FROM THEORY TO PRACTICE

Image: NASA Earth Observatory

www.greenchemistry-toolkit.org
Topics To Be Covered

1. Implementation: Why, What, and How
2. Understanding Context
   • Green Chemistry in the Marketplace
3. Identifying Opportunities
   • Life Cycle and Green Chemistry Principles as a Guide to Finding Opportunity
4. Delivering Innovation
   • Green Chemistry Strategies at All Stages
5. Green Chemistry Assessment Tool
6. How to Proceed: Moving Forward
After several hours of listening to lectures, doing exercises, and viewing case studies, how do you go about implementation and/or dissemination of Green Chemistry?

The process can be summarized in 3 words:

Why → What → How
Why
• Understand Context
  • Business/Market

What
• Identify Opportunities
  • Product/Service

How
• Deliver Innovation
  • Technology
Reasons may vary:
- Reduce cost
- Increase margins
- Increase sale
- Enhance corporate competitiveness
- Improve reputation

Potential roadblocks:
- Resource depletion
- Environmental damage
- Growing population
- Increasing consumption
- Societal attitudes

Why
- Understand Context
- Business/Market
Why

- Understand Context
- Business/Market

Understand Trends & Drivers

Political
- Social services
- Consumer protection
- Tax competition
- Knowledge competition

Environmental
- Climate change
- Extinctions
- Water
- Waste
- Resource constrains

Social
- Urbanization
- Demographics
- Population growth
- Fear

Technology
- Nano
- Molecular biology
- Statistics

Economic
- Globalization
- High value services
- Income
Why

• Understand Context
• Business/Market

Think of an outcome

Generate a problem statement

If only we could _________, then we could ____________
What are we delivering?
- New synthetic route
- New catalyst
- Alternative solvent
- New product

What is the “functional unit”?
- Number of reaction runs
- Performance (yield or atom economy)
- Energy usage per period of time
- Kg of parts cleaned
Use Life Cycle and Green Chemistry Principles as a guide

- Identify Opportunities
- Product/Service
**What**

- Identify Opportunities
- Product/Service

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**GREEN CHEMISTRY**


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<table>
<thead>
<tr>
<th>Material Extraction and Processing</th>
<th>Manufacturing</th>
<th>Use</th>
<th>End of Life</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Prevent waste</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2. Atom economy</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3. Less hazardous chemical synthesis</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4. Designing safer chemicals/products</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5. Safer solvent &amp; reaction media</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6. Design for energy efficiency</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7. Renewable feedstocks</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8. Reduce derivatives</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9. Use of catalysts</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10. Design for degradation</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>11. Real-time monitoring and process control</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12. Inherently safer chemistry</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Raw materials extraction

- Production of waste and energy consumption during raw material extraction
- High impact materials: rare metals, natural extracts (perfume ingredients), bricks, concrete, electronic equipment
Design strategy for raw materials

- Reduce the hazard for the materials used: avoid materials that are persistent, bioacumulative, have high toxicity profile
  
  Use BIOWIN or PBT Profiler (http://www.pbtprofiler.net/default.asp) for persistence/degradation and bioconcentration
  Use ChemHAT, Protox, ChemSpider for toxicity profile
  EcoSAR (not discussed) for ecotoxicity

- Use renewable materials like carbohydrates, lipids, biopolymers
- Use recycled materials or materials from the waste stream
- Reduce the number of raw materials used
- Minimize transportation (locally sourced, or manufacturing shifted onsite)
- Avoid materials that generate a lot of waste or are energy intensive
- Avoid materials produced in environmentally damaging way

How

- Deliver Innovation
- Technology
Manufacturing

- Possibly the greatest impact
- Extensive processing that uses energy and produces a large volume of waste
- Examples include consumer products and chemicals

