About OMICS Group

OMICS Group International is an amalgamation of Open Access publications and worldwide international science conferences and events. Established in the year 2007 with the sole aim of making the information on Sciences and technology 'Open Access', OMICS Group publishes 400 online open access scholarly journals in all aspects of Science, Engineering, Management and Technology journals. OMICS Group has been instrumental in taking the knowledge on Science & technology to the doorsteps of ordinary men and women. Research Scholars, Students, Libraries, Educational Institutions, Research centers and the industry are main stakeholders that benefitted greatly from this knowledge dissemination. OMICS Group also organizes 300 International conferences annually across the globe, where knowledge transfer takes place through debates, round table discussions, poster presentations, workshops, symposia and exhibitions.

About OMICS Group Conferences

OMICS Group International is a pioneer and leading science event organizer, which publishes around 400 open access journals and conducts over 300 Medical, Clinical, Engineering, Life Sciences, Phrama scientific conferences all over the globe annually with the support of more than 1000 scientific associations and 30,000 editorial board members and 3.5 million followers to its credit.

OMICS Group has organized 500 conferences, workshops and national symposiums across the major cities including San Francisco, Las Vegas, San Antonio, Omaha, Orlando, Raleigh, Santa Clara, Chicago, Philadelphia, Baltimore, United Kingdom, Valencia, Dubai, Beijing, Hyderabad, Bengaluru and Mumbai.

Finding the innovation in green chemistry/engineering

John A. Glaser
National Risk Management Research Laboratory
Cincinnati, OH 45268

International Summit on the Past and Present Research Systems of Green Chemistry
Philadelphia, PA

August 25-27, 2014

Innovation

- **Sustainability – meeting the needs of current generations without sacrificing the ability to meet the needs of future generations**
- **Green chemistry – transformative framework**

Guidance

"Green chemistry and engineering seek to maximize efficiency and minimize health and environmental hazards throughout the chemical production process"

Annu Rev Environ Resour 2011

Innovation

- **Clearly, innovation is recognized in the eye of the beholder.**
- **Perspective and context dominate the selection of features related to innovation.**
- **Where innovation is associated with green chemistry/engineering there are limited tools to evaluate the achievement.**
- **Contextually, innovation is a process involving idea formation, evaluation, selection, development of technology designed to provide new or improved products with a reduced environmental footprint.**

Objective

- **Green chemistry/engineering is seen as a leading force directing chemical synthesis and production to the innovative design of processes having features sustaining the environment.**
- **Can the accomplishments of green chemistry/engineering be evaluated in light of the guiding principles to find where innovative success has been attained?**

Why different metrics?

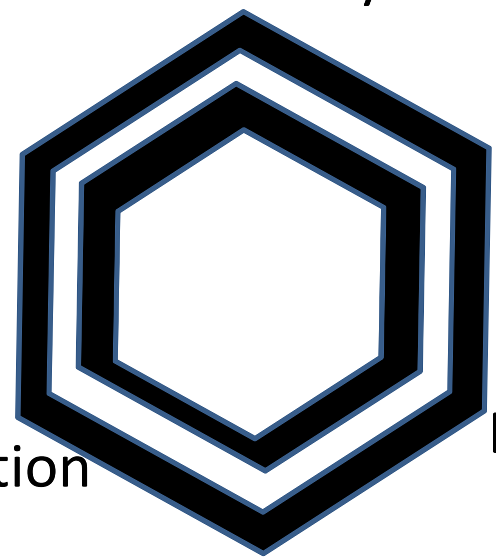
- **Discern the sources of green chemistry/engineering innovations.**
- **Guide the search for new green technology opportunities.**
- **Evaluate the importance of green chemistry/engineering principles to innovation.**

