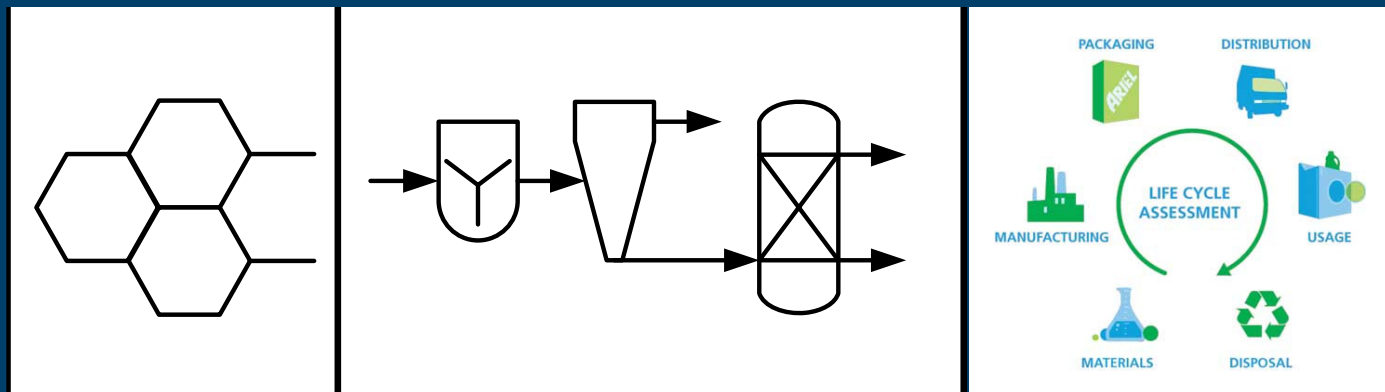


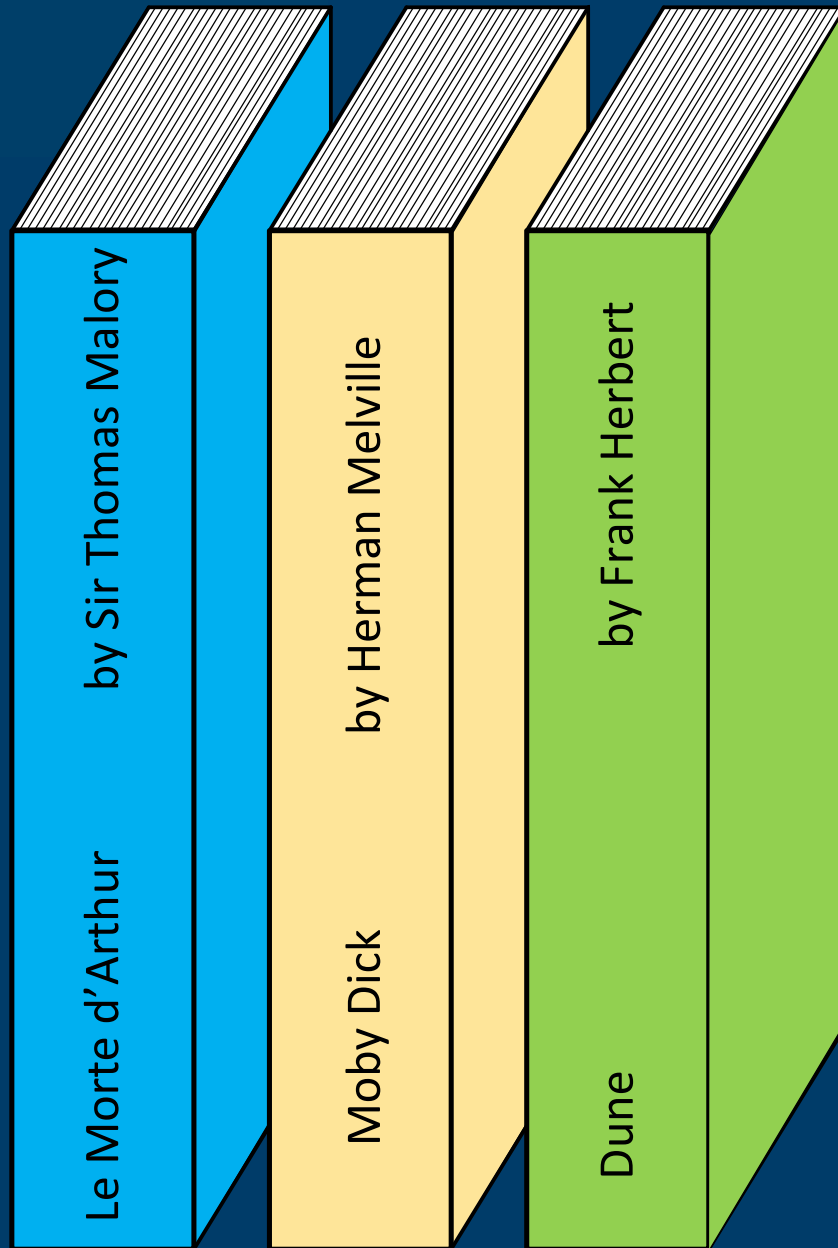
# Evaluating the Sustainability of Manufacturing: Process and Life Cycle Assessments

*Raymond Smith*



# Disclaimer

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.



# Stories of Sustainability

Horses

Whale Oil

“Spice,” i.e., salt

# The Story of Waste

“One man’s waste is another man’s treasure”



Circular Economy



Waste type	Avg. U.S. (%)	Tonnes per year for 100,000 people
Paper and paperboard	27.4	19,834
Glass	4.6	3,344
Metals	8.9	6,469
Plastics	12.7	9,177
Rubber and leather	3.0	2,176
Textiles	5.7	4,142
Wood	6.3	4,573
Food, other	14.5	10,530
Yard trimmings	13.5	9,816
Other materials	1.8	1,329
Misc. inorganic wastes	1.6	1,127
Total	100.0	72,517

# Margins

**Refining margin** (crack spread) is the difference between the value of the products a refinery produces and the value of the crude oil feedstock on a per barrel basis.

For corn to ethanol processes, the **grind margin** is ethanol and co-product net value minus feedstock and energy costs on a per gallon basis.

For MSW to X processes, what's the **X-MSW margin**, or sometimes an **X-RDF** (Refuse-Derived Fuel) **margin**?

# Technologies for Portions of MSW

Facility / Technology Type	Metals	Glass	Paper and Paperboard	Plastics "1" and "2"	Plastics "3" - "7"	Organics			Other Trash
						Food	Fats, Oils and Grease	Yard Waste	
Specific Recycling Process <sup>a</sup>	●	●	●	●	●				
Dirty MRF <sup>b</sup>	●	●	●	●	●	●	●	●	○
Clean MRF <sup>b</sup>	●	●	●	●					
WTE - Anaerobic Digestion <sup>c</sup>			○			●	●	●	
WTE - Gasification <sup>d</sup>			●	●	●			●	
WTE - Fermentation <sup>e</sup>								●	
WTE - Incineration <sup>f</sup>	○	○	●	●	●	●	●	●	●

