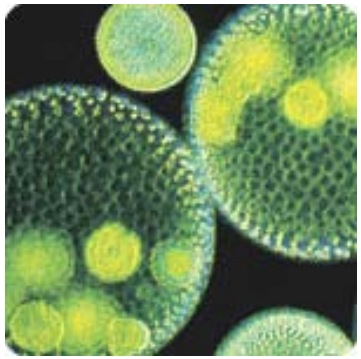
Alternative Analysis in Industry

Don Versteeg, PhD
Environmental Toxicologist & Ecologist

The Good News

- Legislators & regulators are aligned to help identify better chemicals
  - REACH, TSCA Revisions
  - DfE, CA Green Chemistry, etc.
  - Presidential Green Chemistry Awards
- The public is becoming aware
  - DfE, Good Housekeeping, MBDC, blogs, internet, etc.
- Academia is engaged
  - Green chemistry programs
  - Environmental engineering programs
  - West Nyack Elementary

More Good News



- Industry is motivated
  - Toxicologists, chemists, engineers, etc.
  - Green chemistry programs
  - Sustainability initiatives (C2C thinking)
- Green infrastructure
  - Natural power sources
  - Composting
  - Retailer initiatives (WalMart, Home Depot, Target, etc.)

The Rest of the Story

- As a result, significant pressure to move out of CMRs, PBTs, and related chemicals
  - Many alternatives have been found
    - Led to new and improved ingredients & products
    - Reduced impacts
    - Reduced regulatory scrutiny
    - Reduced public pressure
- But, . . .

RISK

High

AA Important and easy

AA Important but difficult

DONE

Importance in Product

Low

High

AA less important and easy

AA less important and difficult

Low

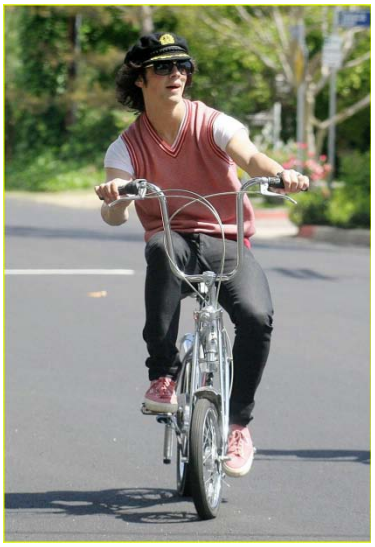
AGENDA

- The Challenge of AA
- Integration of AA into Product Development
- Examples & Issues
- Conclusions

The Challenge of AA

Risk

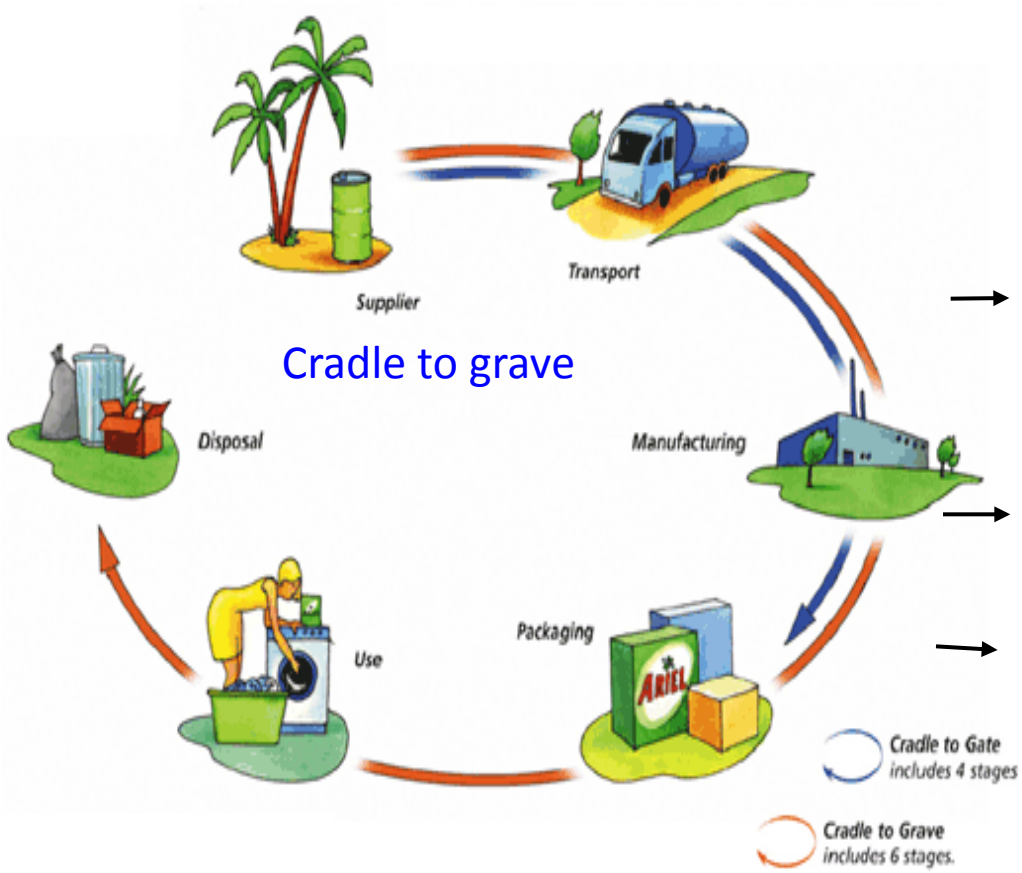
High volume, mid to high toxicity
Low volume, high toxicity
Very high volume, low toxicity