Innovation and the Environment

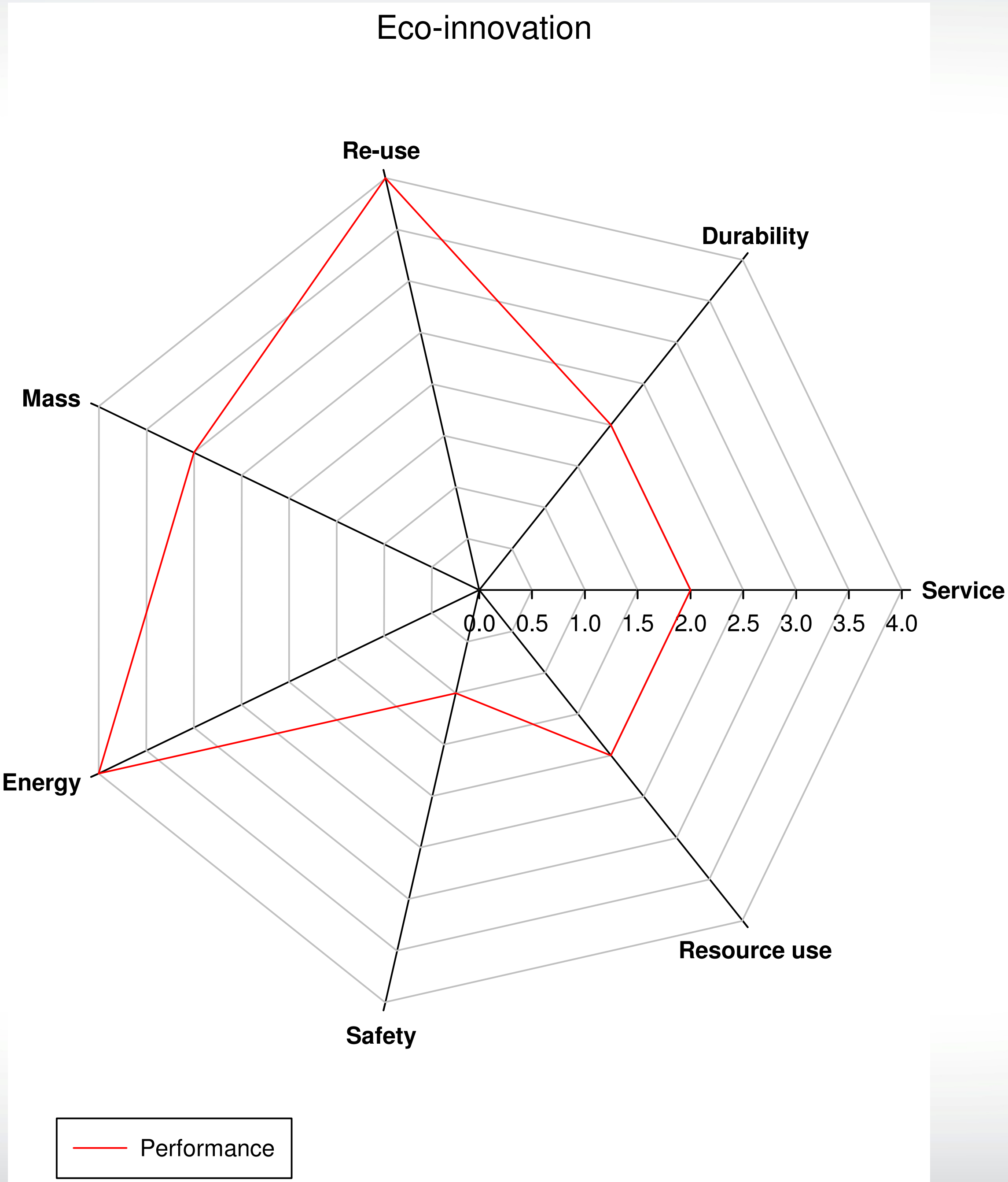
- **Emission cost reduction**
- **Innovation cost and benefits**
- **Policy influence**
  - **Technology progress**
  - **Environmental management**
  - **Innovation induction**
  - **Self regulation**

Worldwatch Institute 2008 *Innovations and the Environment*

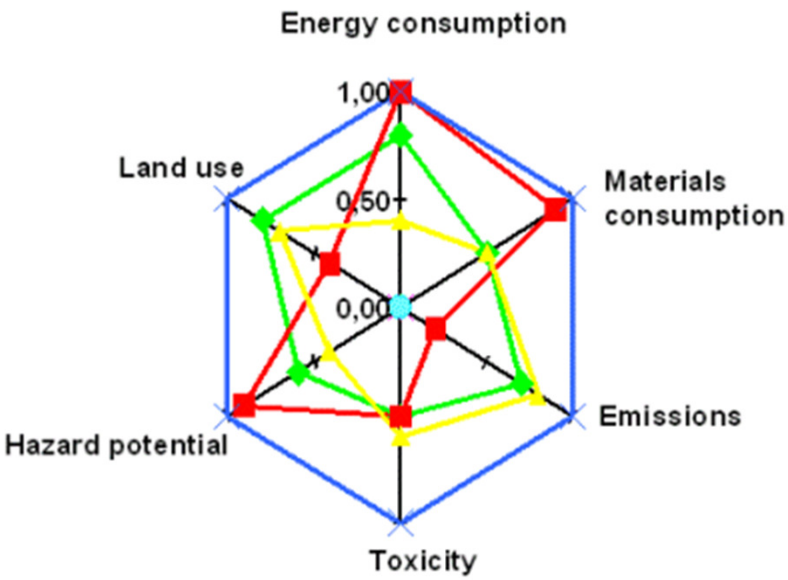
Eco-compass Driving Eco-innovation



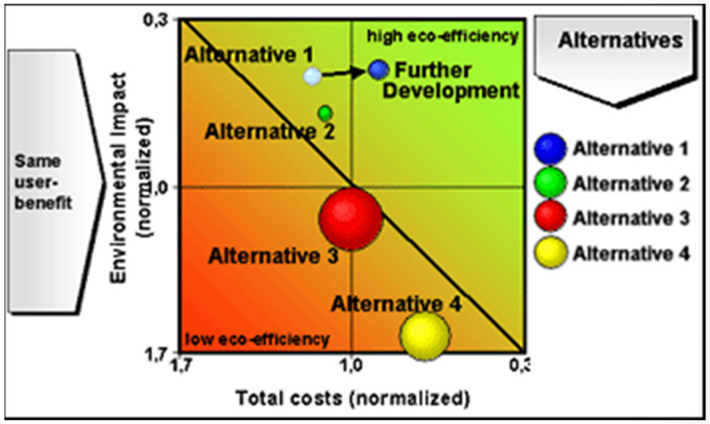
1996 Driving Eco-Innovation


Eco-innovation
Re-use
Durability
Service
Resource use
Safety
Energy
Mass
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
Performance

