# Sustainable Process Design for Biofuel Production Via Syngas Conversion Pathway


Presented by:

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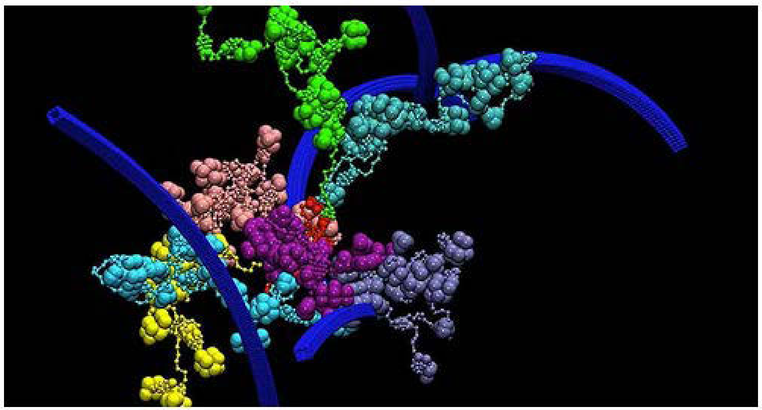
# National Renewable Energy Laboratory (NREL)

- “At NREL, we focus on creative answers to today's energy challenges. From breakthroughs in fundamental science to new clean technologies to integrated energy systems that power our lives, NREL researchers are transforming the way the nation and the world use energy.” (www.nrel.gov)
- 327 acres Golden campus; 305 acres National Wind Technology Center
- National Centers
  - National Bioenergy Center
  - National Center for Photovoltaics
  - National Wind Technology Center
- Nearly 2,200 full- and part-time employees, visiting professionals, postdoctoral researchers, etc.

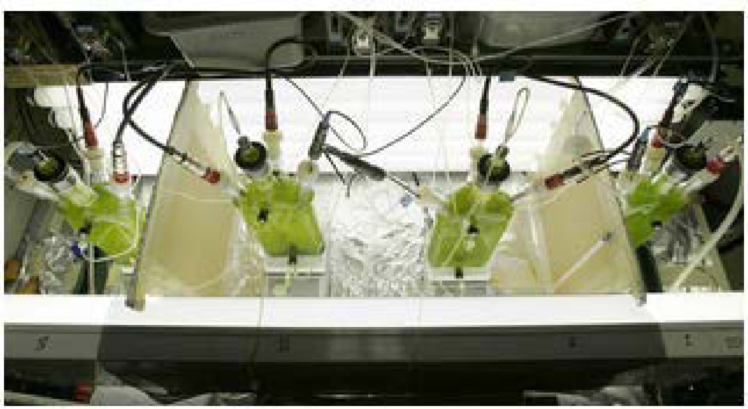
# NREL Bioenergy Research

NREL's bioenergy science and technology group performs a full range of research from exploring biomass at the molecular level through biorefinery process optimization to help bring biofuels and bio-products to market.



