UNITED NATIONS
INDUSTRIAL DEVELOPMENT ORGANIZATION

GREEN CHEMISTRY

FROM THEORY TO PRACTICE

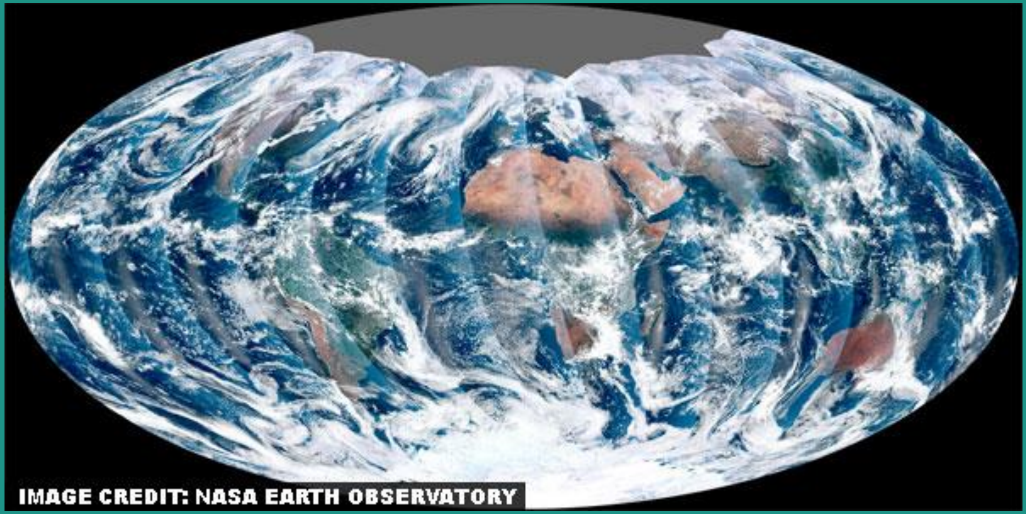

Image: NASA Earth Observatory

DAY 4 SESSION II
4-DAY PRESENTATION

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

Why

- Understand Context
  - Business/Market

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

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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

