Green Chemistry: Possibilities for the Next Generation

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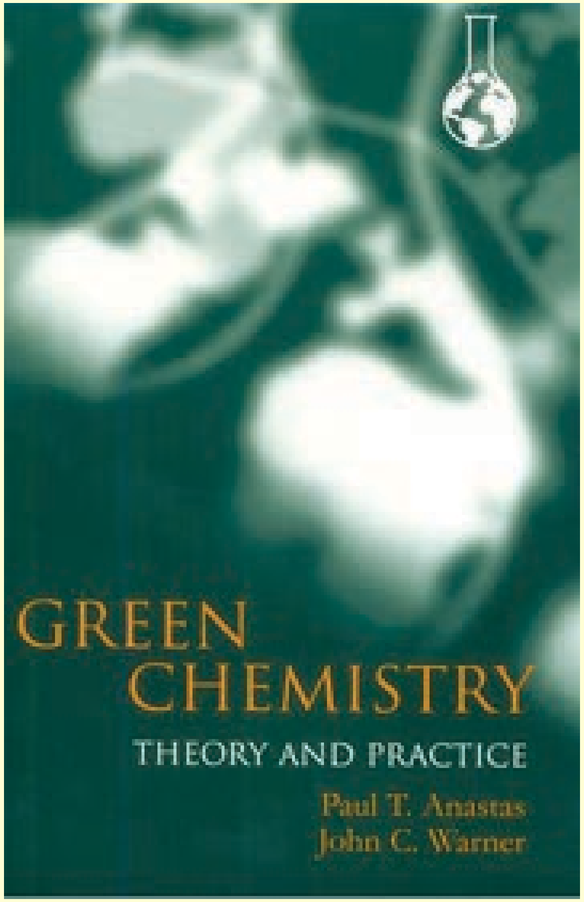
Green Chemistry: 20 Years and counting..



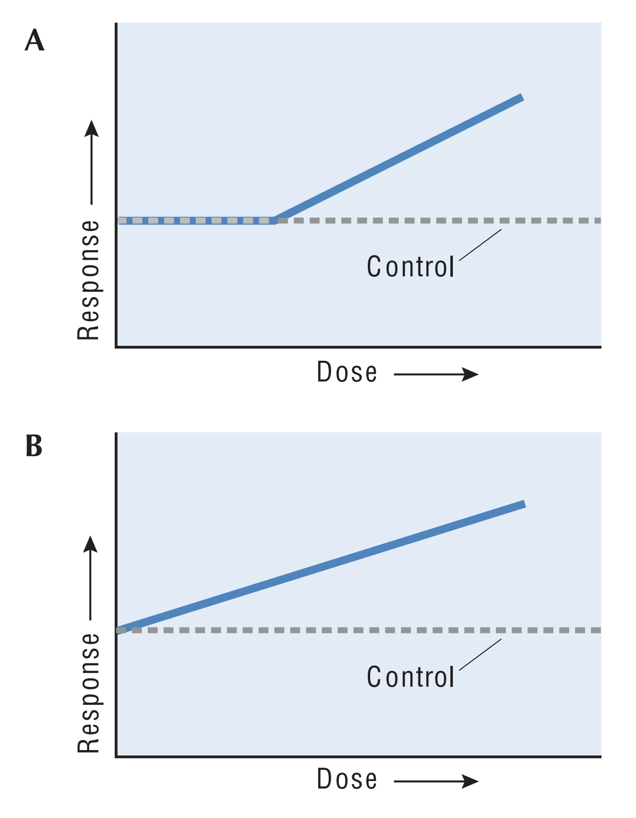
1998

Presidential Green Chemistry Awards (1996)

Green Chemistry: 20 Years on…

- A new way to look at chemistry & engineering
- From cleanup to pollution prevention to hazard reduction
- Along the way,
  - new ways to look at toxicity,
  - tractable tools for life cycle analysis,
  - New technology,
  - profound changes within the business & *investment* community.

New Ways to Look at Toxicity [from *E.J. Calabrese,* EMBO Rep. (2004), 5 (special issue), s37-s40]

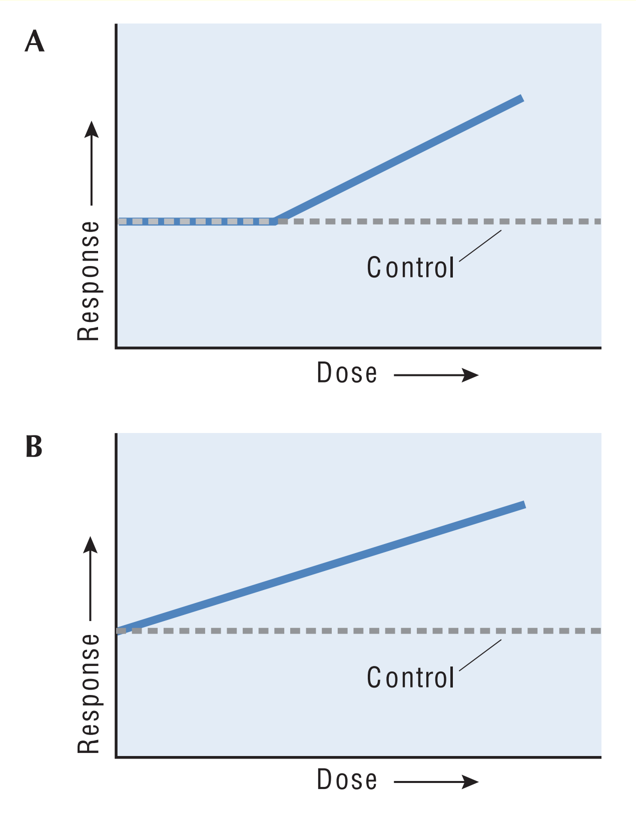


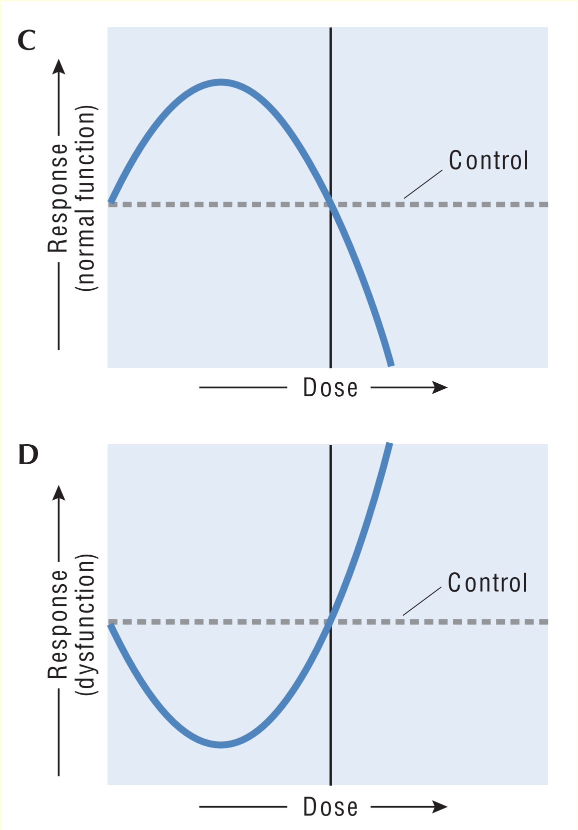
Traditional view, the dose makes the poison, with and without a threshold value…

…carcinogens and radiation assumed to have no threshold

Endocrine disruption, Epigenetics

New Ways to Look at Toxicity [from *E.J. Calabrese,* EMBO Rep. (2004), 5 (special issue), s37-s40]



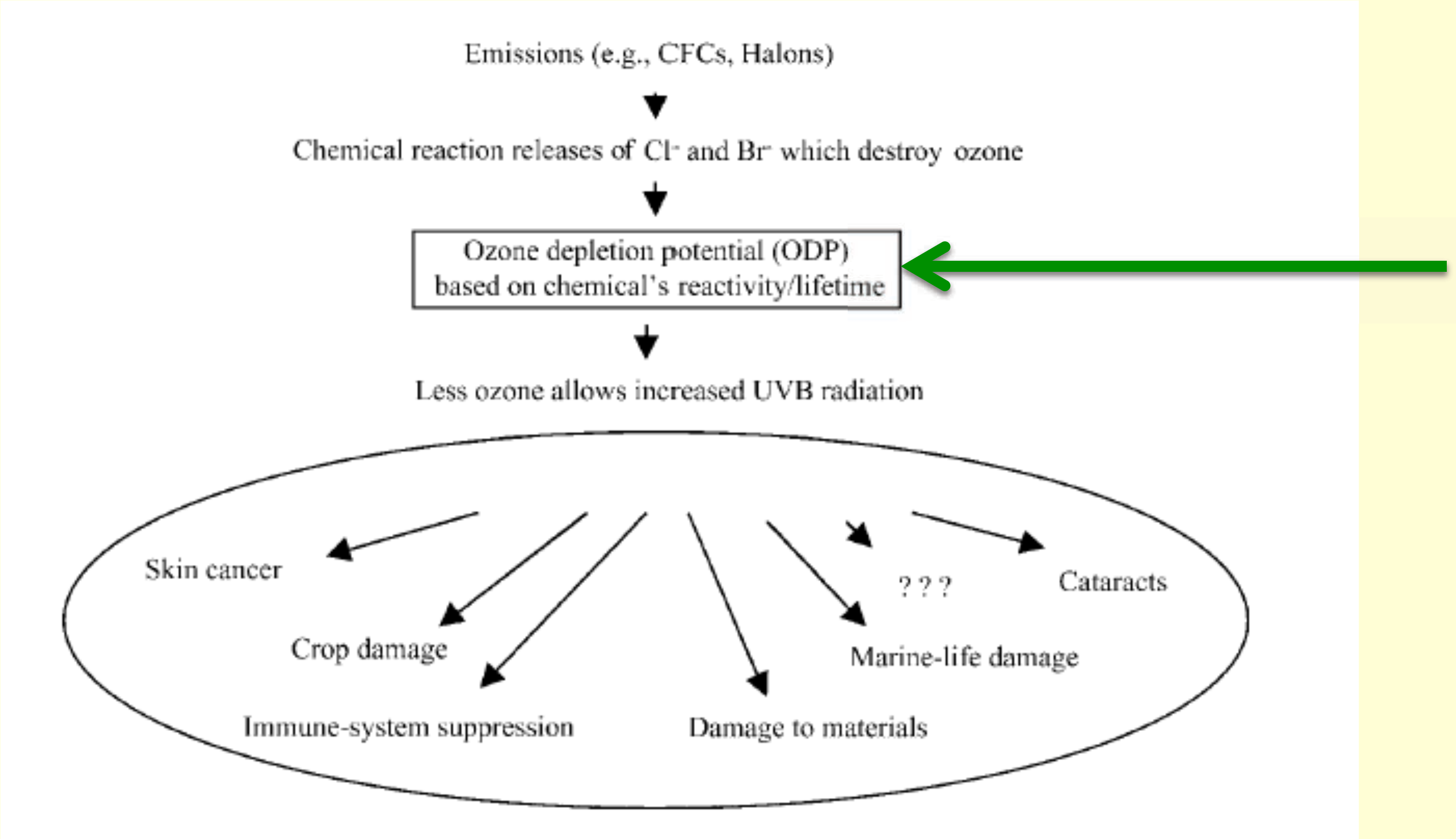


Newer ways to look at toxicity; U and J curves

Endocrine disruption, Epigenetics

Life Cycle Analysis Becomes a Viable Tool

TRACI: Tool for the Reduction and Assessment of Chemical and other Environmental Impacts



See Jane Bare, et al., ***J. Industr. Ecol*****. 2003, 6, 49**

TRACI: Tool for the Reduction and Assessment of Chemical and other Environmental Impacts

- Ozone depletion
- Global warming
- Smog formation
- Acidification
- Eutrophication
- Human health-cancer
- Human health non-cancer
- Human health criteria pollutants
- Eco-toxicity
- Fossil fuel depletion
- Land use
- Water use

