iSUSTAIN™

Green Chemistry Index

A Simple Sustainability Index for the Chemical Industry

Green Chemistry and Commerce Council
April 26, 2010

iSUSTAIN™ Green Chemistry Index is brought to you by:

beyondbenign a warner babcock foundation

CYTEC

sopheon Where innovation means business™

Why develop a new Green Chemistry Index?

- How do your products and projects rank in terms of sustainability?
  - There is a need to measure this
  - With the tool, researchers can plan a strategy to improve
- Publicly available Indices do not focus on green chemistry
  - Don’t allow application across all stages of product development
  - Don’t provide information on raw materials
- Traditional life cycle assessment (LCA) is labor intensive
  - Requires a dedicated specially-trained staff
  - Full LCA information on raw materials is only available for a limited set of compounds
  - Typically takes weeks to prepare one assessment

Our goal was an index we could apply to hundreds of products

Index Basis

- The Index is based on:
  The Twelve Principles of Green Chemistry
- These Principles espouse the concepts of:
  - Minimization of waste
  - Careful design of processes to maximize amount of raw material that ends up in the product
  - Use of safe, environmentally benign substances, whenever possible
  - Greater use of renewable raw materials
  - Incorporation of energy efficient processes

Cytec collaborated with Dr. John Warner, a founder of the field of green chemistry, in developing of the Index

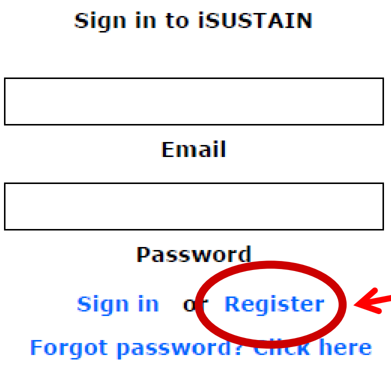
Background & Plans for the Index

- Cytec initially developed the iSUSTAIN™ Sustainability Index as an internal tool
  - **Cytec was encouraged to take the Index public**
- An Alliance was formed between three companies:
  - Cytec Industries Inc.
  - Sopheon PLC, a leading provider of software and services for product lifecycle management
  - Beyond Benign, a non-profit organization dedicated to green chemistry education and training.
- A public web-based version of the new iSUSTAIN Green Chemistry Index has been developed through this Alliance:
  - It's being provided free to all academic users and for a small fee to commercial users.
  - Sopheon will run and support the web version of the Index
  - Beyond Benign will provide training to users and administration of the Raw Material database portion of the Index

Timings

- Launch Date: March 21, 2010 (ACS San Francisco meeting)
- There are currently 4 levels of access:
  - **Public Level**: Free to all users, ability to only save 1 process evaluation and limited output options
  - **Individual Level**: Fee-based access, unlimited saved process evaluations in a secure server area, enhanced sharing and output options
  - **Academic Level**: Free version of the Individual Level
  - **Enterprise Level**: Tiered pricing for multiple seats within an organization; Ability to input proprietary materials (and keep them proprietary); Ability to share scenarios within organization

Accessing the iSUSTAIN™ Green Chemistry Index



- Website:
  - Go to www.isustain.com
- Registration
  - Click the **Register** link

- Fill out the requested information
- Agree to the Terms and Conditions
- Click the Register button
- You'll receive an email from Sopheon
  - Click on the link in it
  - Your registration will be confirmed
- Go back to the main page and Sign In

The iSUSTAIN Index is free to all academic users through the .edu domain name (or international equivalent) in their email address

iSUSTAIN™ Green Chemistry Index

The Index – Home Page

Getting Started | Scenarios | Data Input | My Profile | Log Out

Welcome to the iSUSTAIN™ Green Chemistry Index v2.0

Foreword by Dr. John Warner, Director, Warner-Babcock Institute of Green Chemistry -

> *"Sustainability efforts in institutions across the world have become mainstream and ubiquitous. Although much attention and resources are being spent on such activities, there does not exist a universal understanding of how sustainability can be truly measured and tracked to determine the actual success of any "sustainability endeavor". The iSUSTAIN Sustainability Index provides the user with a CREDIBLE and QUANTIFIABLE assessment of the relative sustainability of a material process."*

The iSUSTAIN™ Index is a tool to generate a sustainability-based score for chemical products and processes. It contains a set of sustainability metrics based on the Twelve Principles of Green Chemistry* and takes into account such factors as waste generation, energy usage, health and environmental impact of raw materials and products, safety of processing steps, and others.