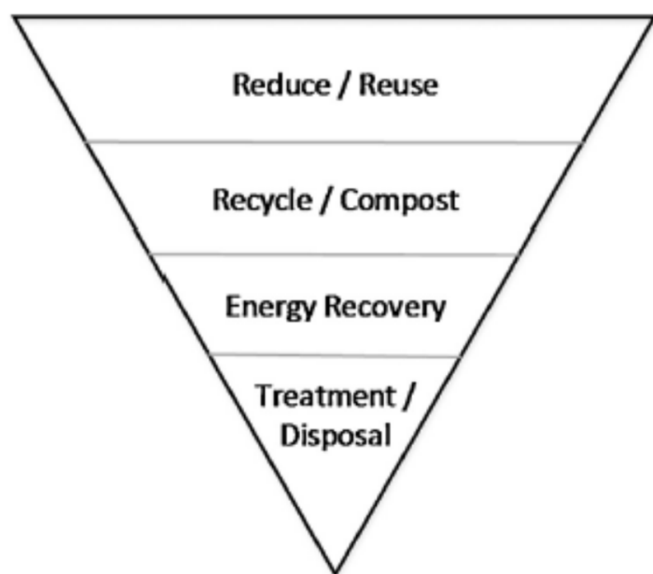
● = commercialized process

● = demonstrated process

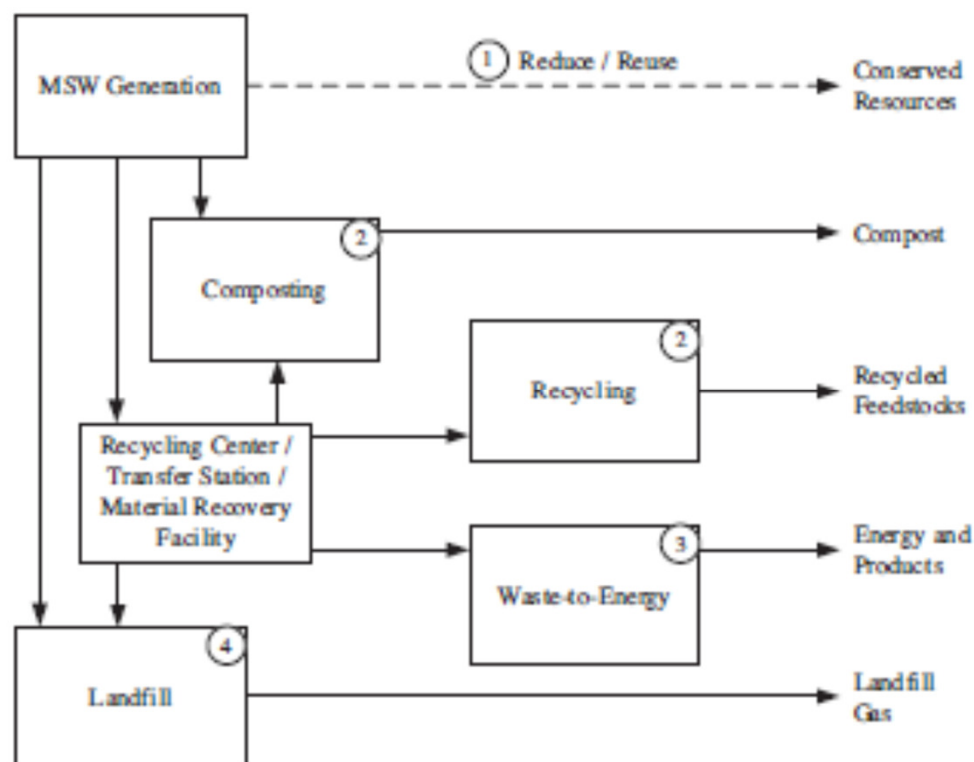
○ = technology that can handle feedstock without using it productively



# Waste Management Options



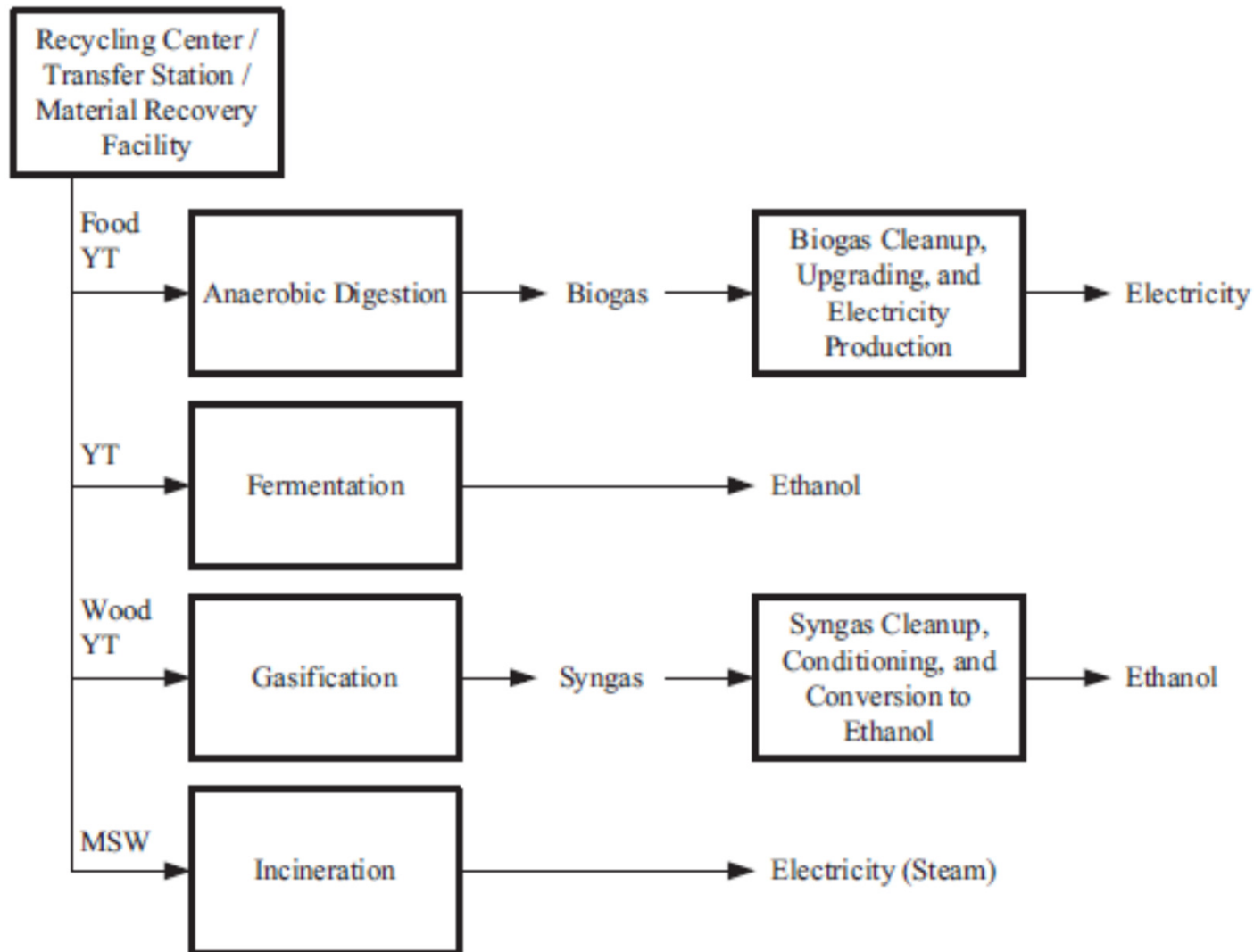
EPA's Waste  
Management Hierarchy





MSW Process	Product(s)	Residuals	Use for Residuals
MSW generation	Compostable and recyclable materials	Non-compostable, non-recyclable materials	Heat value, recycling research opportunity
Composting	Compost	Contaminants (glass, plastics)	Glass and plastic recycling, heat value
Recycling center/transfer station/MRF	Separated recyclable materials	Non-compostable, non-recyclable materials	Heat value, recycling research opportunity
WTE—lignocellulosic fermentation	Ethanol	Lignin; CO <sub>2</sub>	Heat value, products; beverages, algal process
WTE—gasification (with conversion to ethanol)	Syngas, then ethanol	Ash/slag	Construction materials
WTE—anaerobic digestion	Biogas, then power	Digestate slurry	Composting, fertilizer
WTE—incineration	Power	Ash	Construction materials

