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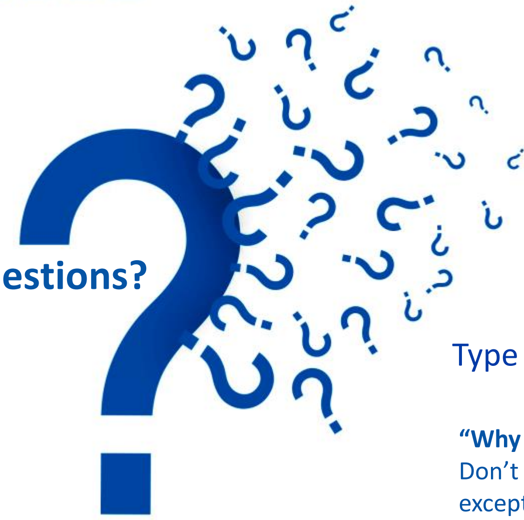

Have Questions?

Type them into questions box!

"Why am I muted?"
Don't worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

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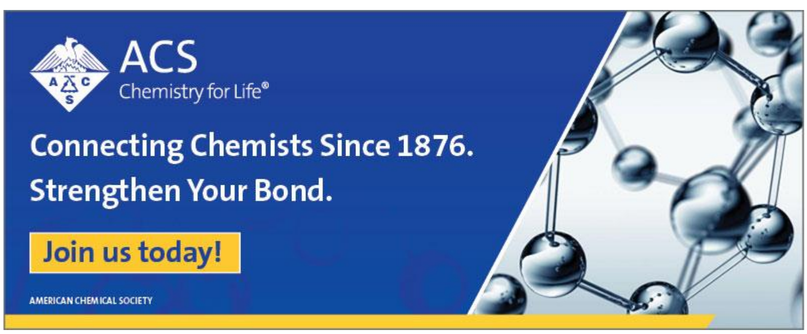

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4

How has ACS Webinars benefited you?

“Great job as usual! It was fascinating to hear about the historical roots of lab safety culture. I hope to see more bite-sized lab safety resources for students in the future.”

http://bit.ly/ChemicalLabSafety

Fan of the Week

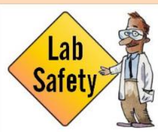
Anna Sitek, CSP
Research Safety Specialist- College of Science & Engineering, Department of Environmental Health and Safety, University of Minnesota

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org

ACS National Meeting Workshops
Boston, MA, August 17 – 19, 2018

ACS Technical Division
Chemical Health & Safety (CHAS)

FRIDAY FULL DAY WORKSHOPS	
Laboratory Waste Management 2018 (click here for workshop description) taught by Russ Phifer, WC Environmental	
Laboratory Safety – Beyond the Fundamentals (click here for workshop description) taught by Jim Kaufman, Lab Safety Institute	

SATURDAY FULL DAY WORKSHOPS	
How to be a More Effective Chemical Hygiene Officer (click here for workshop description) taught by Russ Phifer, Jim Kaufman *(Note that the Chemical Hygiene Officer certification exams are no longer offered at ACS national meetings. These exams are managed by the National Registry of Certified Chemists. Visit their web site at http://www.nrcc6.org for further information.)*	
Reactive Chemical Management for Laboratories & Pilot Plants (click here for workshop description) taught by Neal Langerman, Advanced Chemical Safety and Harry Elston, Midwest Chemical Safety	
Health and Safety Training for Cannabis Businesses (click here for workshop description) taught by Jahan Marcu, Ph.D., Melissa Wilcox, and Julia Bramante	

SUNDAY 3 HOUR WORKSHOP:	
Developing Graduate Student Leadership Skills in Laboratory Safety (click here for workshop description) led by Kali Serrano, and Kaitlin Tyler, University of Illinois at Urbana–Champaign	

Full day workshops begin at 8:30 and finish around 4:00 PM, with a 1 hour (no host) lunch break. The ***Graduate Student Safety Leadership*** workshop will take place on Sunday, beginning at 3:00 PM and ending about 6:00 PM.

https://dchas.org/workshop-registration-page-2

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Recordings are an exclusive ACS member benefit and are made available to registrants via an email invitation once the recording has been edited and posted.

Live Broadcasts of ACS Webinars® continue to be available to the general public every Thursday from 2-3pm ET!

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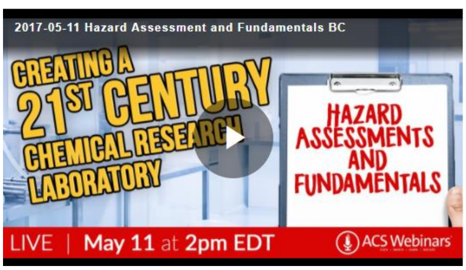
Previous Chemical Safety Webinars

ACS Technical Division
Chemical Health & Safety (CHAS)

Creating a 21st Century Chemical Research Laboratory: Hazard Assessments and Fundamentals



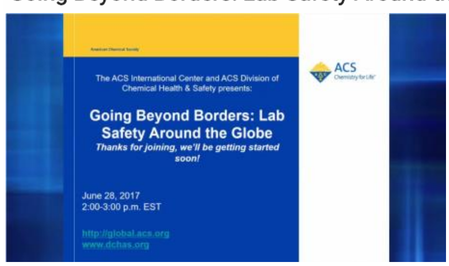
Ralph Stuart
Keene State College

Kendra Leahy Denlinger
University of Cincinnati

Safety in the laboratory requires a full team effort to be successful. When everyone in the laboratory understands how to identify hazards, assess risk, and select the appropriate control measures to eliminate a hazard or minimize risk, accidents, injuries and near misses can be reduced.

http://bit.ly/ACS21stLab

Going Beyond Borders: Lab Safety Around the Globe



Ralph Stuart
Keene State College

Samuella Sigmann
Appalachian State University

Every day, thousands of scientists travel around the globe to engage in scientific exchange, training and collaboration. No matter where you go, learning about the lab safety issues and practices used in the host country should always be a top priority. This webinar will address safety issues while hosting a visiting scholar or issues you may come across as visiting scientist.

https://global.acs.org/acs-international-center-event-webinar-on-global-lab-safety/

An individual development planning tool for you!