BASF Ecological Fingerprint



Eco-efficiency portfolio



Green Principles

Twelve Principles of Green Chemistry

Prevention

Atom Economy

Less Hazardous Chemical Syntheses

Designing Safer Chemicals

Safer Solvents and Auxiliaries

Design for Energy Efficiency

Use of Renewable Feedstocks

Reduce Derivatives

Catalysis

Design for Degradation

Real-time analysis for Pollution Prevention

Inherently Safer Chemistry for Accident Prevention

Twelve Principles of Green Engineering

Inherent Rather Than Circumstantial

Prevention Instead of Treatment

Design for Separation

Maximize Efficiency

Output-Pulled Versus Input-Pushed

Conserve Complexity

Durability Rather Than Immortality

Meet Need, Minimize Excess

Minimize Material Diversity

Integrate Material and Energy Flows

Design for Commercial "Afterlife"

Renewable Rather Than Depleting

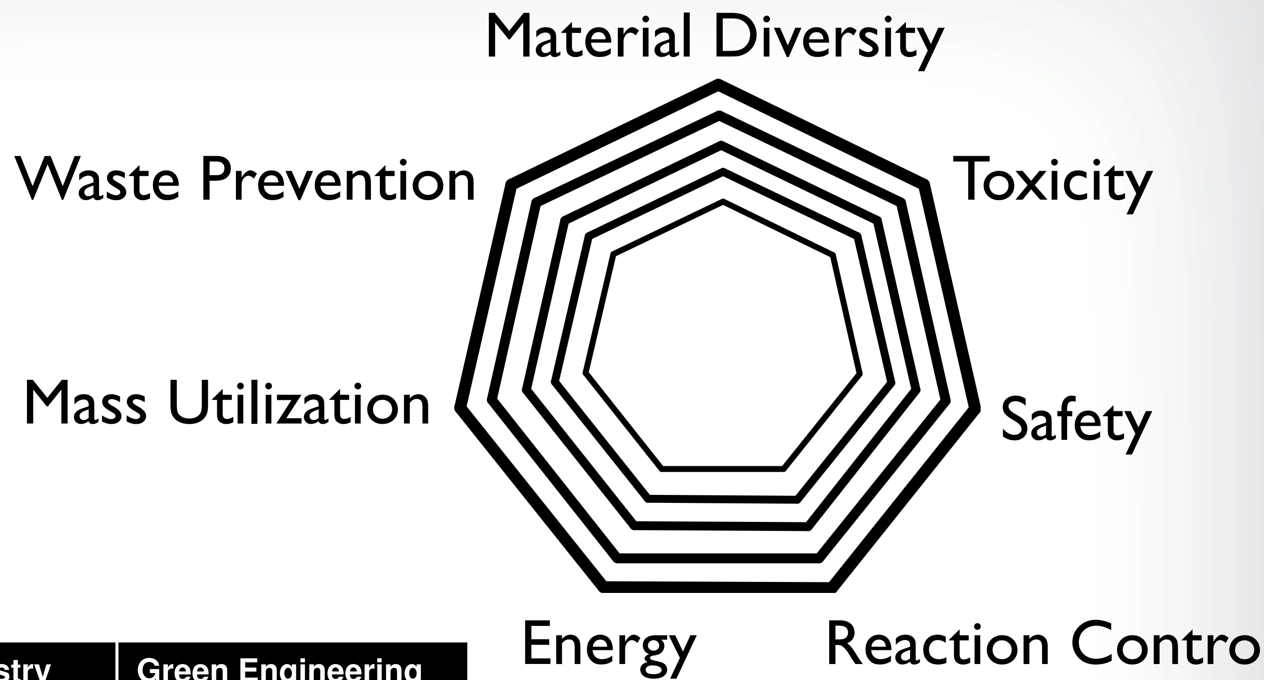
Principles Comparison

Principles of Green Chemistry

P - Prevent wastes
R - Renewable materials
O - Omit derivatization steps
D - Degradable chemical products
U - Use safe synthetic methods
C - Catalytic reagents
T - Temperature, Pressure ambient
I - In-Process Monitoring
V - Very few auxiliary substances
E - E-factor, maximize feed in product
L - Low toxicity of chemical products
Y - Yes it's safe

Principles of Green Engineering

I - Inherently non-hazardous and safe
M - Minimize material diversity
P - Prevention instead of treatment
R - Renewable material and energy inputs
O - Output-led design
V - Very simple
E - Efficient use of mass, energy, space & time
M - Meet the need
E - Easy to separate by design
N - Networks for exchange of local mass & energy
T - Test the life cycle of the design
S - Sustainability throughout product life cycle



	Green Chemistry	Green Engineering
Mass Utilization	E	M,O, E, D,T
Reaction Control	O,V,T,C	V,E
Renewable Materials	R	R
Waste Prevention	P	P,S
Safety	I,D	I
Toxicity		

Innovation Index Development from Green Chemistry/Engineering

Assessment Components

- **Material Diversity**
- **Reaction Control**
- **Mass Utilization**
- **Energy**
- **Safety**
- **Toxicity**
- **Waste Prevention**