The iSUSTAIN™ index is designed to:

• Provide a quantitative measure of the sustainability of products and processes to both develop an initial sustainability baseline and provide guidance for process improvement

• Act as a learning tool for the scientific community to provide increased familiarity with the Twelve Principles of Green chemistry

• Allow use from very early stages in a project's development through to commercialization

A public web-based version of the iSUSTAIN™ Sustainabilty Index has been developed through an alliance between Cytec Industries Inc., a sustainability-aware specialty chemicals and materials company; Sopheon PLC, a leading provider of stage-gate project development software; and Beyond Benign, the non-profit arm of the Warner-Babcock Institute for Green Chemistry. It is being provided for free and without restriction to any and all potential users.

* Anastas and Warner, Green Chemistry: Theory and Practice, 1998, Oxford University Press

Sign in to iSUSTAIN

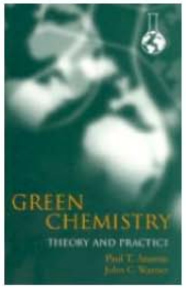
Email

Password

Sign in or Register

Forgot password? Click here

Based on the Book:



Green Chemistry: Theory and Practice

by Paul T. Anastas and John C. Warner

iSUSTAIN is brought to you by:

The Index – Scenarios

Getting Started | Scenarios | Data Input | My Profile | Log Out

Scenarios

Isopropyl Lactate (Sample Scenario)

Actions	Scenario Name	Description	Last Modified
	Isopropyl Lactate (Sample Scenario)	Organic Syntheses Collective Volume 2, Pg. 365, John Wiley & Sons, Inc., NY, 1943	3/3/2010
	What-if Scenario A		3/3/2010
	Research Project 123		3/3/2010
	Development Project XYZ		3/3/2010
	Product ABC		3/3/2010

Add New Scenario Add Sample Scenario

- To use the iSUSTAIN™ Index, the user generates a scenario
- The scenario contains information on
  - The materials going into a process (the BOM In)
  - The materials out of a process (the BOM Out)
  - The conditions used for the various steps in a process (the Process Steps)
- Several alternative scenarios can be generated for the same product/process to see the effect on the overall sustainability score

The Index – Metrics

The Twelve Principles of Green Chemistry

1	Waste Prevention	90
2	Atom Economy	90
3	Safe Raw Materials	60
4	Safe Product	75
5	Safe Solvents	80
6	Energy Efficiency	65
7	Renewables	35
8	Process Complexity	60
9	Catalysis	100
10	Biodegradability	0
11	Process Control	80
12	Safe Process	80

- The Index has a metric for each of the Twelve Principles of Green Chemistry
  - Each metric uses the information in the scenario to generate a score
  - All scores are scaled between zero (the lowest) and 100 (the best)
  - These scores quickly point out the areas in most need of improvement
- Information on over 4,200 raw materials is currently provided in the Index Raw Materials database
  - A request to add a raw material not in the database can be made to Beyond Benign
    - A small fee will be charged for this

Remember: Sustainability is relative – a process isn't inherently Green, but it can be made Greener

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iSUSTAIN™ Green Chemistry Index

The Index – Metric 1

Waste Prevention

Isopropyl Lactate (Sample Scenario)

1 ***It is better to prevent waste then to treat or clean up waste after it is formed.***

DEFINITION

Wastes are assigned to severity classes (see chart). The E^{+}-factor is the sum of each weight of generated waste times its severity class, all divided by the total weight of the end product (on a neat basis – diluents not included in the weight of the final product). It is a useful tool for rapid evaluation of processes based on overall generated waste. Wastes that are used elsewhere to derive some benefit (burning to produce power, byproduct synergy – used as a raw material in another process) are not counted as wastes herein.

Severity Class & Environmental Fate	Severity Multiplier
1 - (Semi) Solid Hazardous Waste Land Disposal/Containment	10
2 - (Semi) Solid Hazardous Waste Incineration	4
3 - (Semi) Solid Non-Hazardous Waste Landfill	2
4 - Waste Water (appropriate to send to treatment plant)	0.5

	Bill of Materials Out	Type of Material	Wt/Batch	% Diluents	Severity Multiplier	Wt times Severity	
	Isopropyl lactate	Product	360	50			
	Azeotrope water	Waste Class 4	24.5		0.5	12	
	Sodium sulfate filter solids	Waste Class 3	13.3		2.0	26	
	Reactors wash	Waste Class 2	129		4.0	516	

Add New

$$E^{+}\text{-Factor (Environmental factor)} = \frac{\Sigma_i (Wt\ Waste_i)(Severity\ Waste_i)}{(Wt.Desired\ Product)(1\text{-}\%\ Diluents/100)} = \mathbf{3.08}$$

Normalized E^{+}-Factor = **70**

The Index – Metric 3

Less Hazardous Chemical Synthesis

Isopropyl Lactate (Sample Scenario)

3 ***Whenever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.***

DEFINITION

Based on available safety, health and environmental information (currently, European Risk Phrases are used), scorings for these impacts and regulatory status for many common raw materials have been developed and provided as available in the iSUSTAIN™ Raw Material database. These separate scorings are combined into a single Raw Material Impact number for each material according to the formula [(Regulatory Status) * (Safety + Health + Environmental Impact)/3/100], which in turn are combined for all of the raw materials in the process according to the equation below to give a final Total Process Raw Material Impact score. If a portion of a material is recycled, then that portion is not counted in this tally. Note that the "% of Total" column is an indication of the relative contribution of each component to the overall process total.