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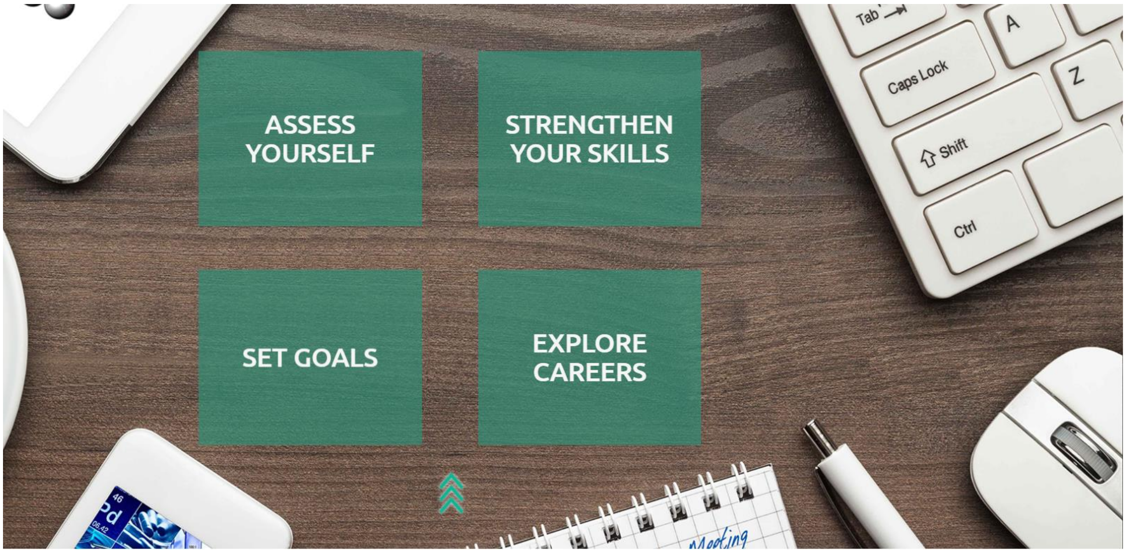

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#gcande **gcande.org/call-for-symposia** @ACSGCI

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Upcoming ACS Webinars

www.acs.org/acswebinars

Thursday, July 26, 2018

How to Optimize Central Nervous System Therapeutics: *Med Chem Strategies, Tactics, and Workflows*

Co-produced with the ACS Division of Medicinal Chemistry and American Association of Pharmaceutical Scientists

Experts

Craig Lindsley
Vanderbilt Center for Neuroscience Drug Discovery

Thursday, August 2, 2018

Cloudiness in Beer: *Considerations and Chemistry*

Co-produced with the ACS Division of Agricultural & Food Chemistry

Experts

Charles Bamforth
UC Davis

Brian Guthrie
Cargill

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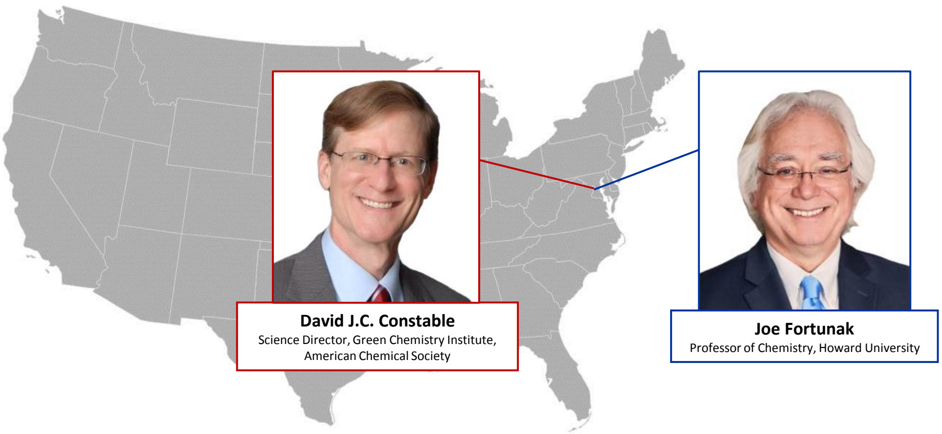
How Sustainable Chemistry is Safer Chemistry



Slides available now and an invitation to view the recording will be sent when available.

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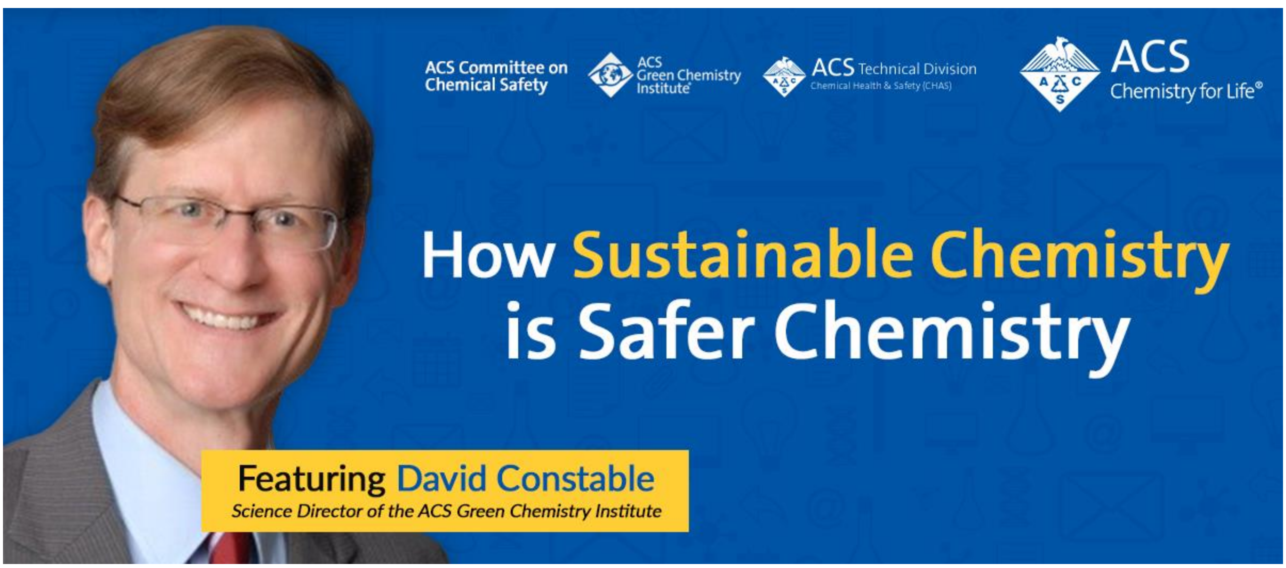
Co-produced with ACS Green Chemistry Institute, ACS Division of Chemical Health & Safety, and the ACS Committee on Chemical Safety



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Engaging *you* to reimagine chemistry and engineering for a sustainable future.

We believe sustainable and green chemistry innovation holds the key to solving most environmental and human health issues facing our world today.

- Advancing Science
- Advocating for Education
- Accelerating Industry

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Why Reimagine Chemistry?