See Jane Bare, et al., *J. Industr. Ecol*. 2003, 6, 49

New Technology: Bio-based materials

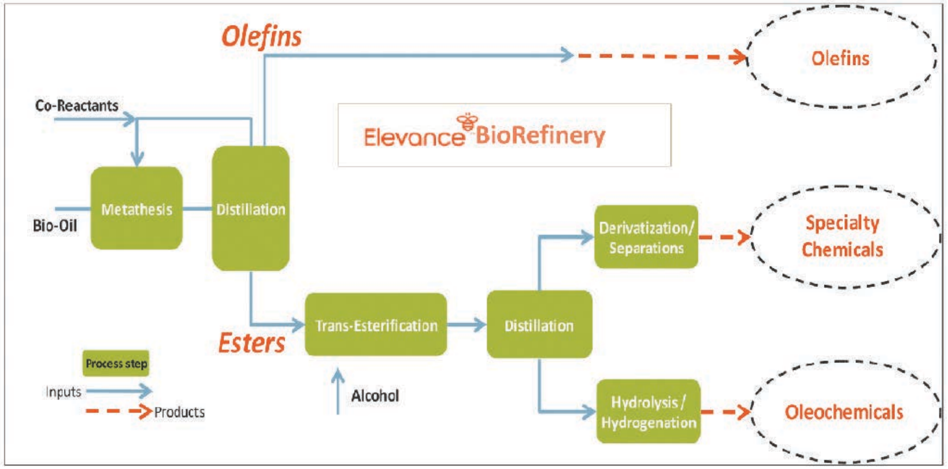
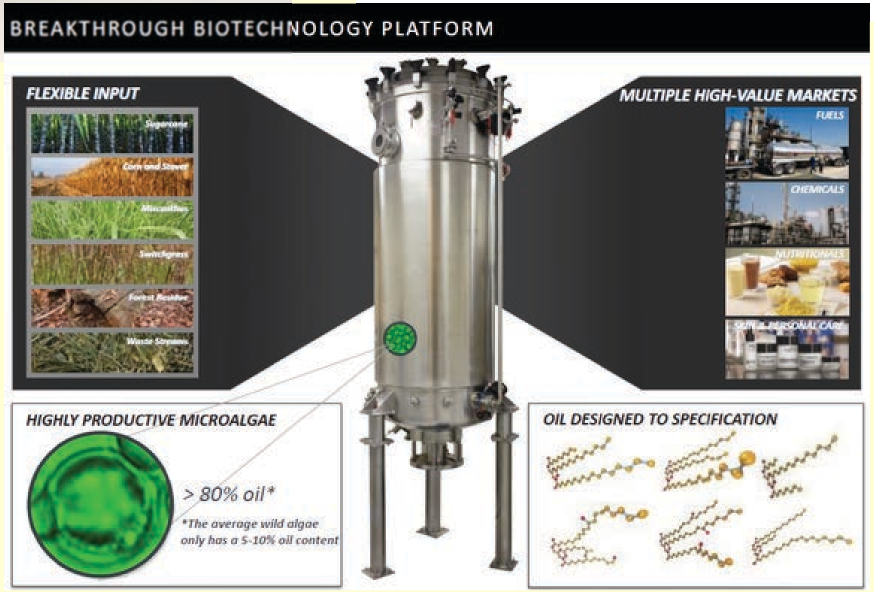


