Recent developments in exposure modeling of "down-the-drain" chemicals across multiple product groups

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Exposure modeling for “down-the-drain” risk assessment

- Wide variety of ingredients (personal care products, pharmaceuticals, biocides, etc.) requiring regulatory assessment are treated and discharged at municipal wastewater treatment facilities

- “Down-the-drain” models can be useful tools for screening-level environmental exposure assessment relevant across multiple product groups

- Presentation will overview recent developments and trends in the “down-the-drain” modeling landscape, with a focus on iSTREEM® (“in-STREam Exposure Model”, American Cleaning Institute).
Developments and trends

Modeling over broad-scale geographies

- Global relevance
- Leveraging best-available data resources
- "Down-the-drain" exposure modeling

- Standard exposure models + custom inputs
- Geo-referenced model input/output
- Open-access via the web
- Transparency and validation
- Diversity of model applications

Global relevance

Diversity of model applications

"Down-the-drain" exposure modeling

Standard exposure models + custom inputs

Geo-referenced model input/output

Open-access via the web

Transparency and validation
Exposure assessment over broad geographies

- Broad-scale capability (regional, national, etc.) is critical for assessment of ingredients in high-volume, widely-distributed products

- “One size fits all” scenario vs. site-specific variability
  - Variability in loading and discharge
  - Variability in treatment processes
  - Variability in in-stream dilution
    - Flow conditions and upstream contributions

- iSTREEM® model was developed specifically to address these issues
  - National (U.S.) point source exposure model originally developed as the “ROUT” model (Procter & Gamble)
  - Models “down-the-drain” concentrations at treatment plants, drinking water intakes, and river reaches for mean and low flow scenarios
  - Chemical-independent
Leveraging best-available data resources and GIS

- **Wastewater treatment facility (WWTP) characteristics**
  - US: USEPA Clean Watersheds NEEDS Survey, Permit Compliance System
    - iSTREEM®: over 10,000 facilities (2004 CWNS, to be updated)
- **Drinking water intakes (DWI)**
  - USEPA Safe Drinking Water Information System (SDWIS)
    - iSTREEM®: ~1700 intakes (2004 SDWIS, to be updated)
- **River network**
  - Flow, other hydrologic characteristics
    - Current iSTREEM®: USEPA RF1
    - Flow updates in 2014
    - Future: NHDPlus v.2 (USEPA/USGS)
- **GIS integration (“GIS-ROUT”)**
  - Points (WWTP, DWI) related along the hydrologic network
Integrating standard exposure models and custom user-driven inputs

U.S. EPA WUI2 model algorithms

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

Model background data (WWTPs, DWIs, rivers)

GIS Routing Model

Extract segment from reach segmentation file

Calculate head-of-reach conc. based on reach boundary type

Extract Intake concentration $C_{in} = C_i$

Add WWTP contributions, if any

$C_r = \sum \frac{Q_i \cdot C_i}{Q} + \frac{\sum L_{WWTP}}{Q} \cdot M$

Calculate influent

$C_e = (1 - C_{WWTP})$

Effluent

$C_{WWTP}$

Loadings to segment

$L_{WWTP} = \sum Q \cdot C_r$

Calculate downstream end-of-reach concentration

Non-dispersive segments

$C = C_r \cdot \exp (-K \cdot L)$

Dispersive segments

$C = C_r \cdot \exp \left( -\frac{v}{2 K \cdot L} \right)$

Downstream segment:

$C_r = C_{prev} \cdot L$

Tributary junction

$C_r = \left( \sum Q_i \cdot C_i \right) / Q_r$

(See Wang et al. 2005 for algorithm details)
Geo-referenced model output

- Ability to import and analyze model output within a GIS
- iSTREEM® output: Modeled concentrations for WWTPs, DWIs, and over 25,000 effluent-impacted river segments (U.S.)
Model access via the web

- Web browser interface for user input, visualization using web mapping services, and accessing and downloading results
- Move towards open-access
  - iSTREEM® web application (www.istreem.org)

iSTREEM Framework
Model transparency and validation

- Enhancing documentation and interaction with user community
- “Validation” datasets and studies for ground-truthing

**iSTREEM® case study:**

- Comparison of national (U.S.) model simulations with available surface water monitoring data (USGS/EPA)
  - Triclosan
  - HHCB
  - DEET

- Subset monitoring data by hydrologic condition (~mean, low flow scenarios)

- Comparison of national concentration distributions

(Example, DEET monitoring data)
Case study: National concentration distributions

- Assessment of conservatism of model output (upper percentiles)

iSTREEM® percentiles based on cumulative % river miles
Case study: Relevance for risk assessment

- Identify spatial trends in modeled output

- “Predicted Environmental Concentration” (PEC, 95th percentile) compared to “Predicted No-Effects Concentration” (PNEC)

<table>
<thead>
<tr>
<th>Chemical</th>
<th>iSTREEM 95th (µg/L)</th>
<th>PNEC (µg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HHCB</td>
<td>0.18</td>
<td>9.7 a</td>
</tr>
<tr>
<td>Triclosan</td>
<td>0.05</td>
<td>0.8 b</td>
</tr>
<tr>
<td>DEET</td>
<td>2.72</td>
<td>43 c</td>
</tr>
</tbody>
</table>

\[ a \text{ chronic concentration of concern (USEPA 2014)} \]
\[ b \text{ HC05 (Lyndall et al. 2010)} \]
\[ c \text{ algal growth ErC50/1000 (KEMI 2010)} \]
Diversity of model applications

