

# An Integrated Tool for Rapid Assessment of Chemical Manufacture Emissions, Treatment, and Sustainability Performance

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# Motivation

- Several industries rely directly or indirectly on the chemical industry
- Several metrics exist for evaluating efficiency for different applications in chemical industry
- Efficiency measures based on optimization are usually driven by cost



Figure 1: Industry dependence

- To assess plant wide performance :
  - (a) Raw material and energy usage (b) Plant productivity
  - (c) Operating costs (d) Waste/Emission generation and treatment
- The methods available to answer the above involve using the proposed integrated GREENSCOPE and Pollution Control Unit (PCU) Analysis tools

# GREENSCOPE FRAMEWORK

- Input data: energy and mass flows, operating and equipment data, properties of addressed component
- GREENSCOPE translates process design and performance data into a set of dimensionless indicator scores
- GREENSCOPE can be used to assess new processes or compare different technologies
- Data availability in terms of quality and quantity is critical for the assessment of results
- Process simulators have the potential for providing required data, but have limitations in emission estimation and challenges in software data transfer

$$\text{Indicator Score} = \frac{|\text{Actual} - \text{Worst}|}{|\text{Best} - \text{Worst}|} \times 100\%$$

\* 100% represents the most sustainable while 0% the least sustainable

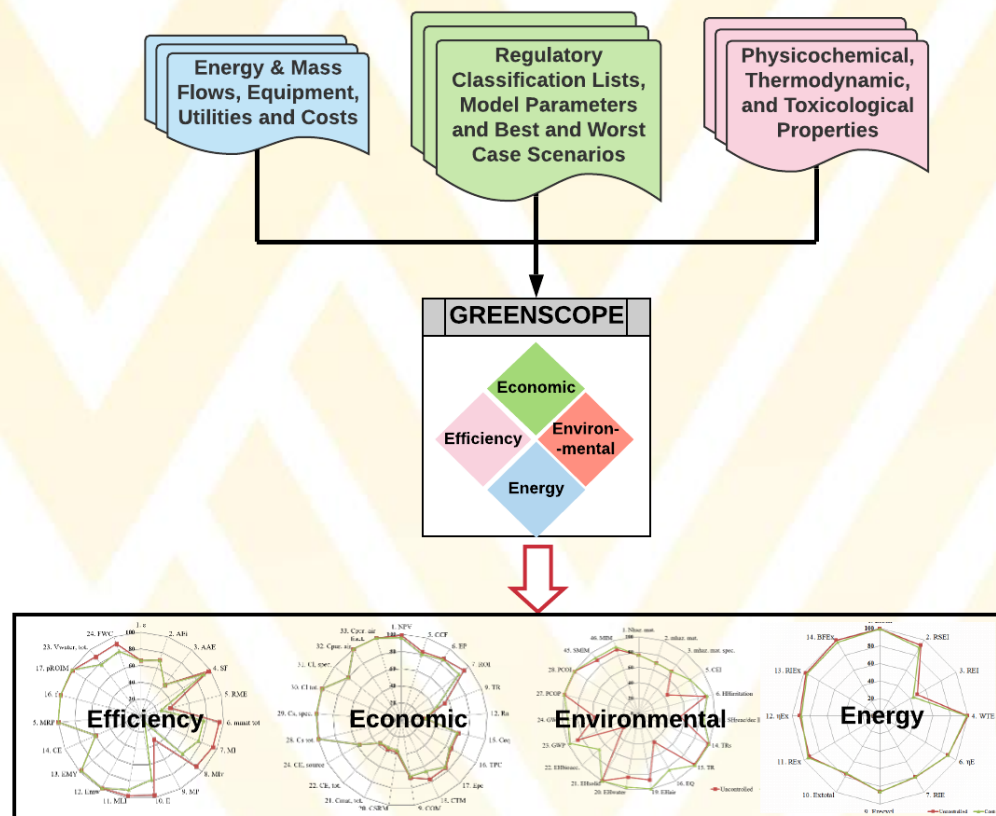


Figure 2: GREENSCOPE Framework

\* Ruiz-Mercado GJ, Smith RL, Gonzalez MA. GREENSCOPE.xlsm User's Guide. Excel Version 1.1 2013