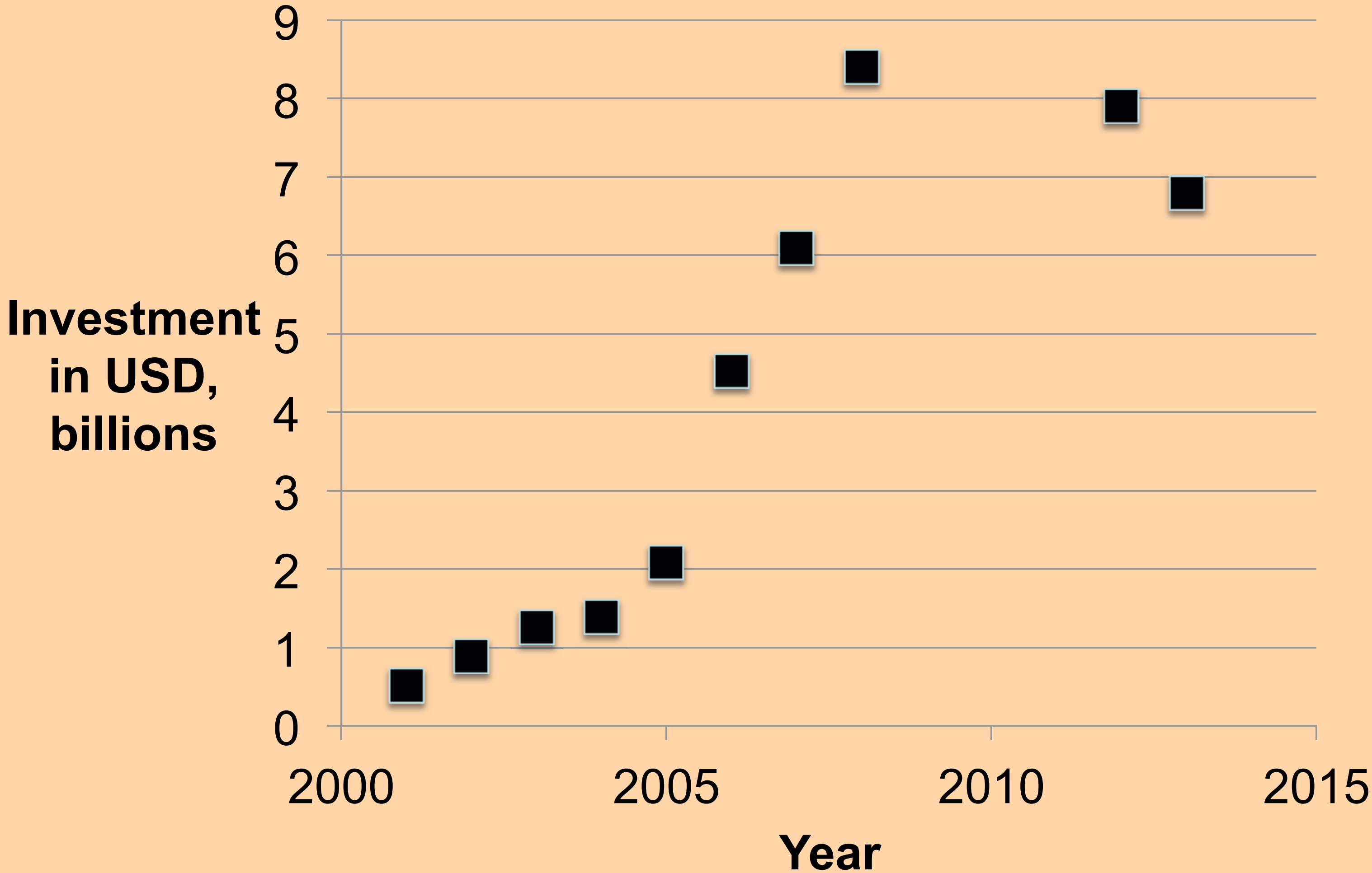
FIG. 7. *Elevance biorefinery.*

Ecovative Design; materials from mushrooms



Solazyme's Bio-oils

The Cleantech Sector Didn't Really Exist Prior to 2000

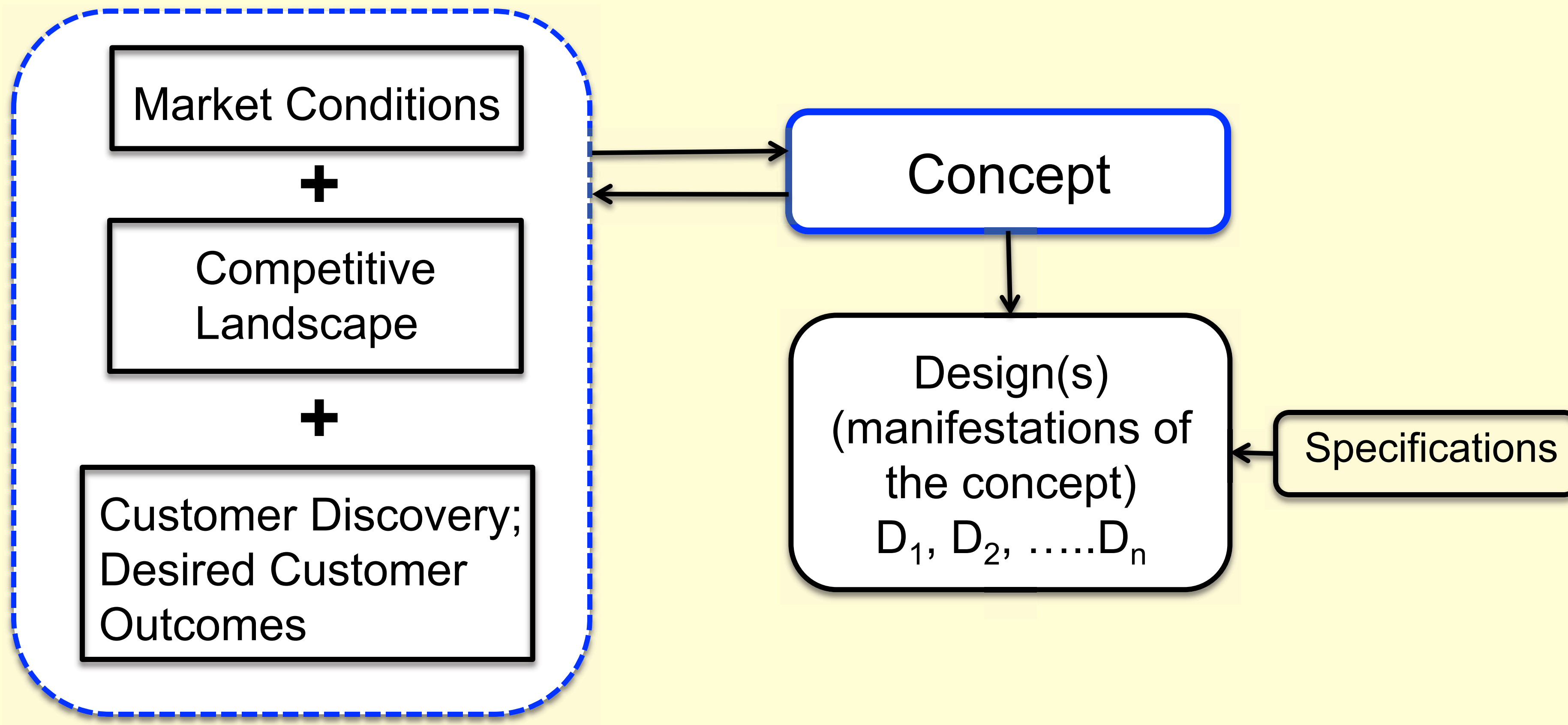


Themes for Today

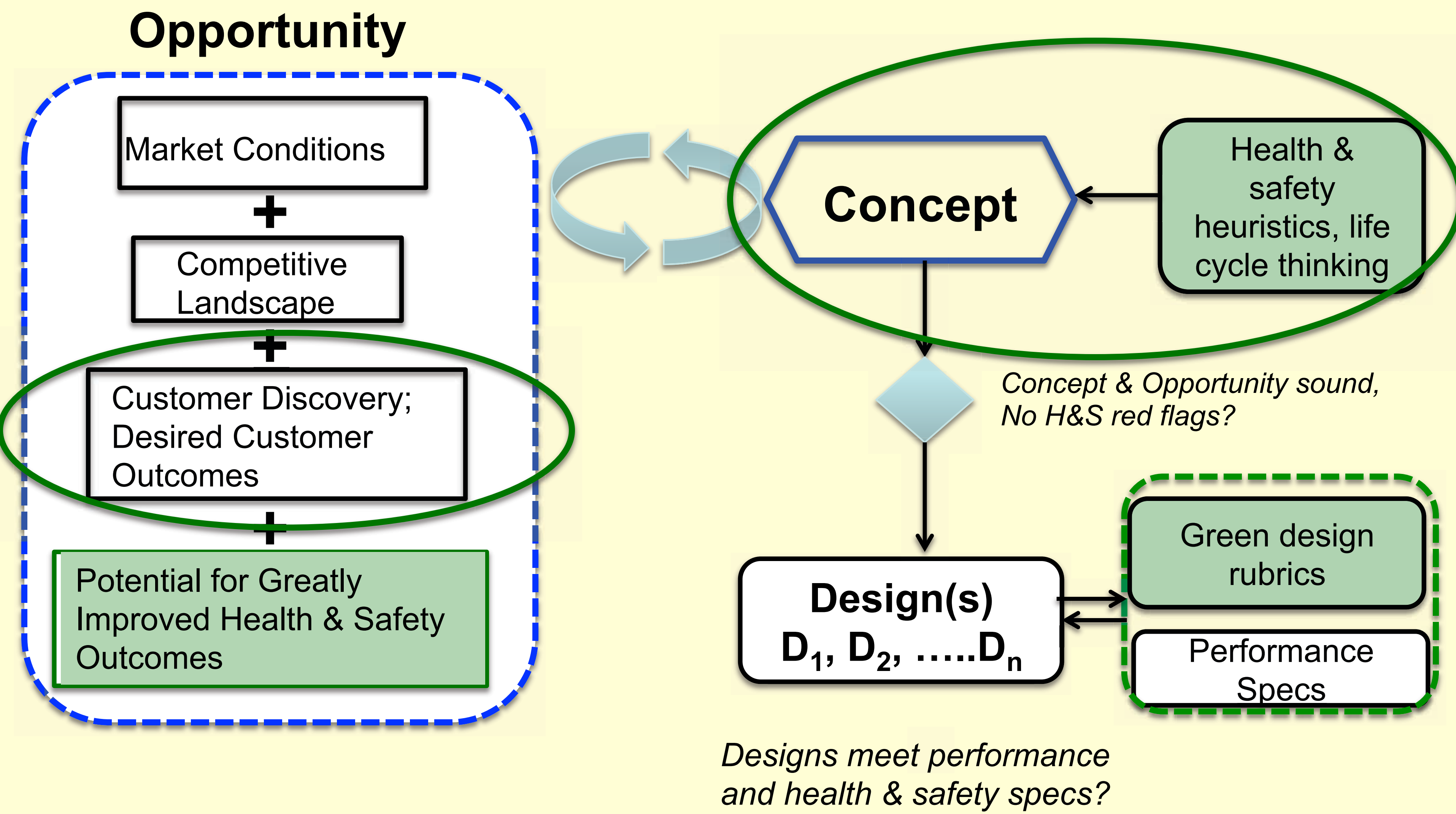
- Eco-Innovation via Customer-Centered Design
- Possible Future Trends (i.e., WAG's)
  - Completely integrated molecular design for chemical products
  - Resilient chemical generation via distributed synthesis
  - Molecular "services"
  - CO_2-based chemical systems

Opportunity, Concept Creation & Design

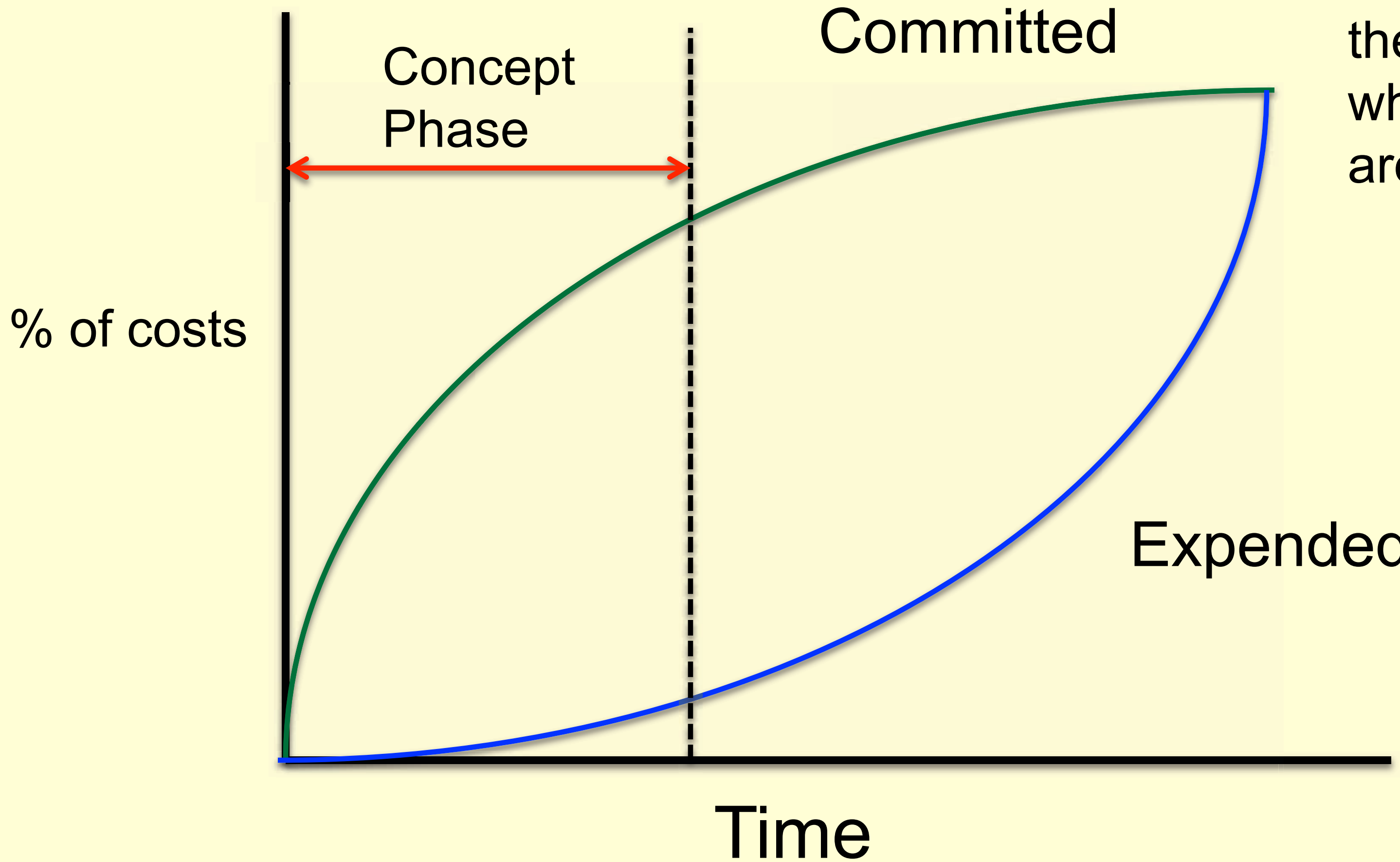
Opportunity



Adding "Green" Thinking to the Process

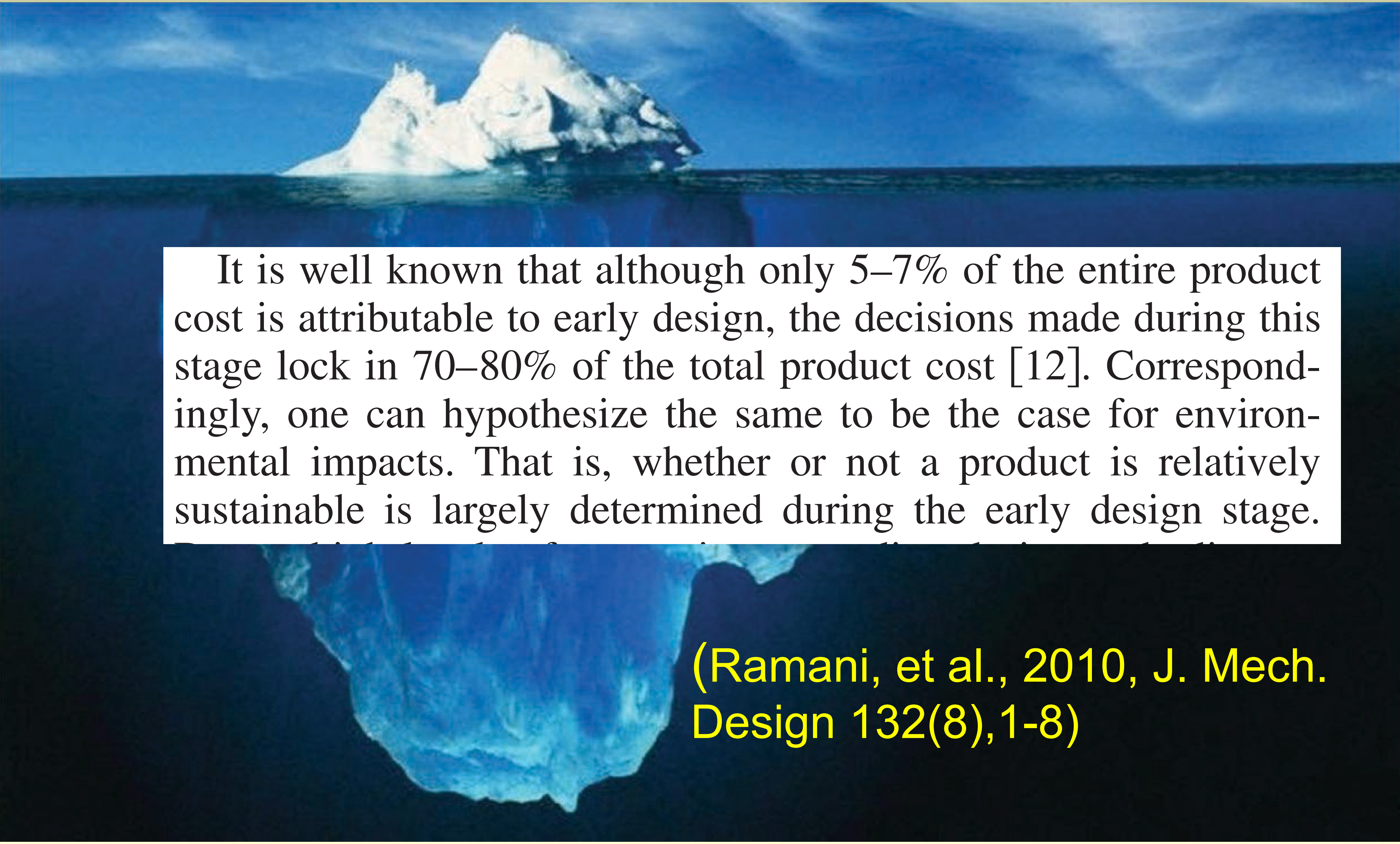


(from Ullman, *The Mechanical Design Process*, 2010).



80% of costs are committed during the concept phase, while only 5-7% are expended

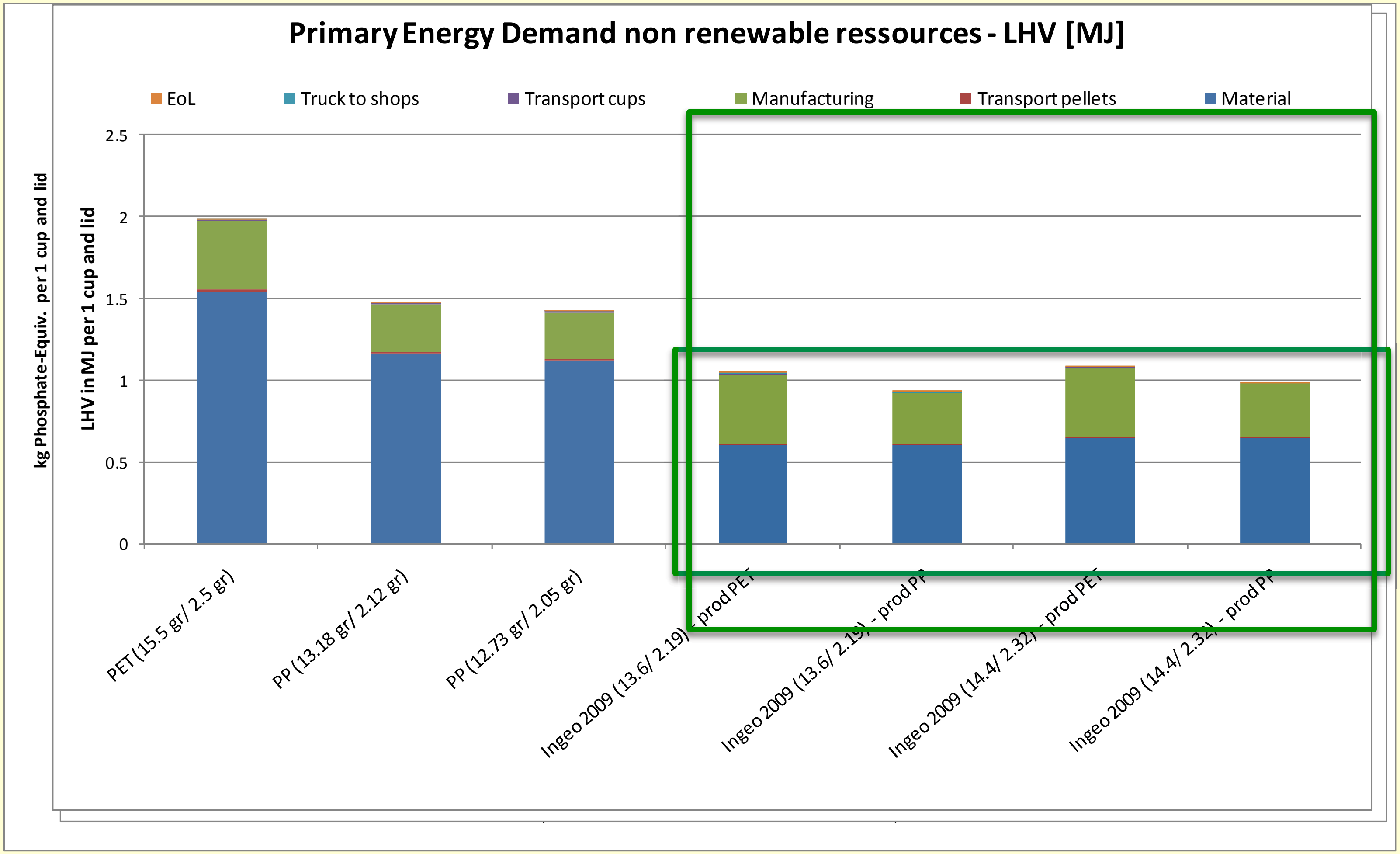
Embedded Impacts Take Shape During the Concept Formation Stage



It is well known that although only 5–7% of the entire product cost is attributable to early design, the decisions made during this stage lock in 70–80% of the total product cost [12]. Correspondingly, one can hypothesize the same to be the case for environmental impacts. That is, whether or not a product is relatively sustainable is largely determined during the early design stage.

