Household Detergents

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AGENDA

- Industry & the TAAG
- Finding New Ingredients
- Green Chemicals/Ingredients
- Hazard vs. Risk
- Case Studies
- Tools: AA, Hazard, Risk, & LCA
- Principles

Why is Industry Involved with the TAAG?

- > 60 years of experience in replacing one ingredient, with another without compromising on safety
  - The search for new ingredients, with an acceptable safety pedigree is alternatives analysis

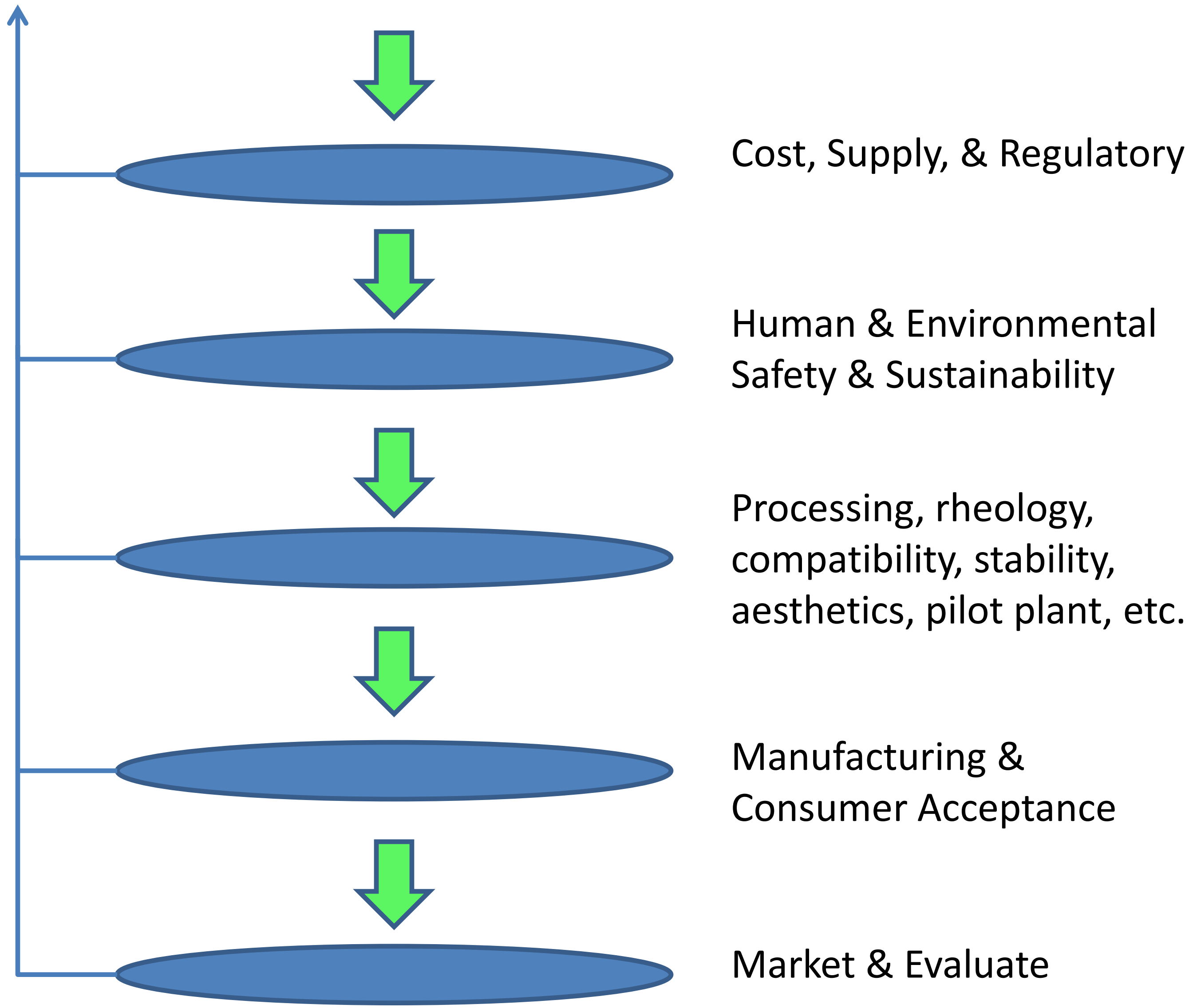
- Similar interest: safer, more sustainable products that improve the lives of consumers now and for generations to come. This includes workers, and all impacts through the lifecycle.