- Methods exist
- General agreement on high and low risk
- History of use in decision-making

Low Volume, mid to low toxicity
Naturally present in food
High volume but low exposure

Life Cycle Assessment (LCA)



Tool to assess env. impact of technologies and products through their entire life cycle

Covers a variety of environmental indicators

Use of resources

Emissions to air

Emissions to water

Emissions to soil

Energy consumption

Water consumption

Solid waste

Global warming

Ozone depletion

Human toxicity

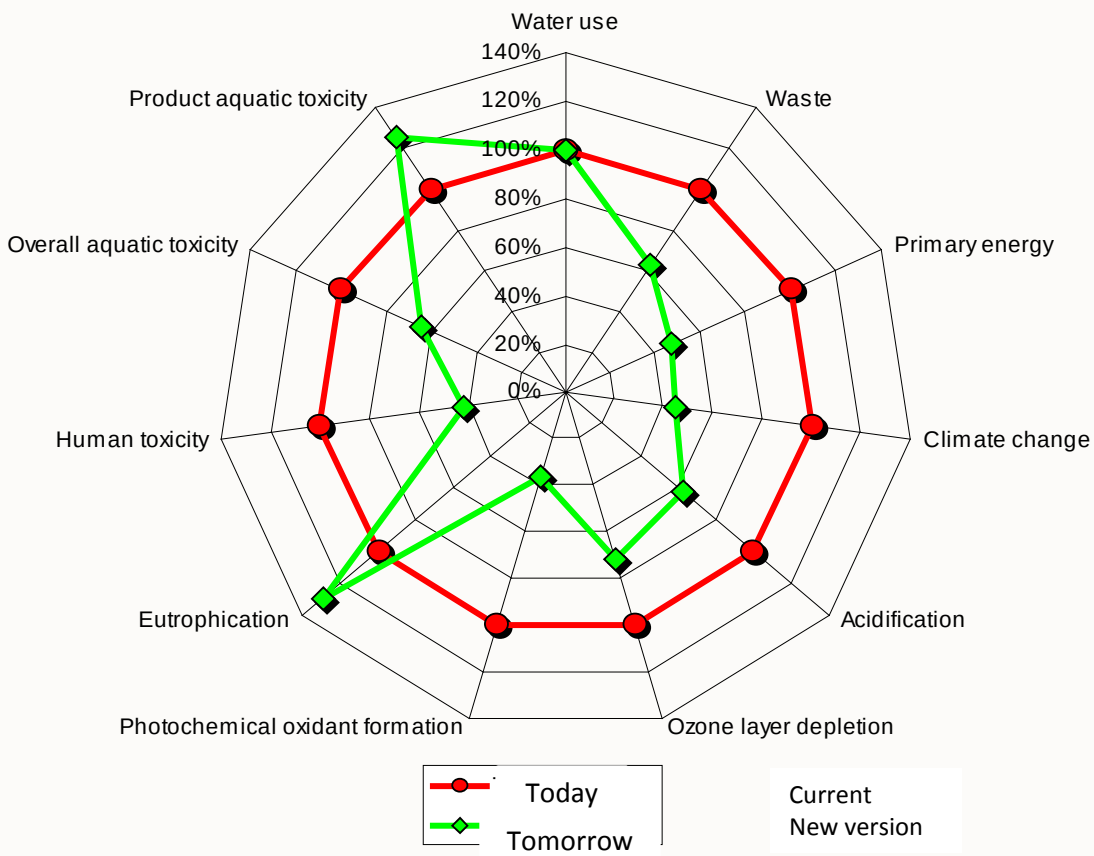
Aquatic ecotoxicity

Acidification

Eutrophication

Summer smog

Integrate LCA with Risk?



