Design for the Environment
Chemical Alternatives Assessments
GC3
May 2012
• Chemical alternatives assessment:
  – Evaluation of chemicals of concern and potentially safer alternatives via **comparative hazard assessment**
  – Complements regulatory actions
  – Involves stakeholders from across the spectrum of interested parties
  – Provides the information on hazard from literature and models
  – Alternate approach to risk assessment or life cycle analysis
    • Consider “functional use” and “life cycle thinking”
1) Determine needs
2) Gather information
3) Involve stakeholders
4) Identify alternatives
5) Assess hazard
6) Apply economic and life cycle context
7) Apply the results

*The intended outcome is informed substitution

Office of Pollution Prevention and Toxics
• **Tetrabromobisphenol A (TBBPA)** in Printed Circuit Boards
  – combustion testing near completion

• **Nonylphenol and nonylphenol ethoxylates (NP/NPE)**
  – final report Spring 2012

• **Bisphenol A (BPA)** in Thermal Paper
  – draft report Spring 2012

• Flame Retardant Alternatives to **decabromodiphenyl ether (decaBDE)** used in many plastics
  – draft report Spring 2012

• Flame Retardant Alternatives to **hexabromocyclododecane (HBCD)** in insulation board
  – draft report Summer 2012

• **Phthalates**
  – list of potential alternatives Summer 2012
### Example Alternatives Assessment

#### Chemicals

<table>
<thead>
<tr>
<th>Chemical</th>
<th>CASRN</th>
<th>Acute Toxicity</th>
<th>Skin Sensitizer</th>
<th>Cancer Hazard</th>
<th>Immunotoxicity</th>
<th>Reproductive</th>
<th>Developmental</th>
<th>Neurological</th>
<th>Systemic</th>
<th>Genotoxicity</th>
<th>Acute Toxicity</th>
<th>Chronic</th>
<th>Persistence</th>
<th>Bioaccumulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tetraethylbisphenol A (TBBPA) (Albemarle, Chemtura, and others)</td>
<td>79-94-7</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>M</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>H</td>
<td>H</td>
<td>M</td>
<td>L</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DOPO (6H-Dibenz[c,e][1,2] oxaphosphorin, 6-oxide) (Samko Co., Ltd. and others)</td>
<td>35948-25-5</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>M</td>
<td>M</td>
<td>L</td>
<td>L</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fyrolflex PMP (Aryl alkylphosphonate) (Supresta)</td>
<td>Proprietary</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>L</td>
<td>H</td>
<td>L</td>
<td></td>
<td></td>
</tr>
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<td>Fyrolflex PMP</td>
<td>Proprietary</td>
<td>L</td>
<td>L</td>
<td>L</td>
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<td>L</td>
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<td>L</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Exposure Considerations

Availability of flame retardants (FRs) throughout the lifecycle for reactive and additive FRs chemicals and resins.

1. **End-of-Life of Electronics (Recycle, Dispose)**
   - Manufacture of FR Resin
   - Manufacture of FR
   - Manufacture of Laminates

2. **Sale and Use of Electronics**
   - Manufacture of PCB and incorporation into Electronics

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**Office of Pollution Prevention and Toxics**
Human Health Toxicity

- Acute mammalian toxicity
- Carcinogenicity
- Mutagenicity/Genotoxicity
- Reproductive Toxicity
- Developmental Toxicity
- Neurotoxicity
- Repeated Dose Toxicity
- Respiratory Sensitization
- Skin Sensitization
- Eye and Skin Irritation/Corrosivity

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- Endocrine Activity

Environmental Fate & Effects

- Aquatic toxicity
- Environmental persistence
- Bioaccumulation

Additional Endpoints

- Physical hazards
- Ecotoxicity
- And more
Criteria derived from GHS, EPA, authoritative lists