'Alternatives Assessment' is a process for identifying and comparing potential chemical and non-chemical alternatives that can be used as substitutes to replace chemicals or technologies of high concern

Identifying New Ingredients

- Suppliers
  - Find supplier knowledgeable in the chemical space
- Brute force approach
  - Focused on appropriate chemistries
  - Test product with new ingredient
- Modeling approach
  - Define the property needed molecular descriptors
  - Search for ingredients optimized for those descriptors
  - Synthesize molecule & test

List of Alternative Chemicals



Availability of Green Chemicals

- Short list of green chemicals
  - Many are conventional chemicals with improvements in supply
- Green Chemistry Principles focus on chemical production
- Evaluate all chemicals for ‘greenness’
  - Criteria & tradeoffs?

Green Detergent	Regular Detergent
Sodium lauryl sulfate	Yes
Laureth-6	Similar
Sodium citrate	Yes
Glycerin	No
Oleic acid	Yes
Sodium hydroxide	Yes
Boric acid	Yes
Calcium chloride	Yes
Fragrance	Yes
Enzymes: protease, amylase and mannanase	Yes
Preservatives: methylisothiazolinone & benzisothiazolinone	Yes

Green detergent contains more naturally based materials.

Regular detergent contained additional ingredients.


What`s the exposure?
What`s the hazard?
What`s the risk?
FAIRY

Tiers in Environmental

- Screening: Some hazards indicated probability of success is low (genotoxicity, LC50< 100ppb). These may be showstoppers.

- Tier 1: Do I have a good chemical analog or good QSARs to support environmental fate and effects predictions?
  - If no, test
  - If yes, evaluate safety
    - If safe, stop, use material
    - If significant risk, stop, do not use material
    - If safety not assured, continue with next tier

- Tier 2: Conduct basic acute toxicity and fate tests, evaluate safety
  - If safe, stop, use material
  - If significant risk, stop, do not use material
  - If safety not assured, continue with next tier

- Tier 3: . . .

Chemicals Eliminated

- High volume surfactants due to risk
- High volume fragrance ingredients due to PBT
- Fluorinated organics due to atmospheric concerns
- Organometallic compounds due to endocrine and toxicity concerns
- Etc.

Historical alternatives efforts

Old	New	When	Trade Off
ABS	LAS	1960	↑ toxic
APE	Alcohol ethoxylates	1970	
Phosphate	DTPA	1970	↓ degradable, ↑ toxic
DTDMAC	Ester-Quat	1995	↑ toxic
MTBE	Ethanol	2000	↑ food prices

Trade-Offs - Preservative/Antimicrobials

Literature Search Results

Compound	Toxicity	Toxicity & Daphnia	River	Endocrine
Current	488	34	400	368
Alt 1	755	6	44	55
Alt 2	279	0	6	29
Alt 3	49	1	7	3
Alt 4	30	0	1	3
Alt 5	97	8	57	75
Alt 6	77	2	2	8

If new chemical needed, then 3-6 years for approval.

