INTEGRATING MASS BALANCE MULTI-MEDIA MODELS
TO LINK NPRI DATA WITH CHEMICAL FATE AND
EXPOSURE IN THE ENVIRONMENT AND THE
POTENTIAL FOR ADVERSE EFFECTS

Liisa Toose\textsuperscript{1}, Alicia Berthiaume\textsuperscript{2}, Jon Arnot\textsuperscript{1}
NPRI Data Users Workshop
February 25, 2020
Montreal, QC, Canada
Outline

- Background
- Objectives and rationale
- Introduction to RAIDAR
- Project tasks
- Results
- Dashboards
- Conclusions
- Future work/next steps
Risk Assessment and Management

Production
Source / Inventory
NPRI

Emission Use

Ecological Exposure
air
water
soil
sediment

Fate, transport, bioaccumulation

Venous Blood
Arterial Blood
Lungs
Adipose tissue
Richly perfused tissues
Poorly perfused tissues
Liver

Risk Evaluation

Toxicology

Biokinetics

Uptake and dose

Decision: refine, regulate, etc.

Human Exposure

Far-field
Near-field

Modified from McKone
Courtesy Embry
Considers chemical impacts on human and non-human organisms, i.e., risk.

Risk includes the hazard posed by a substance and exposure

Risk = Exposure/Hazard

Exposure depends on the amount of substance released and its fate.

Strategies are developed to determine how best to manage “toxic” substances, i.e., potential actions required to mitigate risk of adverse effects.

Social, economic and other factors are integral to risk management.
Project Objectives

- Apply a tool to bridge the gap between NPRI emission estimates and exposures and potential risk to various ecological species and humans.
- Improve understanding of exposure and exposure pathways of NPRI chemicals (can inform possible mitigation steps, if necessary).
- Similar efforts of using mass balance models to link with NPRI data have recently been explored:
  - USETox 2.0
Risk Assessment IDentification And Ranking (RAIDAR)

A continued evolution of fugacity-based, mass balance multi-media models for discrete neutral and ionogenic organic chemicals pioneered by Don Mackay and colleagues

- **RAIDAR** combines environmental fate and food web bioaccumulation models in an evaluative regional-scale environment
- Exposure and risk simulations require chemical-specific information:
  - Partitioning, e.g., Kow, Kaw
  - Medium-specific degradation half-lives, e.g., reaction half-life in air
  - Emission rates, e.g., how much chemical is released to air, water or soil
  - Toxicity thresholds, e.g., LC50s, NOAELs
- Some primary model output of regulatory interest:
  - Fate, Overall Persistence, Long-Range Transport Potential, Bioaccumulation metrics
  - Concentrations in physical environment and biological receptors
  - Exposure potential, and exposure and risk estimates
- Currently coded in Visual Basic for Applications in Microsoft Excel
- Current User Interface is Excel spreadsheets
**RAIDAR model concepts**

Steady state; regional scale; diffuse emissions
RAIDAR hazard and risk-based metrics for ranking chemicals

1. Exposure Assessment Factor (EAF) \( \approx f (P + B) \)

2. Hazard Assessment Factor (HAF) \( \approx f (P + B + T) \)

3. Risk Assessment Factor (RAF) \( \approx f (E + P + B + T) \)

\[ E = \text{Emission rates (NPRI data)} \]
Obtained required chemical input parameters from databases and QSARs.

Two Sets of Simulations:

1. 252 chemicals (RAIDAR input data obtained)
   a. Full chemical emission (release) data unavailable
   b. Therefore only RAIDAR EAF and HAF output provided

2. 137 chemicals (2017 NPRI reporting year, release data only)
   a. NPRI emission estimates used to obtain RAIDAR RAF

RAIDAR Application: NPRI chemicals

2015-2017 NPRI reporting years - 342 NPRI substances
Exposure potential (EAFs) spans 14 orders of magnitude
Results-2

Including NPRI emissions – each point is a facility reported value

Risk (RAF) estimates for these chemicals span 17 orders of magnitude, easy to prioritize chemicals and facilities based on RISK!

log RAF

Rank order
Results-2

RAFs as a function of actual emission rates ($E_A$) for 7000 instances of NPRI data for 135 organic substances based on 2017 reporting data.

Only a weak relationship between chemical release and risk to the environment.
Data presentation using dashboards

- Dashboards help to convey the data and analysis to broader audiences
- Tableau software (www.tableau.com)
- Data analytics
- Distill and compare large datasets of results
- Tabular, graphical, spatial data types
Ranking based on assessment factor

Comparison of different approaches to rank priorities among NPRI release data 2008-2017

- Rank by Quantity released (NPRI data)
- Rank by Exposure Assessment Factor (EAF)
- Rank by Hazard Assessment Factor (HAF)
- Rank by Risk Assessment Factor (RAF) in most sensitive organism

<table>
<thead>
<tr>
<th>Rank</th>
<th>Compound</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Methanol</td>
<td>0.04823</td>
</tr>
<tr>
<td>2</td>
<td>Ethylene glycol</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>n-Hexane</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Xylenes (all isomers)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Toluene</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Styrene</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>Ethylene</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Formaldehyde</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Methyl ethyl ketone</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Isopropyl alcohol</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>Acetaldehyde</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Cyclohexane</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>Benzene</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>1,2,4-Trimethylbenzene</td>
<td></td>
</tr>
</tbody>
</table>