# GREENSCOPE APPLICATION

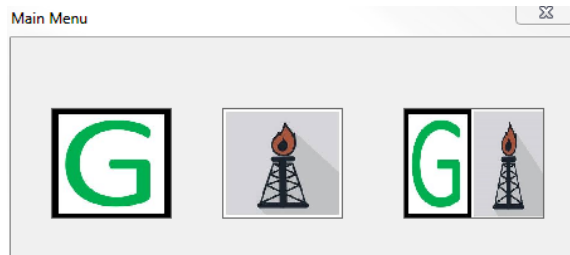


Figure 3:  
GREENSCOPE-PCU  
Main Menu

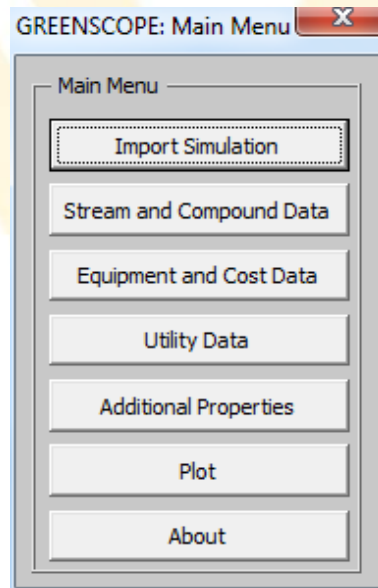


Figure 4:  
GREENSCOPE  
Main Menu

- Users have choices to perform, GREENSCOPE, PCU analysis, or both

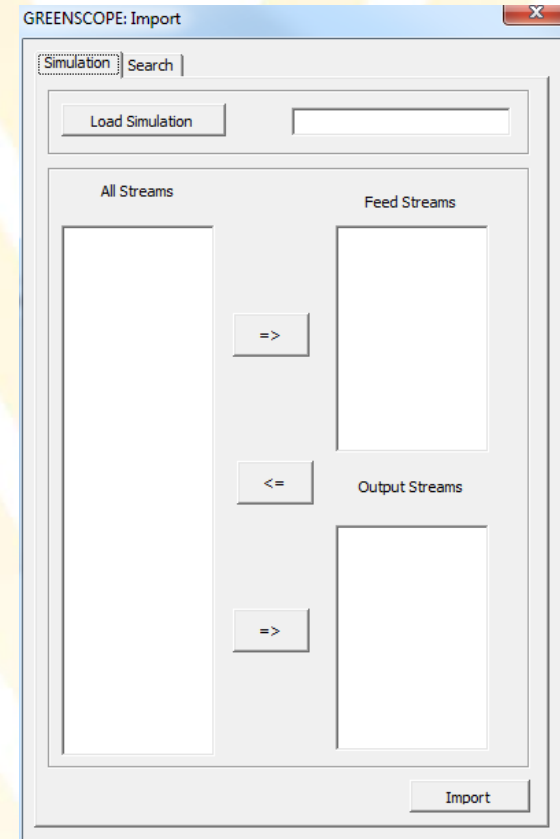


Figure 5: GREENSCOPE  
Import Menu

# GREENSCOPE APPLICATION

GREENSCOPE: Utility Data

Utility Costs and Renewability

Utility type	Utility cost, US\$/kg or US\$/kWh	Utility cost, US\$/GJ	Utility flow rate needs, kg/h, m <sup>3</sup> /h, MJ/h, or kWh/h (Manual input)*	Liquid water type utility in situ produced*
Medium pressure steam at 10 barg 184°C, 1/kg	0.02959	14.83	0	
Moderately low T refrigerated water, T <sub>in</sub> = 5 °C T <sub>out</sub> = 15°C, 1/kg	0.000185	4.43	0	no
Water for process use, makeup cooling tower, washing, etc. 1/kg	0.000067		0	no
Boiler feed water, 1/kg	0.00245		0	no
Potable (drinking) water, 1/kg	0.00026		0	no
Deionized water, 1 / kn	0.001		0	no