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Why

- Understand Context
  - Business/Market

Think of an outcome

Generate a problem statement

If only we could __________, then we could_____________

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What

- Identify Opportunities
  - Product/Service

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

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What

- Identify Opportunities
  - Product/Service

Use Life Cycle and Green Chemistry Principles as a guide

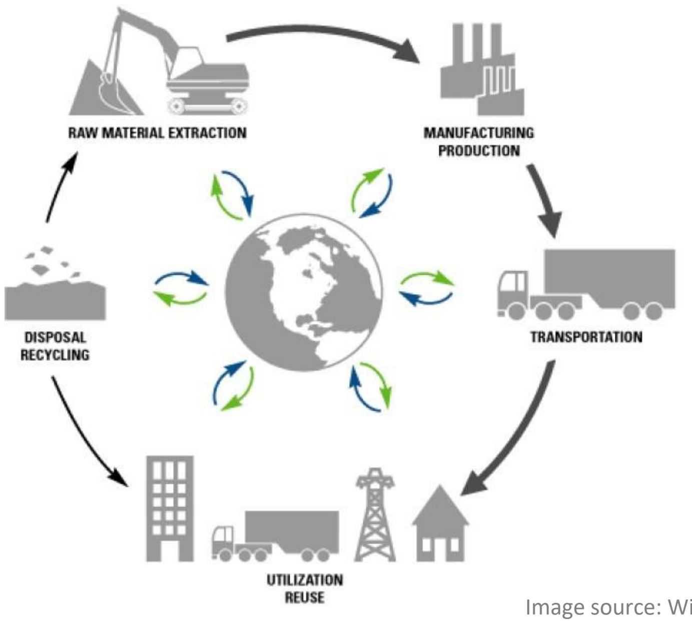

Image source: Wikipedia

What

- Identify Opportunities
  - Product/Service

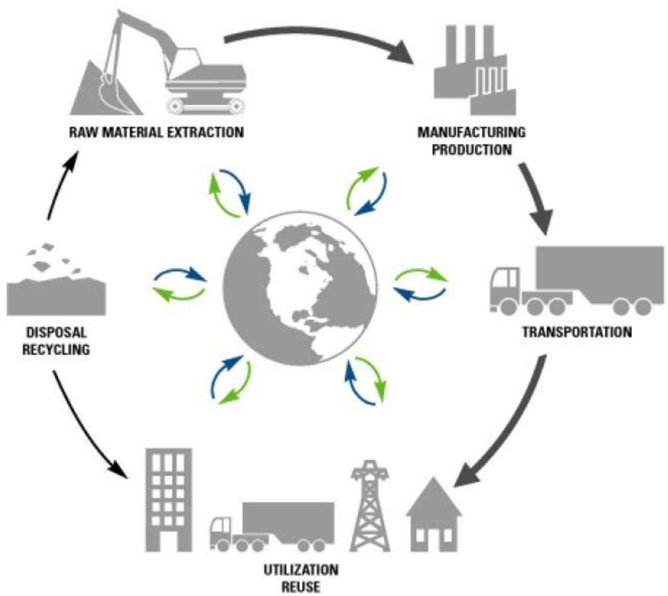

Image source: Wikipedia

Material Extraction and Processing → Manufacturing → Use → End of Life

1. Prevent waste
2. Atom economy
3. Less hazardous chemical synthesis
4. Designing safer chemicals/products
5. Safer solvent & reaction media
6. Design for energy efficiency
7. Renewable feedstocks
8. Reduce derivatives
9. Use of catalysts
10. Design for degradation
11. Real-time monitoring and process control
12. Inherently safer chemistry

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How

- Deliver Innovation
- Technology

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

How

- Deliver Innovation
- Technology

Design strategy for raw materials

- ❑ Reduce the hazard for the materials used: avoid materials that are persistent, bioacummulative, 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)

  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

- ❑ Recycle process materials (solvents)
- ❑ Choose disposal to minimize environmental impact
- ❑ Use waste as a feedstock for another process

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

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How

- Deliver Innovation
- Technology

Use

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

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How

- Deliver Innovation
- Technology

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

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- Based on the life cycle, assess the overall improvement to the process/technology
- Identify if any tradeoffs were made between green chemistry principles

HOW DO OTHERS TRACK THEIR SUCCESS?

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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.

GREEN CHEMISTRY ASSESSMENT TOOL

GREEN CHEMISTRY

- 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

SCORING

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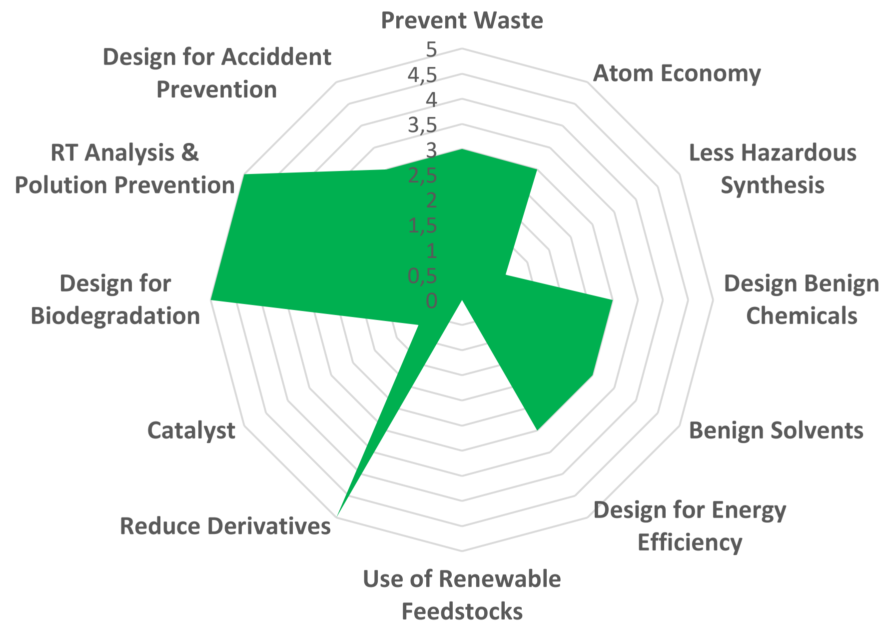
- Each Green Chemistry principle has a scoring system to improve process, operations and products with the purpose of having a positive impact on TBL
- Score for each principle ranges from 0 (worst) to 5 (best)
- *Results are presented in the radar chart