LCA profile of the wash process using a coldwater detergent in cold water compared to a regular detergent following current wash practices.

Comparison of metrics difficult

How do we compare 1 gram of solid waste with 1 gram of CO_2 or 1 mg of phosphate?

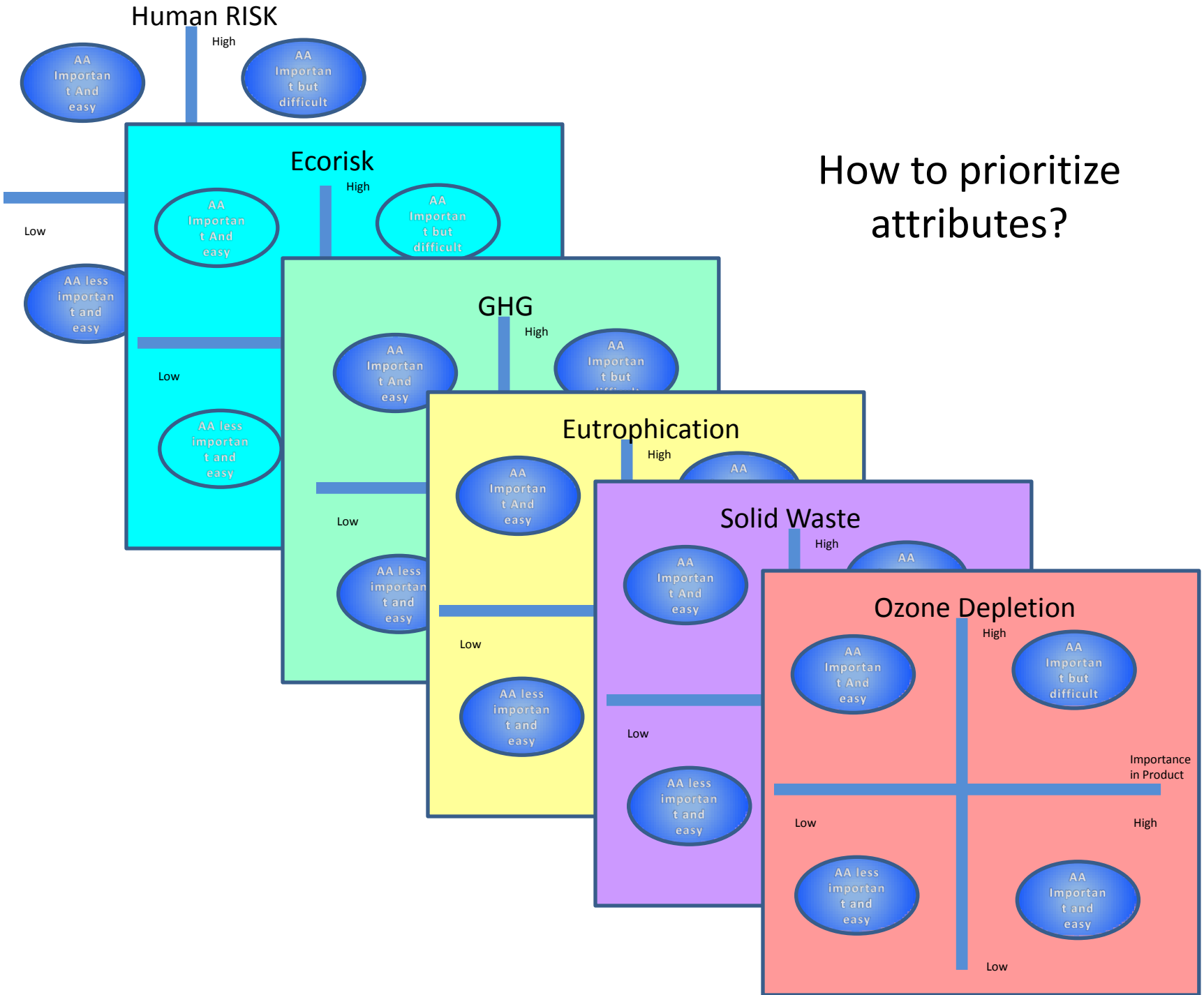
How much additional risk will we take to reduce water use by 10 liters per kg of product?