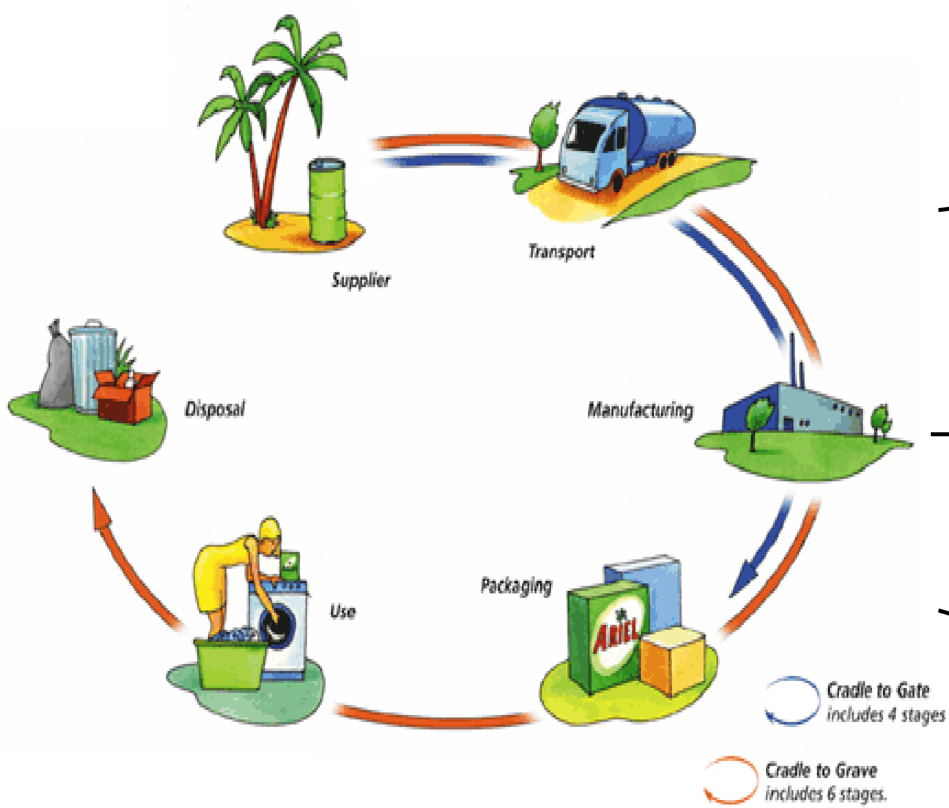
Other experience with AA

- Chelators
  - Chemicals that bind calcium & metals allowing surfactants to work better
  - >35 year search
    - Several new materials developed and commercialized
      - None that adequately replace EDTA, DTPA, phosphates
- Enzyme stabilizers
  - >5 year search
  - PMN needed (multiple years)
  - Capacity

ADW: Nil P Technology Strategy

Area of Consumer Impact	Nil P Technologies
Tough Food Cleaning	4 – 5 materials
Shine	2 materials
Metal Care	2 materials
Stain Removal	2 materials
Gel product aesthetics	1 material