The chemistry enterprise as currently operated is **completely unsustainable**:

- **Feedstocks** (What we start with)
- **Chemicals**
- **Chemistries**
- **Processes**

} (How we put things together)

- **Products**

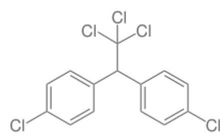
Chemists and chemical engineers are uniquely equipped to do something about making the world more sustainable

"Better Things for Better Living Through Chemistry" - DuPont

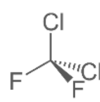
- Ibuprofen, Lipitor, Rogaine, Prozac, Viagra, Prilosec
- Nylon, Dacron, PET, Polystyrene, Acrylics, Teflon, Rayon, Polyaniline
- CRISPR, Recombinant, Technology, PCR

Environmental Disasters

- DDT (Dichlorodiphenyltrichloroethane)



- CFCs (Chlorofluorocarbons)



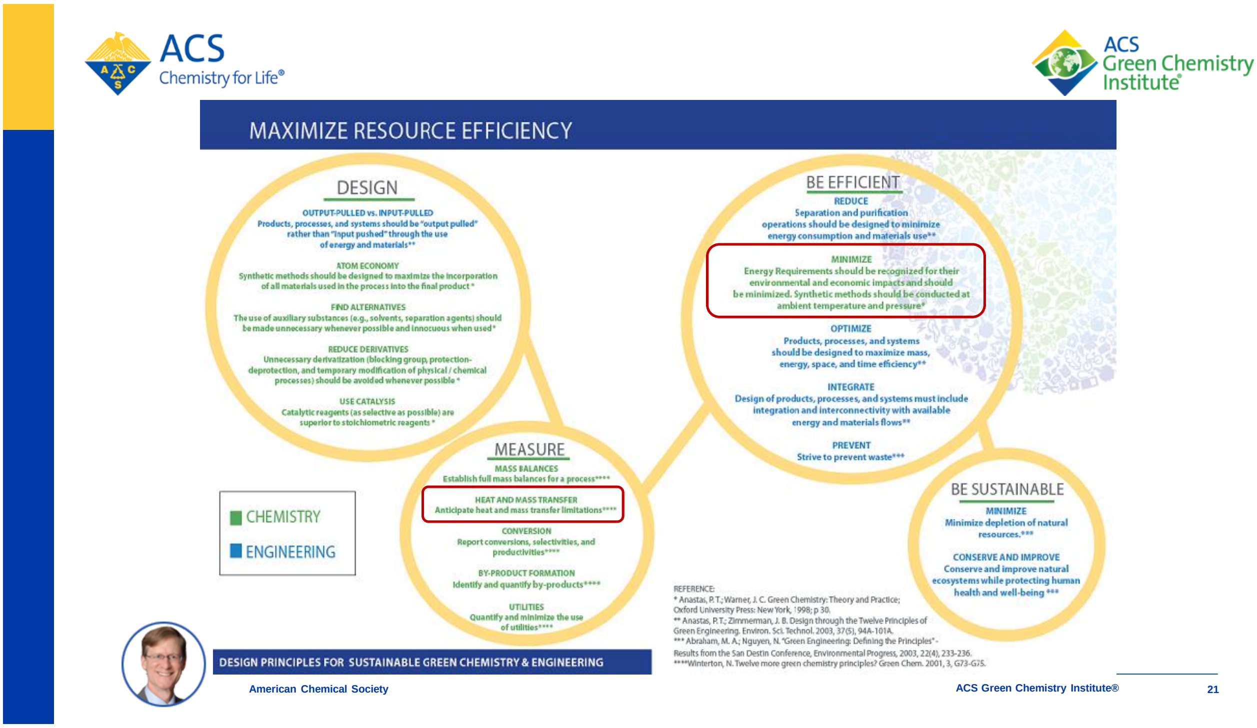
- Cuyahoga River
- Love Canal

Who Do We Blame???

"One day, this will all be your fault."

Who Do We Blame?