Analysis & Characterization

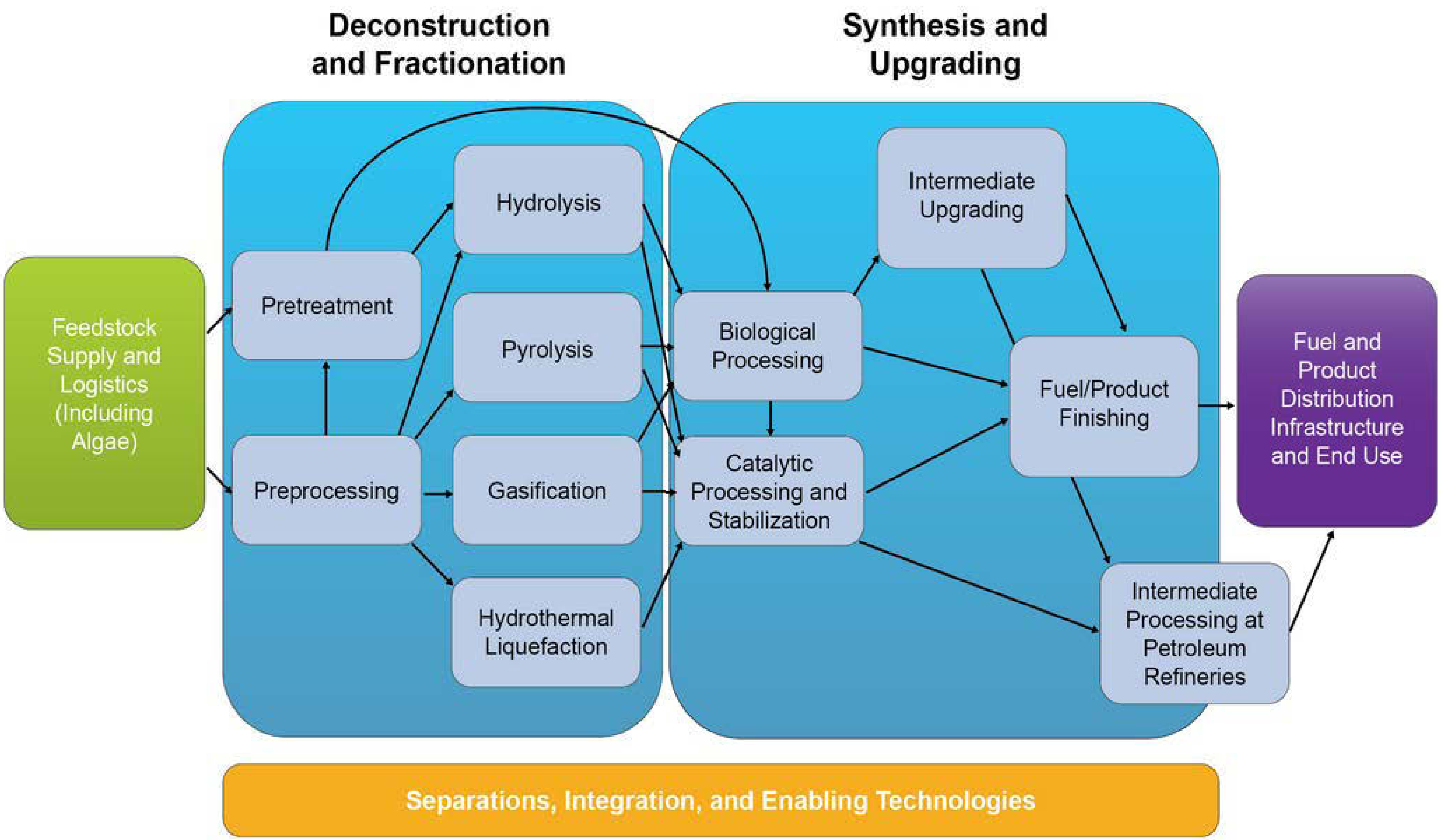
Biochemical Processes



Bioenergetics

Thermochemical Processes

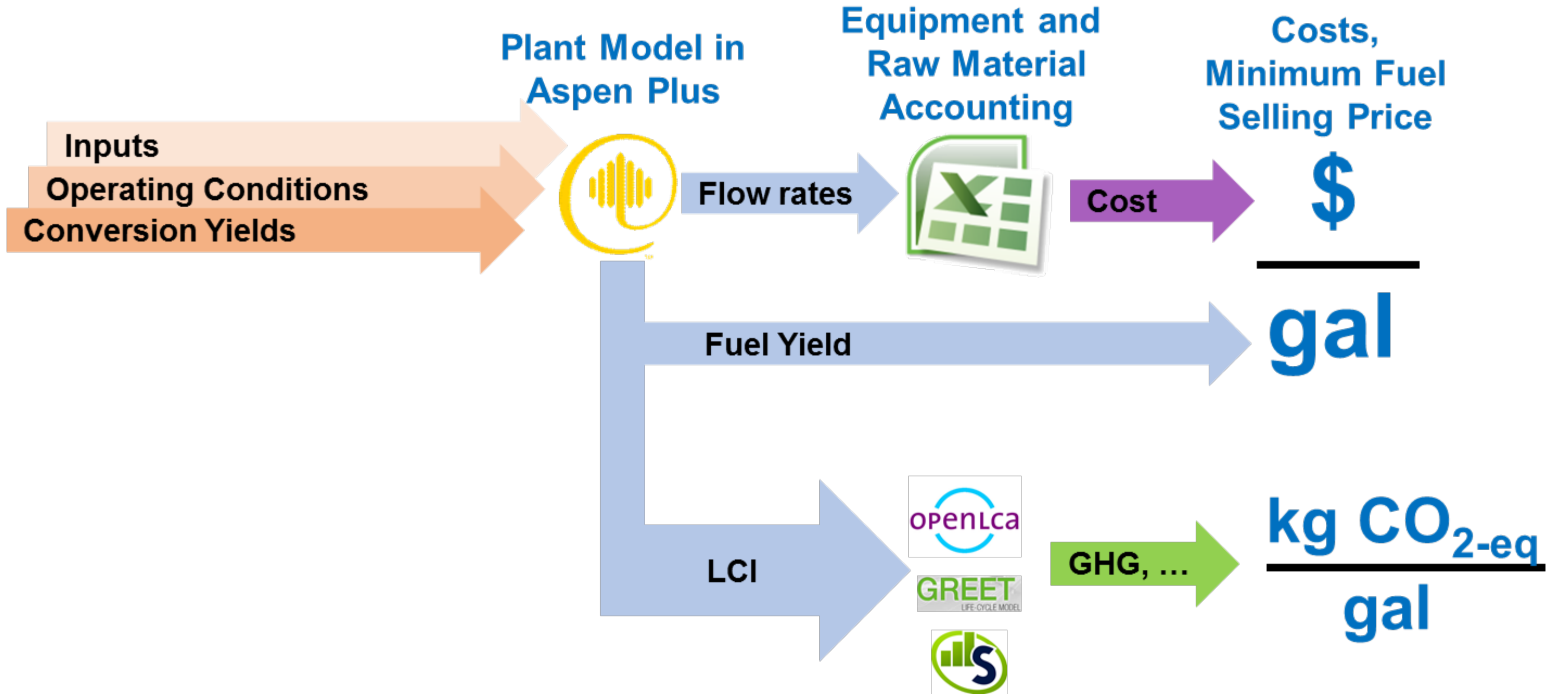
# Biomass-to-fuels conversion pathways




Source: https://www.energy.gov/eere/bioenergy/conversion-technologies

# Conversion Technology Assessment

- Techno-economic analysis
  - Assess the technical and economic viability of new processes and technologies
  - Identify the potential for cost reduction
  - Assess cross-pathway and cross-technology progress, and
  - Provide input into portfolio development and technology validation
- Life-cycle analysis / Supply Chain Sustainability Analysis
  - Estimate the environmental impacts (e.g., GHGs, FEC)



# Objectives and Motivation:

- Integration of sustainability in process design is core to the mission in developing renewable fuels and should be considered a best practice in biorefinery design.