(Ramani, et al., 2010, J. Mech. Design 132(8),1-8)

Why Innovation: Dealing with Trade-offs



Comparative LCA: Ingeo biopolymer, PET, and PP Drinking Cups, PE Americas (2009)

Innovating

Work at the Concept Formation Stage

Let Their Wants & Needs Drive Brainstorming

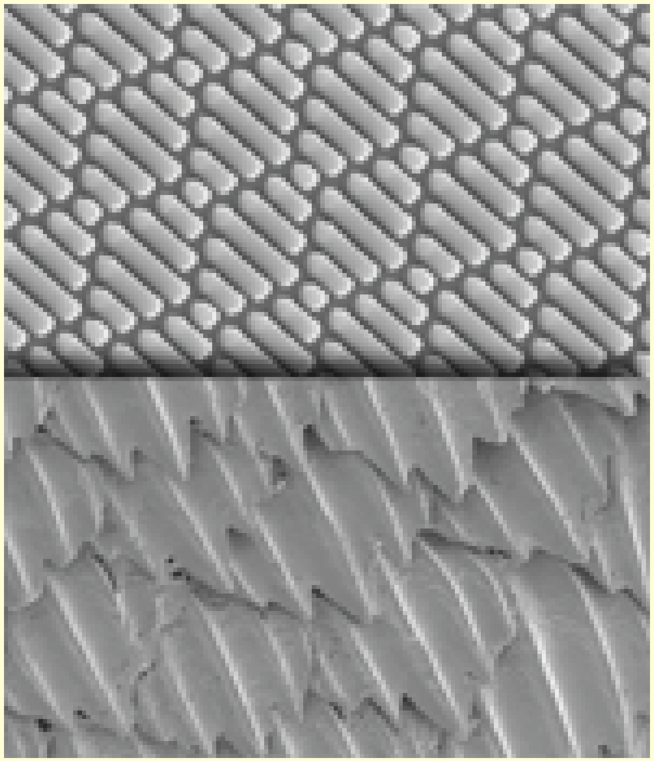
Customers!

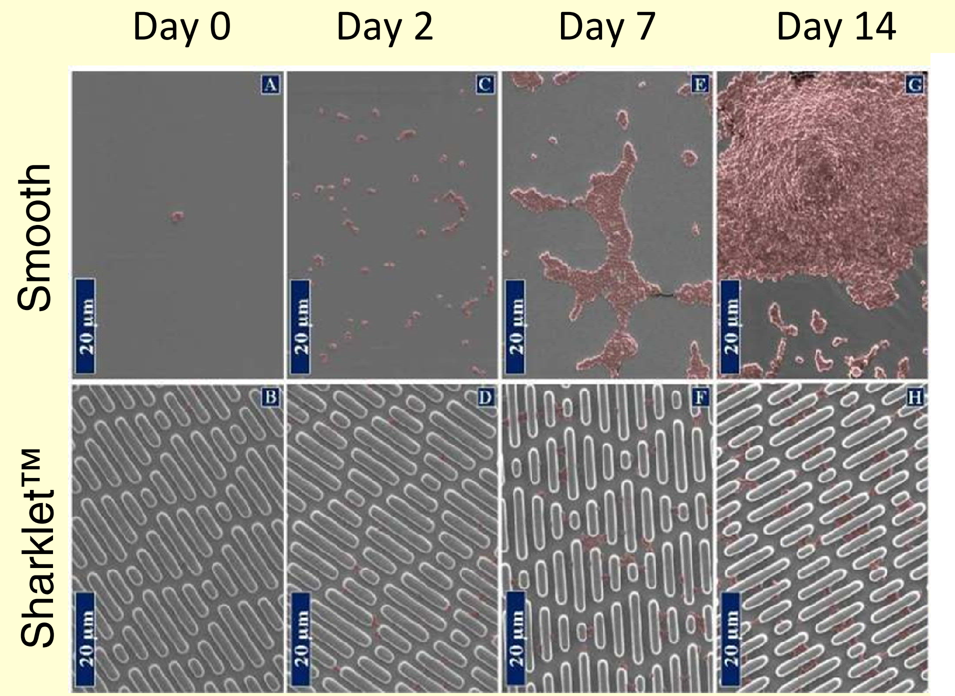
- They don’t sort products neatly into “bins”;
  - Products and services are solutions
  - Tangible, emotional, social
- Oftentimes its hard to tell what they want, but they don’t want hazard.
- True green innovation needs their perspective.
- Its easy to fall into the trap of becoming what we’ve always made.

Customer desired outcome is *no bacteria on surfaces*

Desired outcome is no bacteria

Sharklet Technologies (Aurora, CO) patterned surface

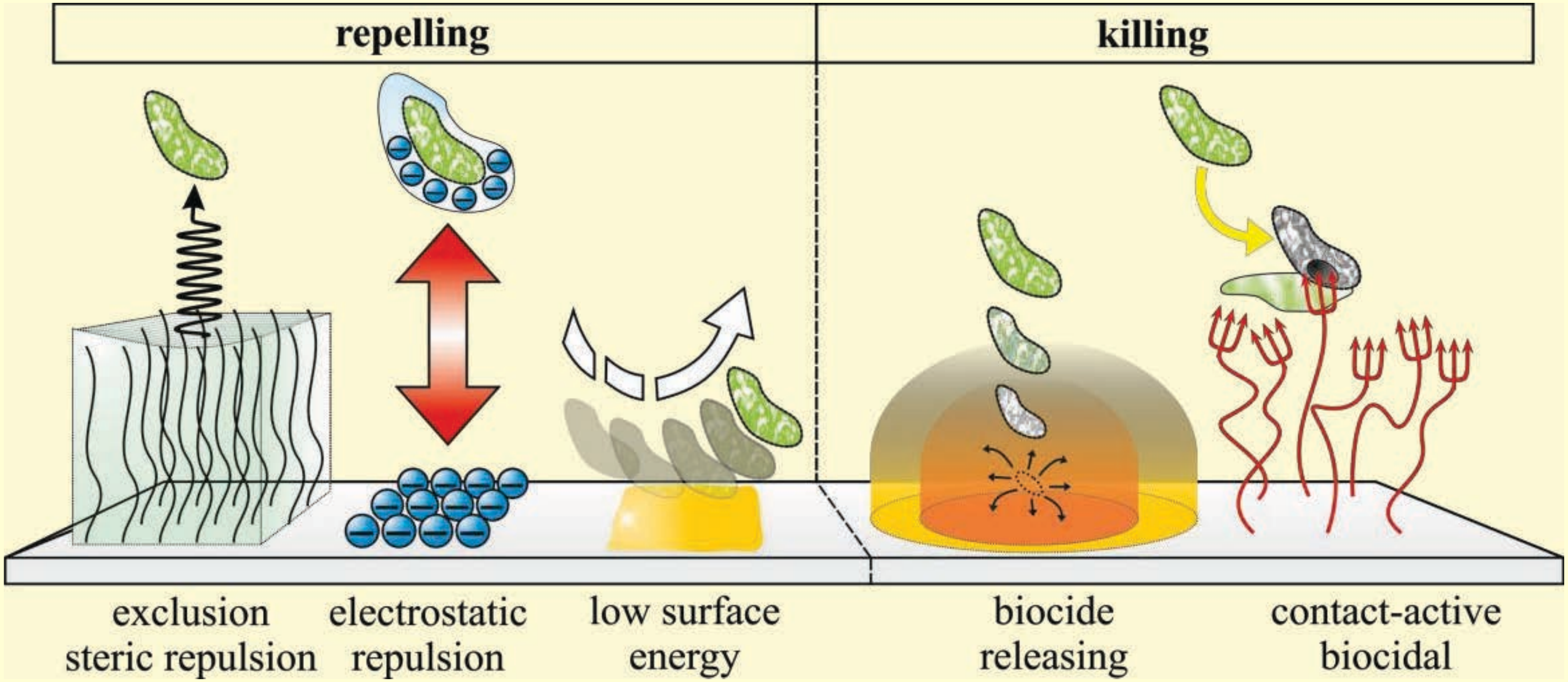




Shark skin: Very low surface frictional drag;

B. Dean & B. Bhushan, *Phil. Trans. Roy. Soc. A* (2010); 368, 4775-4806

Numerous Surface Concepts



Siedenbiedel & Teller, Polymers (2012)

Concepts can be chemical or “non-chemical”

Xenex’s “Violet” robot in an OR at UPMC

Concept versus Design

Example: Desired customer outcome = “no bacteria on surfaces”

Concept 1: = “anti-bacterial spray”

Design 1A = spray of triclosan + ethanol
Design 1B = spray of lactic acid/water

Concept 2: “Anti-bacterial surface”

Design 2A = ammonium *chloride-functional acrylic coating*
Design 2B = Coating impregnated with silver nanoparticles
Design 2C = shark scale mimic (Sharklet, Aurora, CO)