Earth Day, 1971. Walt Kelly, Post-Hall Syndicate, Simon & Schuster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MAXIMIZE RESOURCE EFFICIENCY
DESIGN
OUTPUT-PULLED vs. INPUT-PULLED
Products, processes, and systems should be "output pulled" rather than "input pushed" through the use of energy and materials**
ATOM ECONOMY
Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product *
FIND ALTERNATIVES
The use of auxiliary substances (e.g., solvents, separation agents) should be made unnecessary whenever possible and innocuous when used*
REDUCE DERIVATIVES
Unnecessary derivatization (blocking group, protection-deprotection, and temporary modification of physical / chemical processes) should be avoided whenever possible *
USE CATALYSIS
Catalytic reagents (as selective as possible) are superior to stoichiometric reagents *
MEASURE
MASS BALANCES
Establish full mass balances for a process****
HEAT AND MASS TRANSFER
Anticipate heat and mass transfer limitations****
CONVERSION
Report conversions, selectivities, and productivities****
BY-PRODUCT FORMATION
Identify and quantify by-products****
UTILITIES
Quantify and minimize the use of utilities****
CHEMISTRY
ENGINEERING
BE EFFICIENT
REDUCE
Separation and purification operations should be designed to minimize energy consumption and materials use**
MINIMIZE
Energy Requirements should be recognized for their environmental and economic impacts and should be minimized. Synthetic methods should be conducted at ambient temperature and pressure*
OPTIMIZE
Products, processes, and systems should be designed to maximize mass, energy, space, and time efficiency**
INTEGRATE
Design of products, processes, and systems must include integration and interconnectivity with available energy and materials flows**
PREVENT
Strive to prevent waste***
BE SUSTAINABLE
MINIMIZE
Minimize depletion of natural resources.***
CONSERVE AND IMPROVE
Conserve and improve natural ecosystems while protecting human health and well-being ***
REFERENCE:
* Anastas, P.T.; Warner, J. C. Green Chemistry: Theory and Practice; Oxford University Press: New York, 1998; p 30.
** Anastas, P.T.; Zimmerman, J. B. Design through the Twelve Principles of Green Engineering. Environ. Sci. Technol. 2003, 37(5), 94A-101A.
*** Abraham, M. A.; Nguyen, N. "Green Engineering: Defining the Principles" - Results from the San Destin Conference, Environmental Progress, 2003, 22(4), 233-236.
****Winterton, N. Twelve more green chemistry principles? Green Chem. 2001, 3, G73-G75.
DESIGN PRINCIPLES FOR SUSTAINABLE GREEN CHEMISTRY & ENGINEERING
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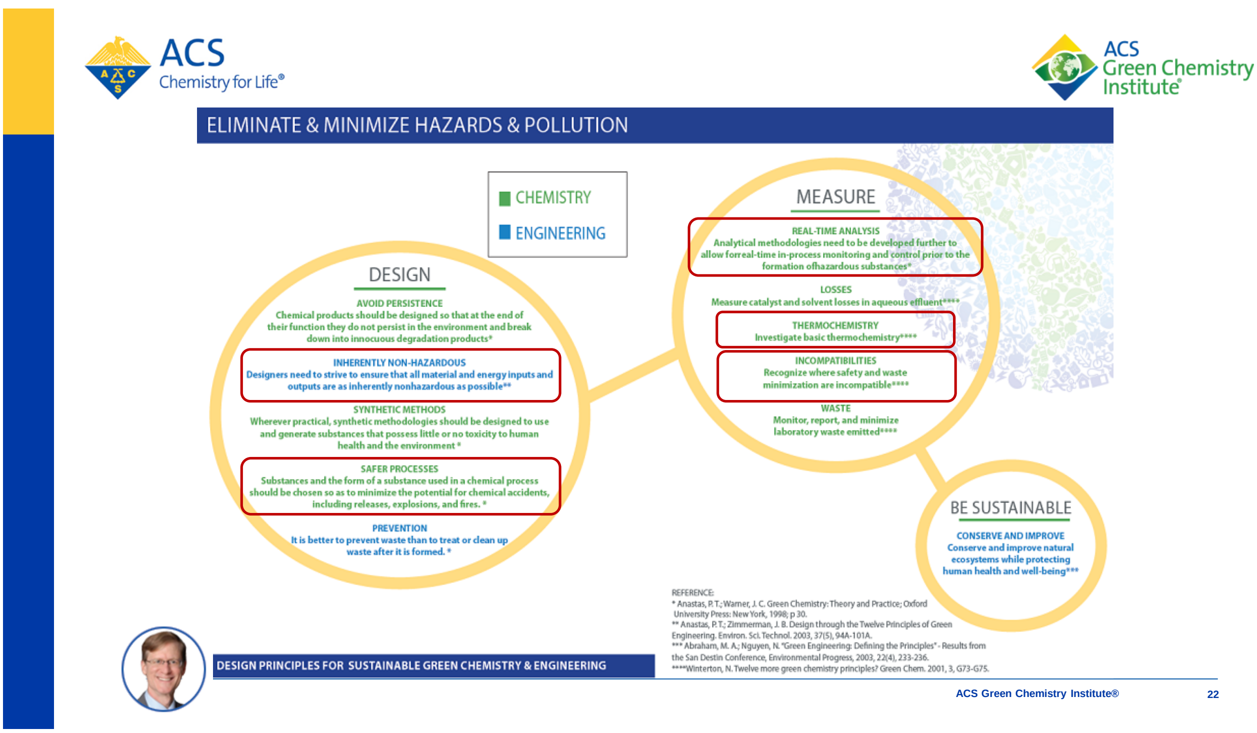
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ELIMINATE & MINIMIZE HAZARDS & POLLUTION
CHEMISTRY
ENGINEERING
DESIGN
AVOID PERSISTENCE
Chemical products should be designed so that at the end of their function they do not persist in the environment and break down into innocuous degradation products*
INHERENTLY NON-HAZARDOUS
Designers need to strive to ensure that all material and energy inputs and outputs are as inherently nonhazardous as possible**
SYNTHETIC METHODS
Wherever practical, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment *
SAFER PROCESSES
Substances and the form of a substance used in a chemical process should be chosen so as to minimize the potential for chemical accidents, including releases, explosions, and fires. *
PREVENTION
It is better to prevent waste than to treat or clean up waste after it is formed. *
MEASURE
REAL-TIME ANALYSIS
Analytical methodologies need to be developed further to allow forreal-time in-process monitoring and control prior to the formation ofhazardous substances*
LOSSES
Measure catalyst and solvent losses in aqueous effluent****
THERMOCHEMISTRY
Investigate basic thermochemistry****
INCOMPATIBILITIES
Recognize where safety and waste minimization are incompatible****
WASTE
Monitor, report, and minimize laboratory waste emitted****
BE SUSTAINABLE
CONSERVE AND IMPROVE
Conserve and improve natural ecosystems while protecting human health and well-being***
REFERENCE:
* Anastas, P.T.; Warner, J. C. Green Chemistry: Theory and Practice; Oxford University Press: New York, 1998; p 30.
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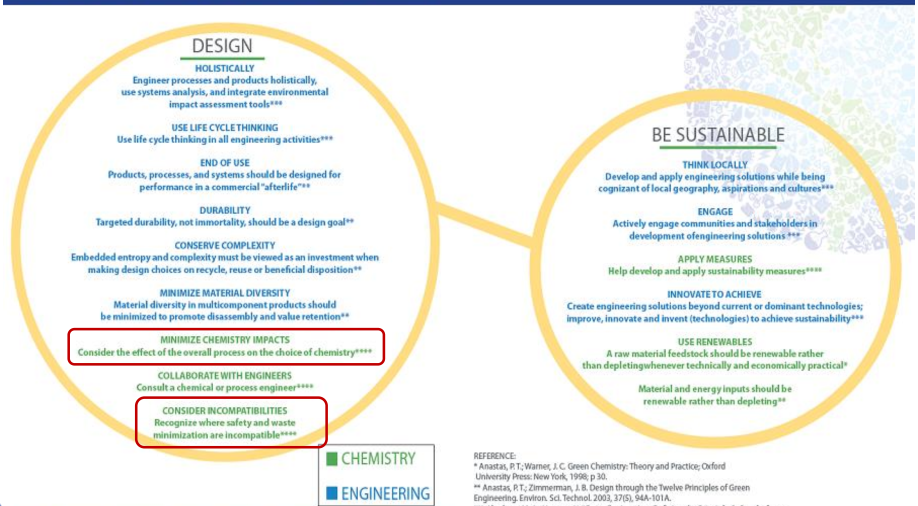
DESIGN SYSTEMS HOLISTICALLY & USING LIFE CYCLE THINKING



DESIGN PRINCIPLES FOR SUSTAINABLE GREEN CHEMISTRY & ENGINEERING

REFERENCE:
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****Winterton, N. Twelve more green chemistry principles? Green Chem. 2001, 3, G73-G75.

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This is not New!