# Waste to Energy Products and Processes

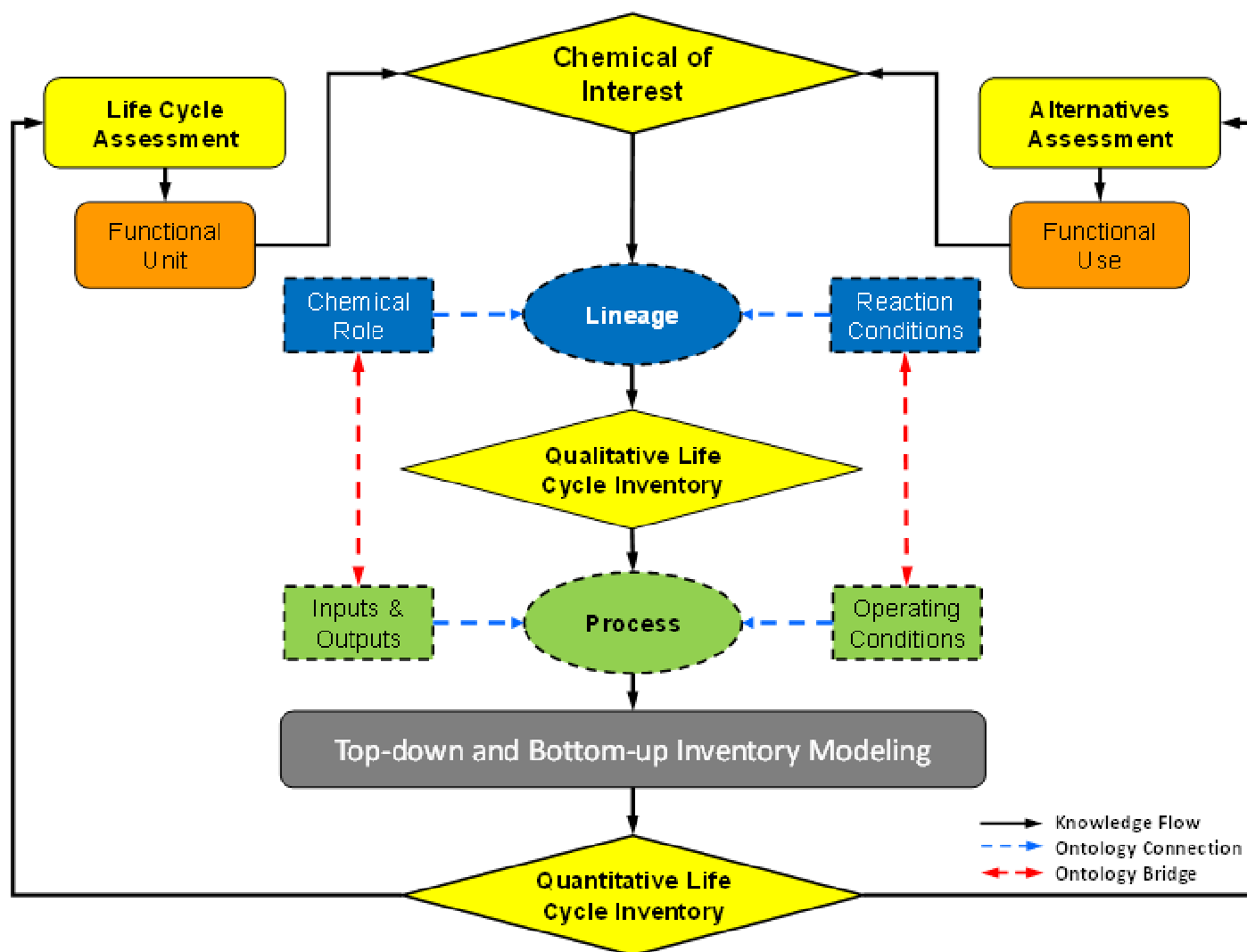


# Sustainable Manufacturing Results

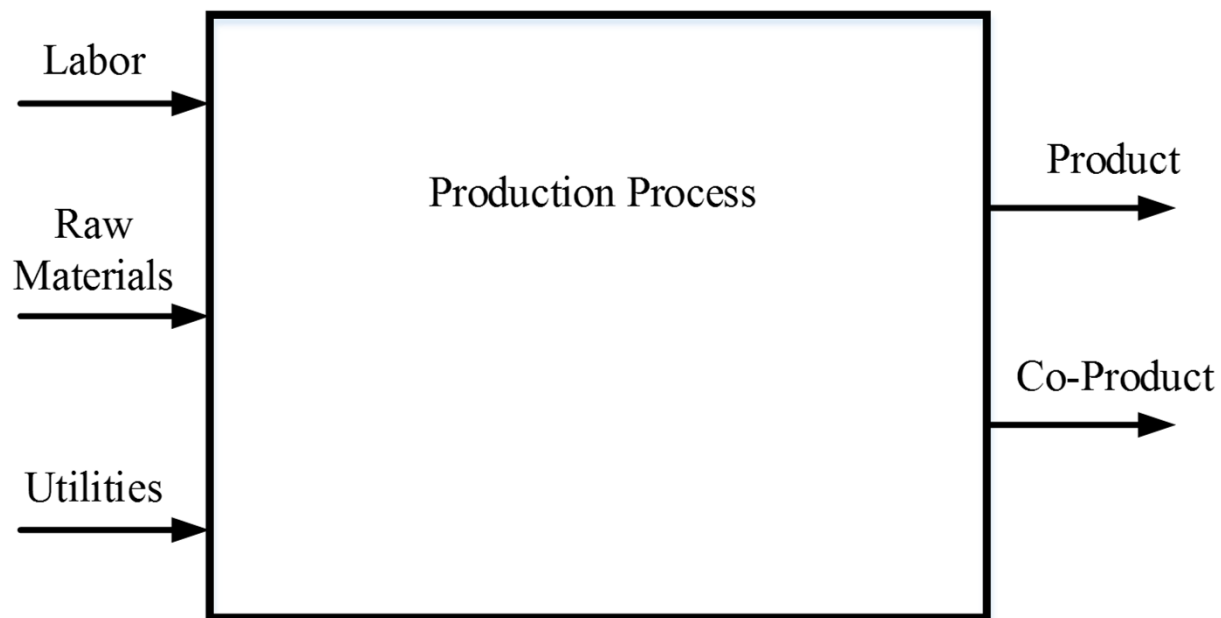
The results of analyses (see publications) show that gasification, anaerobic digestion, and fermentation have positive economics.

Anaerobic digestion improves seven emissions (out of seven explored), while fermentation, gasification, and incineration successively improved fewer emissions.

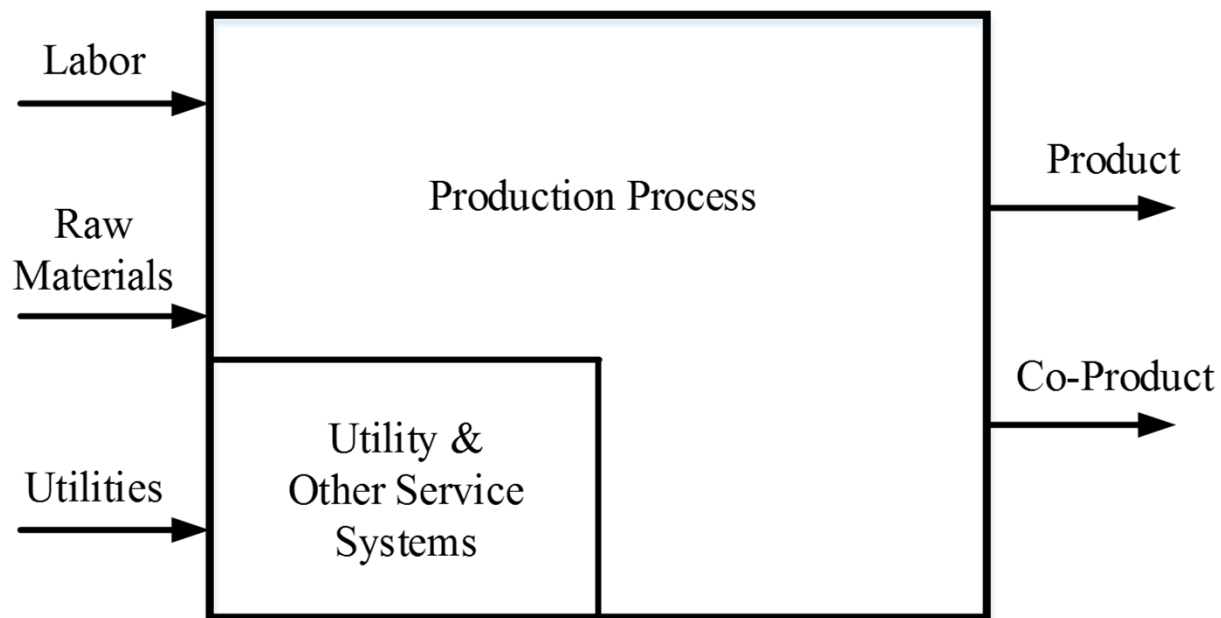
# Identifying Chemicals, Reactions, and Processes in a Life Cycle



