & Gamble Company
• Originally in a mainframe environment but later converted to an enterprise-based intranet system with a GIS interface (GIS-ROUT)
• In 2010 a web-based version of GIS-ROUT has been supported and made available to the public by ACI as iSTREEM®, implemented and hosted by the University of Cincinnati
• In 2013, enhancements to the underlying data, user interface and output were initiated, moved to a new server, and new domain created with access at www.iSTREEM.org
• 2015/6 has seen upgrades in progress to underlying data, and transition to a new hydrologic network based on the NHDPlus dataset: iSTREEM® 2.0 (to be released in Q1 2017)
Model Framework

- Web browser interface for user input, visualization using web mapping services, and accessing and downloading results
- Model runs performed on server, stored for later retrieval
  - iSTREEM® web application (www.istreem.org)
iSTREEM® Model

\[ PEC = \frac{Q \times Cf (1 - R)}{365 \times WW \times POP \times DF} \]

- Q = quantity of substance used \( \rightarrow \) Allow for regional use variability
- \( Cf = 10^6 \); conversion factor (kg to mg)
- R = fraction of chemical removed by WWTP \( \rightarrow \) Allow for variable efficiency for different WWT technologies
- WW = per capita wastewater generation
- POP = population served
- DF = dilution factor of the receiving water \( \rightarrow \) Allow for site specific dilution, and mean & low stream flow

\( \rightarrow \) Calculate dilution factors (concentrations) for 10,000’s of receiving streams and include impact of stream networks
iSTREEM® Model Overview

**Influent to WWTP**
(per capita use x population served)

**Inputs to segment**
- WWTP Effluent
- Upstream Input
- Tributary Input

**WWTP Effluent**
Calculates effluent concentration

**Removal in WWTP**
(e.g., to biosolids)

**Loss within segment**
- Biodegradation
- Adsorption
- Burial

**Calculates concentration for all effluent-impacted streams**

**Calculates concentration for abstraction points (DWI)**
Algorithm

U.S. EPA WUI2 model algorithms

Customized user inputs:
- Per-capita usage
- Treatment efficacy
- In-stream decay

Model background data (WWTPs, river network)

(See Wang et al. 2005 for algorithm details)
Trend and distribution of treatment types in US

- Primary (“less than secondary”) accounts for <2% of 2008 population served
- Secondary: 41%
- Tertiary (“greater than secondary”): 50%
- From 2008 EPA Clean Watershed Needs Survey report to Congress

Figure ES-2. Population served by POTWs nationwide for select years between 1940 and 2008 and projected (if all needs are met), organized by wastewater treatment type. Source: U.S. Public Health Service and EPA Clean Watersheds Needs Surveys
iSTREEM® Wastewater Use at WWTPs

- Comparing population to facility effluent flow
- Facility flow (L/day) / Population = per capita water use
- Assumes influent flow = effluent flow
- Performed at 10,413 facilities

<table>
<thead>
<tr>
<th>Percentile</th>
<th>Water use (L/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>188</td>
</tr>
<tr>
<td>5th</td>
<td>194</td>
</tr>
<tr>
<td>10th</td>
<td>250</td>
</tr>
<tr>
<td>25th</td>
<td>337</td>
</tr>
<tr>
<td>50th</td>
<td>418</td>
</tr>
<tr>
<td>75th</td>
<td>584</td>
</tr>
<tr>
<td>90th</td>
<td>857</td>
</tr>
</tbody>
</table>

E-FAST
388 L/day
iSTREEM® Dilution Factors at WWTPs

- Comparing facility effluent flow to receiving water body flow
- Performed at low and mean flow conditions at 10,413 facilities

![Graph showing dilution factors and corresponding percentiles](image)

<table>
<thead>
<tr>
<th>Percentile</th>
<th>Low Flow DF</th>
<th>Mean Flow DF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st</td>
<td>3.2</td>
<td>1st</td>
</tr>
<tr>
<td>5th</td>
<td>14</td>
<td>5th</td>
</tr>
<tr>
<td>10th</td>
<td>33</td>
<td>10th</td>
</tr>
<tr>
<td>25th</td>
<td>133</td>
<td>25th</td>
</tr>
<tr>
<td>50th</td>
<td>593</td>
<td>50th</td>
</tr>
<tr>
<td>75th</td>
<td>3067</td>
<td>75th</td>
</tr>
<tr>
<td>90th</td>
<td>16061</td>
<td>90th</td>
</tr>
</tbody>
</table>
Stream Dilution Factor