	Cooling water generation	Steam generation	Electricity generation
Total percentage of energy supplied by renewable source, 100%	0.02	2	0.01

Add

Figure 6: Utility Entry Window

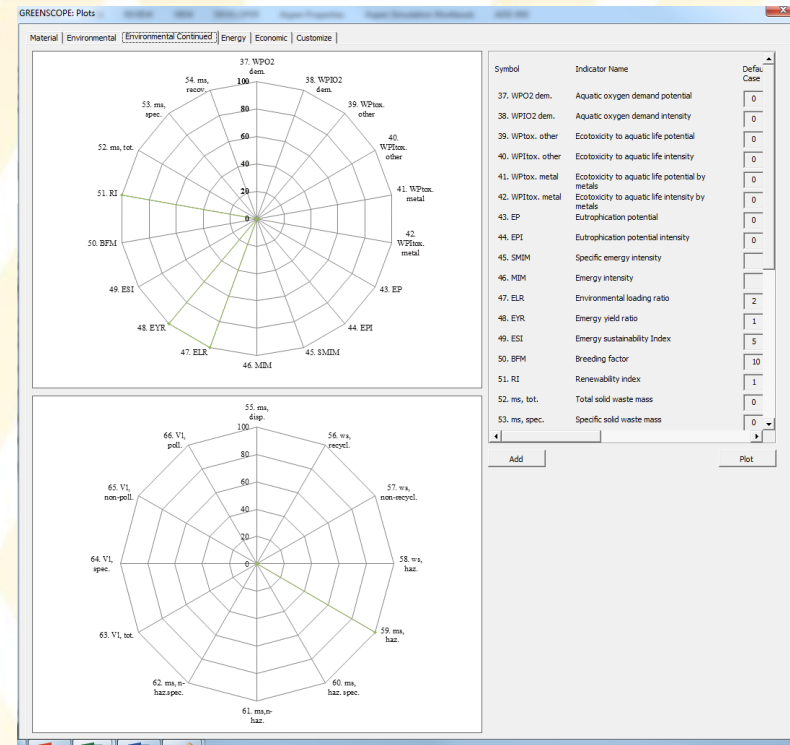


Figure 7: Indicator Plot Window

- Users are able to enter values for different process utilities
- Users can plot all indicators or customize



# PCU FRAMEWORK

- PCU Framework
  - Simulate gas flare calculations
  - Generate results on:
    - Stream composition
    - Equipment size
    - Utility usage
- The current framework has been tailored towards CHEMCAD but this can be extended to Aspen or other process simulators