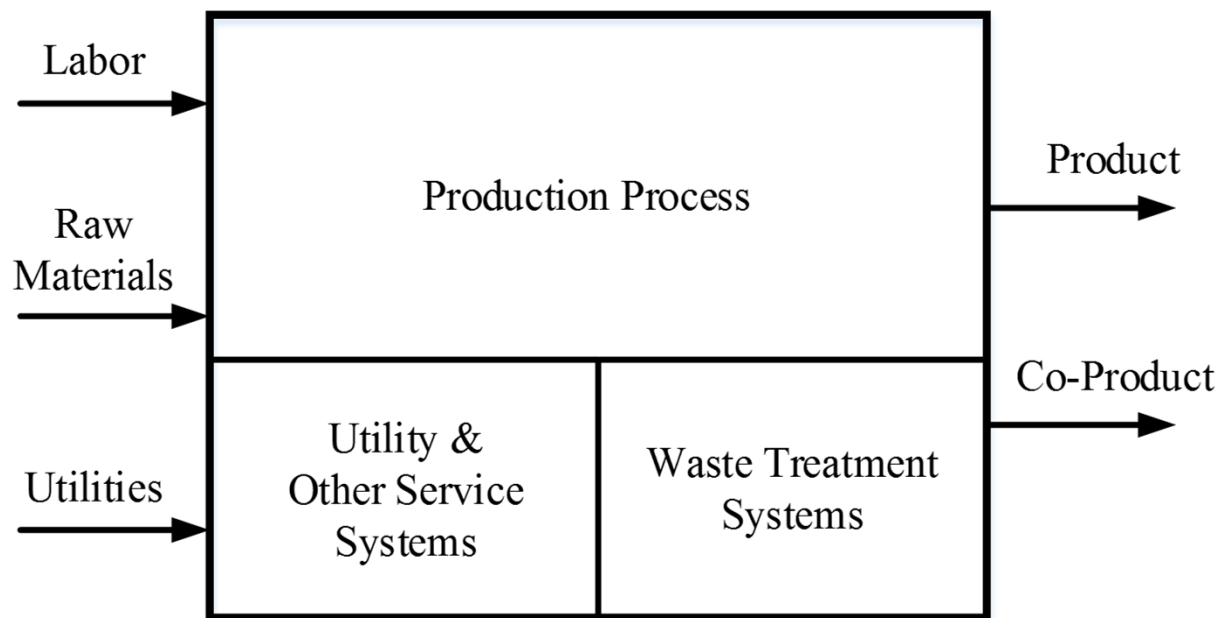
# Process Model



# Process Model

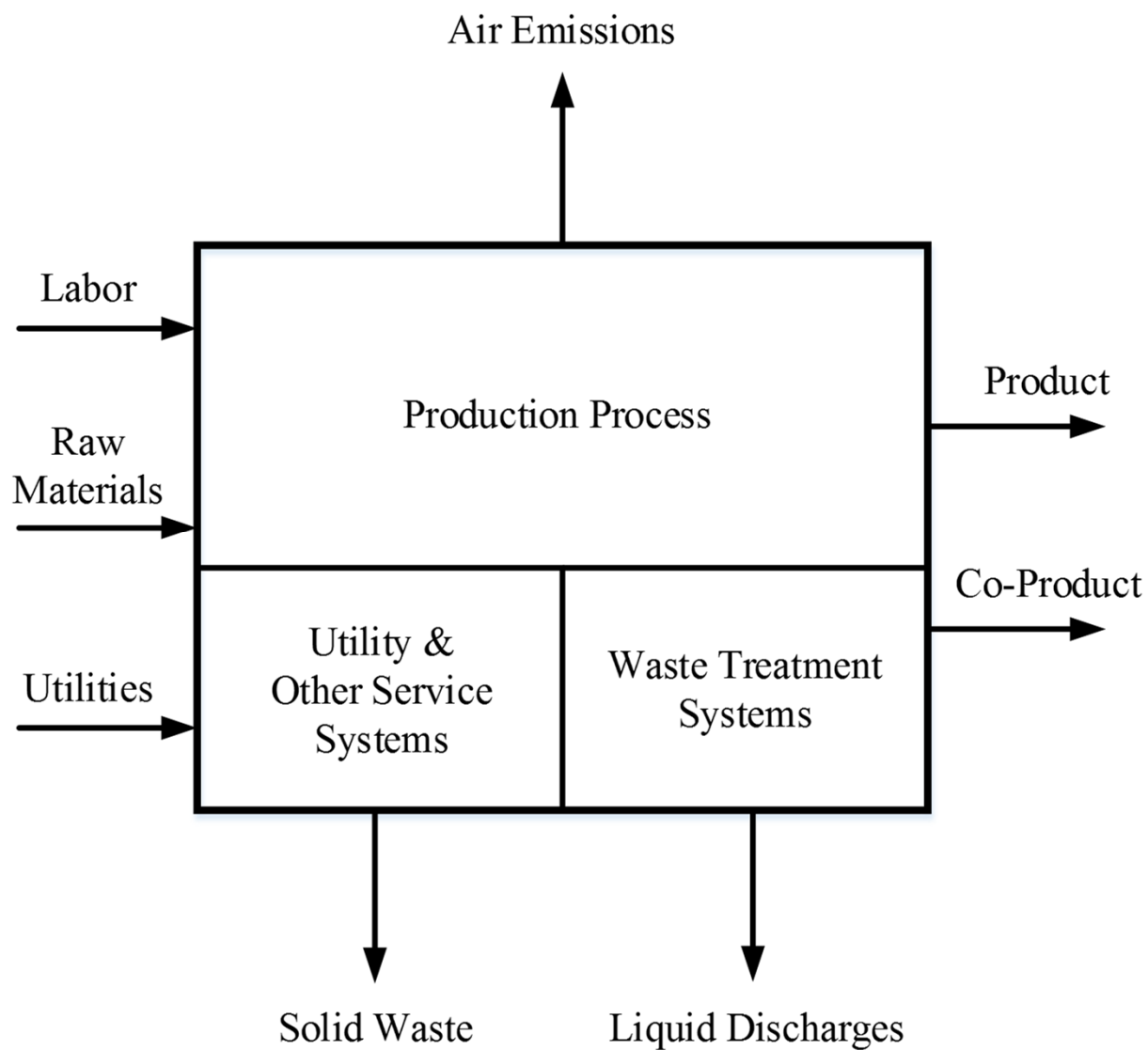


# Process Model

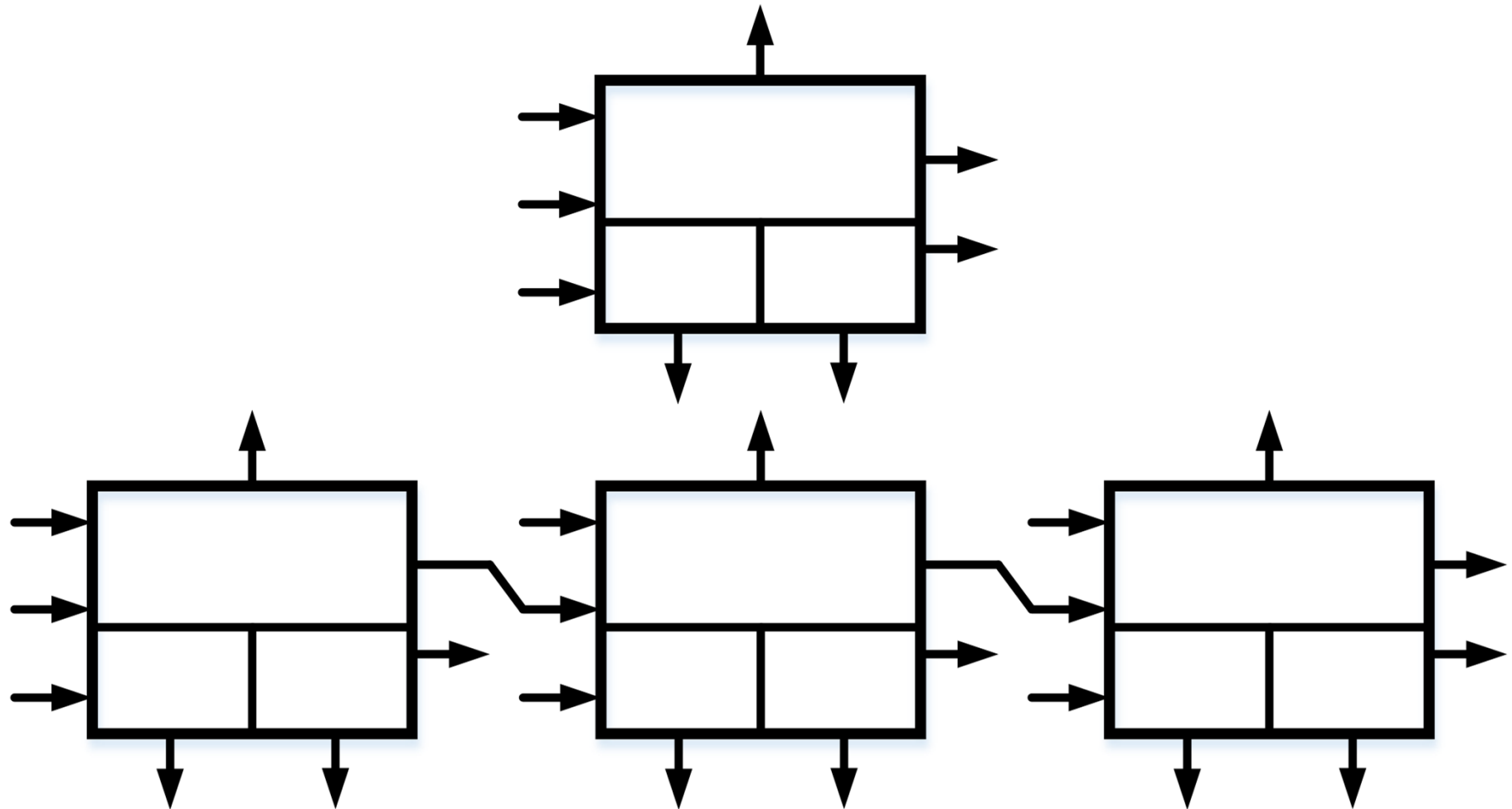




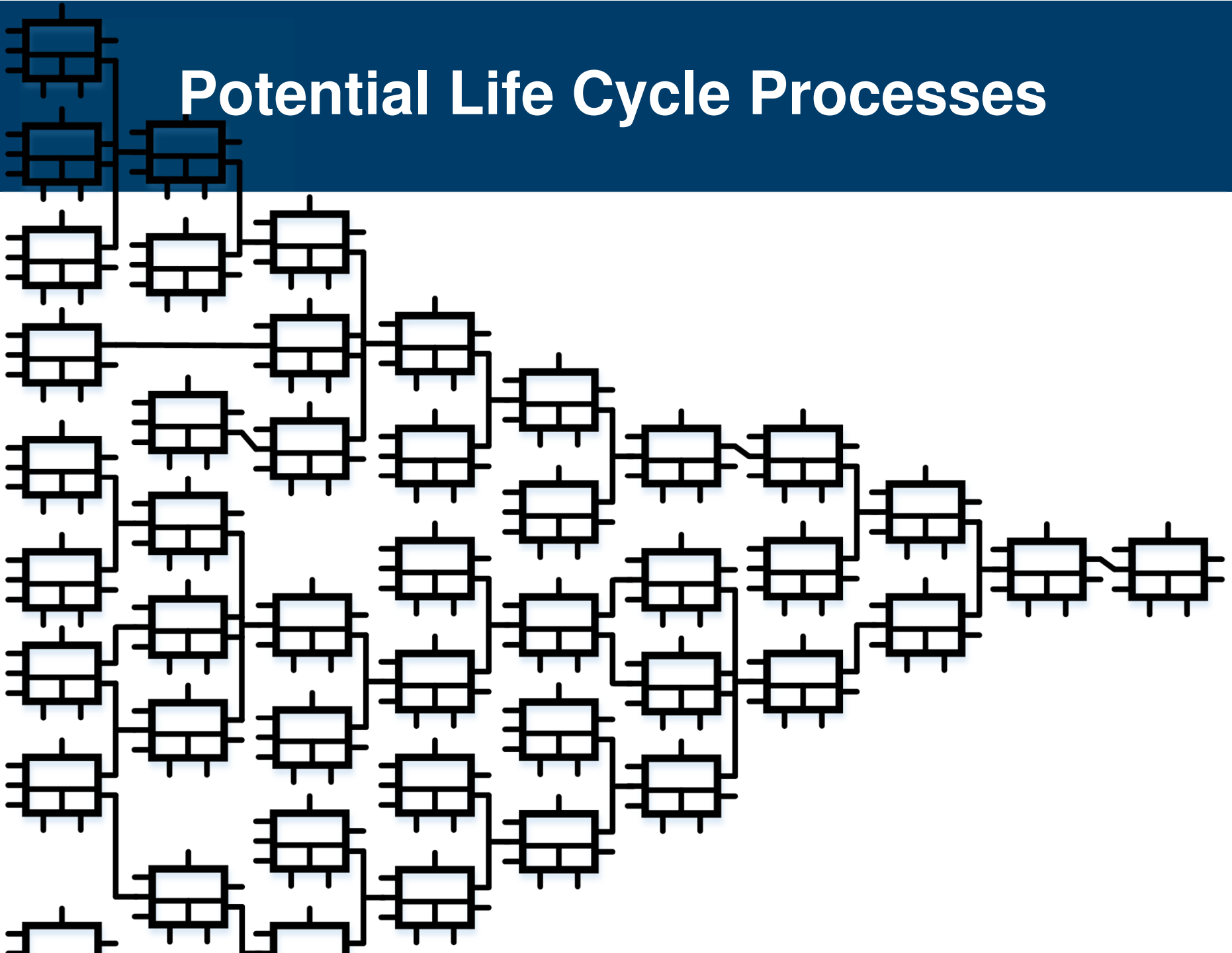
# Process Model



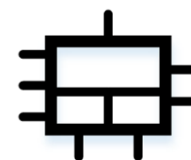