Other Considerations

- Biomonitoring
- Ecological monitoring
- Bioaccumulation or toxic or persistent
- Pseudopersistence
  - 2-methyl-1,4-naphthoquinone

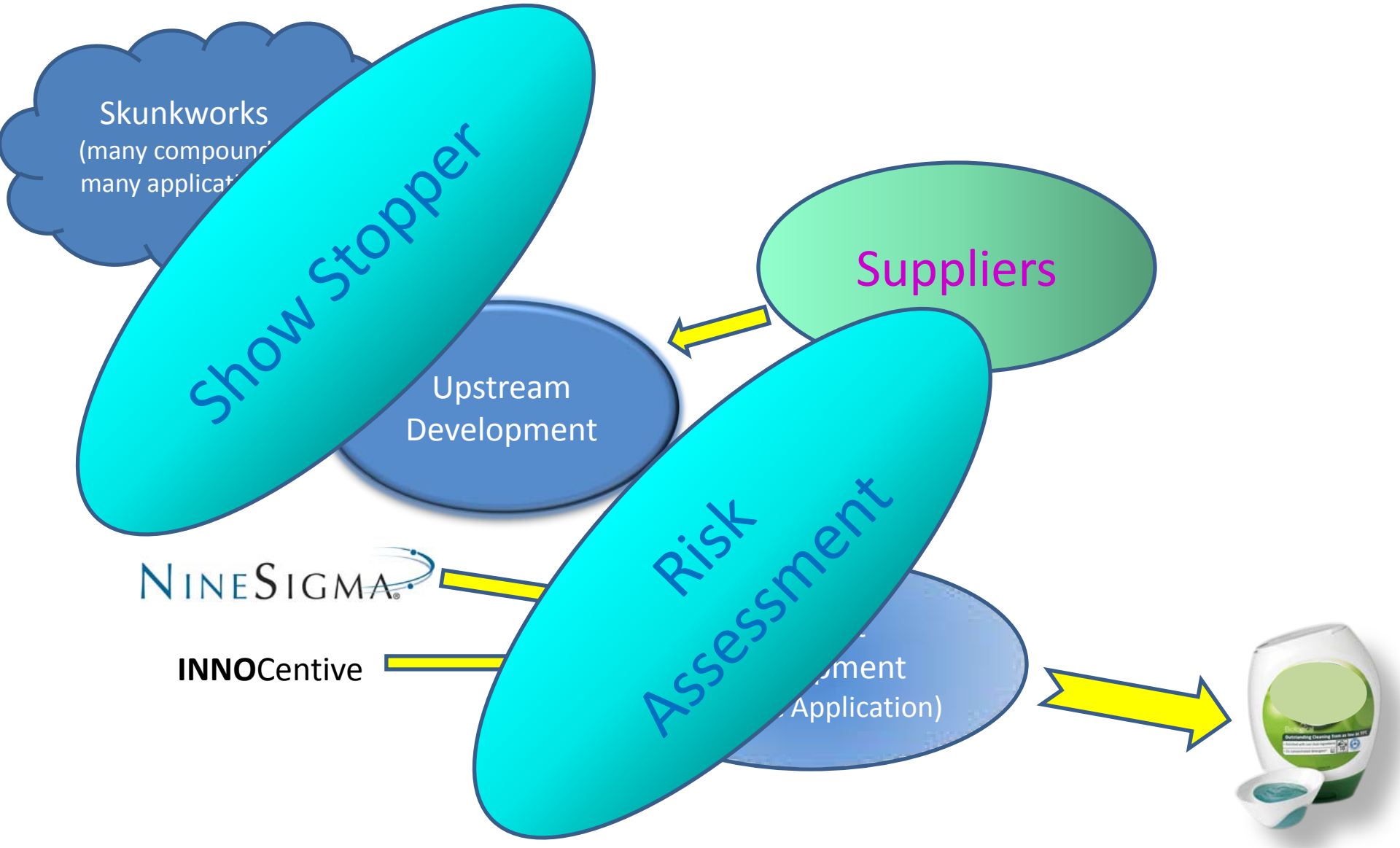
How do we integrate these endpoints into our risk or LCA framework to make a decision?