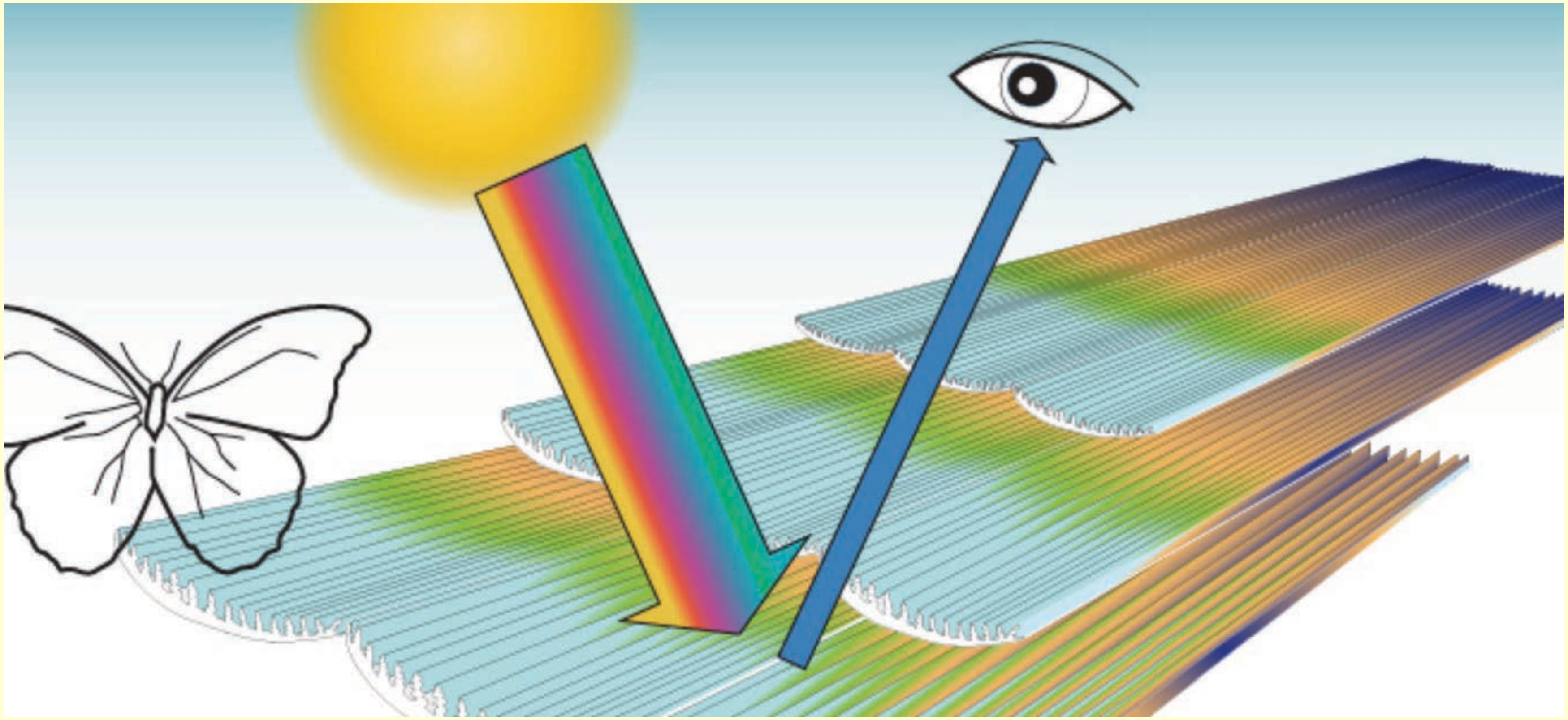
Concept 3: “Radiation”

Design 3A = UV emitting robot

Desired outcome is "color"

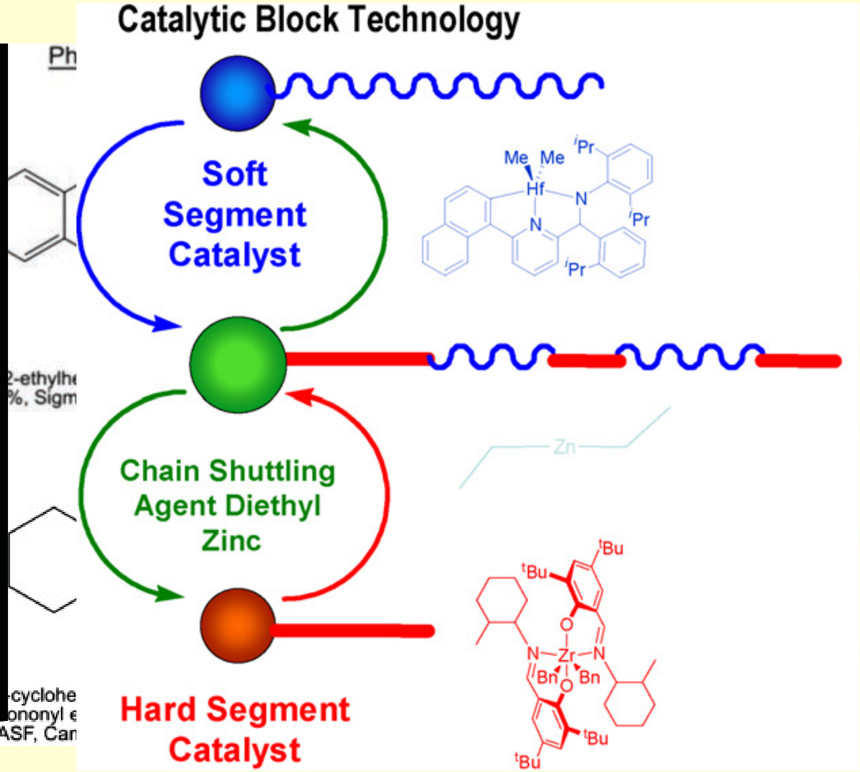
The current method is to employ synthetic organic dyes, mixed-metal pigments (Fe, Cr, Ni, Sb, Ti, Co, Zn)

The Morpho Butterfly



MorphoTex (Teijin Fibers)

Desired Outcome: A soft pliable material safe for use in toys



Dow INFUSE™ Olefin Block Copolymers; bulk density (0.87 g/cm^3) 30% lower than that for plasticized PVC

P.S. Chum & K.W. Swogger, *Progr. Polym. Sci*. (2008), 33, 797-819

Desired Outcome = Clean Clothes

Detergent

Cold-water
Detergent

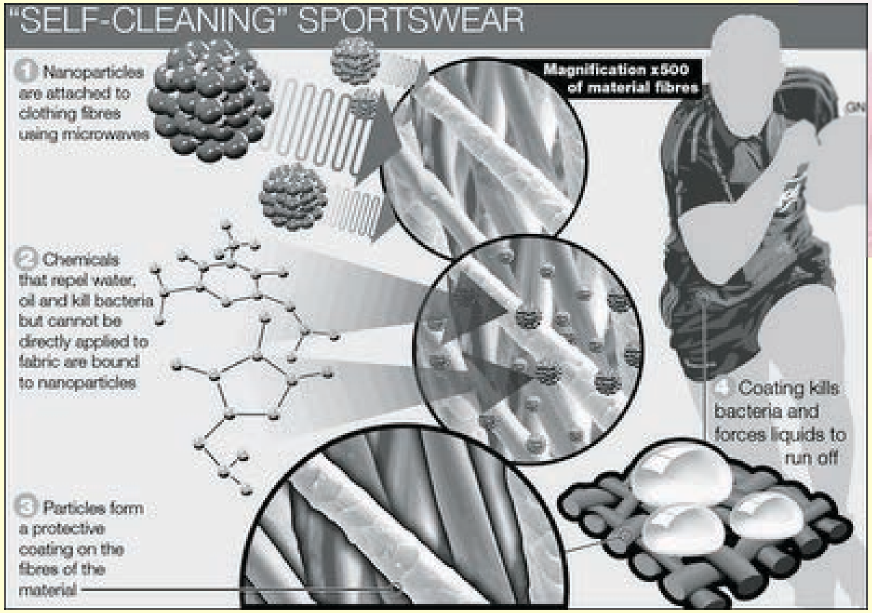
Degradable
Detergent

Perhaps No Detergent: Cleaning with Beads

Perhaps No Cleaning?

Stain-resistant clothing

Disposable Clothing?



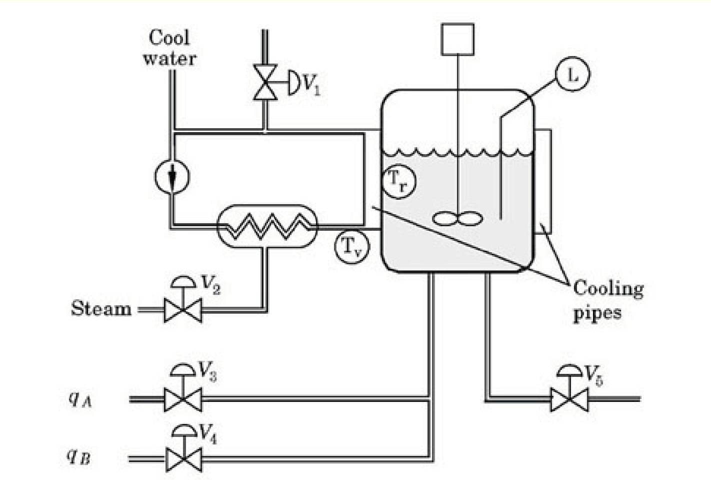
Self-Cleaning Clothing

Next Gen?

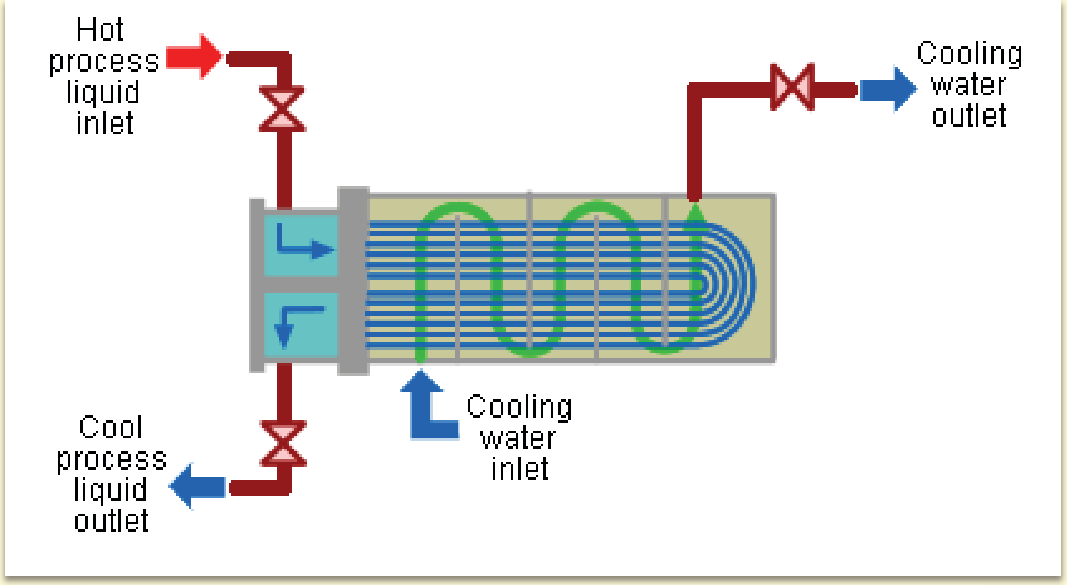
> Completely integrated molecular design for chemical products

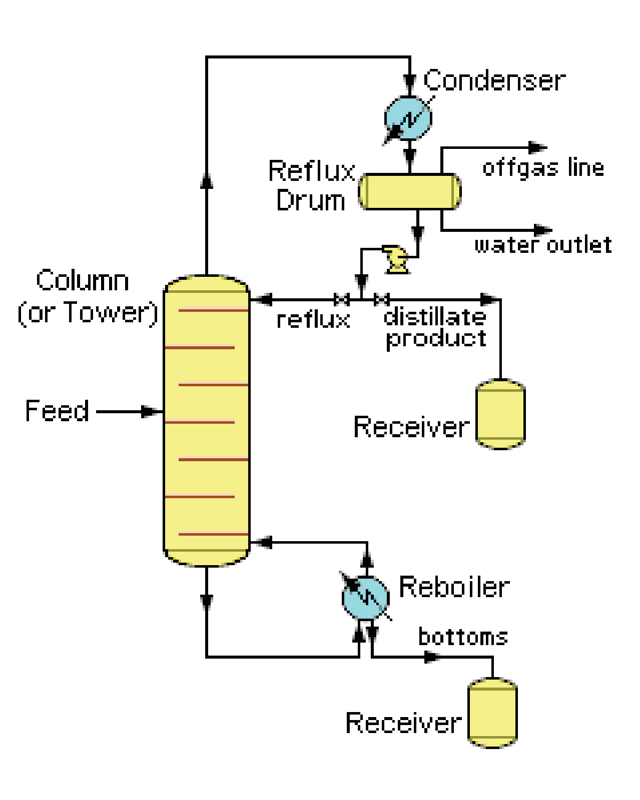
> Resilient chemical generation via distributed synthesis