How
- Deliver Innovation
- Technology
Design strategy for manufacturing

- Improve energy efficiency of the process
- Use technologies which minimize production of waste and emissions
- Use renewable energy
- Avoid hazardous process and auxiliary materials (use safer solvents)
- Recycle process materials (solvents)
- Choose disposal to minimize environmental impact
- Use waste as a feedstock for another process

Use solvent selection guides for better solvent alternative
Identify chemicals of concern: Toxic Release Inventory (https://www.epa.gov/toxics-release-inventory-tri-program)
Use IRIS (https://www.epa.gov/iris) to check human health effect from chemical exposure
Atom economy, E-factor for reaction performance

How

- Deliver Innovation
- Technology
Distribution

- Products which are transported over long distances, are heavy and require a lot of packaging
  - Example includes fresh out of season vegetables shipped to locations around the world

How
- Deliver Innovation
- Technology
Design strategy for distribution

- Minimize packaging per unit of service
- Use returnable packaging
- Avoid PVC and use packaging from renewable feedstocks
- Manufacture product at the point of use
- Use a lower impact transportation
Use

- Products with high durability that go through many cycles are found in this category.
  - Examples include cars, laser printers and dishwashers
Design strategy for use

- Minimize energy efficiency per unit of service
- Can the product be made safer for a human and environment?
- Can the amount of product be automated to avoid losses of product?
- Design out waste and emissions in use or make it environmentally benign
- Minimize auxiliary processes and make materials renewable and recyclable
- Collect and recycle waste

How

- Deliver Innovation
- Technology
Disposal (End-of-Life)

- Products that are toxic or persistent are hard to dispose
  - Example includes batteries

How

- Deliver Innovation
- Technology
Design strategy for disposal

- Design so that manufacturer can recover and reuse the product at end of life
- Design for ease for disassembly
- Can the individual components be recycled at the end of life?
- Avoid harmful substances that could be released at end of life
- Ensure that a toxic substance can be easily extracted from the product
- Design materials that are biodegradable and compostable
CONCLUSIONS

- Based on the life cycle, assess the overall improvement to the process/technology
- Identify if any tradeoffs were made between green chemistry principles
International Flavors & Fragrances Inc (IFF)

- International company employing ~7000 people with manufacturing facilities in 35 countries and current market of $10 billion.

- In Vision 2020, they committed to embed sustainability in the company culture and develop a measurable metrics which will support triple bottom line.

- As a part of this initiative they developed a Green Chemistry Assessment tool, to track their progress.
Internal, easy to apply, uniform and standardized method of analyzing safety, health and environmental impact

Distributed and accepted by scientists and staff across the globe

Sharable with technical and non-technical experts, senior managers, customers and other stakeholders within IFF
Each Green Chemistry principle has a scoring system to improve process, operations and products with the purpose of having a positive impact on TBL.

Score for each principle ranges from 0 (worst) to 5 (best).

*Results are presented in the radar chart.

* Scoring is relative and specifically developed for IFF products. It is not shared publicly.
While IFF uses the scoring system internally, their guidelines may be useful for other companies:

- If a process generates hazardous waste, it is assigned 0
- If the process has over 80% atom economy, then it is assigned 5
Fragrance aroma used in perfumery applications such as personal care and fine fragrances.

New synthesis includes:

**Environmental Benefits**
- Improvement in mass efficiency from 25 – 85%
- Chemical waste elimination up to 80%
- Improved worker safety in reduction of hazardous waste

**Economic benefits**
- 94% reduction in energy cost
- Greater efficiency leading to lower costs for chemical resources
- Reduction for capital cost for equipment
- Reduction of technical failures during scale-up
1. Prevent waste (3→4)  
   • High, non-hazardous waste was reduced by 50 tons
2. Atom economy (3→4)  
   • Yield increased by 10%
3. Less hazardous synthesis (1→4)  
   • Elimination of safety hazards (not defined)
4. Design benign chemicals (3→3)  
   • No change in score
5. Benign solvents (3→3)  
   • No change in score: same non-hazardous solvents used
6. Design for energy efficiency (3→5)  
   • Increase from 8kg/h·m³ to 100kg/h·m³