	Bill of Materials In	Type of Material*	Wt/Batch	Est. % Recycle	% Renew.	Catalyst Mole %	Safety	Health	Envir Impact	Regul Status	MatImp	% of Total	
	Lactic acid [2-hydroxy propionic acid]	Raw	212	20	100	0	100	55	100	100	85	32	
	Isopropanol	Raw	450	80	0	0	55	80	100	100	78	17	

Add New

Total Process Raw Material Impact $= \dfrac{\Sigma_i(MatImp_i)(Wt\ Raw\ Material_i)(100\text{-}\%\ Recycle_i)}{\Sigma_i(Wt\ Raw\ Material_i)(100\text{-}\%\ Recycle_i)} =$ **85**

The Raw Materials Database

- Currently loaded with over 4,200 compounds
  - These materials have scores associated with their Safety, Health, Environmental Impact and Regulatory Status
- Materials Scoring
  - Based on the 126 European Risk Phrase
    - R5 Heating may cause an explosion
    - R35 Causes severe burns
    - R51 Toxic to aquatic organisms
    - R14/15 Reacts violently with water, liberating extremely flammable gases
  - These phrases can be divided into safety, health and environmental categories
  - Each Risk Phrase is given a weighting factor based on its severity
  - For any particular material, its Safety, Health and Environmental Impact scores are determined by the weighting factors for the Risk Phrases assigned to it.
  - The Regulatory Status score is determined by a material's presence or absence on a consolidated regulatory listing of governmental lists of materials of concern (e.g., REACH SIN list and EPA Tri PBT list)

The Raw Materials Database

- Beyond Benign administers the Raw Material Database
  - New materials can be added by users upon request for a nominal fee
  - The ability for subscribers to the iSUSTAIN™ Index to designate materials they add as proprietary will be built into the system in the next upgrade
- Beyond Benign will also lead an Advisory Board of users that will propose changes and/or additions to the Index tool
  - Also under the purview of this Board will be changes to the European Risk Phrase weighting factors, changes to the scoring algorithms and/or changes to the data used for scoring, allowing the Raw Materials database to evolve as more detailed LCA information becomes available for materials
- It is the intent of the Alliance to make the Raw Materials database fully available to the public in the near future

The Index – Metric 6

Design for Energy Efficiency

Isopropyl Lactate (SAMPLE SCENARIO)

6 ***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.***

▼ DEFINITION

Energy Efficiency (EE) roughly accounts for energy usage during heating and cooling and for application of high pressure or vacuum. This has to be assessed for each step of an overall process. Cooling is more costly energetically than heating, but either cooling or heating outside of the range provided by typical equipment becomes quite costly. This is captured in the Temperature Factor table below. This factor is summed with a pressure contribution (high or low pressure) and then multiplied by the average time for application of the temperature, total weight of materials and approximate average heat capacity for each process step, all of which is then divided by the total product weight (diluents included) as in the equation below.

Temperature Ranges (°C)	Temperature Factor (f_T)
< -20	5
-20 to 0 (technical cooling)	3
0 to 10 (ice cooling)	2
10 to 20 (water cooling)	1
20 to 30 (room temperature)	0
30 to 90 (hot water heating)	1
90 to 160 (steam heating)	2
160 to 280 (hot oil or electrical heating)	3
> 280	5

$$\text{Step EE (Energy Efficiency)} = \frac{(f_T + |1\text{-}Pressure(atm)|) * time\ (hrs) * Weight * Heat\ Capacity\ (J/gm{\cdot}°K)}{Wt\ Desired\ Product}$$

	Step	Process Steps	Temp. (deg C)	Time (Hrs)	Pressure (Atm)	Total Weight	Avg. Heat Capacity	Step EE	
	Step 1	Charge reagents and heat-up	80	1	1	1545	2	8.58	
	Step 2	Heat and separate water azeotropically	85	6	1	1521	2	55.77	

	Bill of Materials Out	Type of Material	Wt/Batch	% Diluents	
	Isopropyl lactate	Product	360	50	

Total EE (Energy Efficiency) = $\sum_i Step\ EE_i$ = **77**

Normalized Total EE = **75**

The Index – Metric 7

Renewable Feedstock

Isopropyl Lactate (Sample Scenario)

7 ***A raw material or feedstock should be renewable rather than depleting whenever technically and economically practical.***

DEFINITION

A renewable raw material (RRM) is a raw material from a renewable natural resource. A natural resource qualifies as a renewable resource if it is replenished by natural processes of growth at a rate comparable to or greater than its rate of consumption.