Component Features

Mass utilization
Reduced mass intensity
Recycle options
Efficiency
Availability
Design for degradation

Reaction control
Catalysis
Derivatization control
Process Control
Process intensification
Ambient conditions

Material diversity
Mass Intensity
Recycle options
Efficiency
Availability
Design for degradatiion

Component Features

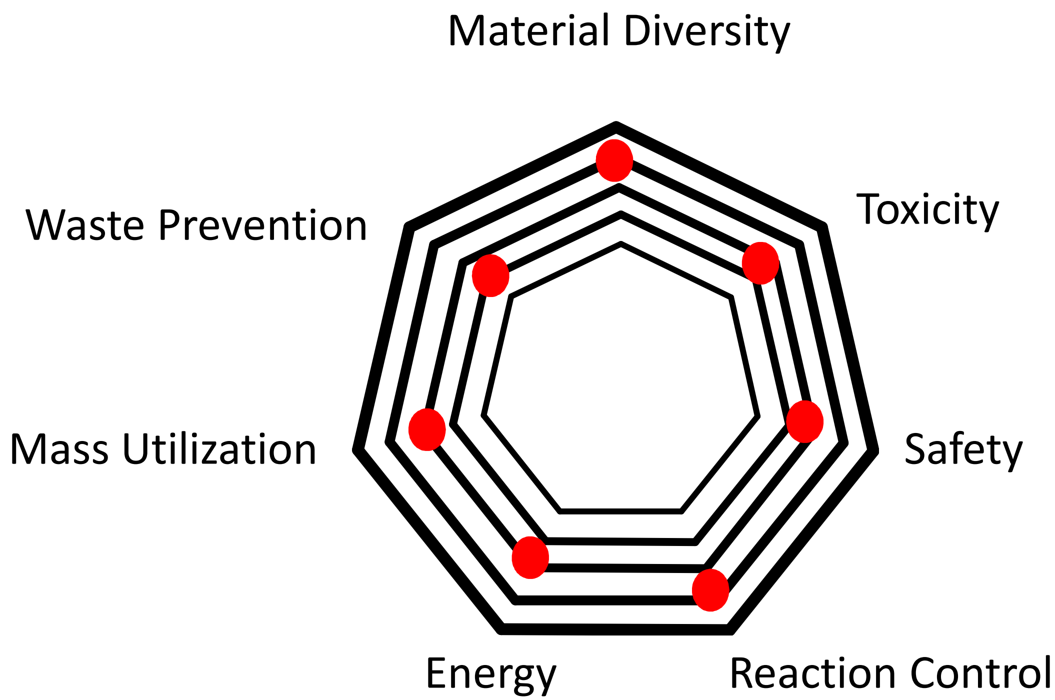
Energy
Renewable/sustainable
Recycle
Efficient
Minimization of impacts
Generation

Waste prevention
Real-time analysis
Design for degradation
Reduced footprint
Reuse
Regeneration

Toxicity
Ecotoxicity
Human health
Reduced emissions
Reduced product toxicity
No bioaccumulation

Safety
Release minimization
Accident prevention
Inherently safer product
Safe reagent/solvent use
Risk based design

Mapping Innovation



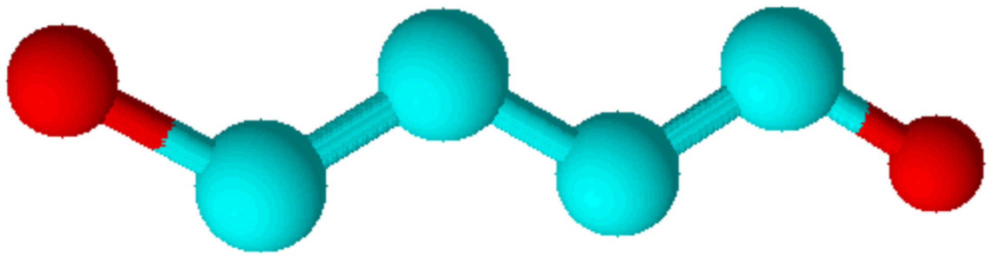
Chemicals from Renewable Feedstocks

- Sustainable chemicals
- Reduced emissions
- Reduced energy use
- Smaller footprint
- Renewable feedstock