SERIOUS REDUCTION OF HAZARDOUS WASTE

For Pollution Prevention and Industrial Efficiency

Chapter 1

Summary and Introduction

SUMMARY

"The major obstacles to increased waste reduction are institutional and behavioral rather than technical." - Serious Reduction of Hazardous Waste. US Congress. 1986

Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

The most important time to integrate green and sustainable chemistry and inherently safer approaches for greener, more sustainable products and processes is:

- After ensuring performance and economic viability
- After you've selected your route
- After you've completed process development but before commercialization
- At the very beginning of design; when you first conceive of the product
- All of the above are appropriate times

25

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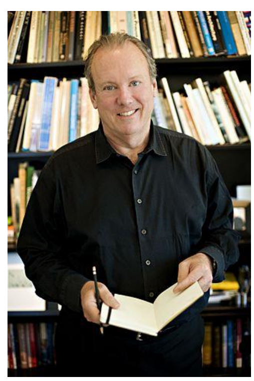
Thinking About Design

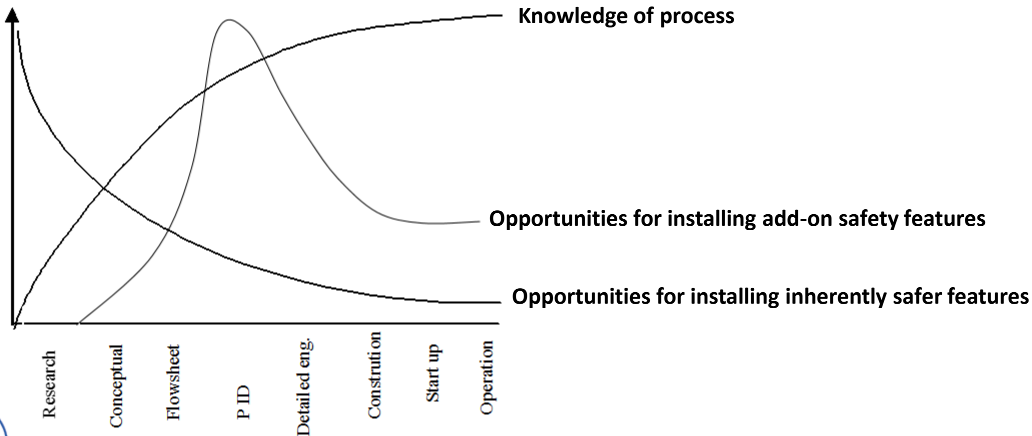
"Design is a signal of intention."



By Lynn Brubaker (Transferred by Kropotkine 113/Original uploaded by HardBoiledWonderland) [CC BY-SA 3.0

"Cradle to Cradle: Remaking the Way We Make Things" William McDonough, 2002

Design and the Inherent Safety Design Paradox



Inherent Safety and Pollution Prevention

Inherent Safety and Pollution Prevention hierarchies are <u>similar</u>.

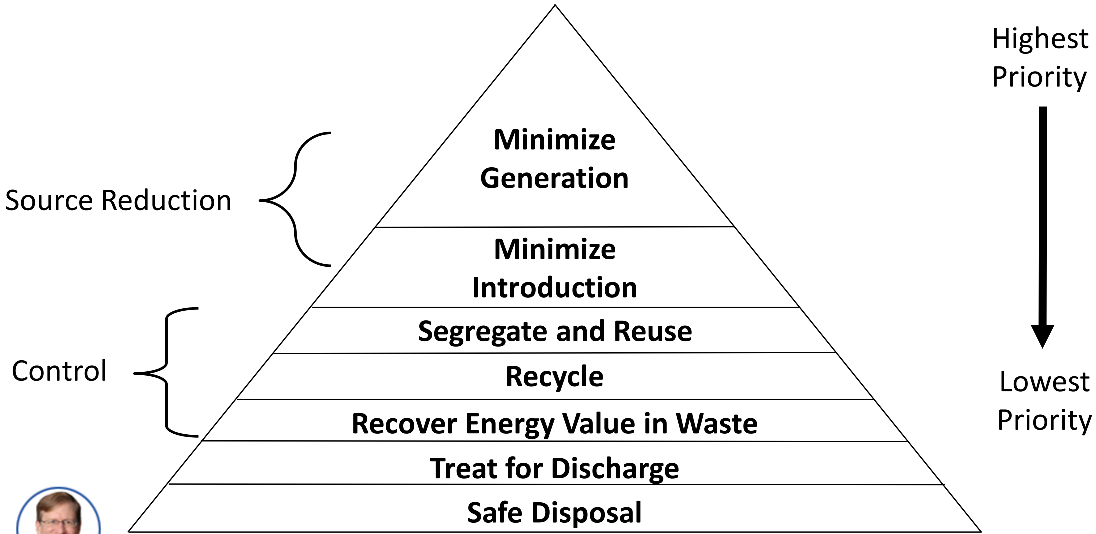
Pollution Prevention:

- Eliminate
- Reduce
- Recycle
- Re-use
- Treat
- Disposal

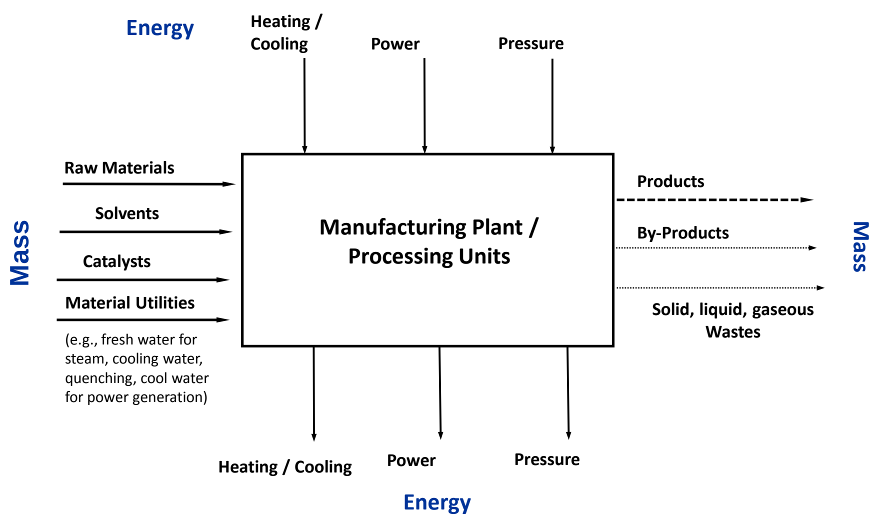
Inherent Safety:

- Minimize
- Substitute
- Moderate
- Simplify
- Control

Pollution Prevention Hierarchy



Mass-Energy Matrix



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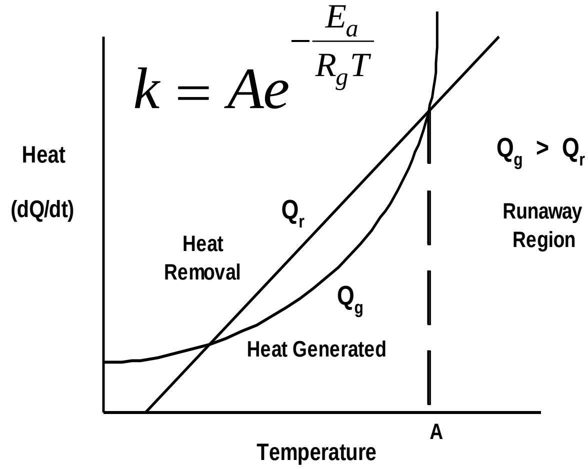
Kinetics and Exotherms