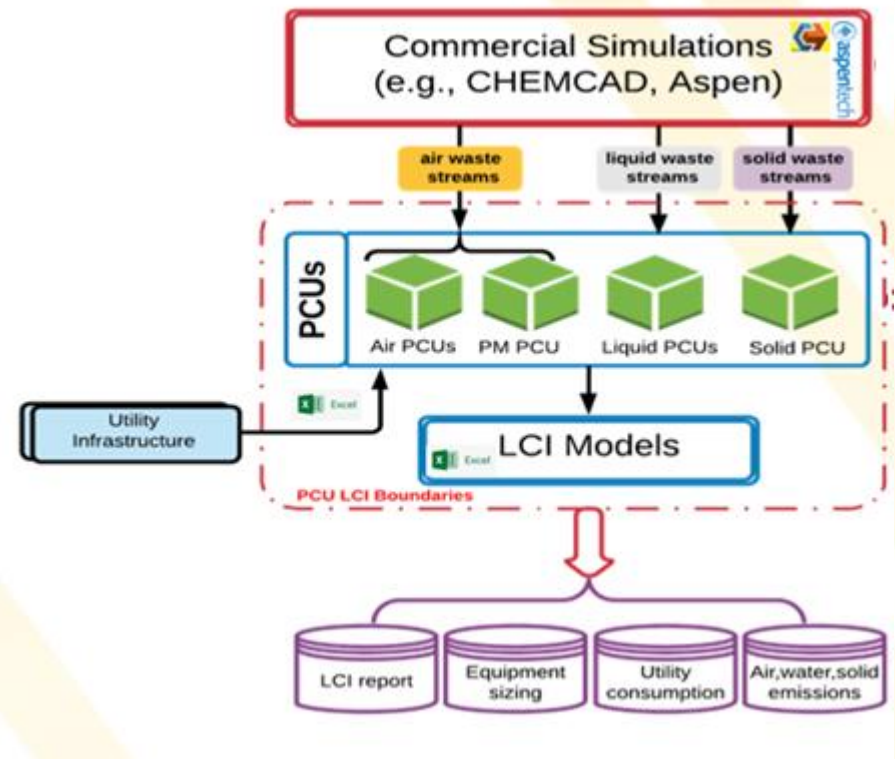


Figure 8: PCU Framework

# PCU APPLICATION

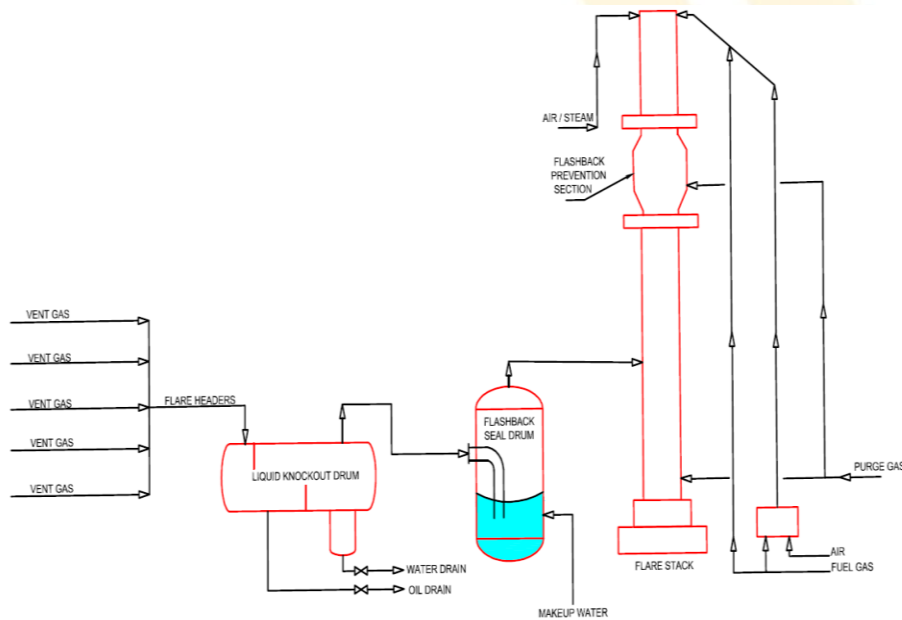


Figure 9: Flare System

Flare Input Data Entry

Vent Gas Flowrate*	1.5	kg/s	Designed Combustion Efficiency*	98	%
Vent Gas Temperature*	100	°C	Designed Wind Velocity*	10	m/s
Vent Gas Pressure*	168.9	kPa	Designed Mach Number*	0.2	
Liquid Mass Fraction	0.05		Maximum Allowable Radiation*	1.58	kW/m²
Liquid Density	795	kg/m³	Radiation Fraction*	0.15	
Flare Type*	Steam-assisted		Horizontal Distance*	50	m

Vent Gas Components

Add a compound  
Methane  
Ethane  
Propane  
Butane  
Pentane  
Heptane  
Octane

Ok Clear Cancel Help

Figure 10: Flare Interface

- This interface allows the user to design a flare system based on maximum estimated flows