# Process Model in the Value Chain



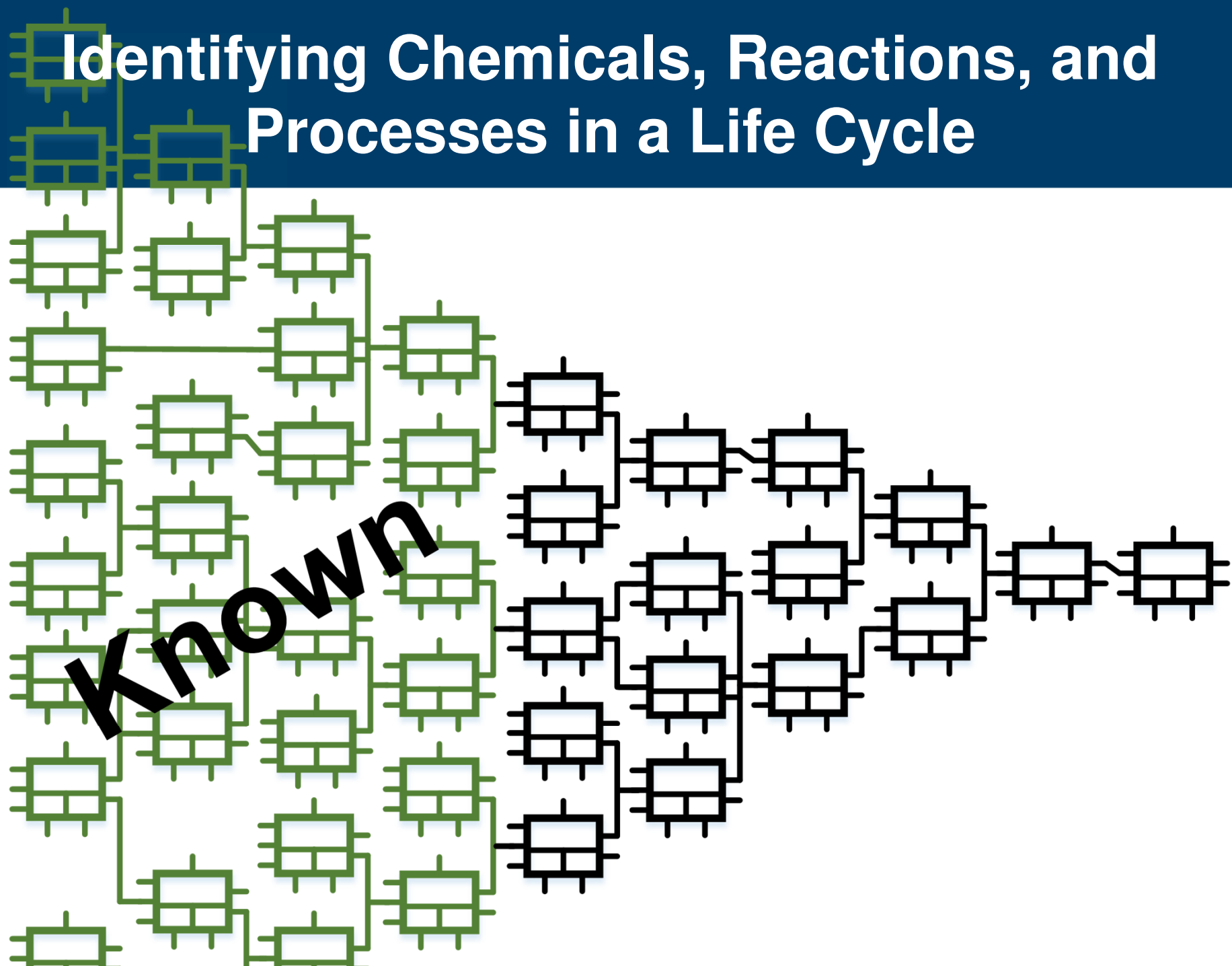
# Potential Life Cycle Processes



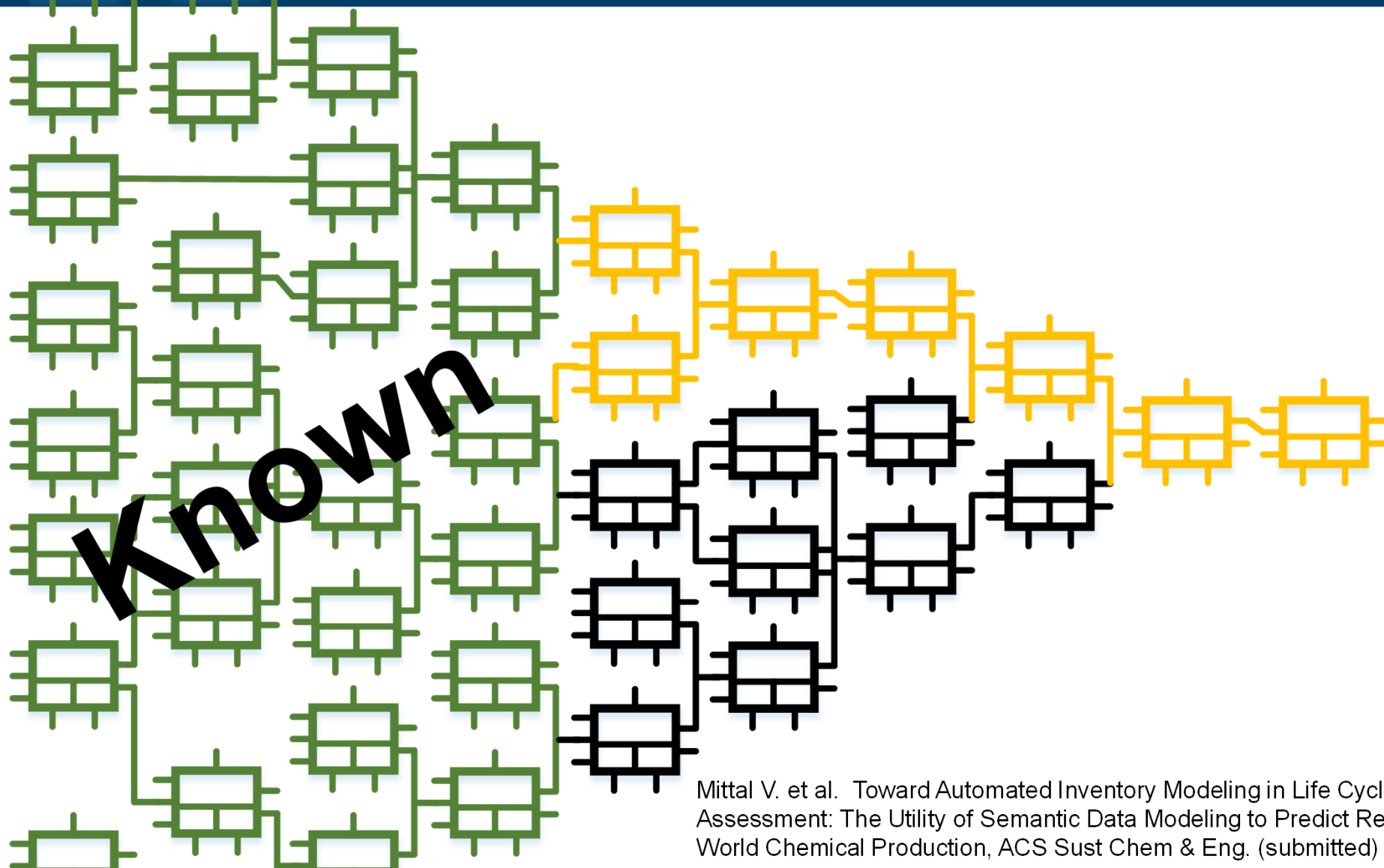
# Identifying Chemicals, Reactions, and Processes in a Life Cycle



