Modelling, monitoring and misinterpretation - the challenges of meaningful exposure assessments

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Key steps in exposure modelling

• Selection and/or modification of appropriate model
• Creation of appropriate scenario(s)
  – Geographic locations
  – Landscape, crop and water body parameters
  – Weather, soil and agronomic data
• Compilation of chemical data
  – Environmental fate (including metabolites)
  – Application data
• Calculation of model results
• Comparison with monitoring data
• Comparison with effects data to assess risk
Evolution of quantitative approaches for creation of modelling scenarios

Expert opinion to estimate major geographic factors  ➔  Use of GIS to quantitate major geographic factors
Approaches to selection of chemical e-fate data

Sources of environmental fate data
- taken from guideline GLP studies
- guidance on kinetic evaluations
- specific endpoints calculated
  - mean / median / geomean
  - specific percentile (80-90)
  - conservative / worst-case

Approaches to selection of modelling results

<table>
<thead>
<tr>
<th>PECsoil</th>
<th>EECsw</th>
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<tbody>
<tr>
<td>Time after last application (days)</td>
<td>Actual PECsoil (pg/kg)</td>
</tr>
<tr>
<td>0</td>
<td>299.0</td>
</tr>
<tr>
<td>2</td>
<td>258.5</td>
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<tr>
<td>4</td>
<td>248.3</td>
</tr>
<tr>
<td>7</td>
<td>233.8</td>
</tr>
<tr>
<td>14</td>
<td>203.1</td>
</tr>
<tr>
<td>28</td>
<td>153.3</td>
</tr>
<tr>
<td>50</td>
<td>98.5</td>
</tr>
<tr>
<td>100</td>
<td>36.1</td>
</tr>
</tbody>
</table>

Deterministic, with a single set of inputs

Probabilistic, with variation in one or more inputs
### Key steps in exposure modelling

**Fixed**
- Selection and/or modification of appropriate model
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### Key steps in exposure modelling

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<tr>
<td><strong>Fixed</strong></td>
<td>• Selection and/or modification of appropriate model</td>
<td></td>
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<tr>
<td><strong>Fixed</strong></td>
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<td>• Comparison with monitoring data</td>
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</tbody>
</table>

*Regulatory*
Key steps in exposure modelling

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USEPA approach to modelling of surface water in drinking water reservoirs

**Tier I Model**

- **FIRST**
  - Compound phys / chem properties
  - Estimated conc in dw reservoir
  - Single reservoir scenario

**Tier II Model**

- **PRZM / EXAMS**
  - Compound phys / chem properties
  - Estimated conc in dw reservoir
  - Scenarios w/ crop, soil, weather, drift

Increased complexity

**BUT greater realism**

Conceptual Tier II drinking water reservoir

- **Legend**
  - Buffer Distance
  - 300
  - 600
  - 1000
  - 1500
  - 2000
  - 3000
  - Crop
  - Forest
  - Grassland
  - 300
  - 600
  - 1000
  - 1500
  - 2000
  - 3000

- **172.8 ha watershed drains into a 5.3 ha reservoir**
Surface water monitoring data

- USGS data
- 12 drinking water reservoirs of various sizes in 12 states of USA
- 178 pesticides and degradation products
- Two years of sampling
- Weekly to quarterly sampling, with higher rate of sampling May to September

Comparison of USEPA Tier I (FIRST) acute surface water modelling to monitoring

Tier I modelling using FIRST is intended to be a screening evaluation of the potential to impact surface water quality

Comparison
- acute modelling results
- maximum monitoring data
(from highly vulnerable reservoirs with 11 to 37 samples per year)
Comparison of USEPA Tier I (FIRST) chronic surface water modelling to monitoring

Comparison
- chronic modelling results
- maximum monitoring data

Extent of overprediction in USEPA Tier 1 acute modelling

Conclusion
Screening modelling using FIRST results in 1-4 orders of magnitude overprediction
Factors contributing to overprediction of USEPA Tier 1 modelling

The most significant factors contributing to overprediction include:
- use of exaggerated chemical application rates in modelling
- use of conservative chemical property data (e.g. longest degradation half-lives)
- selection of worst-case / extreme scenario parameters

For FIRST modelling, the extent of overprediction was moderately correlated with the chemical use rate.