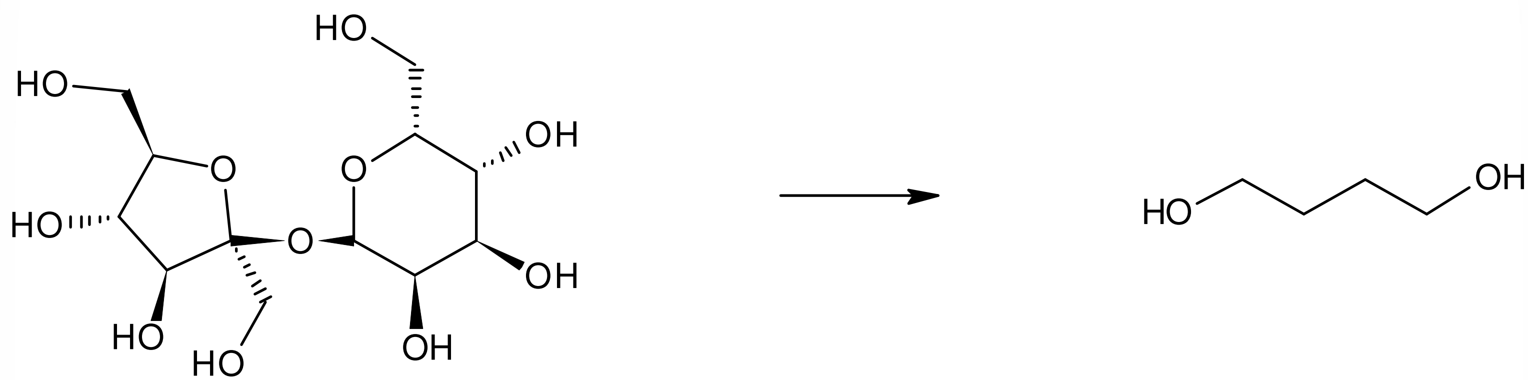
Bioprocess Industrial Chemicals

- Renewable feedstock
- Energy consumption reduction
- CO2 Sequestration
- Source pollutant reduction
- Downstream separation improvements
- Downstream conversion to environmentally attractive chemical products

- **1,4-Butanediol Genomatica**



Process Objective



sucrose

1,4-butanediol

Develop an efficient sustainable process utilizing a microorganism in fermentation to form 1,4-butanediol (BDO)

Pathway design components

- Reaction operator management
- Network calculation
- Integration with simulation software
- Pathway tracing
- Pathway ranking and analysis

Reaction operator management

- **Known chemistry and enzyme class selected or designed**
- **Enhance biopathway predictor database with addition of operators**
- **Identify secondary metabolites for each reaction operator.**

Reaction network calculation

- **Identify target compound in simulator database**
- **Constrain network size**
- **Calculate network**

Automated integration with simulation software

- Involve secondary metabolite in network reactions.
- Employ balanced reactions.
- Use thermodynamic properties to trace energy flow.
- Identify ‘known’ biochemical reactions.

EPA

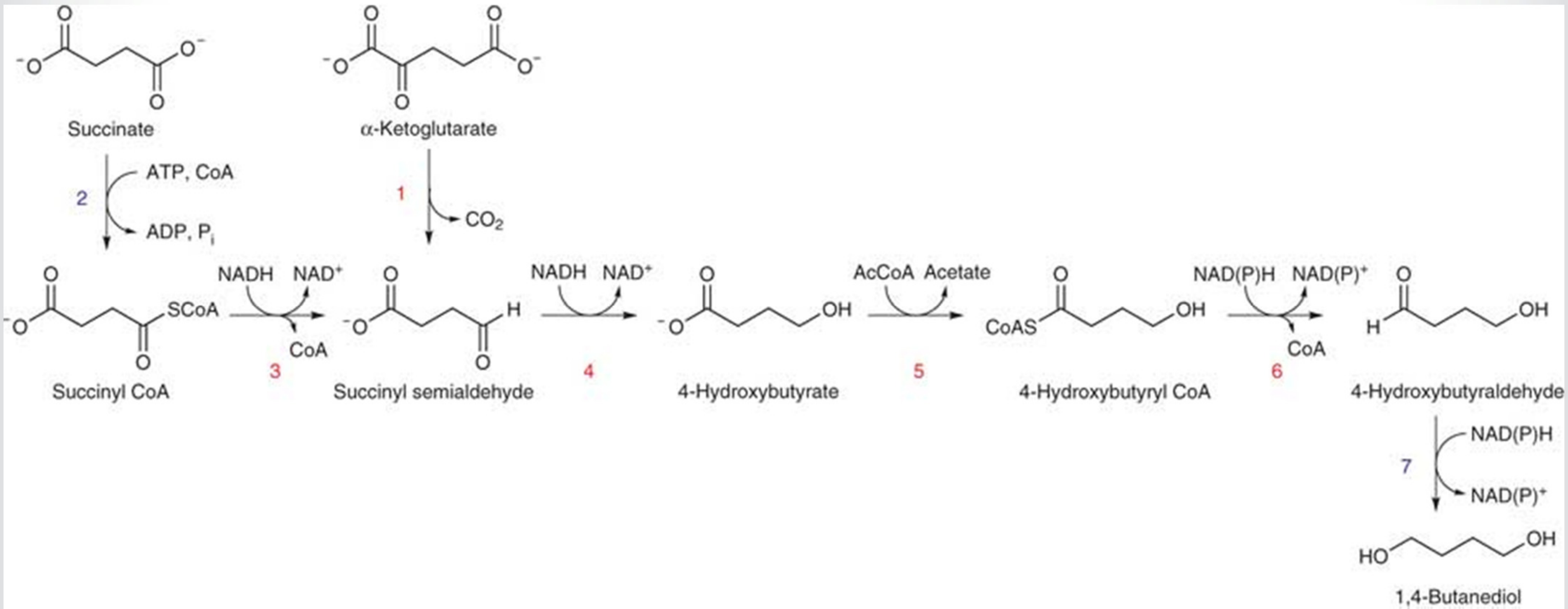
Pathway tracing

- Select starting metabolites from calculated network.
- Select maximum pathway length.
- Trace pathways involving selected starting materials to BDO.
- Thermodynamic evaluation of net reactions and pathways.