LCA– the 1 slide explanation



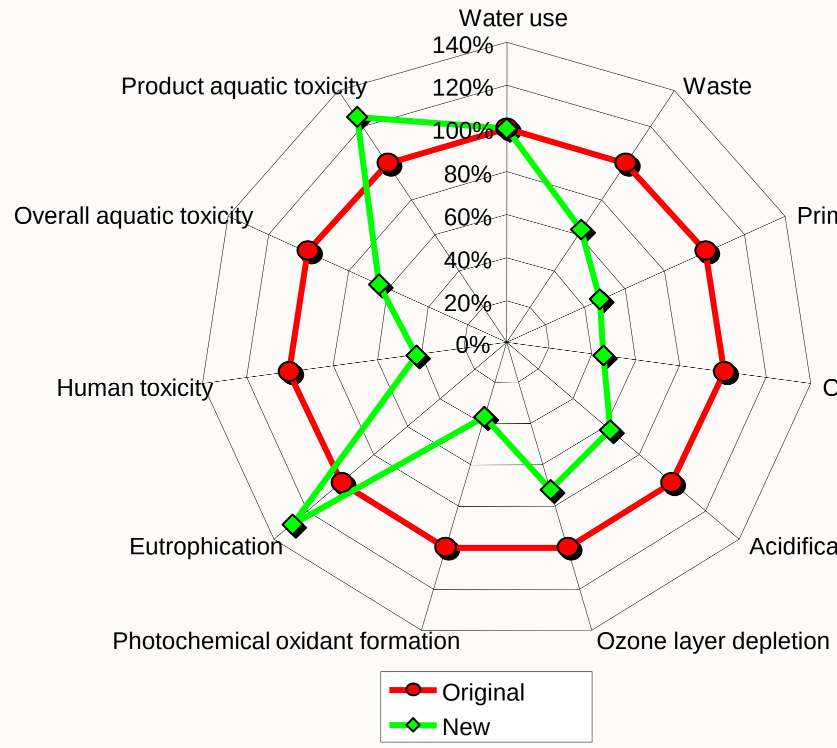
PROCESS

- Use of resources
- Emissions into air
- Emissions into water

IMPACT

- Energy consumption
- Water consumption
- Solid waste
- Global warming
- Ozone depletion
- Human toxicity
- Summer smog
- Acidification
- Eutrophication
- Aquatic ecotoxicity

Typical LCA Output



Comparison of metrics

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

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

No Risk!

Impact Factor	Units	Product 1	Product 2
Energy total	MJ primary	3.2	2.6
Water consumption	liter	1.8	1.8
IPCC GWP 100a	kg CO2 eq	0.15	0.13
Smog	g NOx eq	0.00039	0.00032
Ozone depletion	kg CFC-11 eq	1.0E-08	9.3E-09
Human toxicity	kg toluene eq	2.97	3.28
Respiratory effects	kg PM2.5 eq	0.00021	0.00018
Eutrophication	g N eq	0.00016	0.00049
Ecotoxicity	kg 2,4-D eq	0.22	0.24

Normalization – how important is each factor?

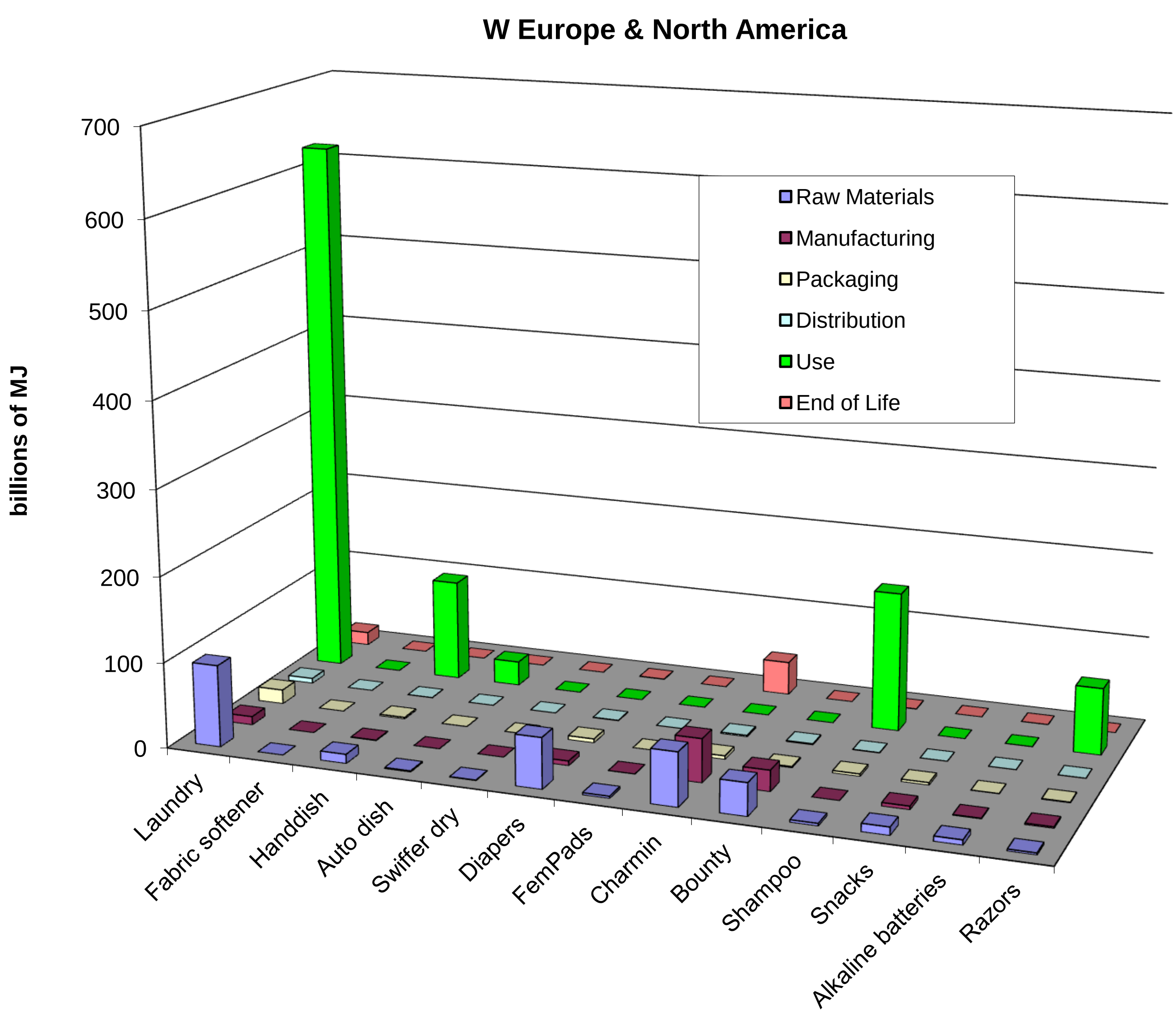
- Difficult to compare an extra 1,000 liters of water used with a reduction of 0.3 kg of air emissions
- We know how much water is used in a region by each average consumer
- We know how much air emissions are released in the region by each average consumer
- Use this information to Normalize the Impacts
  - Convert into people equivalents
    - i.e., amount of that factor used or generated by an average person per year