# Identifying Chemicals, Reactions, and Processes in a Life Cycle



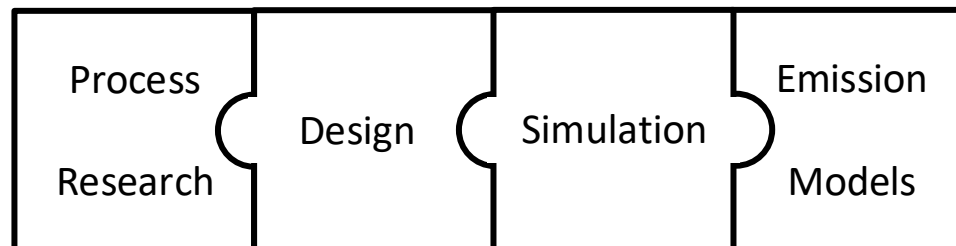
# Identifying Chemicals, Reactions, and Processes in a Life Cycle



Mittal V. et al. Toward Automated Inventory Modeling in Life Cycle Assessment: The Utility of Semantic Data Modeling to Predict Real-World Chemical Production, ACS Sust Chem & Eng. (submitted)

# Rapid Estimation of Life Cycle Inventory

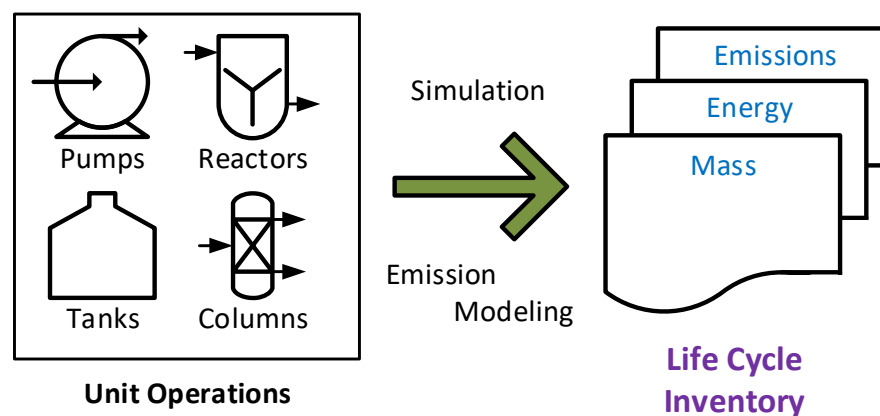
1. Existing inventory databases
2. Top-down inventory data mining
3. Bottom-up inventory development





# Bottom-Up Simulation

**Advantages:** potential for improved LCI; process specific; inputs naturally in results; storage, vent, and fugitive emissions included



ACS  
**Sustainable**  
Chemistry & Engineering

Research Article

[pubs.acs.org/journal/ascecg](https://pubs.acs.org/journal/ascecg)

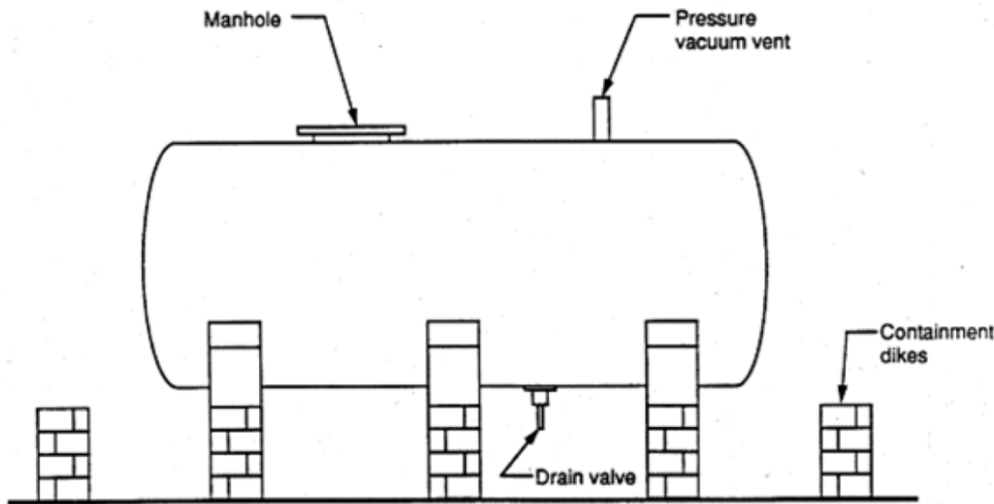
## Coupling Computer-Aided Process Simulation and Estimations of Emissions and Land Use for Rapid Life Cycle Inventory Modeling

Raymond L. Smith,\*<sup>✉</sup> Gerardo J. Ruiz-Mercado, David E. Meyer, Michael A. Gonzalez,<sup>✉</sup> John P. Abraham, William M. Barrett, and Paul M. Randall

National Risk Management Research Laboratory, United States Environmental Protection Agency, 26 West Martin Luther King Drive, Cincinnati, Ohio 45268, United States

**Challenges:** knowledge of engineering design; need for chemical synthesis details; uncontrolled emissions

# Bottom-Up Simulation



## Working Losses

$$L_W = \frac{\dot{V}}{22.4} \left( \frac{273.15}{T} \right) \left( \frac{P_i^{sat}}{760} \right) (MW) K_N K_P$$

## Breathing Losses

$$L_B = 16.3 V_V \left( \frac{273.15}{T} \right) \left( \frac{P_i^{sat}}{760} \right) (MW) \left( \frac{T_R}{T} \right)$$

## Process Vents

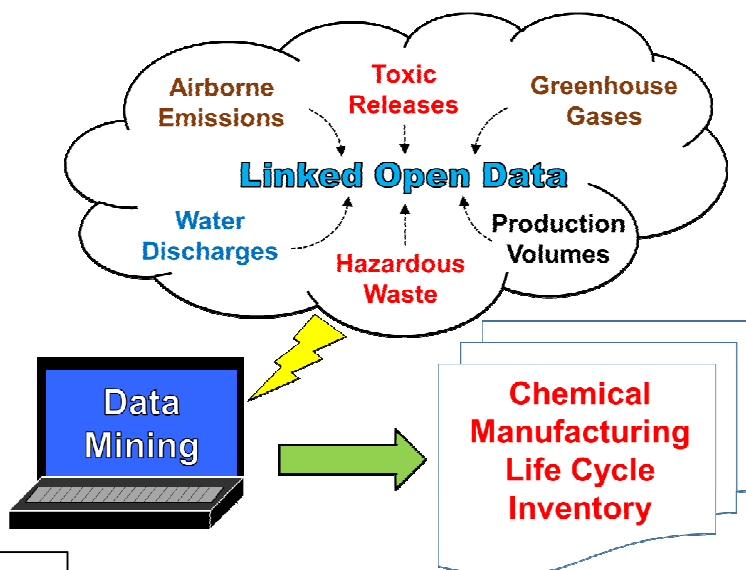
$$S_i = \frac{P_i^b}{x_i \gamma_i P_i^{sat}} = \frac{k_i A}{k_i A + F}$$

$$E_i = \frac{F x_i \gamma_i P_i^{sat}}{RT} S_i (MW_i)$$

Equipment Type	Service	Emission Factor (kg/h/source)
Pumps	Light liquid	0.0199
	Heavy liquid	0.00862
Compressors	Gas	0.228
Valves	Gas	0.00597
	Light liquid	0.00403
	Heavy liquid	0.00023
Connectors (e.g., flanges)	All	0.00183
Open-ended lines	All	0.0017
Sampling connections	All	0.0150
Pressure relief valves	Gas	0.104

# Top-Down Data Mining

**Advantages:** primary data reported by industry and States; detailed release profiles; automation capabilities (linked open data)



Policy Analysis  
pubs.acs.org/est

## Mining Available Data from the United States Environmental Protection Agency to Support Rapid Life Cycle Inventory Modeling of Chemical Manufacturing

Sarah A. Cashman,<sup>†</sup> David E. Meyer,<sup>\*‡</sup> Ashley N. Edelen,<sup>§||</sup> Wesley W. Ingwersen,<sup>‡</sup> John P. Abraham,<sup>‡</sup> William M. Barrett,<sup>‡</sup> Michael A. Gonzalez,<sup>‡</sup> Paul M. Randall,<sup>‡</sup> Gerardo Ruiz-Mercado,<sup>‡</sup> and Raymond L. Smith<sup>‡</sup>