Improvement from assigned value 3 in the traditional reaction to value 4 in the new synthesis
7. Use of renewable feedstocks (0→0)
   • The process does not use renewable feedstock

8. Reduce derivatives (5→5)
   • No derivatives involved

9. Catalysis (1→1)
   • No catalyst used

10. Design for biodegradation (5→5)
    • No change

11. RT analysis for pollution prevention (5→5)
    • Process monitoring and control present

12. Design for accident prevention (3→5)
    • Process hazards eliminated
STEP1: Grignard Addition

**Old process**  **New process**

- Prevent Waste
- Atom Economy
- Less Hazardous Synthesis
- Design Benign Chemicals
- Benign Solvents
- Design for Energy Efficiency
- Use of Renewable Feedstocks
- Reduce Derivatives
- Catalyst
- Design for Biodegradation
- RT Analysis & Pollution Prevention
- Design for Accident Prevention

**Old process** vs **New process**

- **Prevent Waste**: New process is higher than old process.
- **Atom Economy**: New process is slightly lower than old process.
- **Less Hazardous Synthesis**: New process is lower than old process.
- **Design Benign Chemicals**: New process is slightly higher than old process.
- **Benign Solvents**: New process is higher than old process.
- **Design for Energy Efficiency**: New process is slightly higher than old process.
- **Use of Renewable Feedstocks**: New process is slightly lower than old process.
- **Reduce Derivatives**: New process is lower than old process.
- **Catalyst**: New process is slightly lower than old process.
- **Design for Biodegradation**: New process is lower than old process.
- **RT Analysis & Pollution Prevention**: New process is lower than old process.
- **Design for Accident Prevention**: New process is lower than old process.
1. Prevent waste (3→5)
   • Waste reduced by 80%, solvent recyclable between batches

2. Atom economy (1→5)
   • Mass efficiency increased from 25-80%, yield improved by 10%

3. Less hazardous synthesis (3→5)
   • Aluminium isopropoxide and phosphoric acid oxidation replaced by air and catalyst

4. Design benign chemicals (3→3)
   • No change in score

5. Benign solvents (3→5)
   • Acetone replaced by water

6. Design for energy efficiency (4→4)
   • Reaction run at atmospheric pressure and temperature below 100C
7. Use of renewable feedstocks (0→5)
   • New process uses air

8. Reduce derivatives (5→5)
   • No derivatives involved

9. Catalysis (3→5)
   • Use 5% reusable catalyst in place of 66% aluminum isopropoxide

10. Design for biodegradation (5→5)
    • No change

11. RT analysis for pollution prevention (5→5)
    • Process monitoring and control present

12. Design for accident prevention (3→5)
    • New engineering controls in place
STEP 2: Oxidation from alcohol to ketone

- Old process
- New process

Prevent Waste
Atom Economy
Less Hazardous Synthesis
Design Benign Chemicals
Benign Solvents
Design for Energy Efficiency
Use of Renewable Feedstocks
Reduce Derivatives
Catalyst
RT Analysis & Pollution Prevention
Design for Biodegradation
Design for Accident Prevention
No –
  • because metrics is arbitrary and not applied across disciplines
  • Because it limits creativity

But..
  • It allows a systematic evaluation and serves as a guide
  • And it is a good start
With brilliance and optimism.

Science and technology has risen to the challenge and it has the creativity and capability to do it again.
Responsibly.

With power comes responsibility. With all the knowledge, perspective and training you acquire, you also have acquired the ability to impact others – to impact the world. Once you have the power to impact the world, you have the responsibility to impact it for the better.
How to Proceed?

With conviction, courage and commitment.

Green Chemistry and Green Engineering
Because we can.
Because we must
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THANK YOU!

QUESTIONS?

This training material was developed in close collaboration with the Center for Green Chemistry and Green Engineering at Yale University.

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