- From study based on iSTREEM® model
- The dilution factors derived are “combined” dilution factors which account for both hydrologic dilution and cumulative upstream effluent contributions
- The median dilution factors based on in-stream decay rate of zero for POTW mixing zones dominated by domestic wastewater flow:
  - 132 at mean flow
  - 5 at low flow
- Other decay rates range from 24h to 1h

Regional Hotspots

Taking into account variability in treatment efficiency and stream dilution allows for identification of potential regional “hot spots”.

Sites of potential high exposure would suggest locations for a field monitoring campaign.

Further, incorporating variable use rates will lead to emphasis/de-emphasis of certain regions.
Summary

• Tiered system efficiently allocates resources
• Lower tiers use conservative assumptions used to screen out negligible risks
• Tools are readily available to conduct lower tier & higher tier exposure assessment
• Higher tier tools provide distributions of exposure as well as spatial differentiation, linking hydrologic connectivity (i.e., dilution) and allowing for environmental processes (i.e., decay) across different geographies
• The results from these models can provide insights into collection of higher tier data as needed (based on risk)
Exposure and risk assessment for formulated consumer products

MODULE 4: Modeling aquatic environmental exposure using iSTREEM
Overview

• iSTREEM Structure/Data Sources
• Accessing iSTREEM (Logon)
• Running an iSTREEM Simulation
  – Input parameters
• Viewing/Using Model Results
  – Output files
• Charting Data
• Upcoming New Features
iSTREEM® Data Sources

• **US EPA Clean Watersheds Needs Survey** – WWTP data includes NPDES permit numbers, treatment type information, population data, effluent flow, and location data for 2004 → >10,000 WWTP facilities in iSTREEM®

• **EPA Enhanced-River Reach File 1** – 1:500,000 scale; Contains stream data such as reach number, type, name, length, slope, annual/monthly mean and low flows and flow velocities → 30,000 effluent-impacted river reaches in iSTREEM®

• **Drinking Water Supply File** – Contains data for U.S. drinking water facilities: Includes facility code, production volumes, population served, and locations for plant intakes and sources (SDWIS – 2004) → 1,700 drinking water intakes in iSTREEM®

• **Version 2.0 - updated data**
iSTREEM User Inputs

• Chemical per capita use rate (national or regional)

• Chemical fate parameters
  – Primary treatment efficiency
  – Secondary treatment efficiency (activated sludge, lagoon, oxidation ditch, RBC, trickling filter)
  – In-stream loss (first order)

• Geographic scope (national or regional)
Using iSTREEM
Wastewater Treatment Types

- Relative proportion of treatment types (as % total U.S. wastewater flow, and % total U.S. facilities, respectively)
- Based on the facilities in iSTREEM (2004 CWNS)

Tier 2 Dilution Estimation using iSTREEM®

• Considering treatment and dilution variability:
  – Leads to an exposure distribution
  – Illustrates the likelihood (probability) of exceeding a particular concentration
  – Allows identification of regional “hot spots” → providing insights into potential Tier 3 monitoring
Access

http://www.istreem.org/

- User name: any combination of text and numbers, but may be no longer than eight (8) characters, and must contain no spaces
- Password: any combination of text and numbers
New User Registration

• To gain access, input a user name and password
• If the user name and password do not exist, the new user registration screen will appear
• You will be prompted for a user name, password and e-mail address
• You must agree to the terms and conditions of use as well
New User Registration, cont.
Running Simulations

[Image: Diagram of the iSTREEM software interface, showing the Map Window, Operation Panel, and Navigation bar.]
Operation Panel

TABS

• Run Model Tab
  – Initiate a simulation for iSTREEM®

• Model Result Tab
  – Retrieve and review iSTREEM® model output

• Map Tab
  – Display: Select output data
Run Model

- River Reach Parameters
  - Simulation name (no spaces!)
- Chemical Fate Parameters
- Chemical Loading Parameters