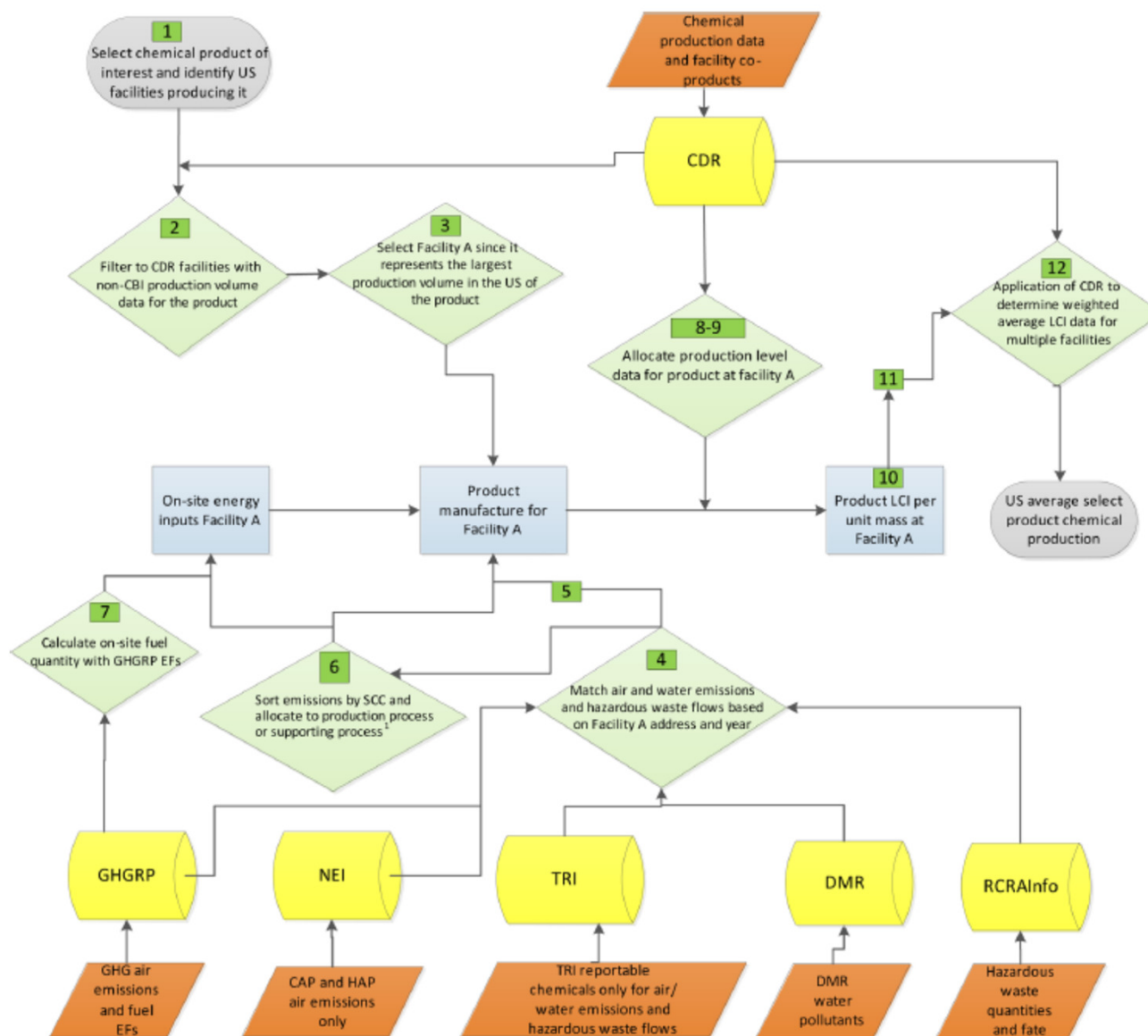
<sup>†</sup>Eastern Research Group, 110 Hartwell Avenue, Lexington, Massachusetts 02421, United States

<sup>‡</sup>United States Environmental Protection Agency, National Risk Management Research Laboratory, 26 West Martin Luther King Drive, Cincinnati, Ohio 45268, United States

<sup>§</sup>Oak Ridge Institute of Science and Education (ORISE) hosted by U.S. Environmental Protection Agency Office of Research and Development, 26 West Martin Luther King Drive, Cincinnati, Ohio 45268, United States

**Challenges:** multi-chemical facility-level allocation; input data gaps; currently limited to TSCA CDR chemicals

# Top-Down Data Mining



# Life Cycle Inventory Methods

Analysis of a chemical of interest leads to identification of the chemical lineage, defining processes of interest.

Methods for bottom-up and top-down life cycle inventories have been developed with capabilities aimed at providing quick and accurate results.

# Return to the Story of Sustainability







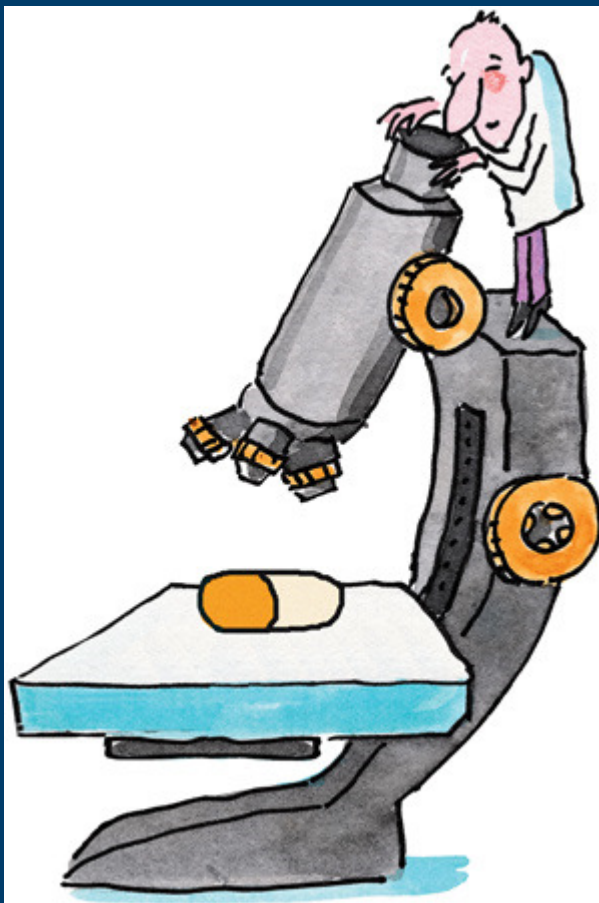


# References

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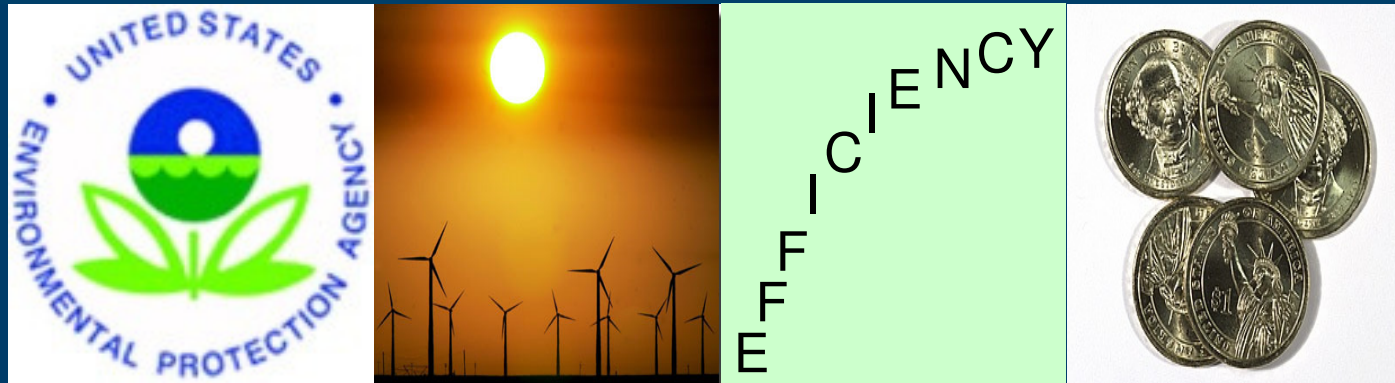
- Smith, R.L. et al. “An Industrial Ecology Approach to Municipal Solid Waste Management: I. Methodology,” *Res. Conserv. Recycl.* 104, 311-316 (2015).
- Smith, R.L. et al. “An Industrial Ecology Approach to Municipal Solid Waste Management: II. Case Studies for Recovering Energy from the Organic Fraction of MSW,” *Res. Conserv. Recycl.* 104, 311-316 (2015).
- Mittal, V. et al. “Toward Automated Inventory Modeling in Life Cycle Assessment: The Utility of Semantic Data Modeling to Predict Real-World Chemical Production,” *ACS Sust Chem Eng* (accepted).
- Smith, R.L. et al. “Coupling Computer-Aided Process Simulation and Estimations of Emission and Land Use for Rapid Life Cycle Inventory Modeling,” *ACS Sust Chem Eng*, 5, 3786-3794 (2017).
- Cashman, S. et al. “Mining Available Data from the United States Environmental Protection Agency to Support Rapid Life Cycle Inventory Modeling of Chemical Manufacturing,” *Environmental Science & Technology*, 50(17), 9013-9025 (2016).