How to prioritize attributes?



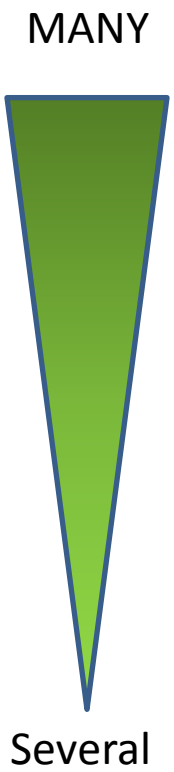
Integration of AA into Product Development

Product Development



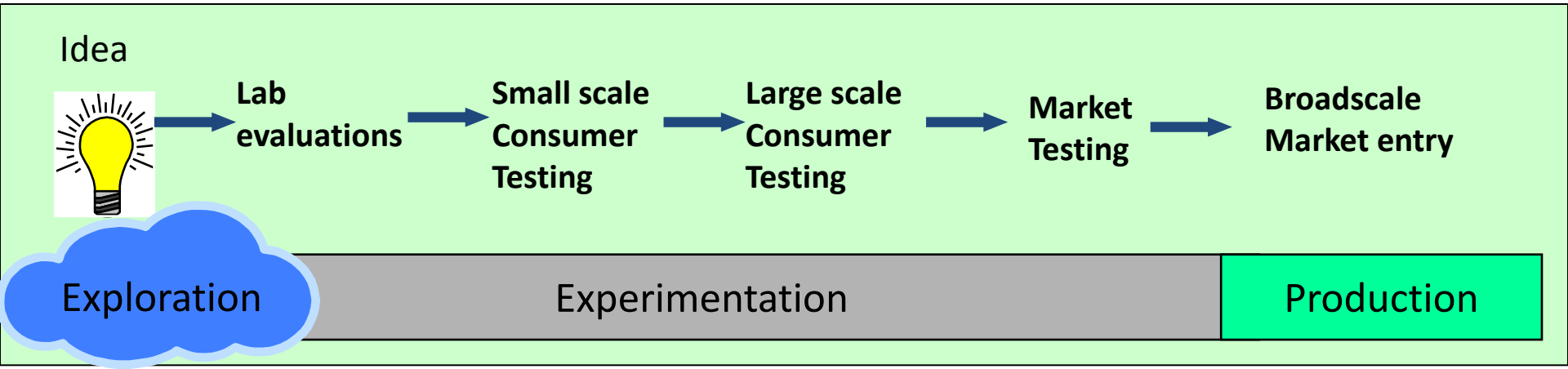
General Approach to AA

Product Development	Safety & Sustainability
New Ingredients Applications undefined	Show Stopper (CMR, PBT)
Specific Application Specific ingredients Cost, supply, processing, etc.	Risk assessment LCA

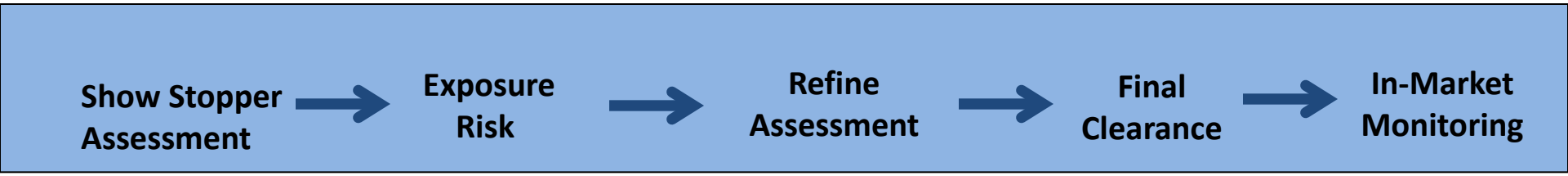


Designing Safety In—*Right from the Start*

Product Development



Ingredient Safety Evaluations



Product LCA

Show Stopper

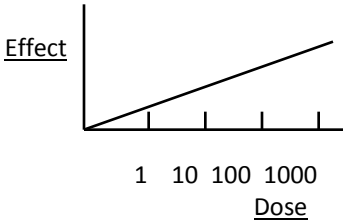
- Human
  - CMRs
  - Sensitization, irritation, overt toxicity
    - Analog analysis, substructural information
  - Metabolism & contaminant
- Environment
  - PBT
  - Overt toxicity
    - QSAR & analog analysis
  - Metabolism considered
- Regulatory
  - Listed in the countries of interest

How do we assess Safety ?