Pathway selection & analysis

- Evaluate all pathways for maximum theoretical yield according to the metabolic model.
- Rank pathways using selection criteria.
- Evaluate results in terms of yield and novel reaction steps.

Pathway introduced into *E. coli*



Pathway Development Features

- **Established a new biochemical pathway.**
- **Developed knowledge of metabolite pathways and metabolism.**
- **Developed a biopathway prediction algorithm.**
- **Model produced metabolic engineering strategies for balancing energy and redox requirement.**
- **Optimized two heterologous pathways for BDO production in *E. coli*.**
- **Renewable feedstock utilization.**

	Material Diversity
X	Mass intensity
X	Recycle options
X	Efficiency
X	Availability
	Design for degradation

	Reaction control
X	Catalysis
	Derivatization control
X	Process Control
	Process intensification
X	Ambient conditions

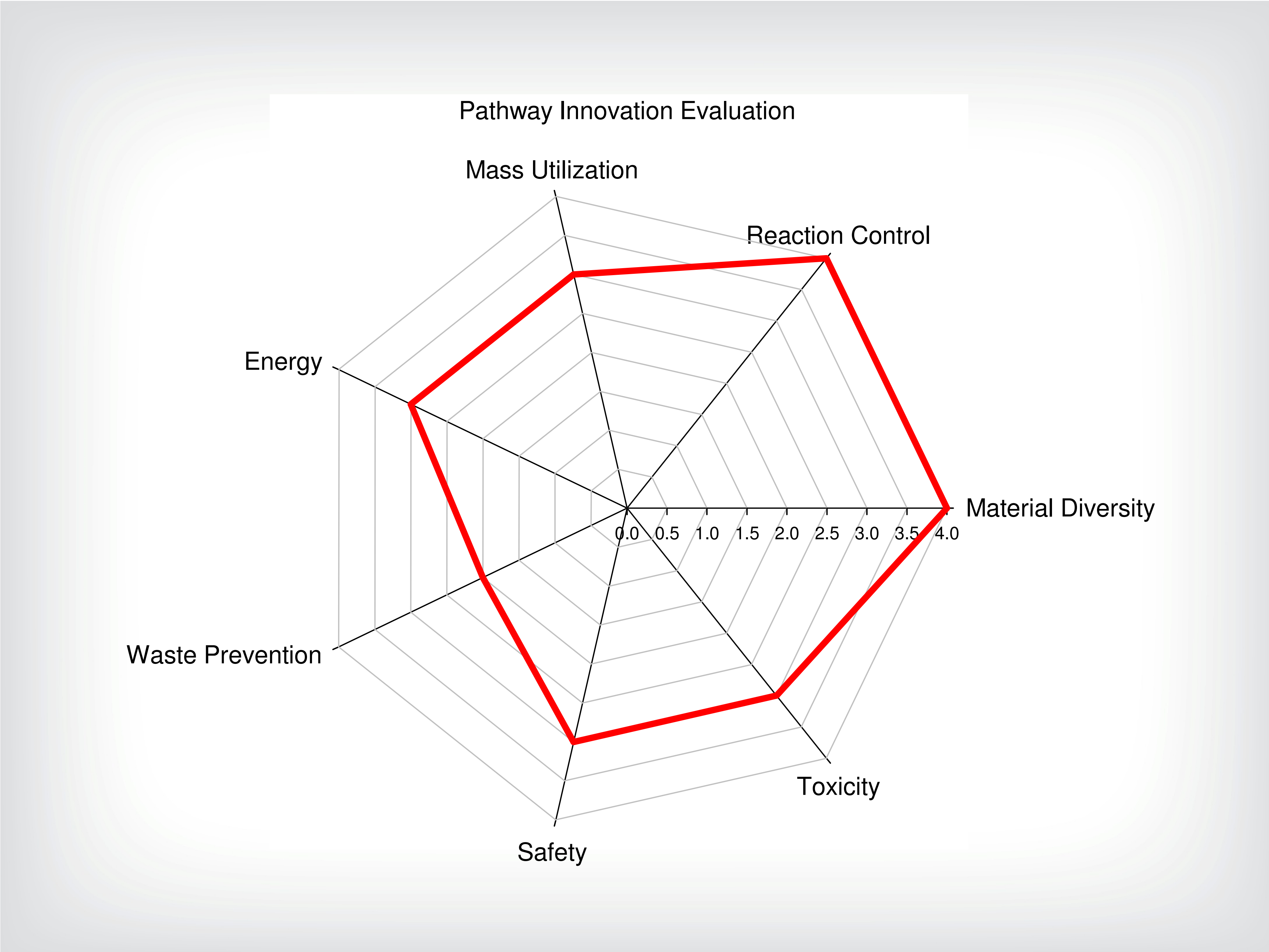
	Mass Utilization
X	Reduced mass intensity
X	Recycle options
X	Efficiency
X	Availability
	Design for degradation