The content of RRM's in a final product is calculated two ways: 1) taking all materials that end up in the product as-sold (raw materials and diluents) and using the full product weight and 2) based on active ingredient, e.g. resin solids or non-volatile materials, meaning on a neat basis (excluding diluents) and multiplying the product weight by (1-% Diluents/100). Water is considered a 100% renewable material.

	Bill of Materials In	Type of Material	Wt/Batch	Est. % Recycle	% Renew.	Catalyst Mole %	% of Total	
	Lactic acid [2-hydroxy propionic acid]	Raw	212	20	100	0	32	
	Isopropanol	Raw	450	80	0	0	17	
	Isopropanol	Diluent	180	0	0	0	34	

Add New

	Bill of Materials Out	Type of Material	Wt/Batch	% Diluents	
	Isopropyl lactate	Product	360	50	

% RRM (as sold basis) - includes diluents $= \frac{\sum_i (Wt\ RRM_i)(1\text{-}\%\ Recycle_i/100)(\%\ Renewable_i)}{Wt\ Product} =$ **45**

% RRM (neat basis) - excludes diluents $= \frac{\sum_i (Wt\ RRM_i)(1\text{-}\%\ Recycle_i/100)(\%\ Renewable_i)}{(Wt\ Product)(1\text{-}\%\ Diluents/100)} =$ **95**

The Index – Metric 12

Safer Chemistry for Accident Prevention

Isopropyl Lactate (Sample Scenario)

(12) *Substance 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.*

Question		Risk	Answer	Points
1.	Are any extreme conditions (pressure ≥ 10 atm., temperature ≥ 200º C. or ≤ -78º C.) used in the process? (20 pts)	High	○ Yes ◉ No	0
2.	Does the potential exist for a runaway exotherm under the process or upset conditions (including violent polymerization)? (20 pts)	High	○ Yes ◉ No	0
3.	Do any of the process materials or mixtures present an explosion hazard (contact, dust and/or peroxide-forming)? (20 pts)	High	○ Yes ◉ No	0
4.	Are there any process materials present initially or formed during this process that might restrict or exclude its use in the intended production facility (other high hazards than mentioned above, strong odor, etc.)? (20 pts)	High	◉ Yes ○ No	20
5.	Is pressure between 1.0 and 10 atm or less than 20 mm of Hg used in this process? (10 pts)	Moderate	○ Yes ◉ No	0
6.	Are temperatures between 150º C. and 200º C. or between -50º C. and -78º C. used in this process? (10 pts)	Moderate	○ Yes ◉ No	0
7.	Is the reaction mixture flammable? (10 pts)	Moderate	◉ Yes ○ No	10
8.	Are any of the process mixtures pyrophoric? (10 pts)	Moderate	○ Yes ◉ No	0
9.	Do any of the process mixtures react violently with water? (5 pts)	Mild	○ Yes ◉ No	0
10.	Is a gas generated in any part of this process? (5 pts)	Mild	◉ Yes ○ No	5
11.	Are any of the process mixtures corrosive (pH ≤ 2 or ≥12)? (5 pts)	Mild	○ Yes ◉ No	0
12.	Are any of the process mixtures irritants or lachrymators? (5 pts)	Mild	○ Yes ◉ No	0