Normalization – annual product use

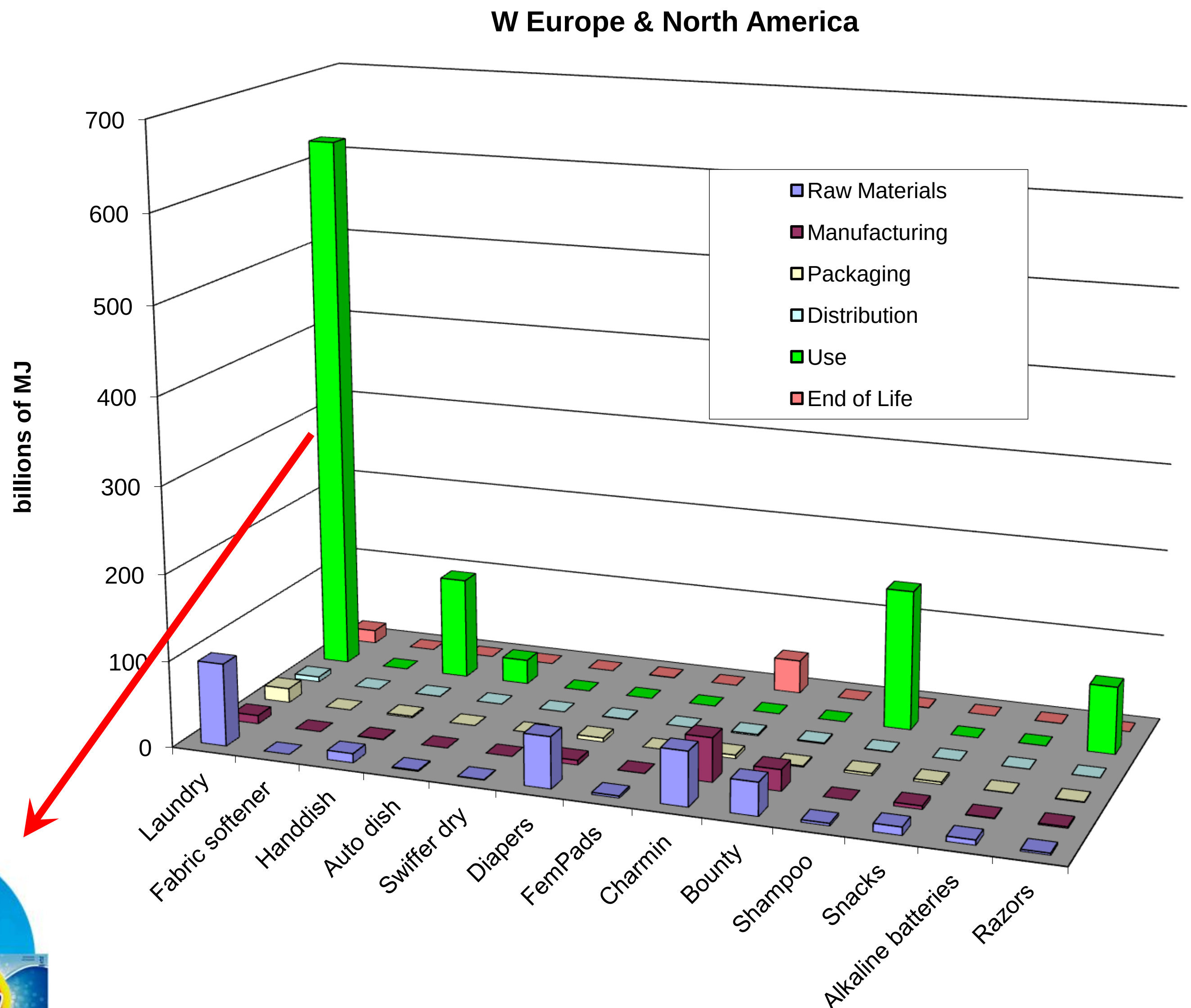
Impact Factor	Product 1	Product 2	People Equivalents*
Energy total	3.2	2.6	-40,000
IPCC GWP 100a	0.15	0.13	-32,000
Smog	0.00039	0.00036	-3,000
Ozone depletion	1.0E-08	9.3E-09	-88
Human Toxicity	2.97	3.28	+16,000
Respiratory effects	0.00021	0.00018	-250
Eutrophication	0.00016	0.00049	+22
Ecotoxicity	0.22	0.40	+3,200