	Energy
X	Renewable/sustainable
	Recycle
X	Efficient
	Min of impacts
	Generation

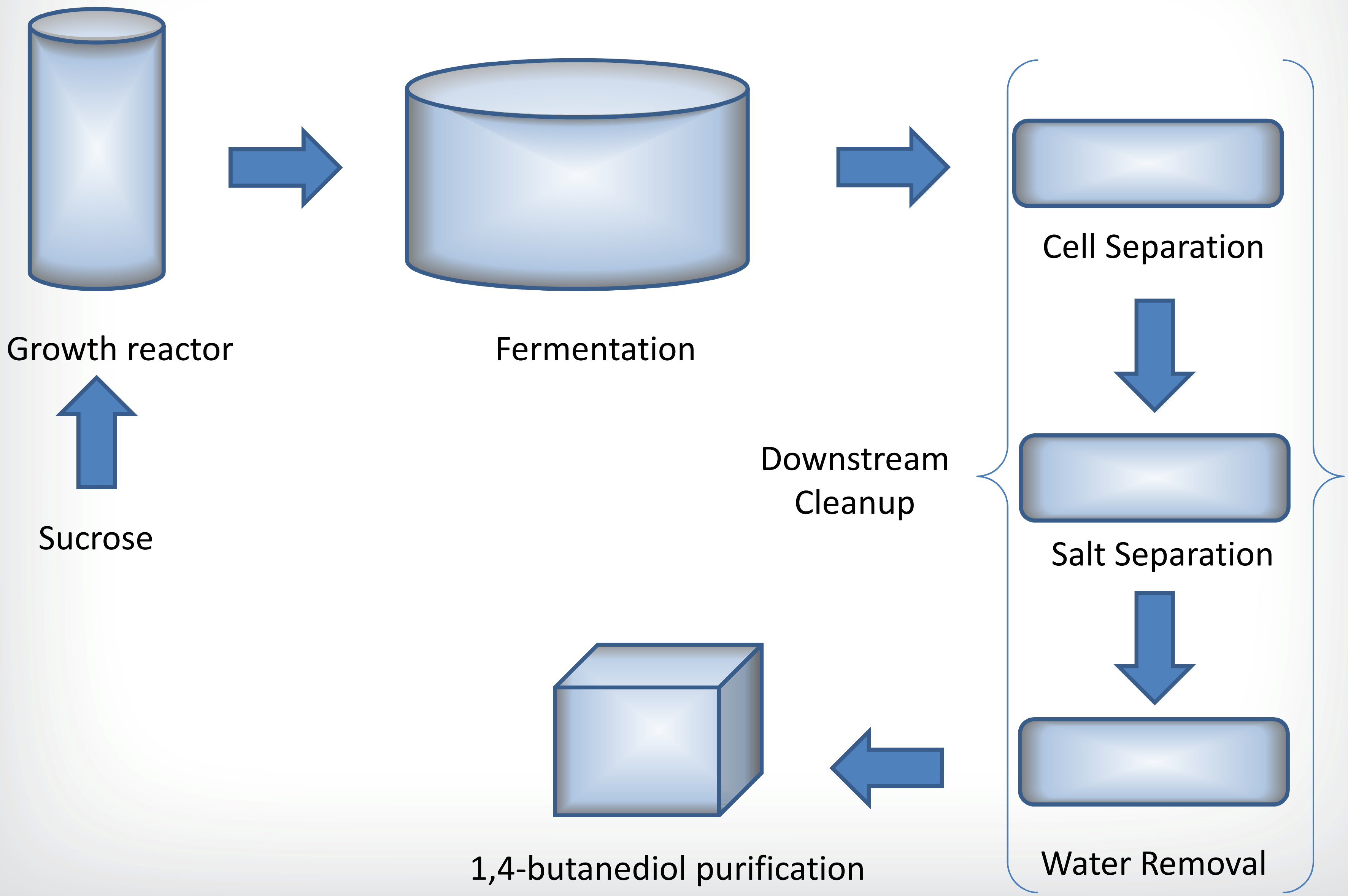
	Waste prevention
	Real-time analysis
X	Design for degradation
	Reduced footprint
X	Reuse
	Regeneration

	Safety
	Release minimization
	Accident prevention
X	Inherently safer product
X	Safe reagent/solvent use
	Risk based design

	Toxicity
X	Ecotoxicity
	Human health
	Reduced emissions
	Reduced product toxicity
X	No bioaccumulation


Pathway Innovation Evaluation
Mass Utilization
Reaction Control
Material Diversity
Toxicity
Safety
Waste Prevention
Energy
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0

BDO Process


Growth reactor
Sucrose
Fermentation
Cell Separation
Downstream
Cleanup
Salt Separation
Water Removal
1,4-butanediol purification

Process Development Features

- Designed for maximum utilization of renewable starting material.
- Credits due from coproducts of steam and energy
- Fewer unit operations.
- Smaller plant footprint.
- Processes engineered for safety.
- Recycle streams are significant to process economics.
- Low particulate emissions.
- Low GHG emissions.
- LCA analyses conducted.