- Comparing modeled concentration distribution to PNECs or other threshold criteria
- Site selection via spatial delineation of “worst-case” scenarios
  - Optimize monitoring efforts
- Concentration and dilution factor distributions for use in probabilistic assessment
- Integration of modeling output with holistic (multiple-stressor) assessment approaches
  - Mixture toxicity
  - Site-specific conditions
  - “Eco-epidemiology”

Above: See poster #MP086 in this session
“Going global”: Extrapolating to new geographies

- Global usage of many products, particularly in developing nations, necessitates extrapolation of methodologies across geographies

- Adaptation of modeling frameworks to accommodate different data sources, data gaps and/or coarser spatial resolution
  - Expansion of iSTREEM® model to portions of Canada (St. Lawrence River Basin)
  - Collaboration and learnings from complementary methodologies and data development strategies
    - Global dilution model, Centre for Hydrology and Ecology (CEH, Keller et al. 2014)
    - ScenAT model (Unilever; Hodges et al. 2012, Holmes et al. in prep.) *see poster #MP085 in this session
### Considerations for model selection (examples)

<table>
<thead>
<tr>
<th>Model characteristic</th>
<th>iSTREEM®</th>
<th>E-FAST2&lt;sup&gt;a&lt;/sup&gt;</th>
<th>PhATE™&lt;sup&gt;b&lt;/sup&gt;,</th>
<th>GREATER-ER&lt;sup&gt;c&lt;/sup&gt;</th>
<th>ScenAT&lt;sup&gt;d&lt;/sup&gt; approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geographic extent</td>
<td>National (U.S.) and portions of Canada</td>
<td>Single national (U.S.) value</td>
<td>11 U.S. watersheds</td>
<td>16 European watersheds</td>
<td>88 countries</td>
</tr>
<tr>
<td>Spatial Resolution</td>
<td>USEPA RF1 Future: NHDPlus 2</td>
<td>Single point of discharge</td>
<td>USEPA RF1</td>
<td>Model-specific river network</td>
<td>County or sub-state/sub-province</td>
</tr>
<tr>
<td>Chemical inputs</td>
<td>&gt;10,000 WWTP facilities; user specifies (g/cap/day) for nation or market</td>
<td>User specifies (kg/yr) for nation and exposure duration (yr)</td>
<td>1302 WWTP facilities; user specifies (kg/yr) for nation</td>
<td>User specifies a per-capita use rate for one or more watersheds</td>
<td>User specifies water use (urban/rural, L/cap/day), product (tonnes/yr) which is distributed by GDP, and product inclusion (%) of chemical of interest</td>
</tr>
<tr>
<td>Inclusion of treatment efficacy</td>
<td>Various treatment types</td>
<td>Single treatment type</td>
<td>Various treatment levels</td>
<td>PDF of treatment removal % (user-specified), and sewer removal</td>
<td>Single treatment type</td>
</tr>
<tr>
<td>Inclusion of flow scenarios</td>
<td>Mean and low (7Q10) flow scenarios</td>
<td>Harmonic mean, 30Q5, 7Q10, 1Q10 flow</td>
<td>Mean and low (7Q10) flow scenarios</td>
<td>Probability density function of flow values</td>
<td>Single flow scenario (mean annual)</td>
</tr>
<tr>
<td>Inclusion of in-stream decay</td>
<td>User specifies first-order in-stream loss (k)</td>
<td>None (point of discharge only)</td>
<td>User specifies first-order in-stream loss (k)</td>
<td>User specifies first-order in-stream loss (k)</td>
<td>User specifies a single removal (%)</td>
</tr>
<tr>
<td>Probabilistic?</td>
<td>Not direct</td>
<td>Y (probabilistic dilution model)</td>
<td>Not direct</td>
<td>Y (Monte Carlo simulations)</td>
<td>Not direct</td>
</tr>
<tr>
<td>Output format</td>
<td>Database (*,dbf), ESRI geodatabase and web map interface</td>
<td>Results generated in tool output interface</td>
<td>Database (MS Access)</td>
<td>Repository interface</td>
<td>Excel and map interface</td>
</tr>
<tr>
<td>Availability</td>
<td>Public</td>
<td>Public</td>
<td>Proprietary</td>
<td>Public</td>
<td>Proprietary</td>
</tr>
<tr>
<td>Application type</td>
<td>Web application</td>
<td>Stand-alone software</td>
<td>Stand-alone software</td>
<td>Stand-alone software and web application</td>
<td>Stand-alone software</td>
</tr>
</tbody>
</table>

<sup>a</sup> USEPA 2007, <sup>b</sup> Anderson et al. 2004, Koormann et al. 2005, <sup>c</sup> Feijtel et al. 1997, Cunningham et al. 2011, <sup>d</sup> Unilever
Conclusions

- “Down-the-drain” exposure models are evolving to meet the expanding needs of risk assessors across sectors and commodity groups

- Various pros/cons across the current modeling landscape are dependent upon needs of a given assessment

- Enhancing understanding, accessibility and collaboration provides opportunity to expand and improve available models and increase their acceptance as a decision-support tool
Thank you!

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