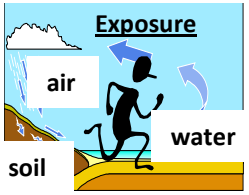
Risk Assessment:

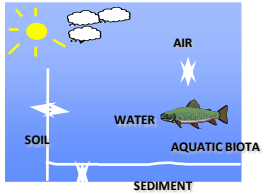
- Hazard identification
  - Use QSAR & Analogs

- Dose response/ effects assessment



- Exposure assessment





- Risk characterization

$$\frac{\text{hazard}}{\text{exposure}} \Rightarrow \text{quantification of Risk}$$

Human Safety

- Safe for use and reasonably foreseen misuse for all (subpopulations included)
  - Sprays vs. Pourable – eyes/respiration vs. dermal
  - Type & severity of effect
  - Food handling, assume use of microwave
  - Assume hand to mouth exposure
    - Food contact
    - Magnitude, frequency, duration

Environmental Safety

- Exposure & effects assessment
  - Internal
    - Fate, effects, risk
      - Terrestrial, sediment, aquatic
  - Regulatory (typically multiple)

Parent & metabolites

Regulatory (US)

Final regulatory evaluation

File new substance application

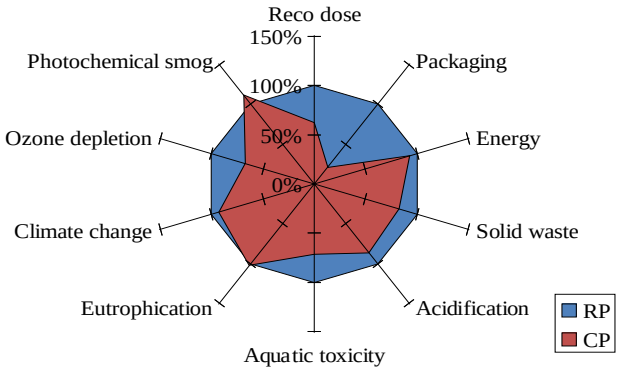
EPA's TSCA

"Any organic or inorganic substances of a particular molecular identity including any combination of such substances occurring, in whole or in part, as a result of chemical reaction or occurring in nature and any element or uncombined radical."

Other Federal Laws Regulating Chemicals

- Federal Insecticide, Fungicide and Rodenticide Act (FIFRA)
- Federal Food, Drug and Cosmetics Act (FFDCA)
- Clean Air Act (CAA)
- Clean Water Act (CWA)
- Resource Conservation and Recovery Act (RCRA)
- Comprehensive Environmental Response, Compensation and Liability Act of 1980 (CERCLA)
- Emergency Planning and Community Right-to-Know Act (EPCRA)
- Occupational Safety and Health Act (OSHA)
- Hazardous Materials Transportation Act (HMTA)
- Consumer Product Safety Act (CPSA)
- Federal Hazardous Substances Act (FHSA)
- Food Quality Protection Act (FQPA)

LCA



- Energy
- Solid waste
- Greenhouse gases
- Ozone depletion
- Smog
- Eutrophication
- Acidification
- Hazardous waste
- Mineral depletion
- Water use
- Toxicity

Many of these LCA impacts can be minimized by optimizing the supply, processing, and formulation chain

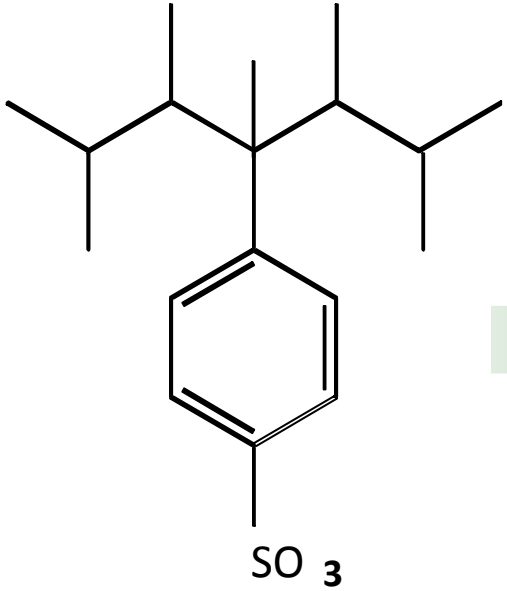
KEY: How much emphasis should be placed on LCA endpoints?