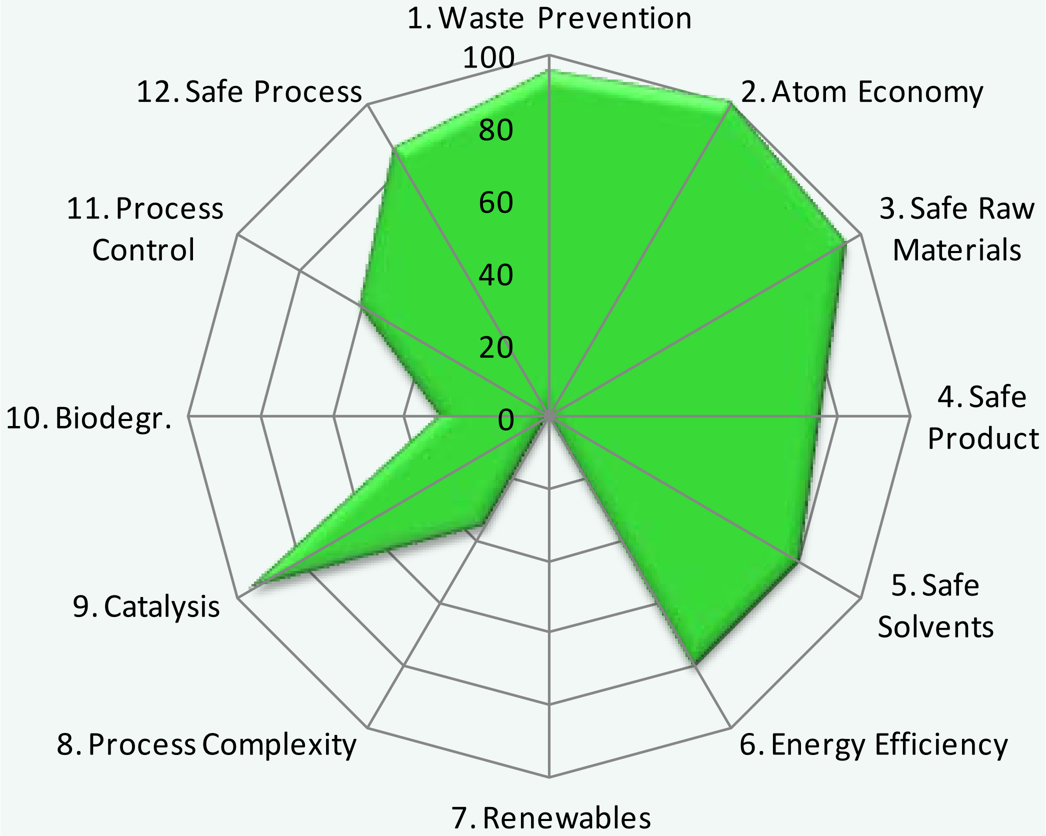
Total Yes answer points = **35**

Safer Chemistry Score = 100 - Total Points = **65**

The Index – Results

Product Improvement

Metric	Product A
1. Waste Prevention	95
2. Atom Economy	100
3. Safe Raw Materials	95
4. Safe Product	75
5. Safe Solvents	80
6. Energy Efficiency	80
7. Renewables	0
8. Process Complexity	35
9. Catalysis	95
10. Biodegradability	30
11. Process Control	60
12. Safe Process	85

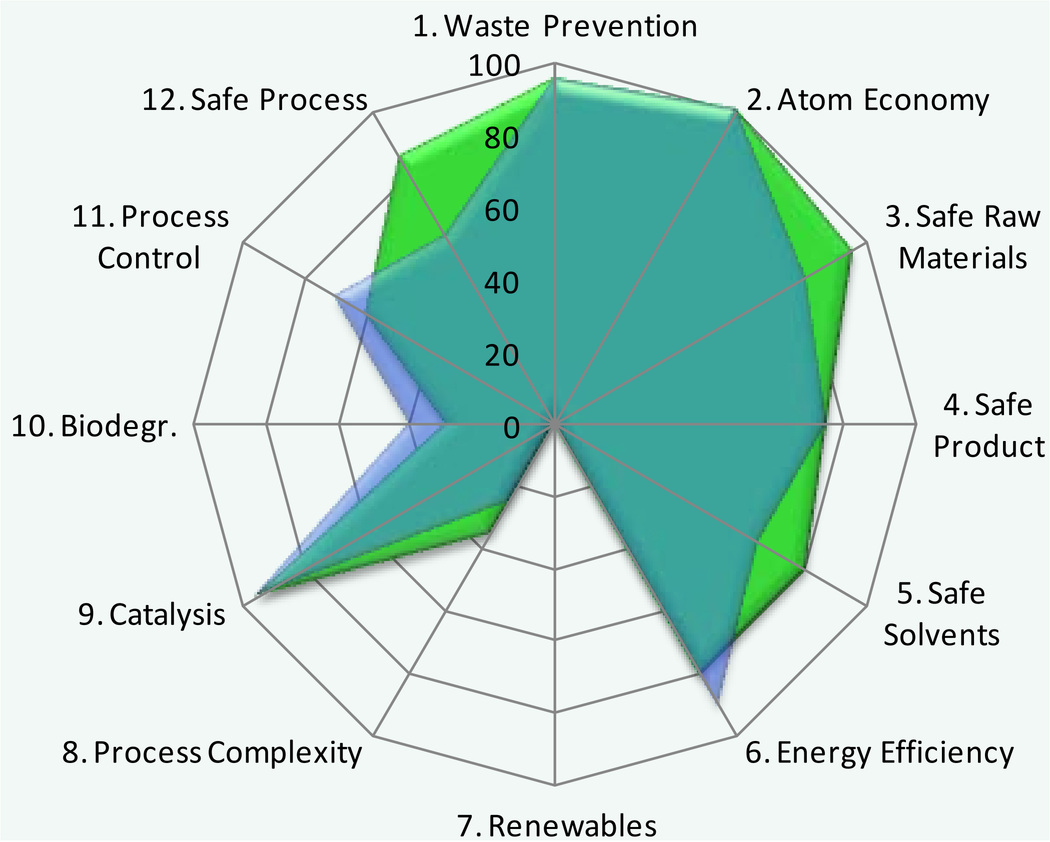


Quickly points out the areas most in need of improvement

The Index – Results

Product Comparison

Metric	Product A	Product B
1. Waste Prevention	95	95
2. Atom Economy	100	100
3. Safe Raw Materials	95	80
4. Safe Product	75	75
5. Safe Solvents	80	65
6. Energy Efficiency	80	90
7. Renewables	0	0
8. Process Complexity	35	25
9. Catalysis	95	95
10. Biodegradability	30	40
11. Process Control	60	70
12. Safe Process	85	60