Green Principles Score



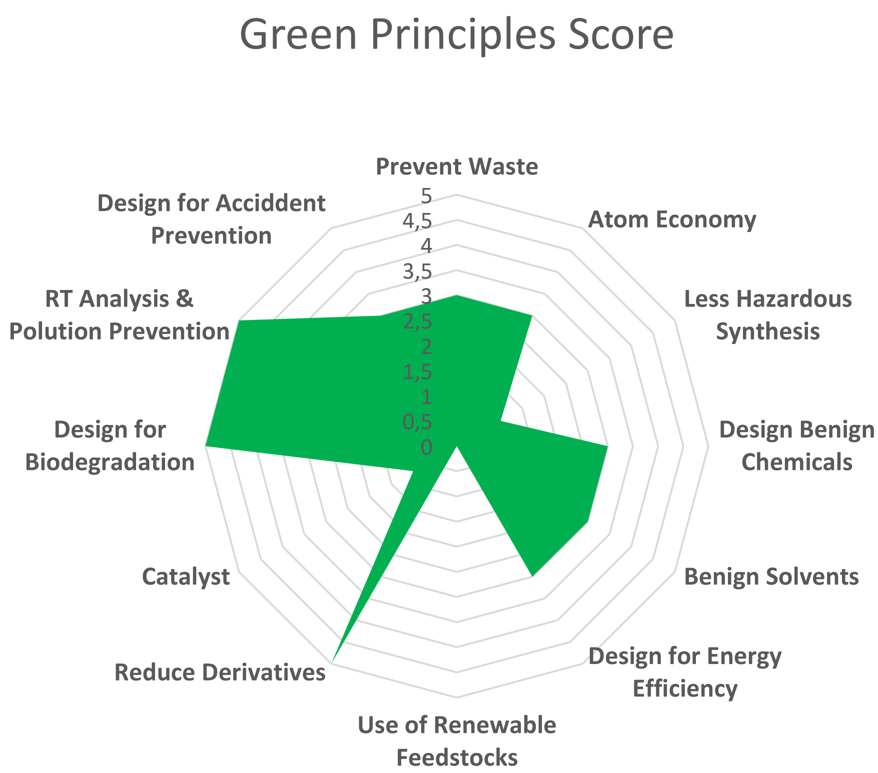
* Scoring is relative and specifically developed for IFF products. It is not shared publically.

SCORING

GREEN CHEMISTRY

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



SYNTHESIS OF VERIDAN

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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

2 reaction steps

IMPROVEMENTS – STEP 1– GRIGNARD ADDITION

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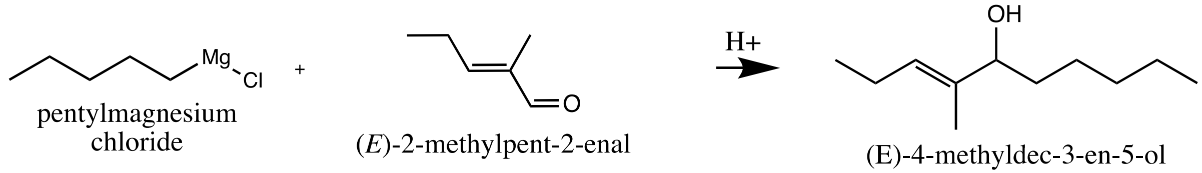

1. Prevent waste (3→4)
   - High, non-hazardous waste was reduced by 50 tons
2. Atom economy (3→4)
   - Yield increased by 10%
3. Less hazardous synthesis (1→4)
   - Elimination of safety hazards (not defined)
4. Design benign chemicals (3→3)
   - No change in score
5. Benign solvents (3→3)
   - No change in score: same non-hazardous solvents used
6. Design for energy efficiency (3→5)
   - Increase from 8kg/h*m^3 to 100kg/h*m^3

Improvement from assigned value 3 in the traditional reaction to value 4 in the new synthesis

IMPROVEMENTS – STEP 1– GRIGNARD ADDITION

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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