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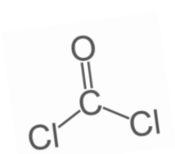
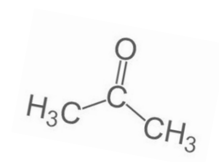
Hazard – A Review

- **An inherent physical or chemical characteristic that has the potential for causing harm to people, the environment, or property** (CCPS, 1992).
- **Hazards are intrinsic to a material, or its conditions of use.**
- **EXAMPLES**
  - **Phosgene** – severe irritant, corrosive, toxic by inhalation
  - **Acetone** – flammable
  - High pressure steam - potential energy due to pressure, high temperature





Dennis C. Hendershot, Rohm and Haas Company, Engineering Division, Bristol, PA

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Inherent

- Eliminate or reduce the hazard by changing the process or materials to materials that are non-hazardous or less hazardous
- Integral to the product, process, or plant - cannot be easily defeated or changed without fundamentally altering the process or plant design
- **EXAMPLE**
  - Substituting water for a flammable solvent (latex paints compared to oil base paints)

Vs.

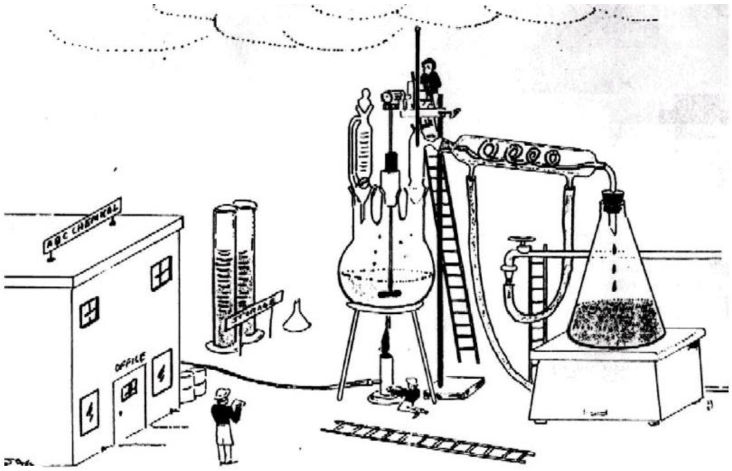
What Is Inherently Safer Design?

- Inherent - "**existing in something as a permanent and inseparable element...**"
  - safety "**built in**", not "**added on**"
- A system may be defined as *inherently safe* if - after a perturbation - it stays in or returns to a safe and stable state without involving human or automatic controls
- Inherently safer - ***eliminate or minimize hazards*** rather than control hazards. *More of a philosophy and way of thinking about design at every level of detail than a specific set of tools and methods*
- "***Safer,"*** not ***"Safe"***

Relationship of Green Chemistry, Engineering, and Inherently Safer Design

- **Green chemistry and engineering – broad consideration of many human and environmental impacts**
  - reaction paths, synthesis routes, raw materials and intermediates
  - implementation of selected synthesis routes
  - Requires fundamental knowledge of physical and chemical processes
- **Inherently safer design – focus on "safety" incidents**
  - Immediate consequences of single events (e.g., fires, explosions, immediate effects of toxic material release)
  - Includes consideration of chemistry as well as engineering issues such as siting, transportation, and detailed equipment design

Inherently Safer Design Strategies



"The bench scale results were so good that we by-passed the pilot plant."

From E. H. Stitt, "Alternative multiphase reactors for fine chemicals: A world beyond stirred tanks," *Chemical Engineering Journal* **90** (2002) 47-60.

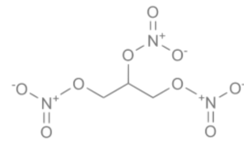
Inherent Safety Principles

- **<u>Intensification or minimization</u>** - *"What you don't have can't leak".*
- **<u>Substitution</u>** - is the use of a safer material in place of a more hazardous one, or the use of less of it.
- **<u>Attenuation or moderation</u>** - is the use of a hazardous chemical under less severe conditions.
- **<u>Limitation of effects</u>** - change designs or process conditions instead of adding on protective equipment that may fail.
- **<u>Simplicity</u>:** Simpler lab set ups/plants are safer than complex set ups/plants

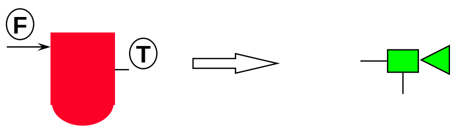
Mannan, M.S., D. Hendershot and T.A. Kletz, "Fundamentals of Process Safety and Risk Management," Encyclopedia of Chemical Processing and Design, ed. R.G. Anthony, vol. 69, Supplement 1, pp. 49-94, Marcel Dekker, Inc., New York, 2002

Intensify or Minimize

- **Use small quantities of hazardous substances or energy**
  - Storage
  - Intermediate storage
  - Piping
  - Process equipment



- **"Process Intensification" -** NAB process for manufacture of nitroglycerine



The Role of Chemistry in Process Intensification

- **Understand what controls a chemical reaction so that equipment design and setup optimizes the reaction**
  - Energy (heat/cool) transfer and removal
  - Mass transfer
    - Mixing
    - Between phases/across surfaces
  - Chemical equilibrium
  - Molecular processes
  - Rate and order of addition

Substitute

- **Substitute a less hazardous reaction chemistry**
- **Replace hazardous materials** with less hazardous alternatives
- **Water based coatings and paints** in place of solvent-based alternatives
  - Reduce fire hazard
  - Less toxic
  - Less odor
  - More environmentally friendly
  - Reduce hazards for end user and also for the manufacturer

Reaction Chemistry - Acrylic Esters

Reppe Process:

$$CH \equiv CH + CO + ROH \xrightarrow[HCl]{Ni(CO)_4} CH_2 = CHCO_2R$$

- Acetylene - flammable, reactive
- Carbon monoxide - toxic, flammable
- Nickel carbonyl - toxic, environmental hazard (heavy metals), carcinogenic
- Anhydrous HCl - toxic, corrosive
- Product - a monomer with reactivity (polymerization) hazards

Propylene Oxidation Process

Alternate Chemistry:

$$CH_2 = CHCH_3 + \frac{3}{2} O_2 \xrightarrow{Catalyst} CH_2 = CHCO_2H + H_2O$$

$$CH_2 = CHCO_2H + ROH \xrightarrow{H^+} CH_2 = CHCO_2R + H_2O$$

Is this process Inherently safe?

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Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Is this process Inherently safe?