Exposure refinement obtained using USEPA Tier 2 (PRZM/EXAMS) modelling

Acute

Chronic
Overprediction obtained using USEPA Tier 2 (PRZM/EXAMS) modelling

Tier 2 - Acute
Overprediction: 1-4 orders of magnitude

Tier 2 - Chronic
Overprediction: 1-3 orders of magnitude

Interpreting the statistical significance of sparse surface water monitoring data

For a single sample, there is a 50% probability that the sample exceeds the 50th percentile of the population - an obvious statistic!
Interpreting the statistical significance of sparse surface water monitoring data

For 10 samples, there is a 99.9% probability that the maximum value sampled will exceed the 50th percentile of the population.

For 10 samples, there is a 90% probability that the highest sample concentration exceeds the 80th percentile of the population.
Interpreting the statistical significance of surface water monitoring data

To obtain a 95% probability that the maximum sampled value exceeds the 95th percentile of the population, it is necessary to have 59 samples.


Experimental study of sampling frequency in a large drinking water reservoir

<table>
<thead>
<tr>
<th>Annual sampling frequency</th>
<th>Percentile of annual mean atrazine concentration (ug/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>50</td>
</tr>
<tr>
<td>4</td>
<td>1.684</td>
</tr>
<tr>
<td>12</td>
<td>1.691</td>
</tr>
<tr>
<td>24</td>
<td>1.703</td>
</tr>
<tr>
<td>120</td>
<td>1.715</td>
</tr>
</tbody>
</table>

Data source: USGS Open-File Report 01-456

**Conclusion:** In this case, quarterly sampling is adequate for determining concentration distributions in drinking water reservoirs. Lower sampling frequencies may provide useful results when the distributions are stable and narrow.
Recommendations to improve interpretation of surface water modelling

- Typically, an unknown degree of conservatism is incorporated into regulatory model simulations as a result of:
  - use of fixed input data (scenarios, e-fate, appln data)
  - reporting of selected modelling results

- To help determine the extent of conservatism, it is appropriate to:
  - determine key factors contributing to predicted concentrations - e.g. drift values, hydrology, buffer width
  - evaluate the magnitude, duration and return frequency of critical value exceedence
  - compare regulatory modelling results with available monitoring data and evaluate possible reasons for differences

Analysis of key factors and exceedence frequency

- Primary issue in this case: runoff due to late spring rain events
- Exceedence appears to be a single event and can be reduced by controlling runoff
- Available monitoring data indicates occasional spring detections
### Higher tier developments in modelling: a groundwater example

- To support higher tier evaluations, it can be useful to express results probabilistically using distributions of key inputs such as chemical properties, time, location, etc.

<table>
<thead>
<tr>
<th>Percentile</th>
<th>PECgw (ug/L)</th>
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<tbody>
<tr>
<td>0</td>
<td>0.04</td>
</tr>
<tr>
<td>10</td>
<td>0.06</td>
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<tr>
<td>20</td>
<td>0.06</td>
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<tr>
<td>30</td>
<td>0.06</td>
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<td>40</td>
<td>0.07</td>
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<tr>
<td>50</td>
<td>0.07</td>
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<td>60</td>
<td>0.07</td>
</tr>
<tr>
<td>70</td>
<td>0.07</td>
</tr>
<tr>
<td>80</td>
<td>0.08</td>
</tr>
<tr>
<td>90</td>
<td>0.08</td>
</tr>
<tr>
<td>100</td>
<td>0.11</td>
</tr>
</tbody>
</table>

### Challenges in development of future surface water modelling

- Improved simulation of potential concentrations in small water bodies may require:
  - better representation of ditch, pond and stream hydrology
  - more realistic water body loading rates
  - a broader range of environmental scenarios

- Simulation of potential concentrations in surface water used as drinking water supplies may require:
  - development and use of watershed-scale models
  - evaluation of chemical use intensity within a watershed

- Finished drinking water concentrations can be impacted by:
  - mixing of source waters
  - filtration and carbon treatment
  - effects of chlorination / ozonation
Acknowledgments

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  Dave Gustafson, Monsanto

• Thank you for your attention!