Reproductive & Developmental Toxicity Criteria

<table>
<thead>
<tr>
<th>Endpoint (LOAEL, NOAEL)</th>
<th>High</th>
<th>Moderate</th>
<th>Low</th>
<th>Very Low</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oral (mg/kg-bw/d)</td>
<td>&lt;50</td>
<td>50-250</td>
<td>&gt; 250-1000</td>
<td>&gt;1000</td>
</tr>
<tr>
<td>Dermal (mg/kg-bw/d)</td>
<td>&lt;100</td>
<td>100-500</td>
<td>&gt;500-2000</td>
<td>&gt;2000</td>
</tr>
<tr>
<td>Inhalation (vapor, mg/L/d)</td>
<td>&lt;1</td>
<td>1-2.5</td>
<td>&gt;2.5-20</td>
<td>&gt;20</td>
</tr>
<tr>
<td>Inhalation (dust, mg/L/d)</td>
<td>&lt;0.1</td>
<td>0.1-0.5</td>
<td>&gt; 0.5-5</td>
<td>5</td>
</tr>
</tbody>
</table>
“BPA is a reproductive, developmental, and systemic toxicant in animal studies and is weakly estrogenic, there are questions about its potential impact particularly on children’s health and the environment.”

(see http://www.epa.gov/opptintr/existingchemicals/pubs/actionplans/bpa.html)

- Shopping receipts
- Credit card receipts
- ATM & banking receipts
- Ultrasound printouts
- EKG & ECG printouts
- Prescription labels
- Deli labels
- Tickets
BPA Alternatives – hazard results

• The results presented at the roundtable are draft – the full BPA report is expected to be released by summer 2012.

• Watch this site for more information:
http://www.epa.gov/dfe/pubs/projects/bpa/index.htm
The Problem:
- All Surfactants have aquatic toxicity by interference with membranes
- Varying rates of biodegradation

Nonylphenol Ethoxylates (NPEs) also have degradants of concern
Safer surfactants degrade quickly to low toxicity degradates.

<table>
<thead>
<tr>
<th>Acute Aquatic Toxicity (L/E/IC50 Value)</th>
<th>Rate of Biodegradation</th>
</tr>
</thead>
<tbody>
<tr>
<td>≤1 ppm</td>
<td>May be acceptable if biodegradation(^1) occurs within a 10-day window</td>
</tr>
<tr>
<td>&gt;1 ppm and ≤10 ppm</td>
<td>Is acceptable if biodegradation(^1) occurs within a 10-day window</td>
</tr>
<tr>
<td>&gt;10 ppm</td>
<td>Is acceptable if biodegradation(^1) occurs within 28 days without products of concern(^2)</td>
</tr>
</tbody>
</table>

\(^1\) Generally, >60% mineralization (to CO\(_2\) and water) in 28 days.

\(^2\) Products of concern are compounds with high acute aquatic toxicity (L/E/IC\(_{50}\) ≤ 10ppm) and a slow rate of biodegradation (greater than 28 days).
<table>
<thead>
<tr>
<th>Chemical Class</th>
<th>Chemical</th>
<th>CASRN</th>
<th>Fate</th>
<th>Aquatic toxicity</th>
<th>Meets DfE Surfactant Criteria?</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Persistence</td>
<td>Degradates of concern</td>
<td>Acute</td>
</tr>
<tr>
<td>Nonylphenol ethoxylate (9EO); NPE9</td>
<td>Nonylphenol ethoxylate (9EO); NPE9</td>
<td>127087-87-0</td>
<td>M</td>
<td>Y</td>
<td>H</td>
</tr>
<tr>
<td>Octylphenol ethoxylate (10EO); OPE10</td>
<td>Octylphenol ethoxylate (10EO); OPE10</td>
<td>9036-19-5</td>
<td>H</td>
<td>Y</td>
<td>H</td>
</tr>
<tr>
<td>Oxirane, methyl-, polymer with oxirane, mono(2-ethylhexyl ether); Ecosurf EH-9</td>
<td>Oxirane, methyl-, polymer with oxirane, mono(2-ethylhexyl ether); Ecosurf EH-9</td>
<td>64366-70-7</td>
<td>L</td>
<td>N</td>
<td>M</td>
</tr>
</tbody>
</table>
Hazard assessment for green chemistry

Continuous improvement towards green chemistry

Challenges necessitate careful decision frameworks
www.epa.gov/dfe
http://www.epa.gov/dfe/alternative_assessments.html

Emma Lavoie
Tel: 202-564-0951

Read more here:
http://dx.doi.org/10.1021/es1015789

The opinions expressed in this presentation are those of the author and do not necessarily represent US EPA policy.