- They're both horrible
- It's much safer
- Need more information to make a decision
- Keep looking for a better alternative process
- Stop making acrylic esters

44

Discussion

While not inherently safe, it is arguably inherently *safer*. Hazards are:

- primarily flammability,
- corrosivity from sulfuric acid catalyst for the esterification step,
- small amounts of acrolein as a transient intermediate in the oxidation step,
- reactivity hazard for the monomer product.

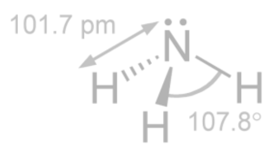
Moderate

- Dilution
- Refrigeration
- Less severe processing conditions
- Physical characteristics
- Containment
  - Better described as **"passive"** rather than **"inherent"**

Dilution

- **Aqueous ammonia** instead of anhydrous
- **Aqueous HCl** in place of anhydrous HCl
- **Sulfuric acid in place of oleum** (a solution of sulfur trioxide in sulfuric acid or sometimes more specifically to pyrosulfuric acid, disulfuric acid)
- **Wet benzoyl peroxide** in place of dry
- **Dynamite** instead of nitroglycerine

Less Severe Reaction Conditions

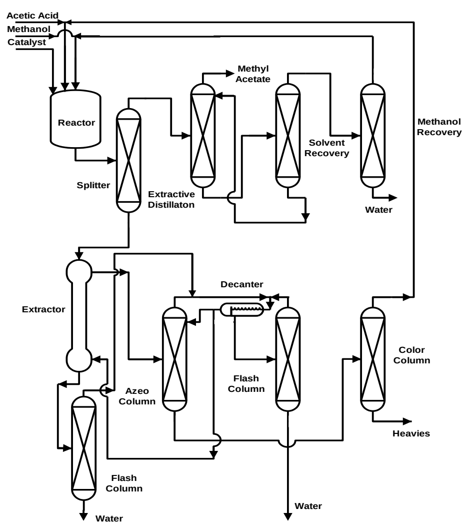


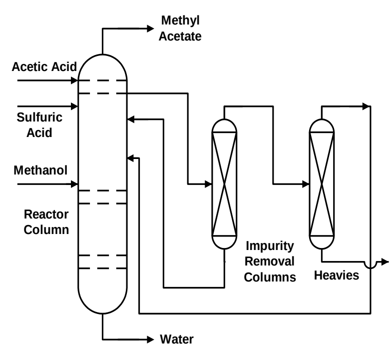
- **Ammonia Manufacture**
  - 1930s - pressures up to 600 bar
  - 1950s - typically 300-350 bar
  - 1980s - plants operating at pressures of 100-150 bar were being built
- Result of understanding and improving the process
- Lower pressure plants are cheaper, more efficient, as well as safer

Simplify

- Eliminate unnecessary complexity to reduce risk of human error
  - **QUESTION ALL COMPLEXITY!** *Is it really necessary?*

Simplify - Eliminate Equipment





Reactive distillation methyl acetate process (Eastman Chemical)

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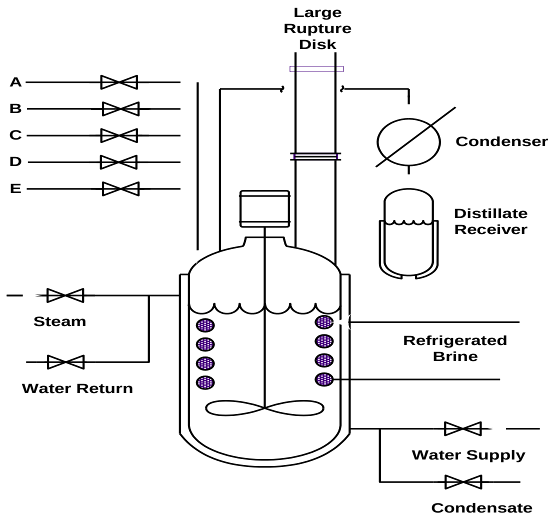
Single, Complex Batch Reactor



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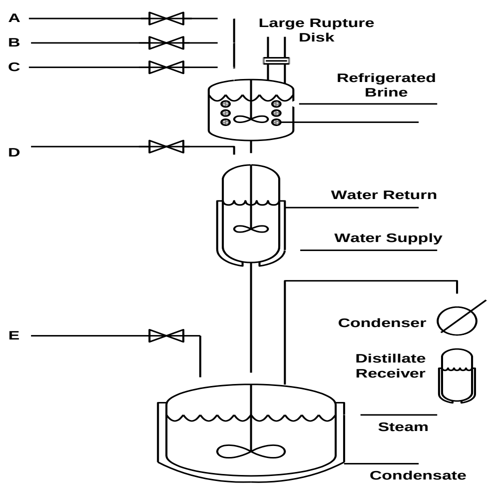
A Sequence of Simpler Batch Reactors for the Same Process

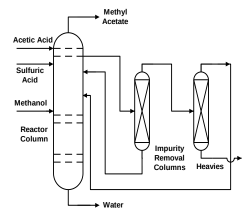


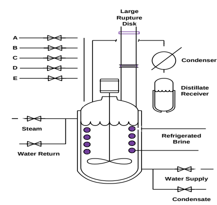
Audience Challenge Question

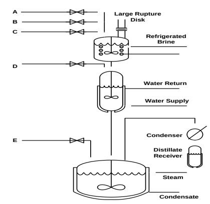
ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

There were 3 process configurations presented. Which of these is simpler?

- The Eastman Reactive Distillation Process
- Complex Batch Reactor
- Series of 3 Batch Reactors
- Each of them have trade-offs







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Simplification Conflicts

- **In the previous example**
  - Each vessel is simpler
- **But:**
  - There are now three vessels, therefore, the overall plant is more complex in some ways
  - Compare to methyl acetate example
- **Need to understand specific hazards for each situation to decide what is best**

Questions a designer should ask when she has identified a hazard

In this order

1. Can I eliminate this hazard?
2. If not, can I reduce the magnitude of the risk?
3. Do the alternatives identified in questions 1 and 2 increase the magnitude of any other risks, or create new risks?

   (If so, consider all hazards and risks in selecting the best alternative.)
4. At this point, what technical and management systems are required to manage the risks which inevitably will remain?

