Exposure hotpots and source apportionment analysis of home and personal care products chemicals in Asia

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Objectives

• Develop and evaluate a flexible multiscale hydrological and multimedia fate model of household chemicals in Asia (China, South Korea, Japan, Pakistan, India, Sri Lanka, Bangladesh, Laos, Thailand, Cambodia, Vietnam, Philippines, Malaysia, Indonesia, Australia, New Zealand)

• Estimate chemical concentrations to identify (sub)catchments hotspots

• Analyse the variability of source-to-receptor pathways, performing an apportionment analysis
A model-based exposure assessment framework

**Chemical use**

- Spatial environmental emissions (ScenAT)
- Wastewater treatment plant model (SimpleTreat)
- Multiscale multimedia fate model (Pangea)
- Hotspot identification & source apportionment

Spatial exposure estimates in the environment (water, sediments, ...)

**Introduction**

**Pangea**

**Prediction**

**Evaluation**

**Hotspots & source app.**

**Outlook**
SCENAT+SimpleTreat spatial emissions [mg/m$^2$/day]
1 – Build grids, define geometry, topology, connections, project spatial data: 1 – 20min (substance independent)

2+3 – Build abstract compartmental model, solve fate at steady-state + exposure: 5s – 1min per substance
Environmental models: **Pangea**
global, multi-scale, multimedia, flexible

**Water layer**

\[ \log_{10}(\text{discharges}) \]  
\[ [\text{m}^3/\text{s}] \]

- 4.7
- 2.9
- 1.2
- 0.6
- n/a

**Multiscale air layers**
## Results for 13 substances

<table>
<thead>
<tr>
<th>CAS #</th>
<th>Name</th>
<th>Use function</th>
</tr>
</thead>
<tbody>
<tr>
<td>68411-30-3</td>
<td>Linear alkylbenzene sulfonate (LAS)</td>
<td>Anionic surfactant</td>
</tr>
<tr>
<td>3380-34-5</td>
<td>Triclosan (TCN)</td>
<td>Antimicrobial / preservative</td>
</tr>
<tr>
<td>2682-20-4</td>
<td>Methylisothiazolinone (MIT)</td>
<td>Antimicrobial / preservative</td>
</tr>
<tr>
<td>541-02-6</td>
<td>Decamethylcyclopentasiloxane (D5)</td>
<td>Emollient</td>
</tr>
<tr>
<td>79261-49-7</td>
<td>Ibuprofen (IBU)</td>
<td>Pharmaceutical</td>
</tr>
<tr>
<td>52645-53-1</td>
<td>Permethrin (PERM)</td>
<td>Insecticide</td>
</tr>
<tr>
<td>6197-30-4</td>
<td>Octocrylene</td>
<td>UV filter</td>
</tr>
<tr>
<td>5466-77-3</td>
<td>2-ethylhexyl 4-methoxycinnamate (OMC)</td>
<td>UV filter</td>
</tr>
<tr>
<td>131-57-7</td>
<td>Benzophenone-3 (BP-3)</td>
<td>UV filter</td>
</tr>
<tr>
<td>94-13-3</td>
<td>Propyl Paraben</td>
<td>Antimicrobial / preservative</td>
</tr>
<tr>
<td>99-76-3</td>
<td>Methyl Paraben</td>
<td>Antimicrobial / preservative</td>
</tr>
<tr>
<td>134-62-3</td>
<td>Diethyl toluamide (DEET)</td>
<td>Insect repellant</td>
</tr>
<tr>
<td>8001-54-5</td>
<td>Benzalkonium chloride (BAC)</td>
<td>Cationic surfactant / Antimicrobial</td>
</tr>
</tbody>
</table>
Triclosan concentration in freshwater [mg/L]

Water layer

$log_{10}(C_{SS})$ [mg/L]

-30 -25 -20 -15 -10 -5 0

$n/a$
13 predicted concentrations
Yangtze river catchment

\( \log_{10}(C_{ss|0}) \) [mg/L] - MODEled for Asia

~99.5th percentile
75th percentile
50th percentile (median)
25th percentile
~0.5th percentile
Data collection

- Literature review of ~50 papers in Asia with monitoring data of select chemicals
- 1600 georeferenced freshwater/sediment measured concentrations extracted from literature
- ~15 different watersheds across Thailand, China, India, Japan, South Korea
- Standard error on the log:

\[
S_e = \sqrt{\frac{\sum_{i=1}^{n} \left( \log(C_{i}^{\text{predicted}}) - \log(C_{i}^{\text{observed}}) \right)^2}{n}}
\]
Model evaluation Triclosan

DT50 water = 23d, TSS = 1500mg/L

India
- Cauvery
- Vaigal

China
- Huang He
- Song Hua
- Xi Jiang
- Yangze

\[ SE = 6.91 \times 10^{-1} \]
Sensitivity study for Triclosan as a function of half-life in freshwater

**DT$_{50}$ water = 2.6d**

- SE = 1.01e+00

**DT$_{50}$ water = 26d**

- SE = 6.91e-01

**DT$_{50}$ water = 256d**

- SE = 7.56e-01

**DT$_{50}$ water = 10d**

- SE = 7.16e-01
Model evaluation - across substances

\[ \log_{10}(C_{ss>0}) \text{ [mg/L]} - \text{MODEled vs MONitored for Asia} \]
Introduction

Hotspot identification: Triclosan

Ying River, a tributary of the Huai River. Interestingly this is one of the Chinese rivers classified with the poorest grade (V+) for macro indicators of water quality.
Triclosan hotspots = medium emission level, low volume of dilution equivalent

Volume of dilution equivalent
\[ V \times k_{adv} \left(1 + k_{tot\ elim}/k_{adv}\right) \]
Source apportionment: which sources contribute most to the concentrations in Yangtze terminal cell?

LAS: only a few adjacent cells substantially contribute, 63% of the concentration due to direct emissions in terminal cell.

Triclosan only 1.2% of the concentration in terminal cell due to direct emissions, 5% from neighbouring Shanghai, remaining 94% coming from more than 220 cells spread over 2000 km upstream in the Yangtze River catchment.
Conclusions

- **Pangea** - an efficient multiscale model to run multiple chemicals for entire Asia, accounting for multi-compartmental transfers
- Ongoing evaluation with monitored freshwater concentrations for multiple sites and substances (reasonable initial results)
- Hotspots correspond to region with medium/high emissions and low equivalent volume of dilution
- Source apportionment shows that concentrations may be related to contribution of multiple sources upstream.
Next steps

HydroBasins
Collaboration with Dr Bernhard Lehner, McGill

+ New data collection on the Songhua river with Harbin Inst. of Technology