Clear graphical assessment of which is the greener product

Resources

- To learn more about the iSUSTAIN™ Index:
  - Go to the web site at www.isustain.com to use the Index or become a subscriber
  - For information about the Raw Materials database and services offered by Beyond Benign, use the links on the iSUSTAIN™ web site

FAQ's

Q. Of what potential value is the iSUSTAIN™ Index to commercial users?

A. Most companies are being asked for information on sustainability by their customers. The iSUSTAIN Green Chemistry Index provides a consistent and clearly defined language to use.

Q. Can users of the iSUSTAIN™ Index be assured of the security of their proprietary information?

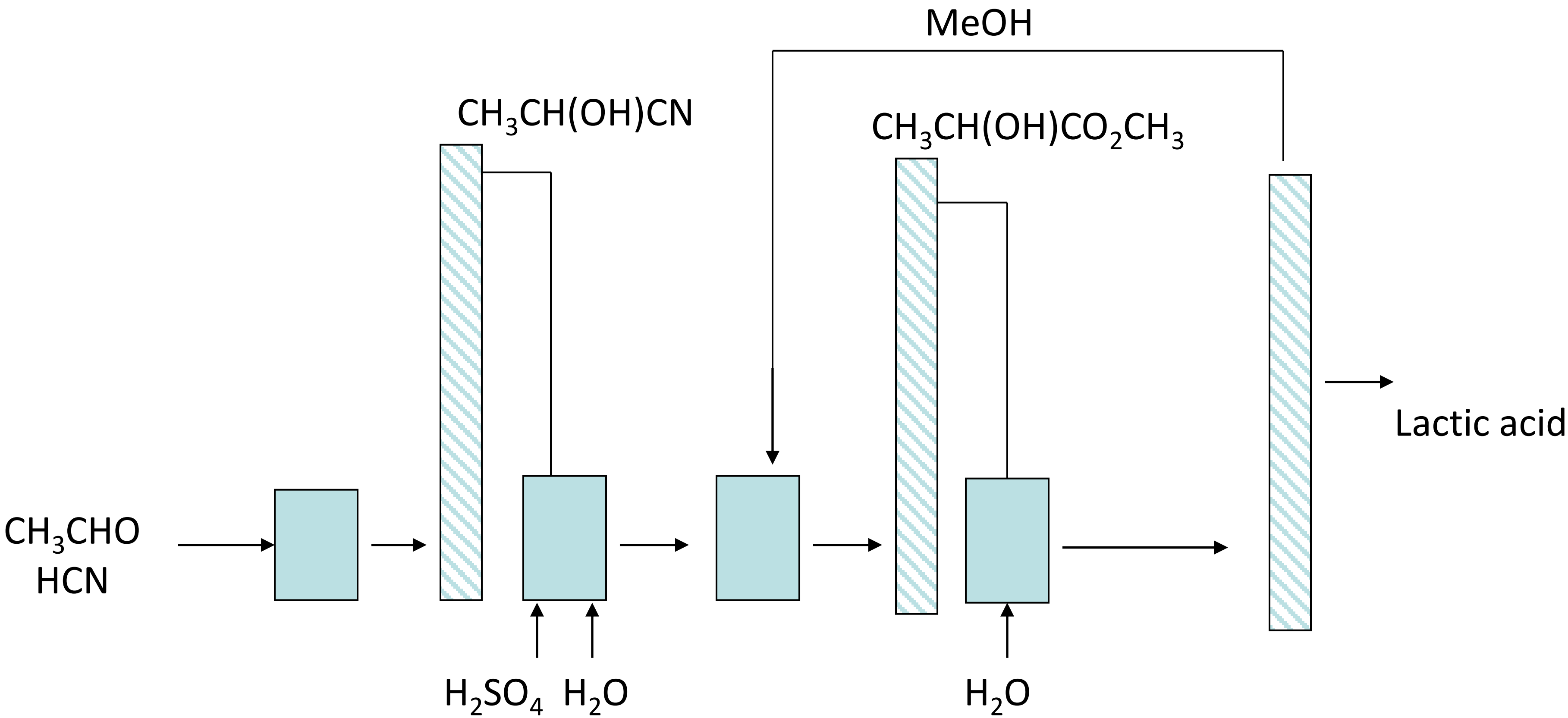
A. Definitely. Each user is given a secure directory space accessible only to them. Sopheon uses the latest industry-standard measures to safeguard the security of that information.