8 Reaction Process Design Considerations

1. Rapid reactions (but not too rapid, especially if they are endo or exothermic) are desirable
2. Avoid batch processes in which all of the potential chemical energy is present in the system at the start of the reaction step
3. Use gradual or reverse addition, “semi-batch” processes, or micro-reactors/alternative reaction spaces for exothermic reactions
4. Avoid using control of reaction mixture temperature as the only means for limiting the reaction rate

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8 Reaction Process Design Considerations

5. Account for the impact of reactor/reaction space size/volume on heat generation and removal capabilities
6. Use multiple temperature sensors, in different locations in the reaction vessel for rapid exothermic reactions
7. Avoid feeding a material to a reaction vessel at a higher temperature than the boiling point of the reactor contents
8. Pay careful attention to ensure good mixing, especially for heterogeneous or multi-phase reactions

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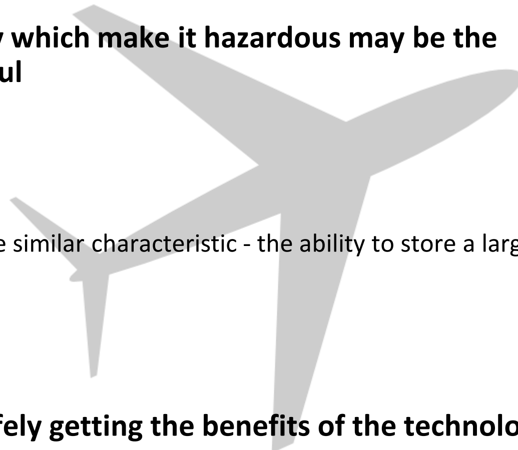
Conflicts and Tradeoffs

Some Problems



- **The properties of a chemical or technology which make it hazardous may be the same as the properties which make it useful**
  - Airplanes travel at 600 mph
  - Gasoline is flammable
    - Any replacement for gasoline must have one similar characteristic - the ability to store a large quantity of energy in a compact form
      - a good definition of a hazardous situation

  - Chlorine is toxic but it is chemically useful
- **Control of the risk is the critical issue in safely getting the benefits of the technology**

Multiple Hazards

- **Everything has multiple hazards and risks**
  - Automobile travel
    - velocity (energy), flammable fuel, exhaust gas toxicity, hot surfaces, pressurized cooling system, electricity......
  - Chemical process or product
    - acute toxicity, flammability, corrosiveness, chronic toxicity, various environmental impacts, reactivity.......

Inherently Safer ≠ Safer

Air Travel

- several hundred people
- 5 miles up
- control in 3 dimensions
- 600 mph
- thousands of gallons of fuel
- passengers in a pressure vessel
- ....

Automobile Travel

- a few people
- on the ground
- control in 2 dimensions
- 60 mph
- a few gallons of fuel
- might even be a convertible
- ....

- ***Automobile travel is inherently safer***
- ***But, what is the safest way to travel from Washington to Los Angeles?***
- ***Why?***
  - ***Primarily because of active and procedural engineering features of the air transportation system***

Chemical Hazard Identification

Approaches and Tools

Chemical Hazard Identification – Tools, Resources – Theoretical and Computational Screening

- Safety data sheet (SDS) and manufacturer's data
- Chemical compatibility matrix
- Literature reactivity data such as Bretherick's handbook, NFPA hazard ratings, etc.
- Incident data
- Chemical structure
- Formation energies; can be estimated from group contributions (Benson, NIST Database 25) or quantum mechanics (Gaussian 94)
- Heat of reaction, decomposition, solution
- Computed adiabatic reaction temperature at constant pressure and/or volume, CART
- Oxygen balance
- Software tools such as the ASTN CHETAH, NASA CET89, SuperChems, TIGER, etc.

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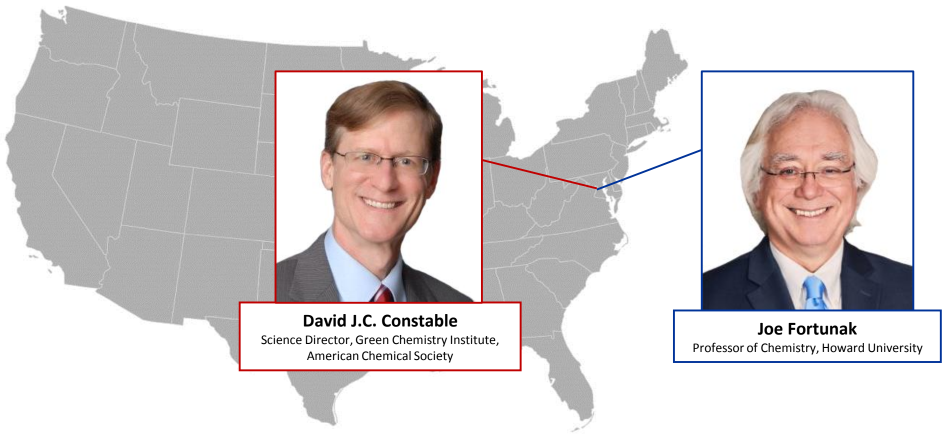

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Experts

Craig Lindsley
Vanderbilt Center for Neuroscience Drug Discovery

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Experts

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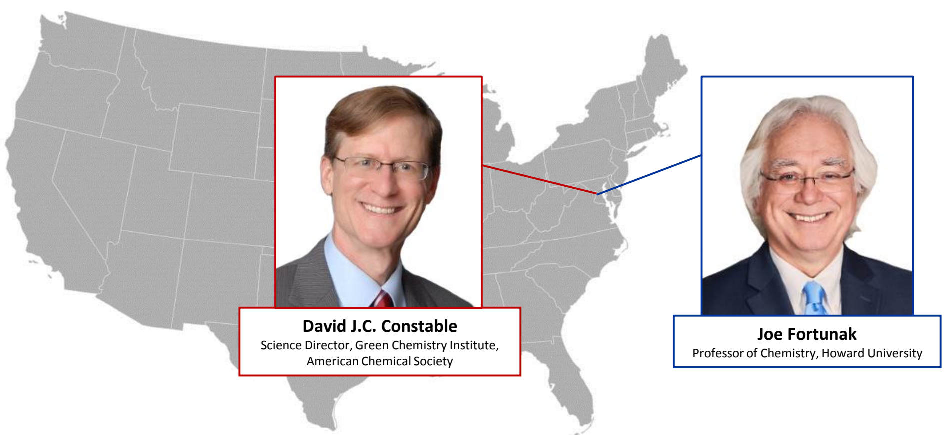

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Final Thoughts

- Chemists have a duty to recognize and minimize the potential economic, societal and environmental risks that are a part of chemistry
- Design is the most important activity a chemist can do to reduce or eliminate sustainability risks
- Green chemistry, inherent safety, pollution prevention begins at the route design level
- Process flow sheets are invaluable in highlighting continued opportunities to reduce or eliminate waste and unsafe practices or potential for accidents.
- There is an overwhelmingly clear business case for green and sustainable chemistry.

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"Great job as usual! It was fascinating to hear about the historical roots of lab safety culture. I hope to see more bite-sized lab safety resources for students in the future."

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Anna Sitek, CSP
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