Traditional plant engineering: integration of various unit operations

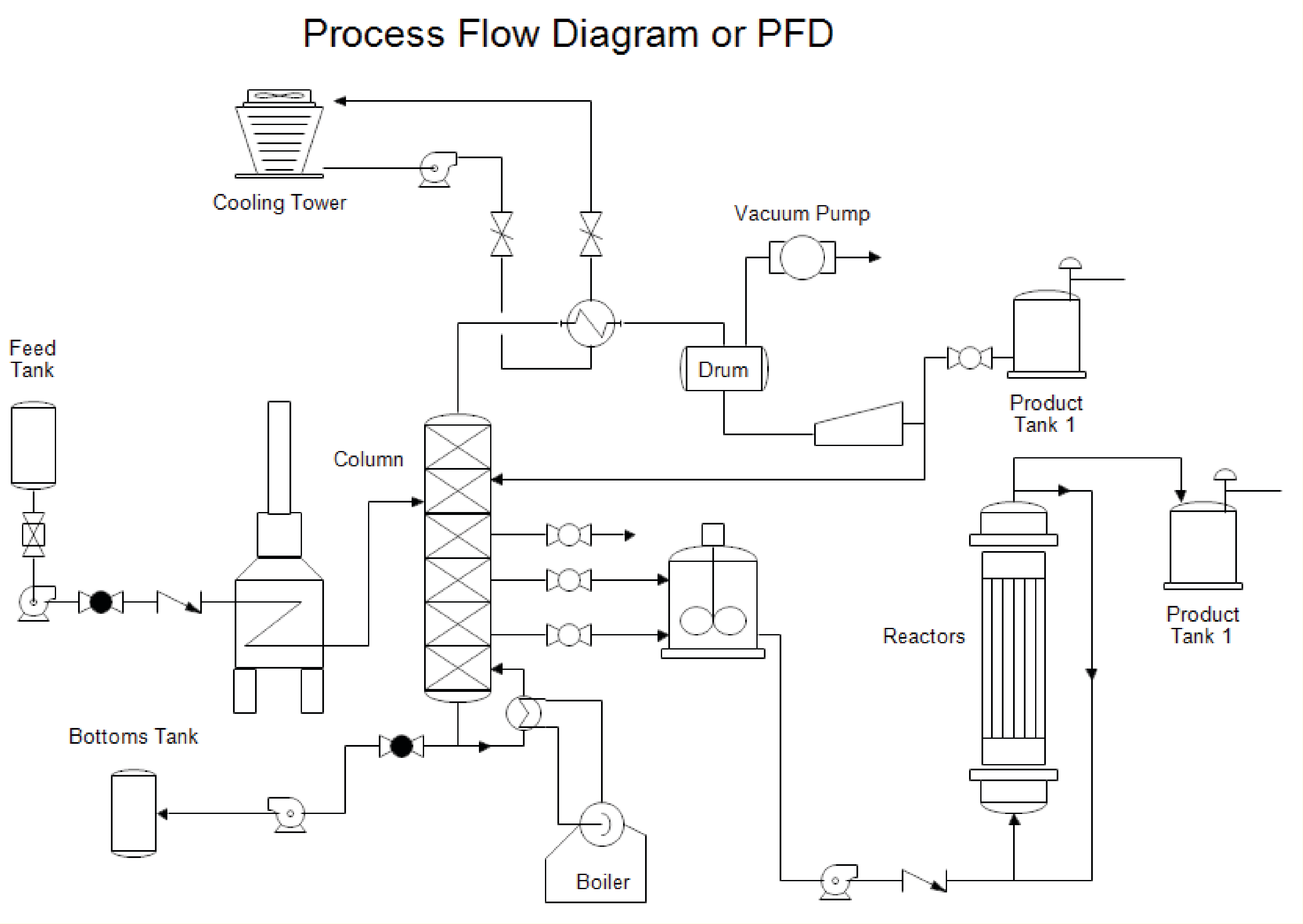


Reactors, Columns, Heat Exchangers, Pumps, etc.





Ultimately an optimized plant is designed



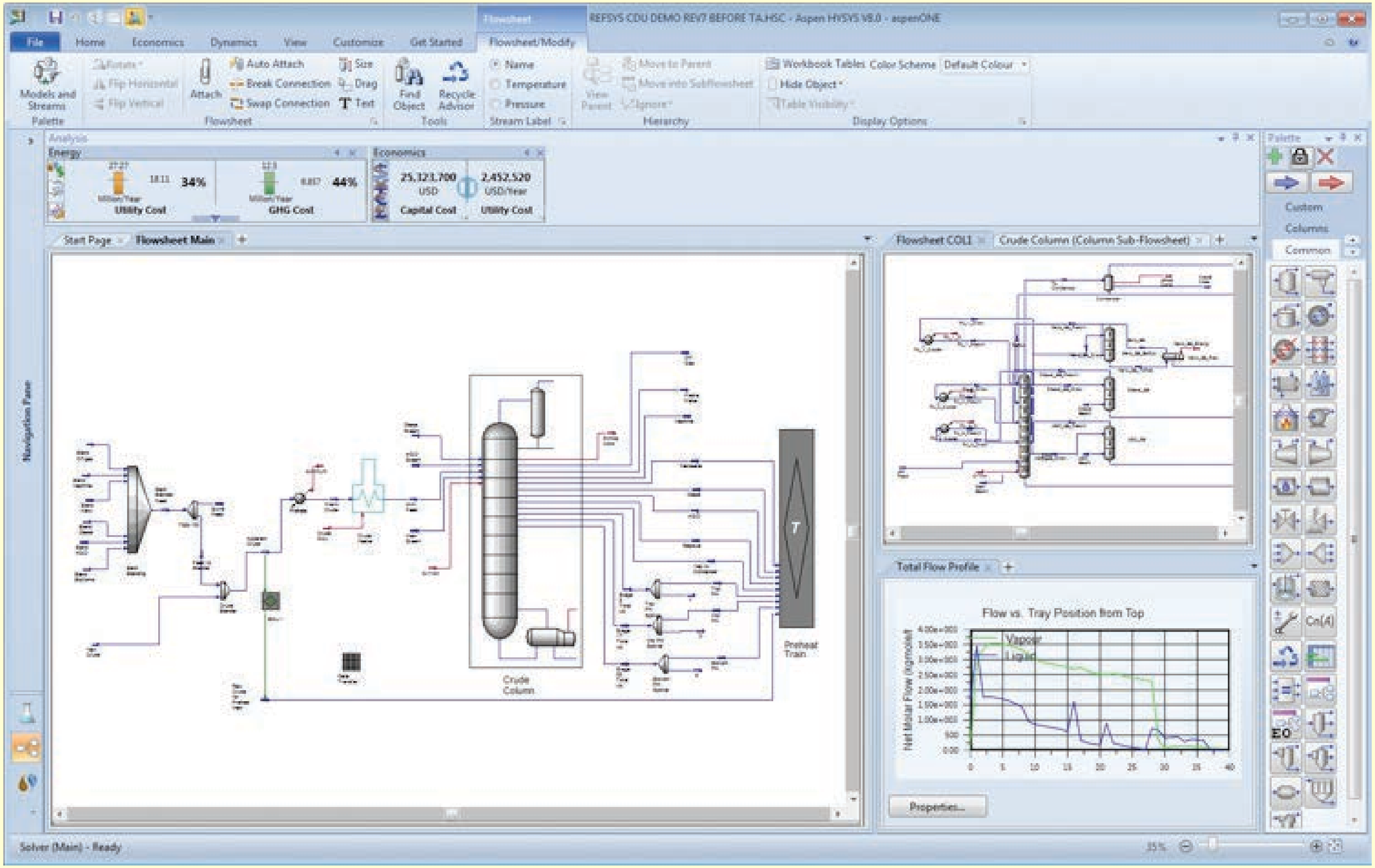
Now, with advances in computing power, undergraduate engineering students can design plants

+

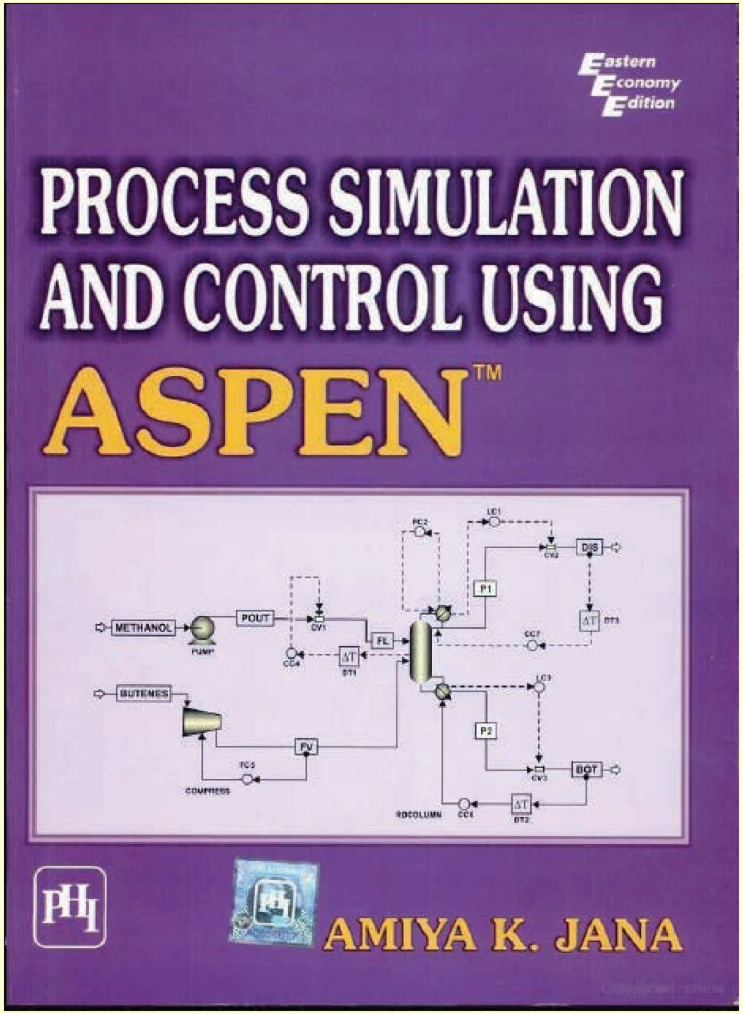
+

= ....

Provided they have access to ASPEN or HYSIS or another process simulator



Provided they have access to ASPEN or HYSIS or another process simulator



Plants can be designed, costed, and visualized if the fundamentals are available *or even if they're not*

With capital and operating costs, energy use, raw material needs and waste.

Computationally-Supported Product Design

Computational Molecular Design

Computationally-based toxicology & ecotoxicology

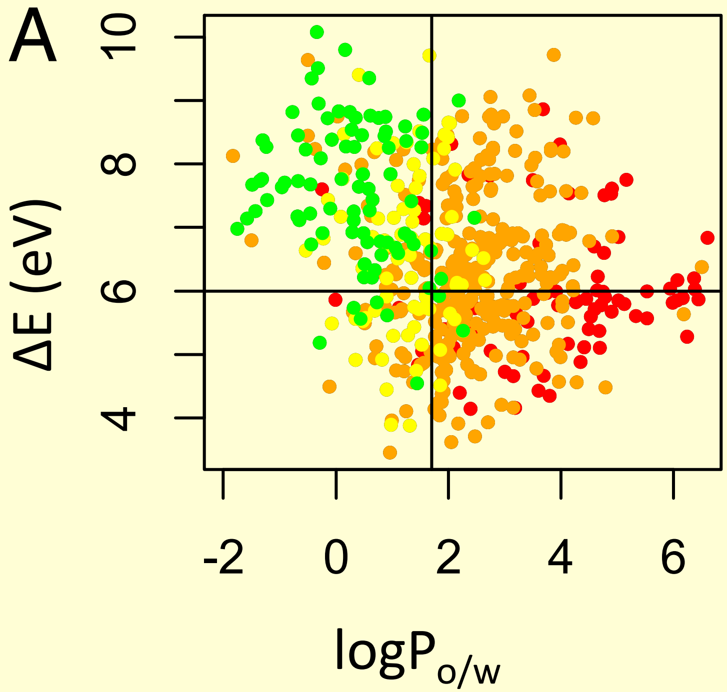
Green Product Design

Computational Formulation Design

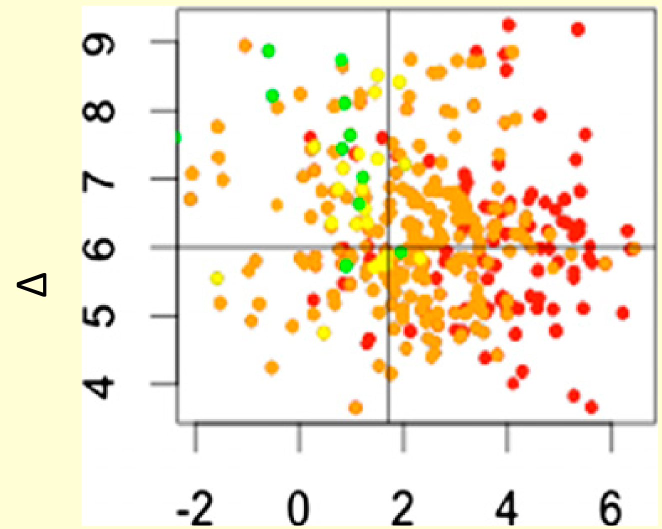
Computational Life Cycle Impact Analysis