- Online Help and Sample input available to assist in parameter selection
River Reach
Parameters
### Chemical Fate Parameters

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>Input your value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>Ingredient</td>
<td></td>
</tr>
<tr>
<td>Oxidation Ditch Removal %</td>
<td>0</td>
</tr>
<tr>
<td>Activated Sludge Removal %</td>
<td>0</td>
</tr>
<tr>
<td>Lagoon Removal %</td>
<td>0</td>
</tr>
<tr>
<td>Trickling Filter Removal %</td>
<td>0</td>
</tr>
<tr>
<td>RBC Removal %</td>
<td>0</td>
</tr>
<tr>
<td>Primary Removal %</td>
<td>0</td>
</tr>
<tr>
<td>Decay(K1)</td>
<td>0</td>
</tr>
<tr>
<td>River Temperature(C)</td>
<td>20</td>
</tr>
<tr>
<td>Scenario</td>
<td>Present.Pop</td>
</tr>
<tr>
<td>Flow Type Indicator</td>
<td>Mean Flow</td>
</tr>
</tbody>
</table>

- **Input required**
- **Input required**
- **Treatability by secondary treatment**
- **In-stream 1\(^{st}\) order loss (e.g., sorption, biodegradation, etc.)**
- **Present Pop = 2004, Future Pop = 2008**
- **Mean River Flow or Low Flow = 7Q10 (worse-case, sometimes 100% effluent)**
Chemical Loading Parameters

![Map of the United States with market regions labeled: West Market, Plains Market, Great Lakes Market, Midwest Market, Southeast Market, California Market, North East Market.]

Loading factor (G/Cap/Day): National: 0
Market Region:
- California: 0
- Great Lakes: 0
- Midwest: 0
- Plains: 0
- South Central: 0
- Southeast: 0
- West: 0

Notes:
- Sample
- Clear
- Submit
Complete Simulation Data for Model Run

Simulation name:

- Required
- Ten (10) character maximum!
- No spaces
- No special characters: 
  
  ![special_characters](image)

- System will confirm that an acceptable simulation name is used
Run Model

- Default parameters
- Reset parameters
- Run Model

Sample  Clear  Submit

Done
Run Model Dialogue

Depending on the river reach parameters selected, it may take a few minutes up to 45 minutes to complete the model run.
Model Results
Checking Progress of Model Run

Simulation complete

Simulation running (pending)

When simulation is complete, Load Output to view on Map
Viewing Model Results

- **Classification methods**
  - quantile (same number of records in each category)
  - natural break (records are clustered)

- **Category**
  - 4-6

- **Color**
  - Red
  - Green
  - Blue
  - Purple
  - Gray
Three-Panel Main User Interface

Note “+” sign on “iSTREEM Output” when simulation is loaded.
Map Control Panel

• Results
  – Selected concentrations

• Map Contents
  – GraphicsLayer (not used)
  – iSTREEM Output
    • River
    • WWTP
    • DWI
  – BaseMap
    • Contextual layers
View of Model Results
Map Window Navigation Bar

- Zoom in
- Zoom out
- Pan
- Zoom to Full Extent (National view)
- Back to Previous Extent
- Forward to NextExtent
- Open/Hide a Magnifier
- Identify the feature attributes of an iSTREEM Output layer
- Measure distance on the map
- Open/Hide an Overview Map
- Print the current map
- Clear map
- Adjust scale
Map/Display/Select Feature
Download Model Result

- **Model Configuration**
  - Review input

- **Model Results**
  - dbf Format
    - DWI
    - WWTP
    - River
  - Input Parameters
    - Enables statistical analyses, graphing, use in GIS
Model Results
WWTP File
(10,400 WWTPs)

• CUSEGSEC – identifier of associated river reach
• P_SERVED – Population served by the plant
• TREATMENT_TYPE – Facility treatment technology (primary, activated sludge, oxidation ditch, lagoon, RBC, trickling filter)
• FLOW – Effluent discharge volume (million gallons/day)
• ICONC – Influent concentration (µg/L)
• CONC – Effluent concentration (µg/L)
• DILF – Dilution factor
RIVER File
(29,700 Stream Segments)