Examples & Issues

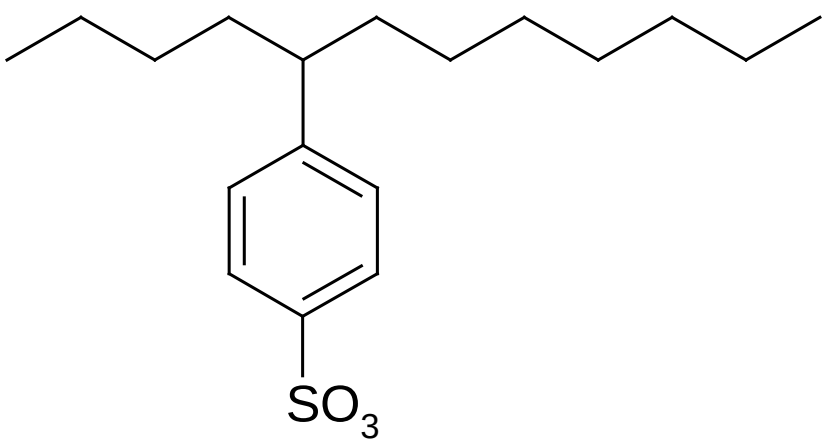
Sustainable Innovation: Inventing Technologies that Improve Environmental Quality

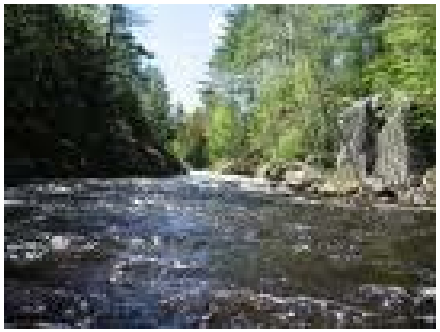
Old Technology	Replacement Technology	Why change?
ABS	LAS	Anionic surfactant Foaming in rivers/improved biodeg profile
APE	AE	Nonionic surfactant Marginal to complete biodeg, toxicity & EDC issues
DTDMAC	DEEDMAC	Fabric softener active Non-biodegradable to biodegradable
Anionic surfactants	HSAS	Anionic surfactants with superb environmental pedigree replaced; cold water wash need

Alkylbenzene Sulfonate



Linear Alkylbenzene Sulfonate (LAS)

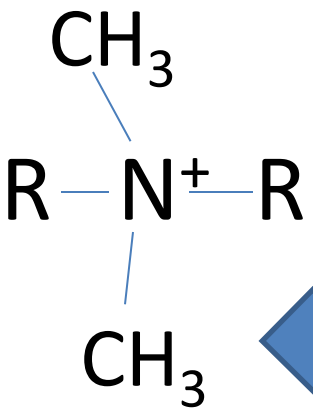




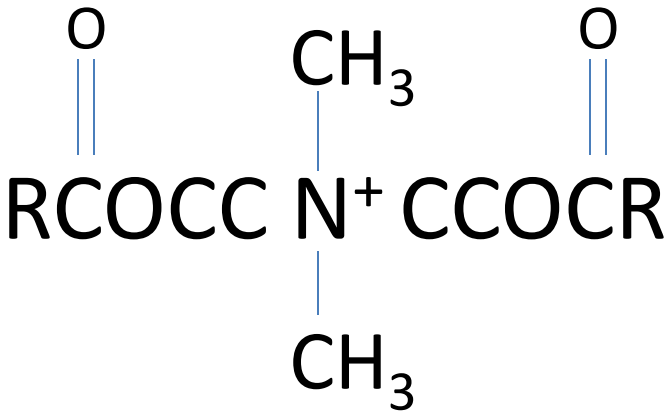
APE - > AE

- Alkyl phenol ethoxylates
  - Degrade to alkylphenols
  - More toxic (EDC), less biodegradable than parent
- Major manufacturers have replaced
- Smaller companies slower to change
  - Store brands
- Alternatives like linear AE more expensive