Q. Are Scores from the Index meant to be used externally?

A. The main intent and design of the Index is for internal use within an organization to drive continuous improvement towards greener processes.

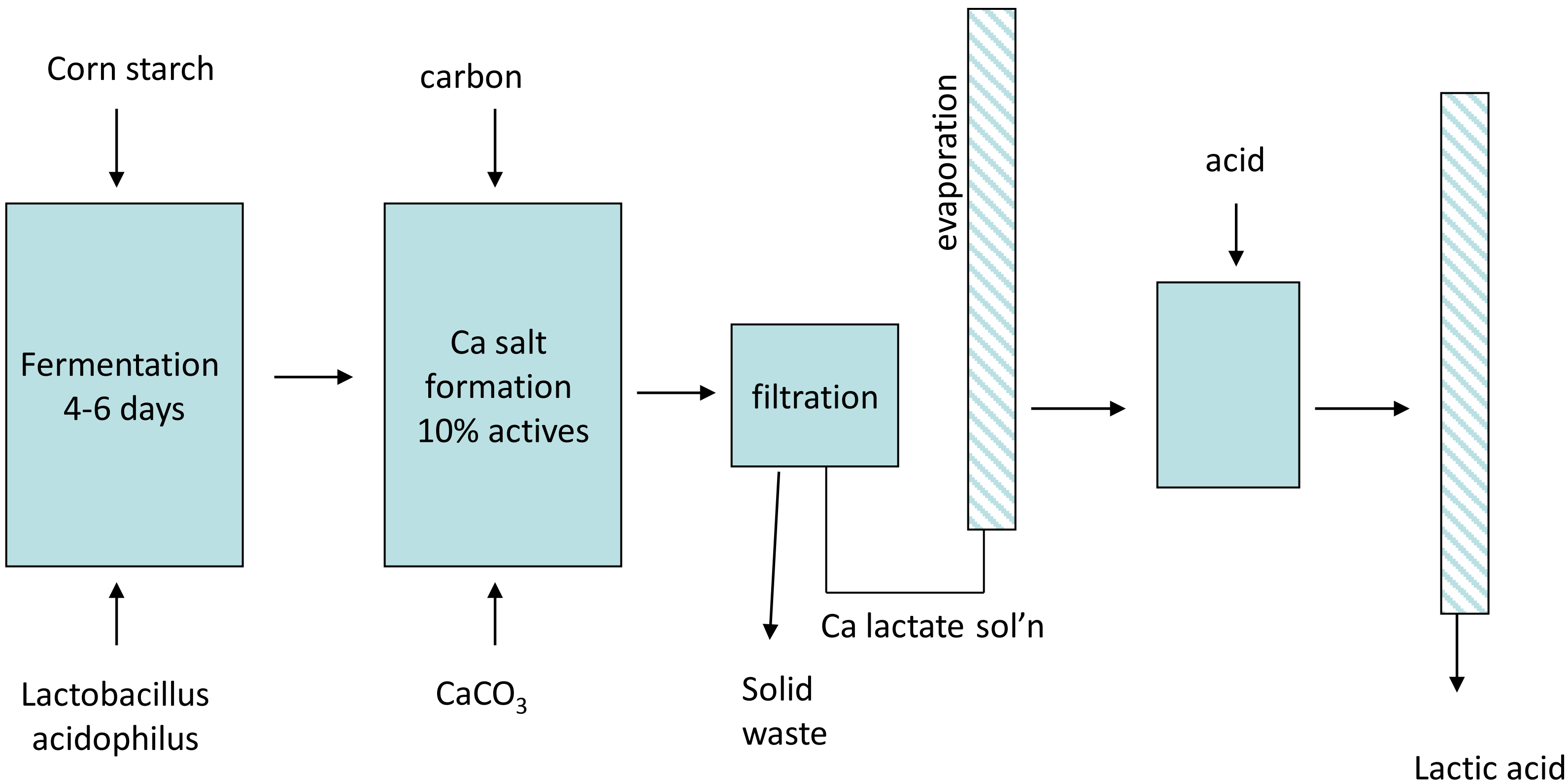
However, the iSUSTAIN™ Index is being released complete with a certification process, whereby Beyond Benign, an internationally recognized non-profit third party will certify upon request that the information contained in an iSUSTAIN™ Index scenario conforms to appropriate standards and procedures.