• CUSEGSEC – identifier of associated river reach
• CFLOW – Flow rate of stream segment (feet\(^3\)/second)
• POTWQ – WWTP effluent flow on this reach (feet\(^3\)/second)
• CI – Concentration at beginning of segment (µg/L) – mixing zone concentration for segments with a WWTP discharge
• CL – Concentration at end of segment (µg/L)
• CA – Average concentration of segment (µg/L)
• CLOAD – Amount of daily chemical discharge from WWTP (lb)
• Remove records with CA = 0 (~5,000)
DWI File
(1,700 DWIs)

- CUSEGSEC – identifier of associated river reach
- NPDES – Facility permit number
- P_SERVED – Population served by the plant
- CONC – Concentration at intake (µg/L)
Model Results - Charting

- Ranked distribution of concentrations

Comparison to E-FAST (no-decay)
Model Results - Mapping

Test run, Low Flow, No decay

Modeled concentration (ng/L)
- Non-impacted (zero concentration)
- 25th-centile (0.84 ng/L)
- 50th-centile (3.04 ng/L)
- 75th-centile (9.71 ng/L)
- 90th-centile (19.85 ng/L)
- 95th-centile (32.93 ng/L)
- 99th-centile (224.09 ng/L)
Development of iSTREEM® 2.0

• Updated underlying data in model to contain best available information
  • WWTP attributes (CWNS 2008 & 2012)
    • location data, population served, flow
    • 28% increase in number of facilities
    • 34% increase in population
    • 20% increase in flow
  • River network (USGS/US EPA 2014)
    • Based on NHD Plus v 2, segments increased 9x, and a 16% increase in river miles
    • 1:100,000 scale (compared to 1:500,000)
Summary 2.0 changes

- Lower dilution factors – inclusion of intermittent streams and more periods of drought in the dataset
- Higher resolution river network adds new streams into the model
- Some WWTP moved to new segments given the new network contains more streams
More on version 2.0

Spatial improvements leading to advances in down-the-drain chemical exposure modeling with iSTREEM® 2.0

Wednesday November 9th, 2016 1:20 PM
Room F2
Environmental exposure and risk assessment for formulated consumer products

MODULE 5: Case Studies
US COMPARISON OF MEASURED AND MODELED DATA
Case Study

• Comparison of iSTREEM® national modeled exposure estimates to best available monitoring data (USGS/EPA)
  o Musk fragrance HHCB (1,3,4,6,7,8-Hexahydro-4,6,6,7,8,8,-hexamethylcyclopenta-γ-2-benzopyran)
  o Insect repellent ingredient DEET (N,N-Diethyl-m-toluamide)

• These chemicals were chosen to represent consumer products having broad use patterns across the U.S. and different usage (loadings) and chemical properties

• Complete details in:
DEET model inputs

Exposure:

<table>
<thead>
<tr>
<th>Treatability Parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxidation Ditch</td>
<td>56.9%</td>
</tr>
<tr>
<td>Activated Sludge</td>
<td>56.9%</td>
</tr>
<tr>
<td>Lagoon</td>
<td>56.9%</td>
</tr>
<tr>
<td>Trickling Filter</td>
<td>56.9%</td>
</tr>
<tr>
<td>Rotating Biological Contactor</td>
<td>56.9%</td>
</tr>
<tr>
<td>Primary</td>
<td>0%</td>
</tr>
</tbody>
</table>

Decay (d-1)                     | 0.0234 |
River Temperature               | 20°C   |
Scenario                        | Present Population |
National Loading factor (g/capita/day) | 0.0318 |

Effects:

- The most conservatively predicted aquatic species no-effect concentration (PNEC) for DEET is 43 µg/L (derived as the algal median value for growth inhibition [ErC50] divided by 1000 (KEMI, 2010).
DEET monitoring data

- Available surface water (streams or rivers) monitoring data (both filtered and unfiltered) from USGS National Water Information System

- Specific flow conditions were used in retrieval
  - “Stable, Normal Stage” used to represent mean flow conditions
  - “Stable, Low Stage” used to represent low flow conditions

- Average chemical concentrations for each respective flow condition were computed per monitoring location.

- Monitoring data spanned a time period of 2001 to 2014, with up to 535 monitoring locations spread over a large extent of the conterminous U.S.