# GREENSCOPE Tool



Gauging Reaction Effectiveness for ENvironmental Sustainability  
of Chemistries with a multi-Objective Process Evaluator

# GREENSCOPE Tool



- Spreadsheet and online software tool, capable of calculating ~140 different indicators.
- User can choose which indicators to calculate.
- User can redefine indicator limits to fit circumstances.

# Sustainability Framework

Identification and selection of two reference states for each sustainability indicator:

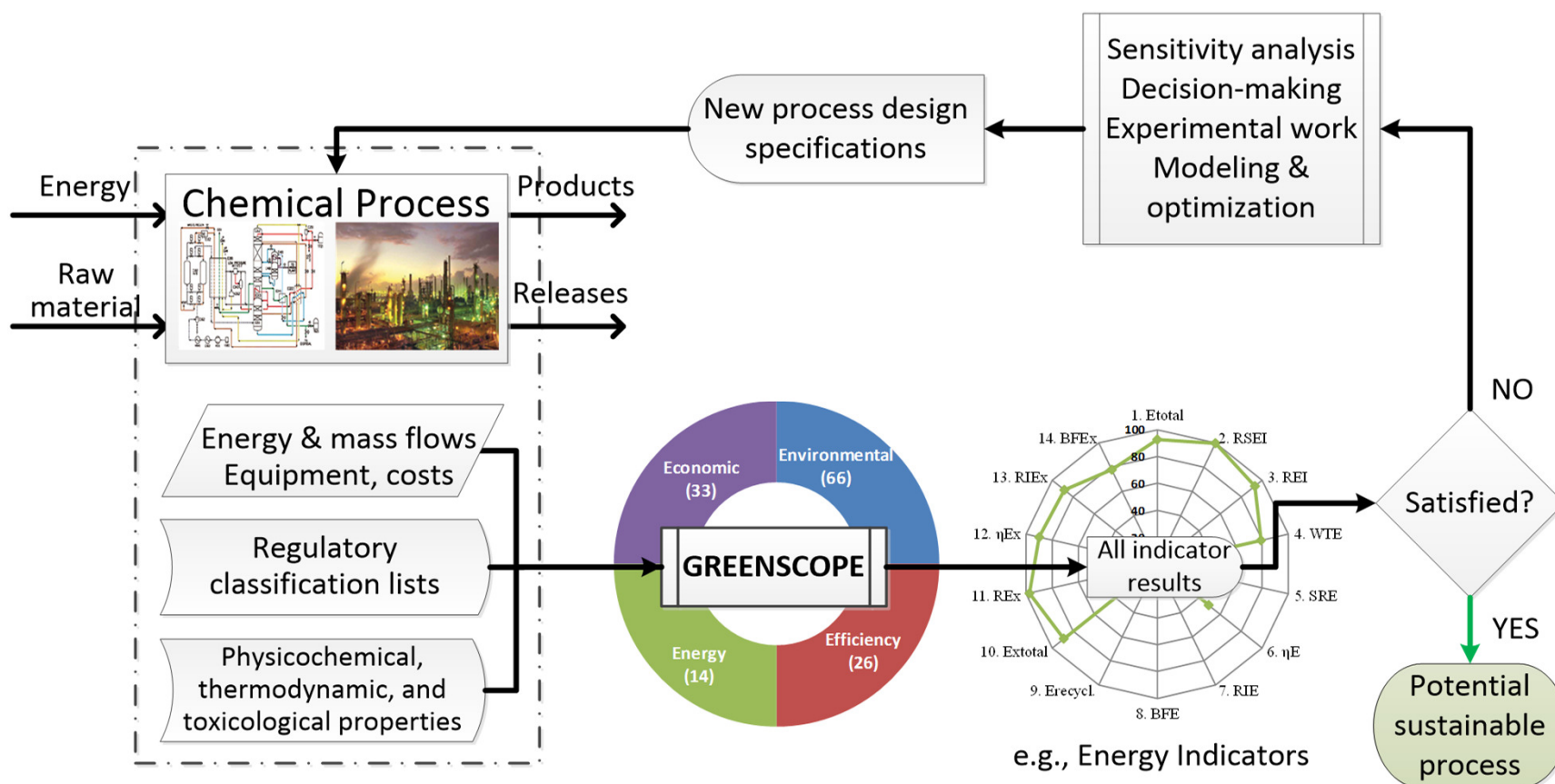
- Best target: 100% of sustainability
- Worst-case: 0% of sustainability

Two scenarios for normalizing the indicators on a realistic measurement scale

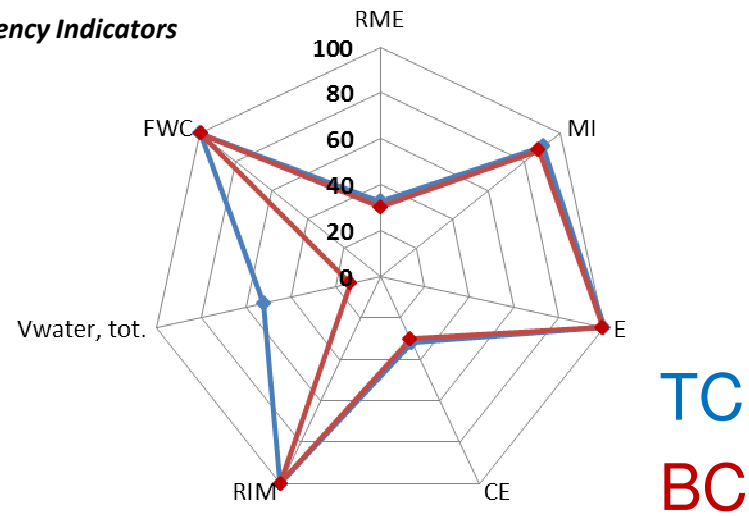
Dimensionless scale for evaluating a current process or tracking modifications/designs of a new (part of a) process

$$\text{Percent Score} = \%G_i = \frac{(\text{Actual-Worst})}{(\text{Best-Worst})} \times 100\%$$

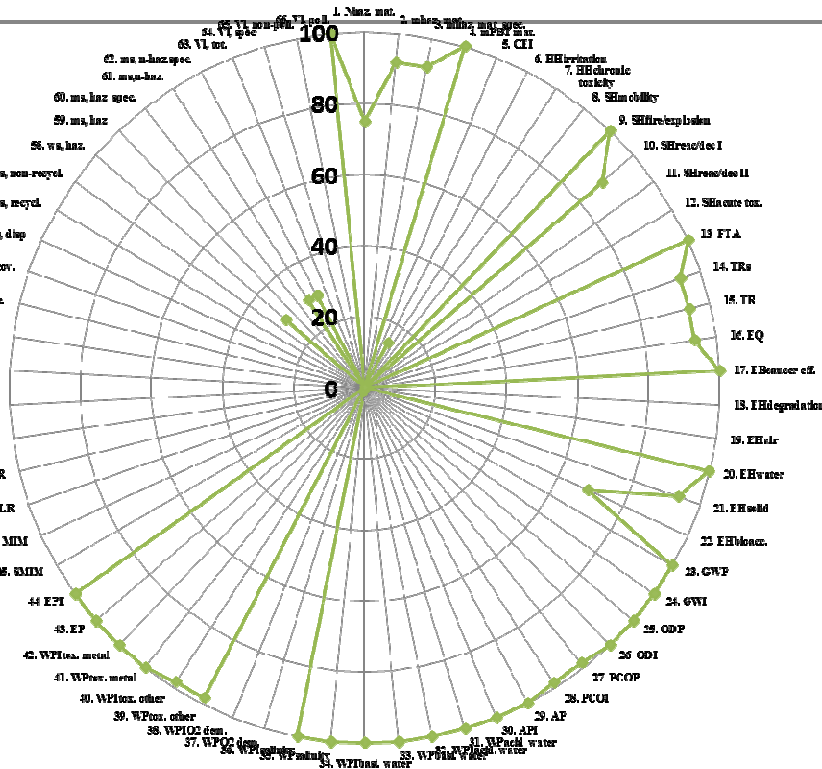
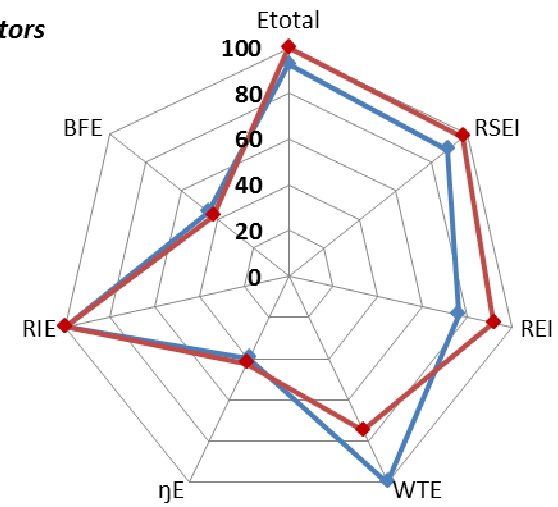
# Using GREENSCOPE



### Efficiency Indicators



### Energy Indicators



### Economic Indicators