*Difference between products 1 & 2, converted to people equivalents, annualized

Energy Usage from Life Cycle Perspective



Energy Usage from Life Cycle Perspective



Warm vs. Cold Water Surfactant

Property	Warm Surf	Cold Surf
Persistence	Ready	Ready
Bioaccumulation	Low	Moderate
Toxicity (aquatic)	Moderate	↑ toxic

- The warm water surfactant wins in a hazard assessment

- But, both compounds are **safe** based on risk assessment and the cold water surfactant is needed for cold water solubility = energy & GHG savings

Is Bio-PE Better than Petro-PE for use in a Shampoo Bottle?

- Sugar ($C_6H_{12}O_6$) → Plastic $(CH_2)_x$
  - ↑ energy
- Petroleum (CH2) → Plastic $(CH_2)_x$
  - ↓ Energy

Is Bio-PE Better than Petro-PE for use in a Shampoo Bottle?

	Bio vs. Petro-PE
Total Energy	↑

Is Bio-PE Better than Petro-PE for use in a Shampoo Bottle?

	Bio vs. Petro-PE
Total Energy	↑
Fossil Energy	↓
GHG Emission	↓

Is Bio-PE Better than Petro-PE for use in a Shampoo Bottle?

	Bio vs. Petro-PE
Total Energy	↑
Fossil Energy	↓
GHG Emission	↓
Land Occupation	↑
Eutrophication	↑
Terrestrial Acidification	↑

Site & resin specific!

Tools

- Alternatives Analysis – identifies list of potential ingredients
  - Describes entire process of analyzing information & making a decision
  - aka – Product Development
- Hazard Assessment – initial screening of alternatives
  - Screening tests, related materials, structural alerts,
  - Narrows list of alternatives – no absolute rules
- Risk Assessment – defines safety
  - Definitive tests needed
  - Select list of acceptable alternatives
- LCA – defines impacts through the lifecycle
  - Not good for risk (not temporally or spatially explicit)
  - Identifies sustainability issues & opportunities

Principles

- Do no harm
  - Carefully select materials to replace
- Involve experts
  - Retired R&D & Process Engineers?
- Flexibility
  - Toys, electronics, cars, pesticides, cleaning products
- Include the life-cycle
  - Establish rules for trade-offs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