Computational Process Synthesis

Computational Toxicology: Voutchkova, et al., PNAS (2014)



555 chemicals arranged by HOMO-LUMO difference versus LogP; colors represent degree of toxicity towards the fathead minnow



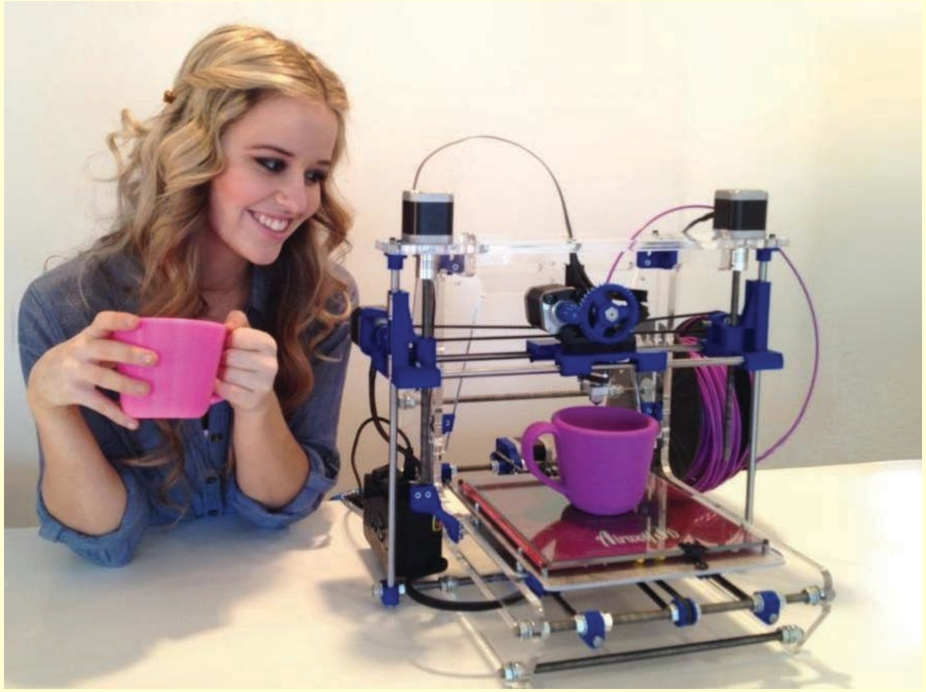
Similar plot for toxicity towards Daphnia Magna

Distributed Manufacturing & Green Chemistry?

Power Generation: Kids, don't try this at home

3D Printing – The Ultimate Distributed Manufacturing?

3D Printing (aka Additive Manufacturing): Distributed production – no shipping or packaging?



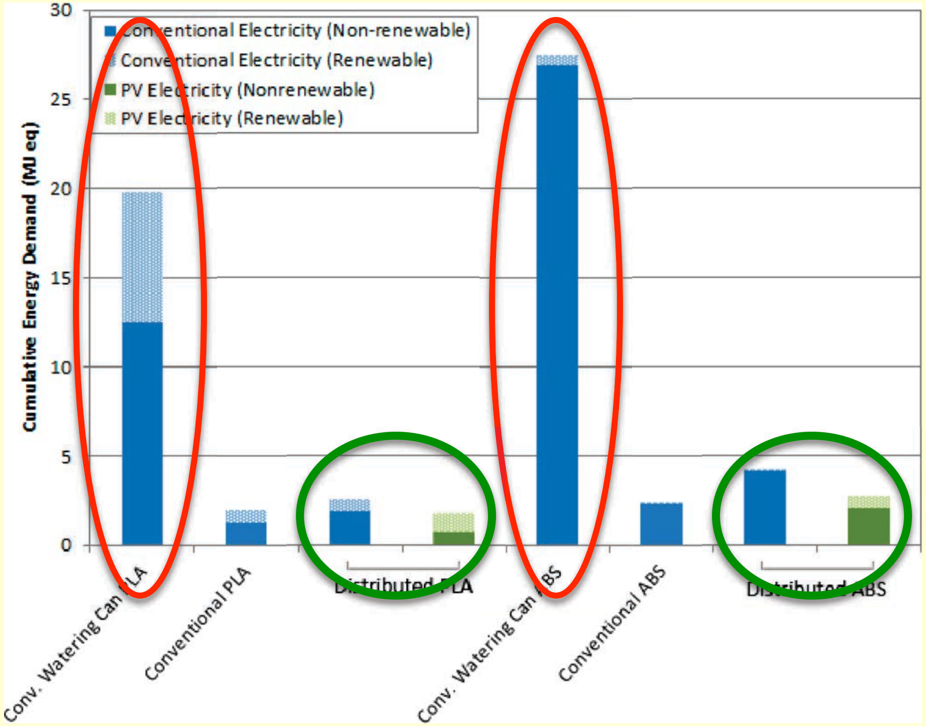


Figure 6. CED showing a typical watering can in PLA and ABS, and values for the spout in conventional PLA and ABS at 100% fill and distributed PLA and ABS at 100% fill, along with the effect of PV electricity.

M. Krieger & J.M. Pearce, *ACS Sust. Chem.& E*ng. (2013) dx.doi.org/ 10.1021/sc400093k

Chemical Manufacturing: The Conventional Wisdom

Reducing Risk Via Armoring

Sufficiently commonplace that we almost don't notice

Mitsui Chemicals (Japan), 2015

Garland, Tx, 2012

Louisiana, 2013

Chlorine spill, Graniteville, SC (2005)

(Dunn & Oswalt, Northern Arizona University)

January 6, 2:40 AM

- Someone forgets to toggle a line switch
- Freight train leaves main line onto spur at 47 mph
- Freight train crashes into parked train on spur, 3 engines and 18 cars derail
- 60 tons of Cl_2 released

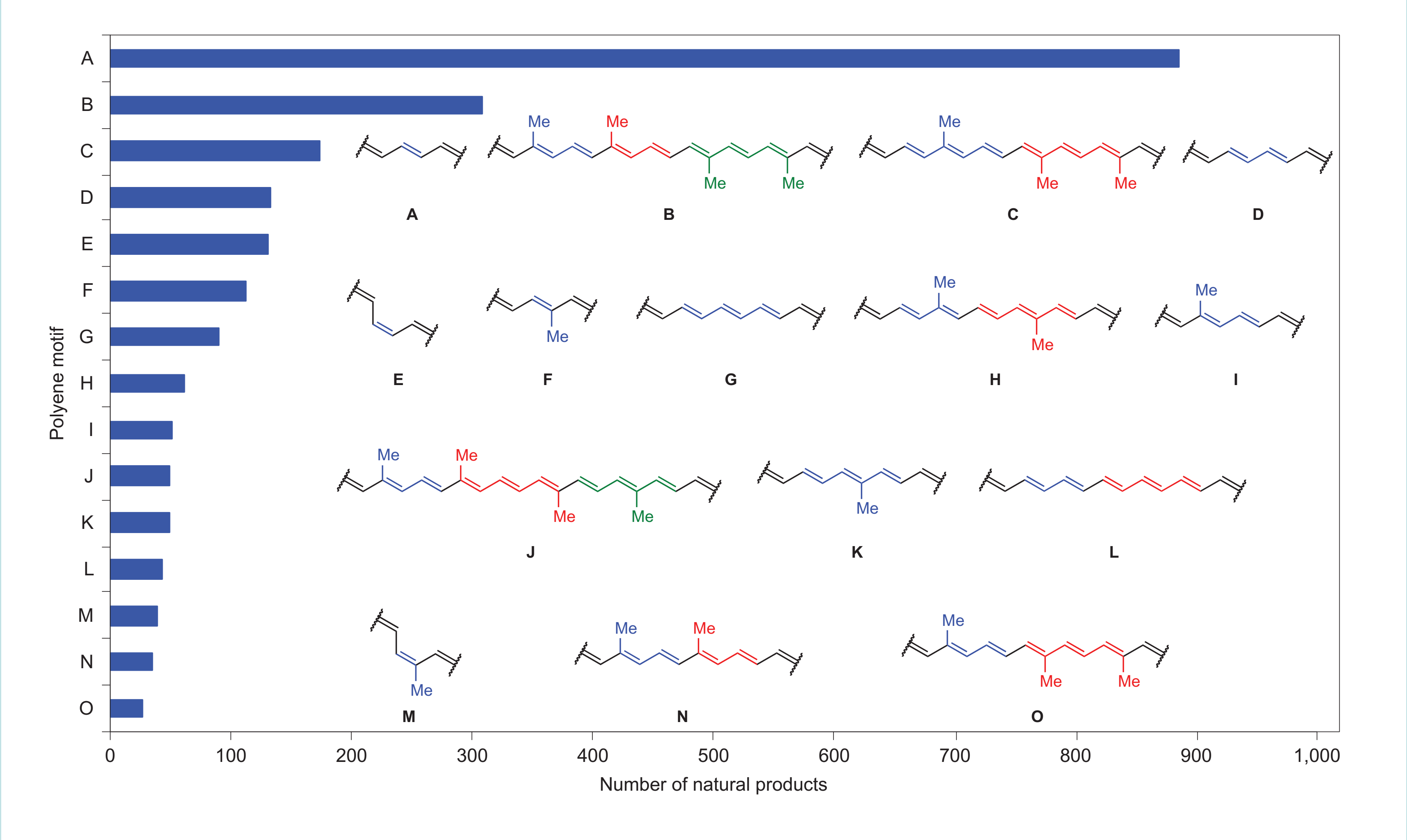
9 dead, 550 to hospitals

Distributed Synthesis: Why & How

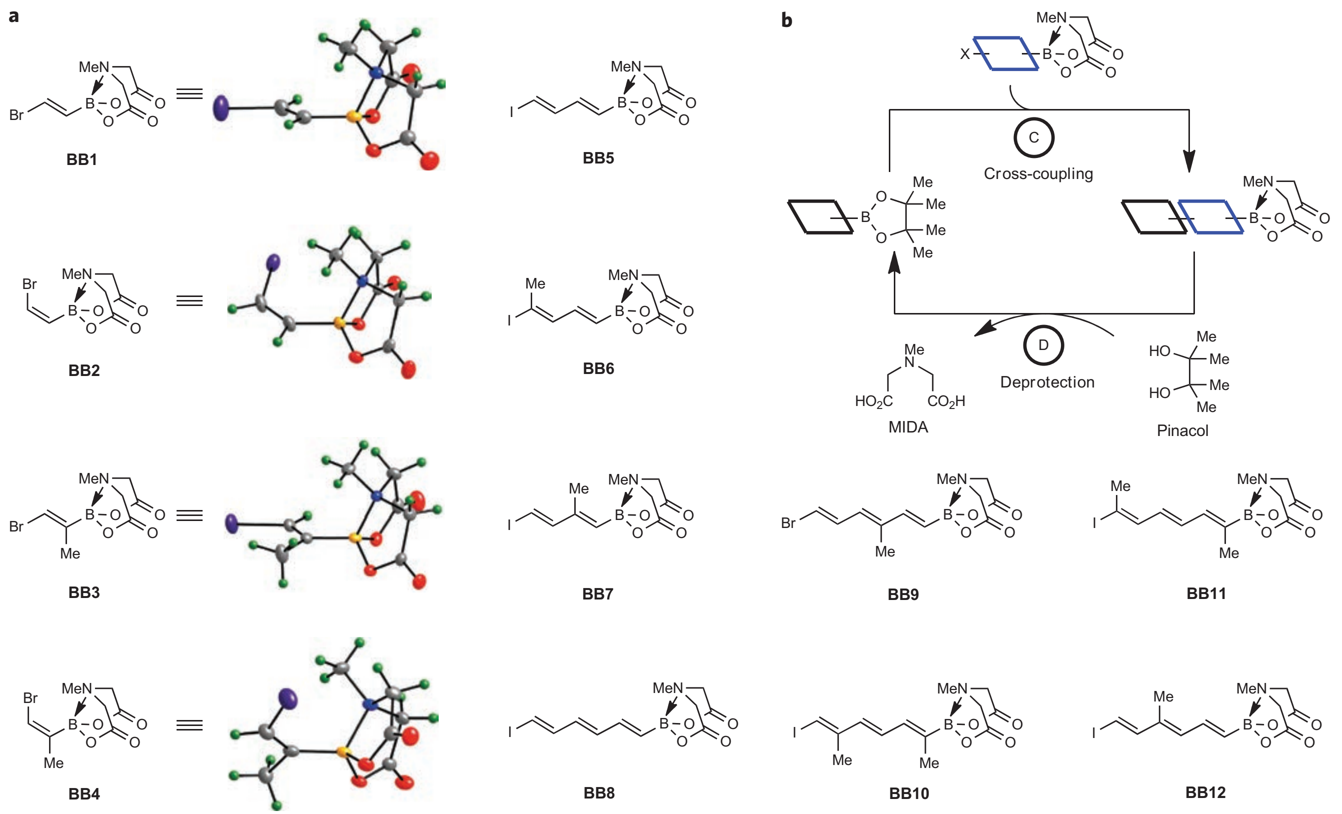
- Why distributed
  - Desire for personalization
  - Resilience/safety

