Design for the Environment

Chemical Alternatives Assessments

GC3

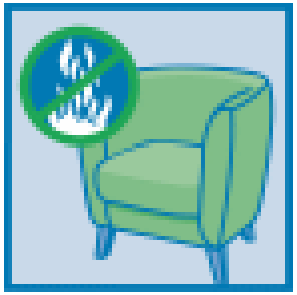
May 2012

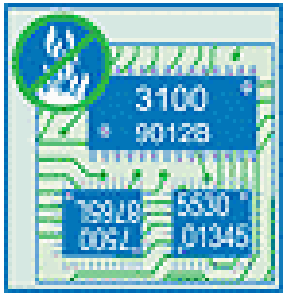
DfE Chemical Alternatives Assessment

- 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”

What is a Chemical Alternatives Assessment?

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

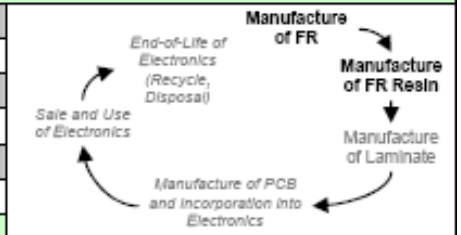
DfE Alternatives Assessments for Priority Chemicals

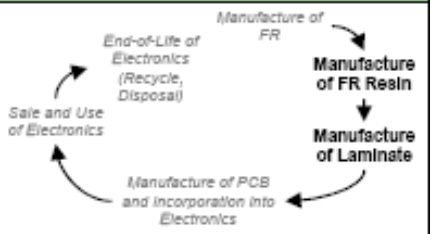
- **Tetrabromobisphenol A (TBBPA)** in Printed Circuit Boards
  - combustion testing near completion
- **Nonylphenol and nonylphenol ethoxylates (NP/NPE)**
  - final report Spring 2012
- **Bisphenol A (BPA)** in Thermal Paper
  - draft report Spring 2012
- Flame Retardant Alternatives to **decabromodiphenyl 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

Human Health Hazard Concern | **Ecotoxicity Hazard Concern** | **Persistence Hazard Concern**

Chemical	CASRN	Human Health Effects: Acute Toxicity	Skin Sensitizer	Cancer Hazard	Immunotoxicity	Reproductive	Developmental	Neurological	Systemic	Genotoxicity	Aquatic Toxicity: Acute	Aquatic Toxicity: Chronic	Environmental: Persistence	Environmental: Bioaccumulation	Exposure Considerations: Availability of flame retardants (FRs) throughout the lifecycle for reactive and additive FRs chemicals and resins
Reactive Flame Retardant Chemicals[2]															
Tetrabromobisphenol A (TBBPA) (Albemarle, Chemtura, and others)															
TBBPA	79-94-7	L	L	L	L	L	M	L	L	L	H	H	M	L	
DOPO (6H-Dibenz[c,e][1,2] oxaphosphorin, 6-oxide) (Samko Co., Ltd. and others)															
DOPO	35948-25-5	L	L	L	L	L	L	L	L	L	M	M	L	L	
Fyrolflex PMP (Aryl alkylphosphonate) (Supresta)															
Fyrolflex PMP	Proprietary	L	L	L	L	L	L	L	L	L	L	L	H	L	
Reactive Flame Retardant Resins[2]															
Reaction product of TBBPA - D.E.R. 538 (Phenol, 4,4'-(1-methylethylidene)bis[2,6-dibromo-, polymer with (chloromethyl)oxirane and 4,4'-(1-methylethylidene)bis[phenol]) (Dow Chemical)															
D.E.R. 538	26265-08-7	L	M	M◊	L	M◊	M◊	L	L	M	L	L	M	L	
Reaction Product of DOPO - Dow XZ-92547 (reaction product of an epoxy phenyl novolak with DOPO) (Dow Chemical)															
Dow XZ-92547	Proprietary	L	M	M◊	L	M◊	M◊	L	L	M◊	L	L	H	L	
Reaction product of Fyrolflex PMP with bisphenol A, polymer with epichlorohydrin (Representative Resin)															
Representative Fyrolflex PCB Resin	Unknown	L	L	M◊	L	M◊	M◊	L	L	M◊	L	L	H	L	





DfE Alternatives Assessment Criteria Endpoints

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

- Endocrine Activity

Environmental Fate & Effects

- Aquatic toxicity
- Environmental persistence
- Bioaccumulation

Additional Endpoints

- Physical hazards
- Ecotoxicity
- And more

EPA DfE Criteria

- Criteria derived from GHS, EPA, authoritative lists

Reproductive & Developmental Toxicity Criteria

Endpoint (LOAEL, NOAEL)	High	Moderate	Low	Very Low
Oral (mg/kg-bw/d)	<50	50-250	> 250-1000	>1000
Dermal (mg/kg-bw/d)	<100	100-500	>500- 2000	>2000
Inhalation (vapor, mg/L/d)	<1	1-2.5	>2.5-20	>20
Inhalation (dust, mg/L/d)	<0.1	0.1-0.5	> 0.5-5	5

BPA Alternatives in Thermal Paper Partnership

"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

http://www.zimbio.com/pictures/RD7q8nFOyKs/Jessica+Alba+Out+Beverly+Hills/Hndv07-2WS4/Meter+Maid

http://www.jpihealthcare.com/ultrasound-paper

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

Surfactants

- The Problem:
  - All Surfactants have aquatic toxicity by interference with membranes
  - Varying rates of biodegradation

- Nonylphenol Ethoxylates (NPEs) also have degradants of concern

Surfactants

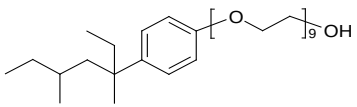
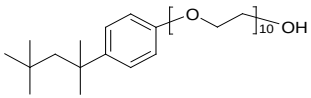
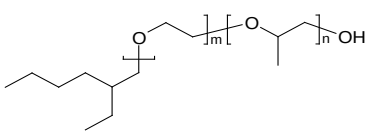
- Safer surfactants degrade quickly to low toxicity degradates.

Acute Aquatic Toxicity (L/E/IC50 Value)	Rate of Biodegradation
≤1 ppm	May be acceptable if biodegradation[1] occurs within a 10-day window
>1 ppm and ≤10 ppm	Is acceptable if biodegradation[1] occurs within a 10-day window
>10 ppm	Is acceptable if biodegradation[1] occurs within 28 days without products of concern[2]

[1] Generally, >60% mineralization (to CO_2 and water) in 28 days.

[2] Products of concern are compounds with high acute aquatic toxicity ($L/E/IC_{50} \leq 10ppm$) and a slow rate of biodegradation (greater than 28 days).

Nonylphenol Ethoxylates and Alternatives

Chemical Class		Fate		Aquatic toxicity[1]			
Chemical	CASRN	Persistence	Degradates of concern[2]	Acute	Chronic	Degradate Aquatic toxicity	Meets DfE Surfactant Criteria?
Nonylphenol ethoxylate (9EO); NPE9 	127087-87-0	M	Y	H	M	VH	N
Octylphenol ethoxylate (10EO); OPE10 	9036-19-5	H	Y	H	*H*	VH	N
Oxirane, methyl-, polymer with oxirane, mono(2-ethylhexyl ether); Ecosurf EH-9 	64366-70-7	L	N	M	*M*	L	Y

AA based substitution

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

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Read more here:

Lavoie, E. T., L. G. Heine, et al. "Chemical Alternatives Assessment: Enabling Substitution to Safer Chemicals." Environmental Science & Technology 44(24). 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.