DTDMAC → Ester Quats



- DTDMAC – nonbiodegradable, but not very toxic
- Ester quats – biodegradable, but more toxic, more expensive
- Major manufacturers used alternative, smaller manufacturers stayed with DTDMAC
- Alternative more expensive



R=C16-18

AS → HSAS

- HUGE LCA/Energy Savings – 3% of Kyoto CO_2 goals

- Longer chain alkyl sulfate
  - Alternative to short chain alkyl sulfate
- Balancing solubility, toxicity and biodegradability key to being able to safely wash in cold water

Chelators

Phosphate - Eutrophication issue

Synthetic chelants - EDTA, DTPA, Phosphonates

Biodegradable chelants – EDDS, GLDA, IDS

Excellent in some applications!!

But, poor chelators for some impt metals, thus, need to use 10-100x more (eliminates advantage of biodegradation)

Alternatives from Green Labels

- Recommended new solvent
  - Hazardous waste
- Low molecular weight amine
  - Would create a new material
    - 4-7 years to get approved by EPA PMN Office

Barriers

- Lack of understanding of new chemicals
  - “Old” chemical, high knowledge→ new chemical, limited knowledge

- Regrettable substitution
  - Chlorinated solvents in CA
  - DDT
  - Chlorine disinfection
  - Pb → MTBE

Out of the Box Thinking

- Enzymes
- Fluorescent whitening agents

- Nanoparticles
- “Gene” therapy
  - Preservatives, drugs & pesticides

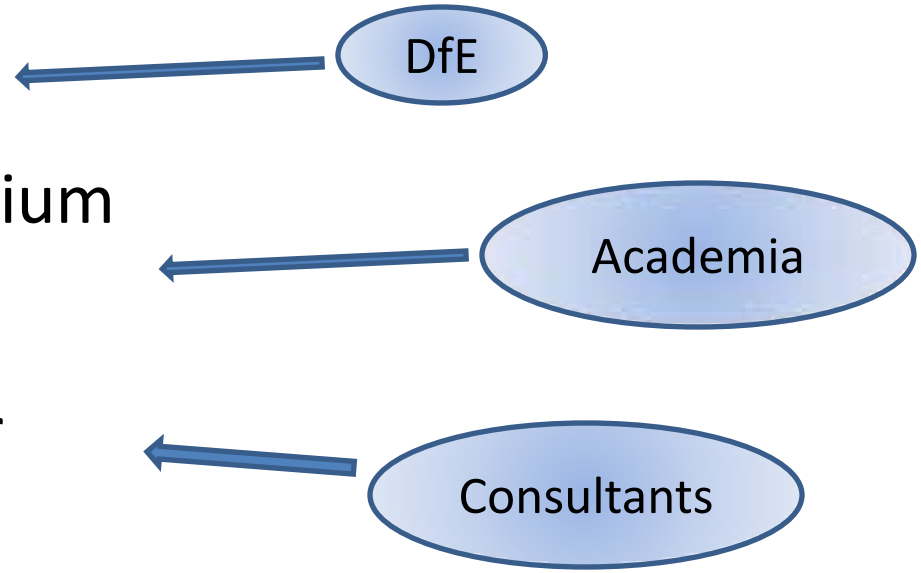
Ingredient Performance
Ingredient Supply
Ingredient Cost
Performance + Price = Consumer Satisfaction
Ingredient Compatibility
Ingredient Safety
Ingredient Aesthetics
Ingredient Sustainability
Chemical Hazard

AA Personnel Needed

- Product development
- Manufacturing processes
  - Company & process specific
- Purchasing
- Regulatory expert
- Human safety
- Environmental safety
- Worker safety
- LCA

AA Practioners?

- Nonproprietary
  - Industry led consortium
- Proprietary
  - Single manufacturer



- Experience with product, production, product compatibility, cost, supply, safety, etc.
  - Consumer knowledge

Conclusion

- Alignment on pursuit of a sustainable future
- Long history of successful AA in industry
- AA should be risk based, then LCA
  - May not need to replace all uses
  - May not have technology to replace all uses
- AA is complex, resource intensive, multidisciplinary
  - Technology owners need to be involved in AA

Versteeg.dj@pg.com