- Methanol 17.641602
- Isopropyl alcohol 1.040837
- Formaldehyde 0.097128
- N-Propylacetic acid (and its salts) 0.004227
- N-Methyl-2-pyrrolidone 0.003548
- Nonylphenol and its ethoxylates 0.003058
- Indeno(1,2,3-cd)pyrene 0.001800
- Anthracene 0.001616
- 2-Mercaptobenzothiazole 0.001385
- Phenol (and its salts) 0.001078
- Acrolein 0.000759
- Peracetic acid (and its salts) 0.000753
- Benzof[g,h]perylene 0.000465
- Pyrene 0.000569

Legend:
- Total Air
- Total Land
- Total Water
- Total Organism

- Forest vegetation
- Crop vegetation
- Plant
- Water vegetation
- Water
- Soil
- Building and structure
- Air

Note: The table and graph show the ranking of compounds based on different assessment factors, with Methanol being the highest ranked.
Ranking based on release pattern

Comparison of different approaches to rank priorities among NPRI release data 2008-2017

<table>
<thead>
<tr>
<th>Match to RAIDAR?</th>
<th>Reporting Year</th>
<th>Release type</th>
<th>Most Sensitive Orga.</th>
<th>Release type by Quantity</th>
<th>Colour legend - Release.</th>
<th>Most Sensitive Organism</th>
<th>Colour legend - Most Sensitive Organism</th>
</tr>
</thead>
<tbody>
<tr>
<td>True</td>
<td>All</td>
<td>All</td>
<td>All</td>
<td>Total Air</td>
<td>Total Air</td>
<td>Placental Fish</td>
<td>Most Sensitive Organism</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Rank by Quantity released (NPRI data)</th>
<th>Rank by Exposure Assessment Factor (EAF)</th>
<th>Rank by Hazard Assessment Factor (HAF)</th>
<th>Rank by Risk Assessment Factor (RAF) (in most sensitive organism)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>121 HCF1-123 (all isomers)</td>
<td>136 Ethylene</td>
<td>Ethylbenzene</td>
</tr>
<tr>
<td>Ethylene glycol</td>
<td>122 HCF-142 (all isomers)</td>
<td>137 1,2-Dichloroethane</td>
<td>45 Benzyl peroxide</td>
</tr>
<tr>
<td>n-Hexane</td>
<td>123 1,2-Dichloroethane</td>
<td>138 HCF-142b</td>
<td>46 Dimethyline</td>
</tr>
<tr>
<td>Xylene (all isomers)</td>
<td>124 Butylene</td>
<td>139 Vinyl chloride</td>
<td>47 Acrylic acid (and its salts)</td>
</tr>
<tr>
<td>Toluene</td>
<td>125 2-ethyl-1,3-dimethoxyethanol</td>
<td>140 Dimethylamine</td>
<td>48 Octylphenol and its ethoxylates</td>
</tr>
<tr>
<td>Styrene</td>
<td>126 Toluene</td>
<td>141 Toluene</td>
<td>49 Toluene</td>
</tr>
<tr>
<td>Ethylene</td>
<td>127 1,2-Dichloropropane</td>
<td>142 Acrylamide</td>
<td>50 7,8-Dihydroxy-2-oxo-5H-chromene</td>
</tr>
<tr>
<td>Formaldehyde</td>
<td>128 HCF-142</td>
<td>143 1,4-Dioxane</td>
<td>51 Bis(2-ethylhexyl) adipate</td>
</tr>
<tr>
<td>Methyl ethyl ketone</td>
<td>129 Catechol</td>
<td>144 Propylene oxide</td>
<td>52 Pththalic anhydride</td>
</tr>
<tr>
<td>Isopropyl alcohol</td>
<td>130 Chloroform</td>
<td>145 Diethanolamine (and its salts)</td>
<td>53 Xylen (all isomers)</td>
</tr>
<tr>
<td>Acetophenone</td>
<td>131 Hydroquinone (and its salts)</td>
<td>146 Isocyanate</td>
<td>54 Dibenzotriphenine</td>
</tr>
<tr>
<td>Acetylaldehyde</td>
<td>132 N-Methyl-2-pyrrolidone</td>
<td>147 HFC-22</td>
<td>55 Pyridine (and its salts)</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>133 Dimethyl phthalate</td>
<td>148 Formic acid</td>
<td>56 1,2,4-Trimethylbenzene</td>
</tr>
<tr>
<td>Benzene</td>
<td>134 Chloroacetic acid (and its salts)</td>
<td>149 Propylene</td>
<td>57 Diethyl phthalate</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Ranking based organism of interest
Conclusions

- Successful “proof of concept” linking NPRI data with mass balance models for fate and exposures and potential risk of discrete neutral and ionogenic organic chemicals to biological receptors in Canada.

Possible future work

- Improved spatial simulation of release, exposure and risk
  - Determine “hotspots” for not only emissions, but for risk
  - Parameterize RAIDAR for regional-specific environments in Canada

- Evaluate model predicted environmental concentrations with monitoring data in these regions (partnerships with other government agencies)

- Consider using NPRI disposal data (not currently modelled in RAIDAR) using EASE Suite which includes a chemical life cycle emissions module (CiP-CAFÉ)
Acknowledgments

- Environment and Climate Change Canada, National Pollutant Release Inventory Program for funding and collaboration.

- The RAIDAR model and other tools can be found at www.arnotresearch.com

- Please contact liisa.toose@gmail.com, jon@arnotresearch.com or Alicia.Berthiaume@canada.ca for more information
Impact of industry type
Trends in emissions and risk