	Material Diversity
X	Mass intensity
X	Recycle options
X	Efficiency
X	Availability
X	Design for degradation

	Reaction control
X	Catalysis
	Derivatization control
X	Process Control
X	Process intensification
X	Ambient conditions

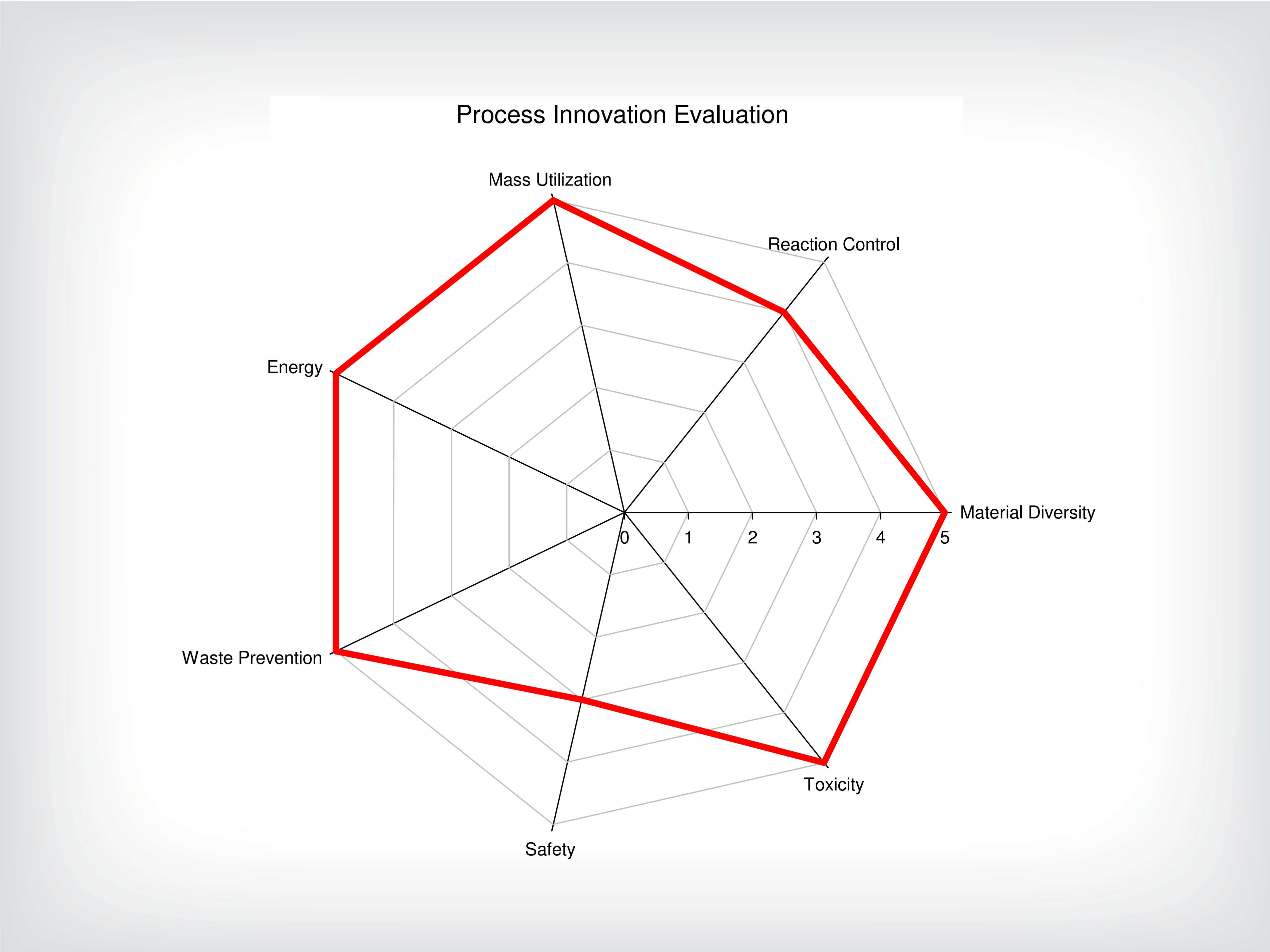
	Mass Utilization
X	Reduced mass intensity
X	Recycle options
X	Efficiency
X	Availability
X	Design for degradation

	Energy
X	Renewable/sustainable
X	Recycle
X	Efficient
X	Min of impacts
X	Generation

	Waste prevention
X	Real-time analysis
X	Design for degradation
X	Reduced footprint
X	Reuse
X	Regeneration

	Safety
X	Release minimization
X	Accident prevention
X	Inherently safer product
X	Safe reagent/solvent use
X	Risk based design

	Toxicity
X	Ecotoxicity
X	Human health
X	Reduced emissions
X	Reduced product toxicity
X	No bioaccumulation


Process Innovation Evaluation
Mass Utilization
Reaction Control
Energy
Material Diversity
Waste Prevention
Toxicity
Safety
0
1
2
3
4
5

Measuring Innovation

- **New ways to use traditional indicators**
- **New experimental indicators providing insight into new areas of devoted research.**
- **Gap and challenge measurement**
- **Supports a forward looking research agenda**

Expected Results

- Increase of new ideas.
- Idea quality improvement.
- Efficient optimization of quality ideas.
- Success derived from the efficient implementation of new ideas.
- Emulation of successful innovation strategies.
- Exploration of green chemistry/engineering principles for new developmental opportunities.

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