# GREENSCOPE-PCU FRAMEWORK

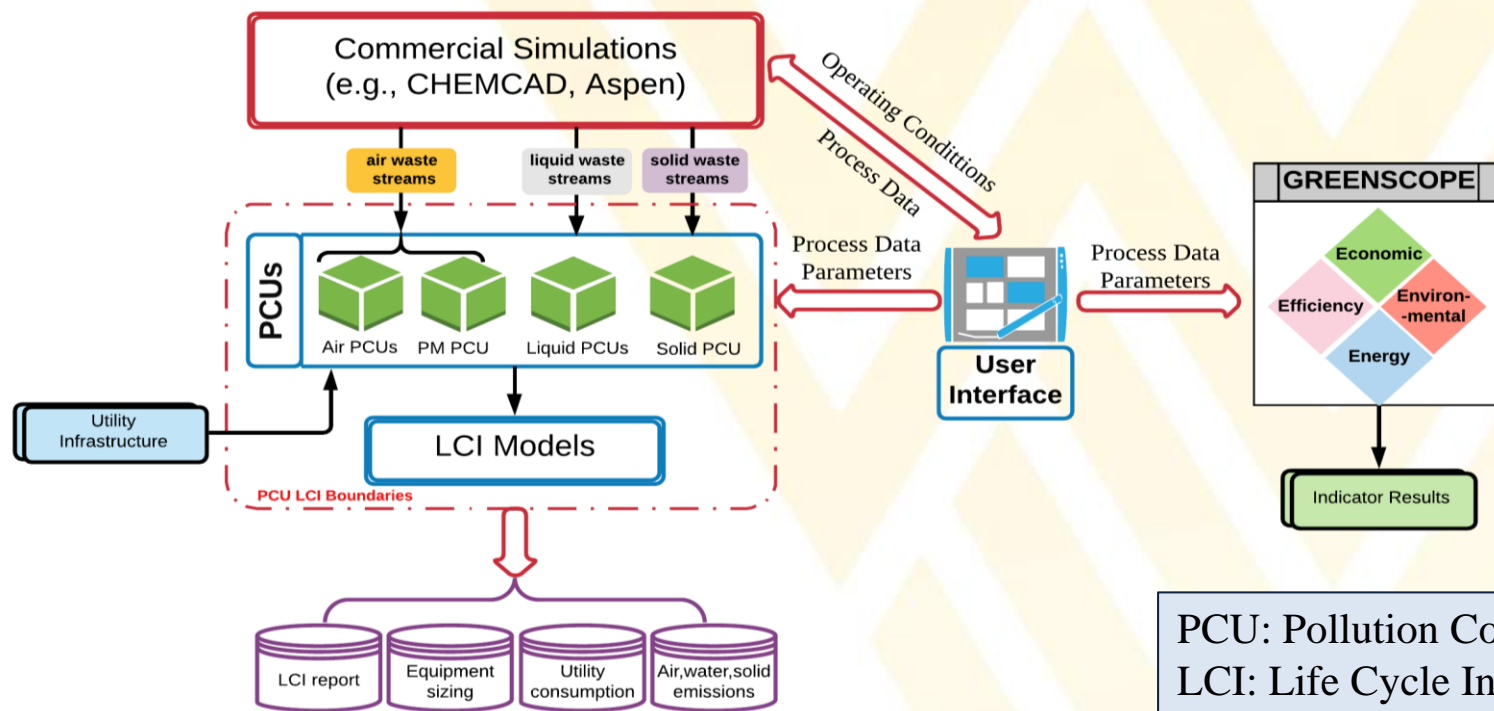