DEET monitoring data summary

- **Number of sites (and samples)**

<table>
<thead>
<tr>
<th>Stage</th>
<th>Filtered</th>
<th>Unfiltered</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stable, normal stage</td>
<td>535 (1628)</td>
<td>306 (1040)</td>
</tr>
<tr>
<td>Stable, low stage</td>
<td>236 (314)</td>
<td>97 (231)</td>
</tr>
</tbody>
</table>

- **Number of non-detects**

<table>
<thead>
<tr>
<th>Stage</th>
<th>Filtered</th>
<th>Unfiltered</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stable, normal stage</td>
<td>24%</td>
<td>20%</td>
</tr>
<tr>
<td>Stable, low stage</td>
<td>32%</td>
<td>24%</td>
</tr>
</tbody>
</table>

- **Detection levels**

<table>
<thead>
<tr>
<th>Stage</th>
<th>Filtered</th>
<th>Unfiltered</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stable, normal stage</td>
<td>0.06, 0.1, 0.14, 0.2, 0.5, 0.51, 0.67, 0.82, 0.85, 5</td>
<td>0.04, 0.06, 0.2, 0.37, 0.63, 1</td>
</tr>
<tr>
<td>Stable, low stage</td>
<td>0.06, 0.1, 0.11, 0.14, 0.2, 0.5</td>
<td>0.04, 0.2, 0.24, 0.32, 0.34, 0.39, 0.5</td>
</tr>
</tbody>
</table>
Handling non-detections in data

- Two approaches to handling non-detection data points
  1. Assign non-detect samples the value of the limit of detection (LOD), or the lower reporting limit when applicable
     - Most conservative representation of potential exposure
  2. Interpolate values using ProUCL 5.0, a statistical package developed for analyzing datasets with non-detect observations
     - Used the lognormal regression on order statistical method (ROS) in ProUCL
     - This has been found to be useful for datasets having multiple detection limits

- Sample data (detections and interpolated) were averaged by monitoring location for each data subset

\(^1\)USEPA, http://www.epa.gov/osp/hstl/tsc/software.htm
\(^2\)Perez et al. 2013
DEET national concentration distributions

Top = Data not interpolated
Bottom = Data interpolated

Dark dashed line = iSTREEM® mean flow modeled concentration
Light dashed line = iSTREEM® low flow modeled concentration
Dark points = USGS monitoring data, stable normal stage
Light points = USGS monitoring data, stable low stage
Vertical solid line = Predicted No Effect Concentration (PNEC)
iSTREEM® 95th-%ile mean flow Predicted Environmental Concentration (PEC) = 2.7 µg/L for all impacted river segments (i.e., those below WWTP facilities)

The most conservatively predicted aquatic species no-effect concentration (PNEC) for DEET is 43 µg/L

- Derived as the algal median value for growth inhibition [ErC50] divided by 1000 (KEMI, 2010)
Spatial trends in modeled DEET output

Mean flow, DEET
Modeled concentration (ug/L)
- Zero concentration
- 25th centile
- 50th centile
- 75th centile
- 95th centile
- >95th centile
Exposure:

- **Effects:**
  - The EPA chronic aquatic Concentration of Concern is 9.7 ug/L

<table>
<thead>
<tr>
<th>Treatability Parameters (Simonich at al, 2002)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxidation Ditch</td>
<td>90%</td>
</tr>
<tr>
<td>Activated Sludge</td>
<td>90%</td>
</tr>
<tr>
<td>Lagoon</td>
<td>99%</td>
</tr>
<tr>
<td>Trickling Filter</td>
<td>80%</td>
</tr>
<tr>
<td>Rotating Biological Contactor</td>
<td>80%</td>
</tr>
<tr>
<td>Primary</td>
<td>30%</td>
</tr>
<tr>
<td>Decay (d-1)</td>
<td>0.24</td>
</tr>
<tr>
<td>River Temperature</td>
<td>20°C</td>
</tr>
<tr>
<td>Scenario</td>
<td>Present Population</td>
</tr>
<tr>
<td>National Loading factor (g/capita/day)</td>
<td>0.0149</td>
</tr>
</tbody>
</table>
National concentration distributions of HHCB