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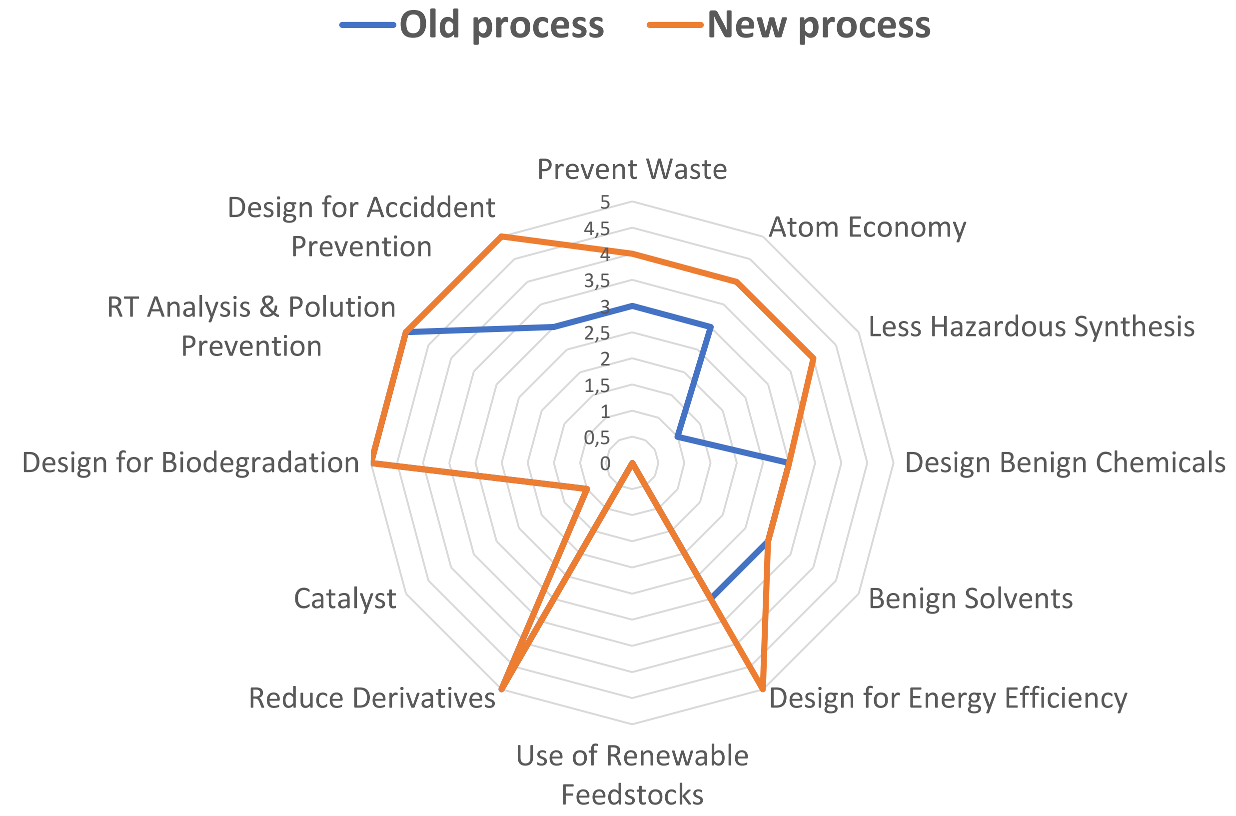
STEP1: Grignard Addition



IMPROVEMENTS – STEP 2– OXIDATION FROM ALCOHOL TO KETONE

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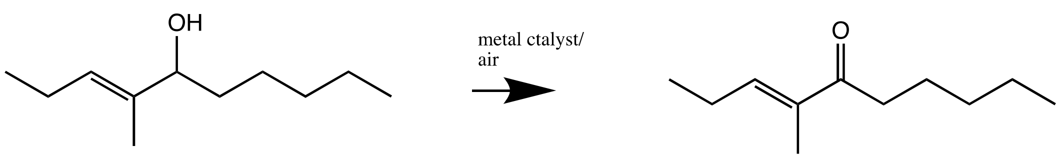