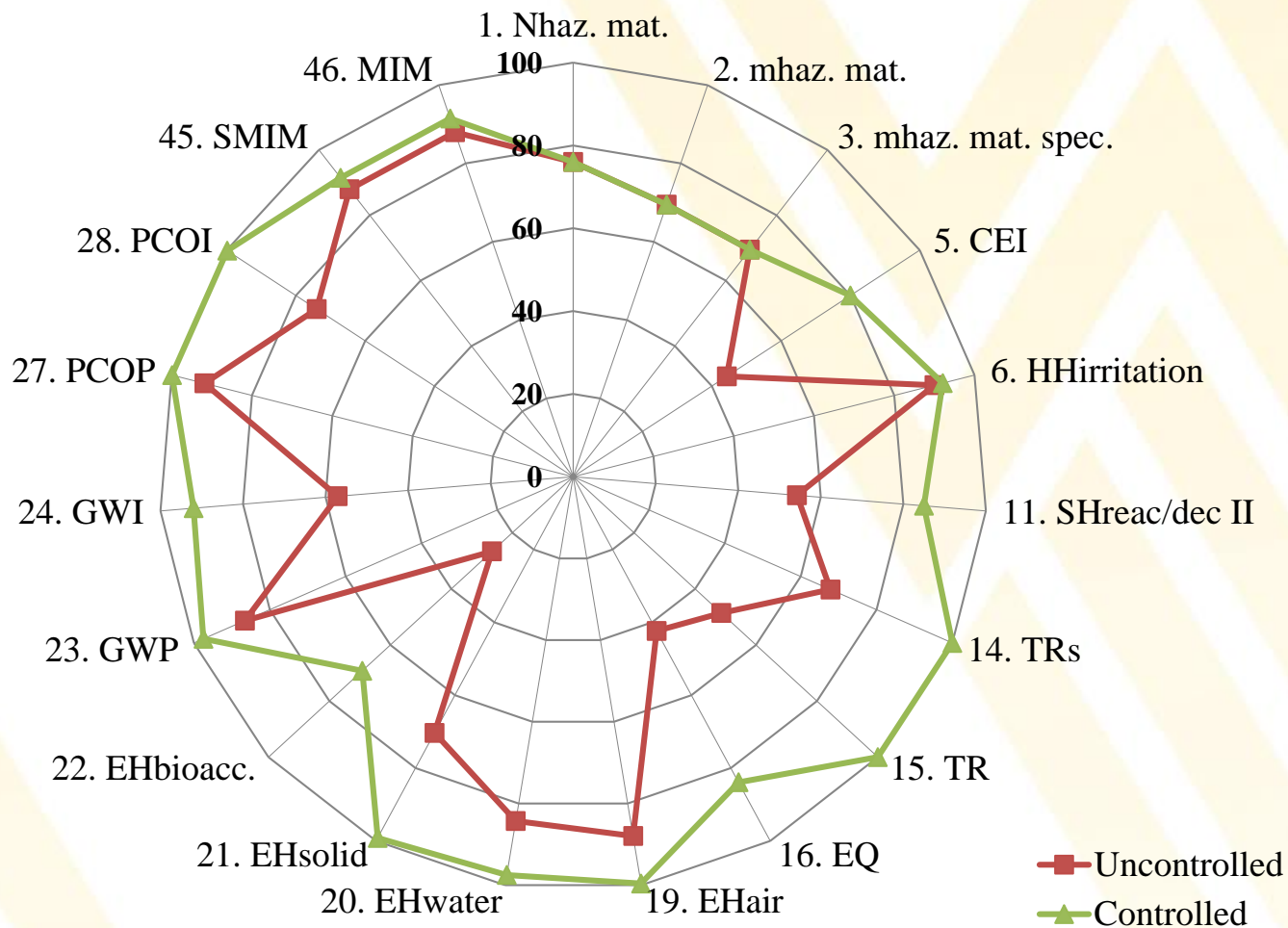