Lactic Acid Production: Chemical route



$(NH_4)_2SO_4$ by-product
Extremely high purity product
3 distillation steps

Lactic Acid Production: Fermentation route

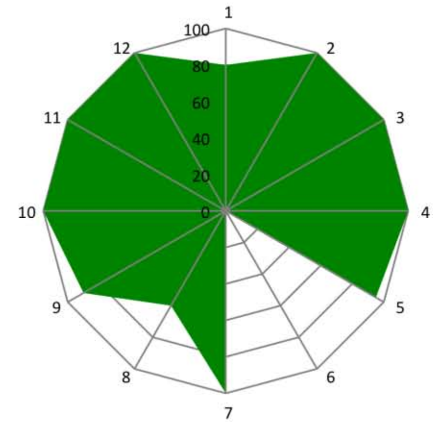


Renewable feedstocks
Amt of product per unit of reactor volume is low (Ca lactate 10%)
Evaporation step
Solid waste, calcium sulfate waste

Scenario: **Lactic Acid: Fermentation Route**
Description: Based on industrial process of production of lactic acid from glucose fermentation

User: **Amy Cannon**
Exported: **4/23/2010**

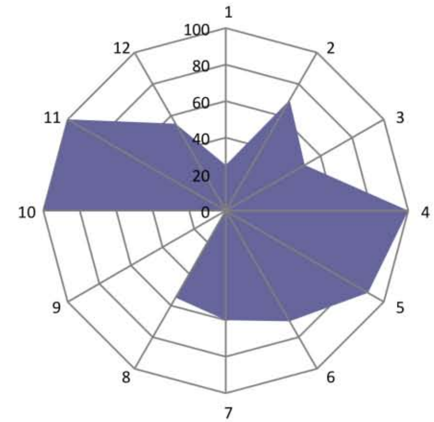
1. Waste Prevention	80
2. Atom Economy	100
3. Safe Raw Materials	100
4. Safe Product	100
5. Safe Solvents	95
6. Energy Efficiency	0
7. Renewables	100
8. Process Complexity	60
9. Catalysis	90
10. Biodegradability	100
11. Process Control	100
12. Safe Process	100



Scenario: **Lactic Acid: Chemical Route**
Description: Based on actual 7 step chemical route to lactic acid. Some assumptions made: pressure/temperature conditions, % conversion

User: **Amy Cannon**
Exported: **4/23/2010**

1. Waste Prevention	25
2. Atom Economy	70
3. Safe Raw Materials	50
4. Safe Product	100
5. Safe Solvents	90
6. Energy Efficiency	70
7. Renewables	60
8. Process Complexity	55
9. Catalysis	0
10. Biodegradability	100
11. Process Control	100
12. Safe Process	55



iSUSTAIN™ Green Chemistry Index

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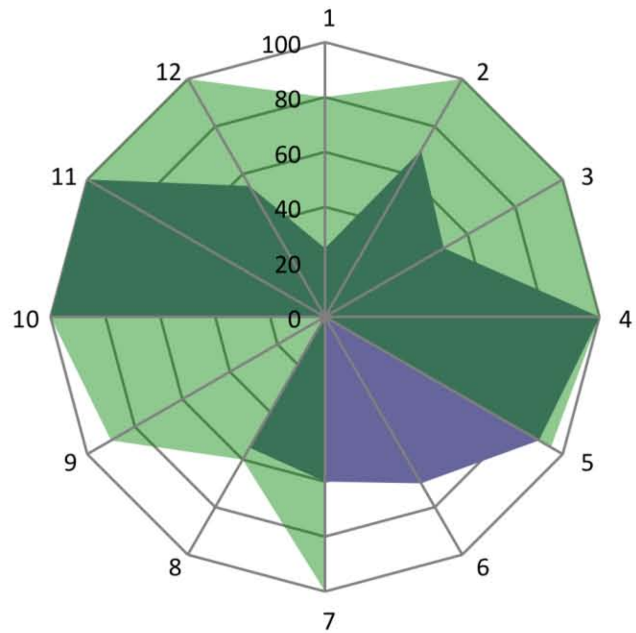
Scenario: **Lactic Acid: Chemical Route**

Description: Based on actual 7 step chemical route to lactic acid. Some assumptions made: pressure/temperature conditions, % conversion

User: **Amy Cannon**

Exported: **4/23/2010**

	Chemical	Fermentation
1. Waste Prevention	25	80
2. Atom Economy	70	100
3. Safe Raw Materials	50	100
4. Safe Product	100	100
5. Safe Solvents	90	95
6. Energy Efficiency	70	0
7. Renewables	60	100
8. Process Complexity	55	60
9. Catalysis	0	90
10. Biodegradability	100	100
11. Process Control	100	100
12. Safe Process	55	100



For more information:

www.isustain.com

Amy_Cannon@beyondbenign.org

http://www.beyondbenign.org/isustain/isustain.html