(E)-4-methyldec-3-en-5-ol → (E)-4-methyldec-3-en-5-one

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

IMPROVEMENTS – STEP 2– OXIDATION FROM ALCOHOL TO KETONE

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

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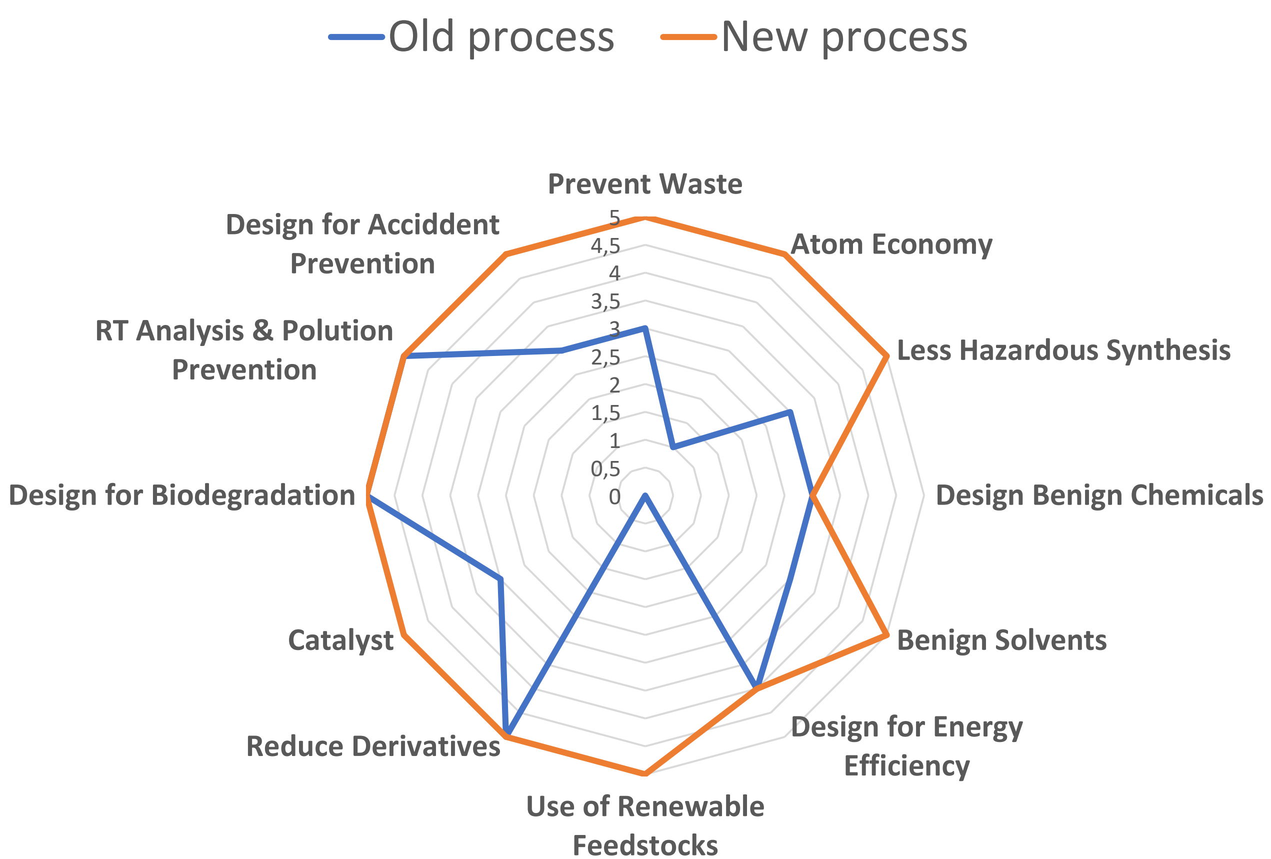
STEP 2: Oxidation from alcohol to ketone



IS GREEN CHEMISTRY ASSESSMENT TOOL A SOLUTION?

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

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With brilliance and optimism.

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

HOW TO PROCEED?

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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.

GREEN CHEMISTRY

How to Proceed?

With conviction, courage and commitment.

Green Chemistry and Green Engineering

Because we can.

Because we must

TOPICS TO BE COVERED

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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.

www.greenchemistry-toolkit.org