Figure 11: GREENSCOPE-PCU Framework



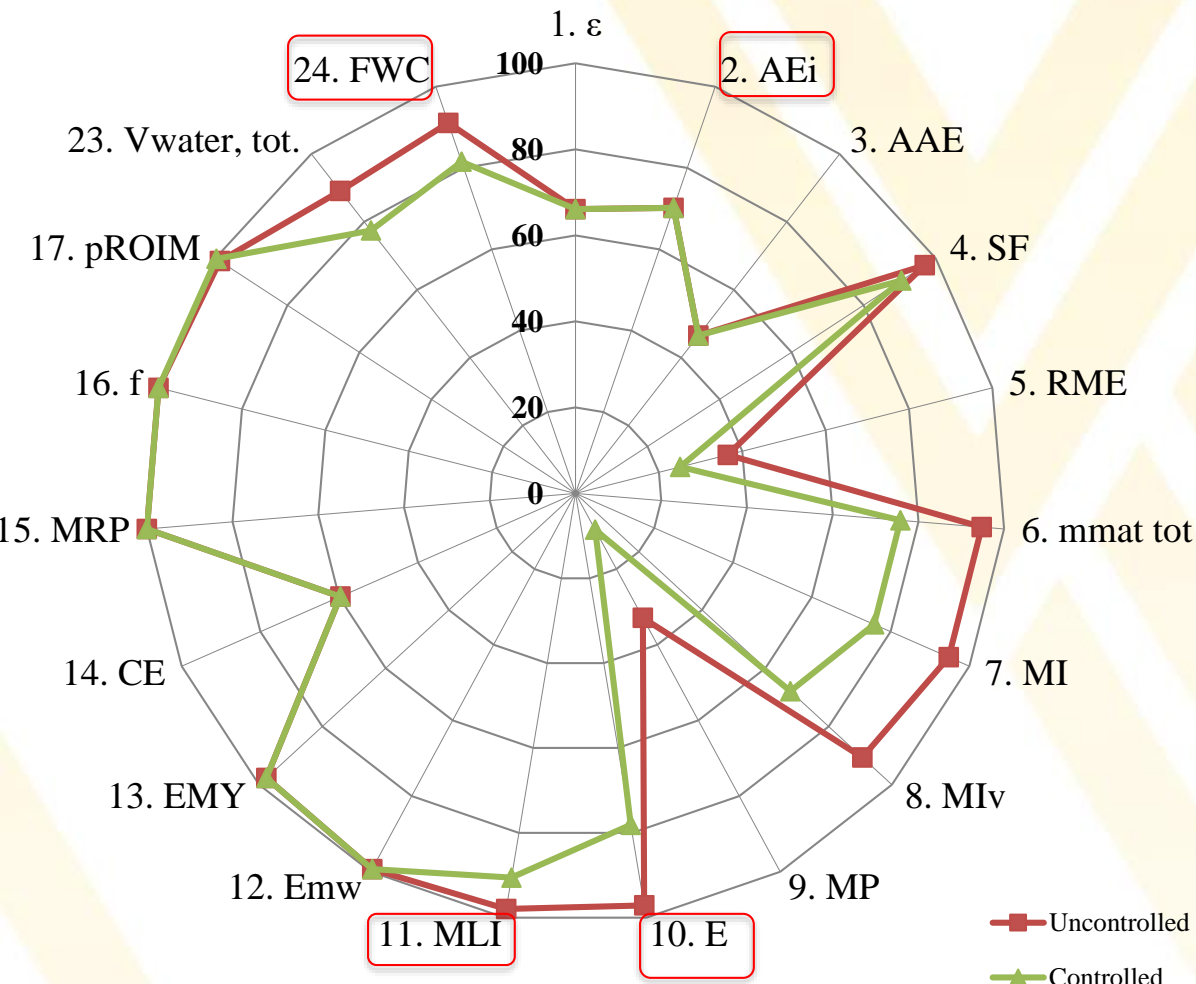
# Results



- CEI (Chemical Exposure Index), EQ (Environmental Quotient), GWI (Global Warming Intensity) increased 35.65%, 41.56%, 34.93%, respectively, due to the controlled emissions by PCUs

Figure 12: GREENSCOPE-PCU Framework

# Results



- Radar plot shows that some efficiency indicator scores decrease when pollution treatment units are added to the process
- total material consumption ( $m_{mat.,tot.}$ ), Mass Intensity (MI), dropped 18.94%, 19.98%, respectively

Figure 13: GREENSCOPE-PCU Framework

# CONCLUSIONS

- GREENSCOPE was used to estimate indicators and improve plant performance
- The PCU package is a great tool for estimating and simulating treatment operations and designs
- The motivation for the integration of these frameworks is due to their reliance on the same dataset
- Proposed framework can bridge existing gaps between *sustainability assessment*, *pollution control*, and *process modeling* (commercial simulators)



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Thank you!



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