- How to allow distributed synthesis?
  - Safe building blocks and products
  - Selective chemistry, high yield
  - Minimize separations (byproduct as benefit)
  - Programmable
  - No solvent or entirely benign solvent

Burke & colleagues, *Nature Chem* 2014



Burke & colleagues, *Nature Chem* 2014



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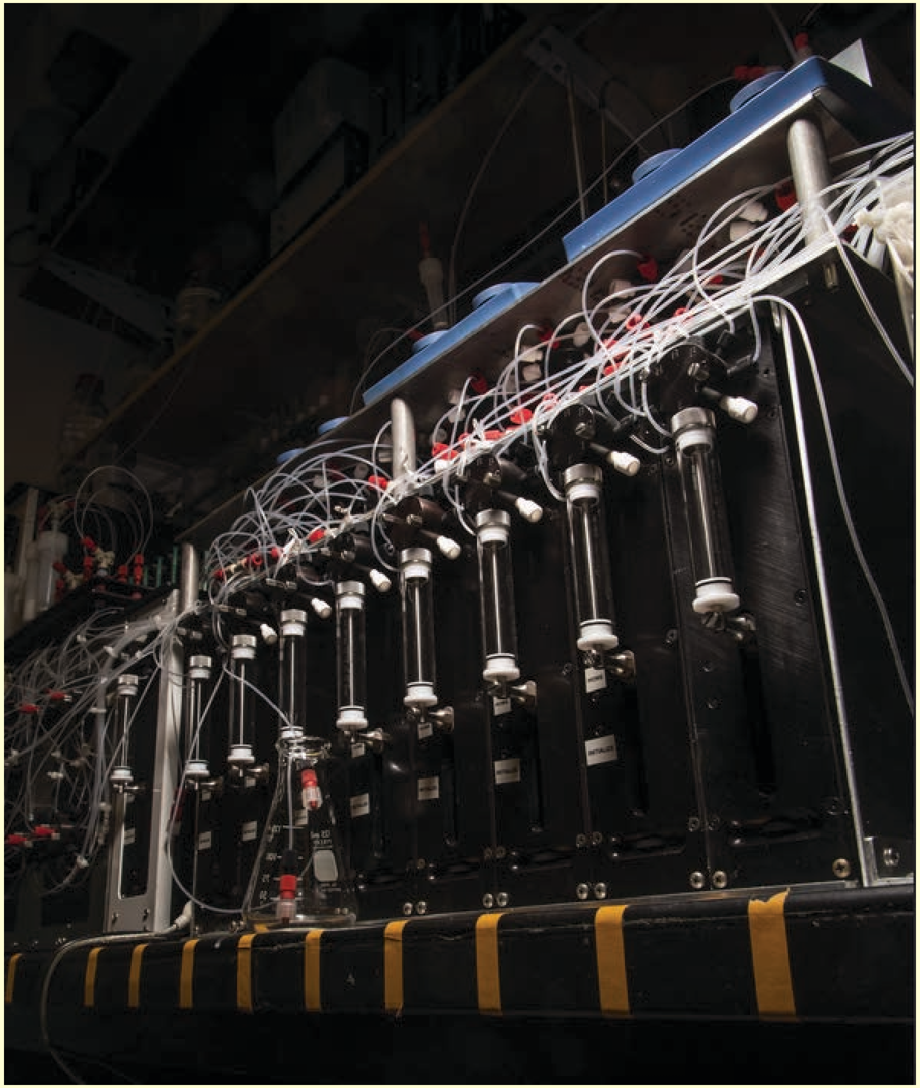

Cronin and colleagues, 2013

Chemical Science

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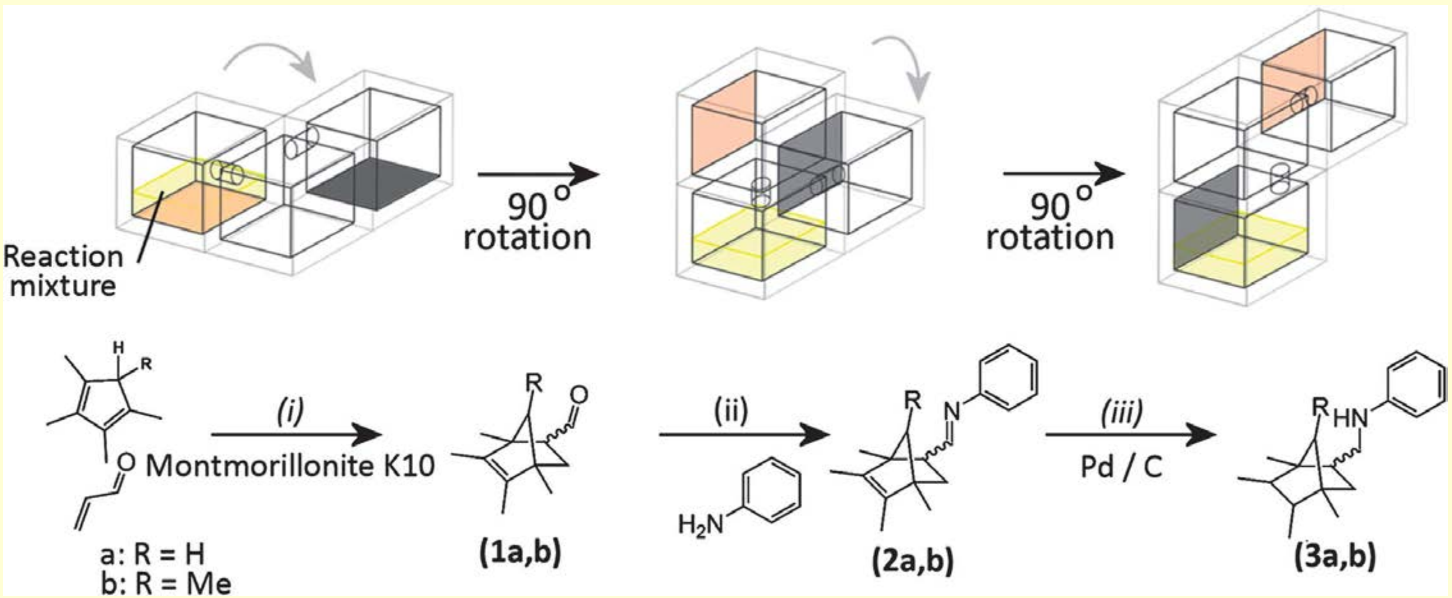
Cite this: *Chem. Sci.*, 2013, **4**, 3099

Combining 3D printing and liquid handling to produce user-friendly reactionware for chemical synthesis and purification†

Philip J. Kitson, Mark D. Symes, Vincenza Dragone and Leroy Cronin*

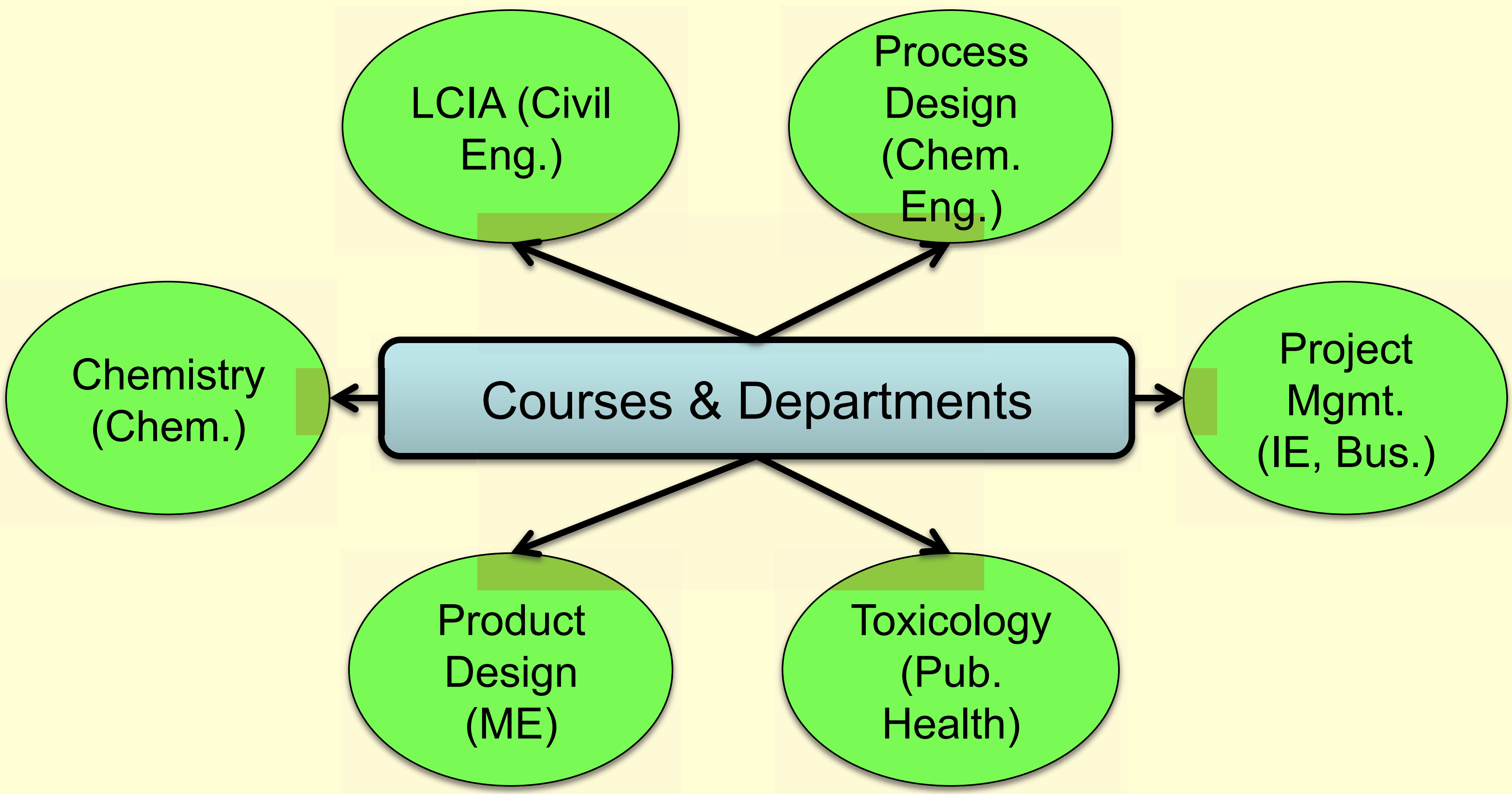


Future Chemistry? Chemicals for personal care a possible target?

Programmable, personalized, and safe

Next Gen for Academia?

Academia: Let's say you're a student who wants to learn about green chemical product design.



Computationally-Supported Product Design

Computational Molecular Design

Computationally-based toxicology & ecotoxicology

Green Product Design

Computational Formulation Design

Computational Life Cycle Impact Analysis

Computational Process Synthesis

What academia can do

- The option to explore integrated product design
- Options for chemistry & chemical engineering UG's to explore entrepreneurial opportunities (entrepreneurs tend to drop out).
- Options for graduate students to more easily work across silos.

Summary

- The first 20 years (or so) of green chemistry have seen a sea change in the way the chemical enterprise operates.
- It’s not just about chemistry anymore – we’re overlapping other disciplines whether we like it or not.
- Just as radical & disruptive innovation has driven changes in our digital & home lives, the same should hold true for green chemistry in the next 20 years.
- The educational enterprise needs to keep pace with the chemical (business) enterprise.

"It's tough to make predictions, especially about the future."

Yogi Berra

Thank you!