Mean flow:
90th and 95th centiles:
0.09 μg/L
0.20 μg/L

Low flow:
90th and 95th centiles:
3.19 ug/L
8.83 ug/L
Spatial trends in modeled HHCB output

iSTREEM Model, Low Flow
Modeled concentration (ug/L)

- Non-impacted (zero conc)
- 0.000001 - 0.022362 (25th-centile)
- 0.022363 - 0.124856 (25th-50th-centile)
- 0.124857 - 0.719101 (50th-75th-centile)
- 0.719102 - 8.827680 (75th-95th-centile)
- 8.827681 - COC of 9.7 (95th-95.26th-centile)
- >COC 9.7 (>95.26th-centile)
Relevance for risk assessment

• At low flow conditions (7Q10), 95.26% of the predicted concentrations were below the concentration of concern
• During mean flow conditions, 99.9% were below 9.7 ug/L
• Neither of the filtered nor unfiltered datasets measured nationally reached or exceeded the benchmark of 9.7 ug/L
• The concentrations of HHCB predicted for US rivers are well below concern levels for aquatic toxicity established by US EPA
• Results of the this screening level assessment using iSTREEM® are consistent with the conclusion of US EPA, which found no aquatic risk.
Conclusions

• iSTREEM® provides the ability to predict concentrations of user-defined chemicals in wastewater effluent and receiving streams on a national scale or a watershed scale

• Concentration data from iSTREEM® are easily represented as a distributions which can be compared to a regulatory or biological endpoint threshold (e.g., 90th or 95th centiles)

• iSTREEM ® provides conservative aquatic exposure estimates and the results may be used to conduct screening level risk assessments of chemicals found in formulated consumer products
GRAND RIVER WATERSHED, CANADA
Grand River Watershed

- A local exposure assessment of sucralose at the Grand River watershed was conducted using iSTREEM® to compare against available measured data.

- Available monitoring data for four artificial sweeteners (sucralose, cyclamate, saccharin, and acesulfame) in the Grand River Watershed were obtained from Spoelstra et al., 2013.


- The use rate for sucralose was increased by a factor of four (4x) as a surrogate for the three other sweeteners for which use data was not available: cyclamate, saccharin, and acesulfame.

Figure 1. Grand River Watershed (6,800 km²), Ontario, Canada. Numbered circles and red squares indicate the 23 sampling sites and 30 WWTPs, respectively. Site numbering starts in the headwaters and increases downstream.

Comparison of flow data

- Before comparing concentrations, flow should be examined.
- iSTREEM® mean and 7Q10 low flow data were compared to the flow measured at the study sites during the 3 different time periods.
  - September 2007 flows were lowest in study.
- iSTREEM® mean flow was comparable to April 2009 flow.
- iSTREEM® 7Q10 low flow was much lower than all study periods.
- In order to model the iSTREEM® low flow scenario, measured gage data from the Water Survey of Canada was accessed to estimate flow for all river segments in the watershed.
  - These flows subsequently used in the modeling.
Flow Comparison

[Graph showing flow comparison with various data points and labels.]
iSTREEM® Predicted Concentrations

- Modeled with no WWTP removal and no in-stream decay
- Highest concentration of sweeteners near study sites 11-14 (~140-175 km downstream)
Comparison of iSTREEM® predicted concentrations of sucralose surrogate and measured concentrations

Figures adapted from Spoelstra et al., 2013
Conclusions

• Mean flow in iSTREEM® comparable to 2009, but 7Q10 low flow not comparable to study flows. Developed custom flow data for model.
• iSTREEM® mean and September 2007 flow scenarios predicted the highest concentration of sweeteners ca. 140-175 km downstream
  – This is consistent with the areas of highest measured concentrations
• Comparison of concentrations produced variable results
  – iSTREEM® overestimation for saccharin & cyclamate compared to monitoring
  – iSTREEM® was comparable for acesulfame
  – Differences likely due to assumptions about use rate (i.e., each sweetener modeled with the same overall volume)
• Results support iSTREEM® model results as comparable or conservative to real world data, even at a local scale
  – However, custom flow data was important for modeling low flow monitoring conditions

Acknowledgments to Raghu Vamshi, Megan Sebasky, Katherine Kapo and Duane Huggett from Waterborne Environmental