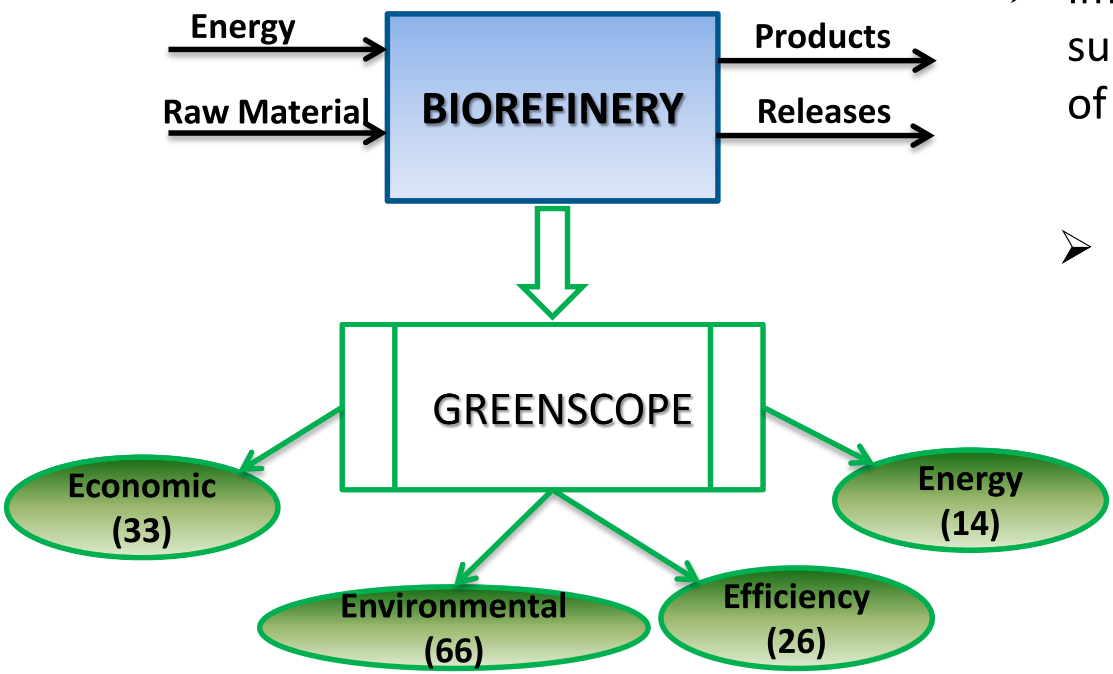
- Consider a wider range of sustainability metrics (beyond only costs, GHGs) that allow for more comprehensive direct comparison when evaluating design modifications and alternatives.

- Integrate a systematic framework in biorefinery process design
  - Understand impact of design variation
  - Evaluate alternative technologies
  - Track progress (vs baseline)

- Capture the multi-dimensional aspect of process design and operation

- Answer key questions like:
  - What process areas are in need of sustainability improvement?
  - What are the challenges and opportunities for achieving the best possible sustainability targets?
  - Where to allocate the resources?

# Approach: GREENSCOPE Sustainability Framework



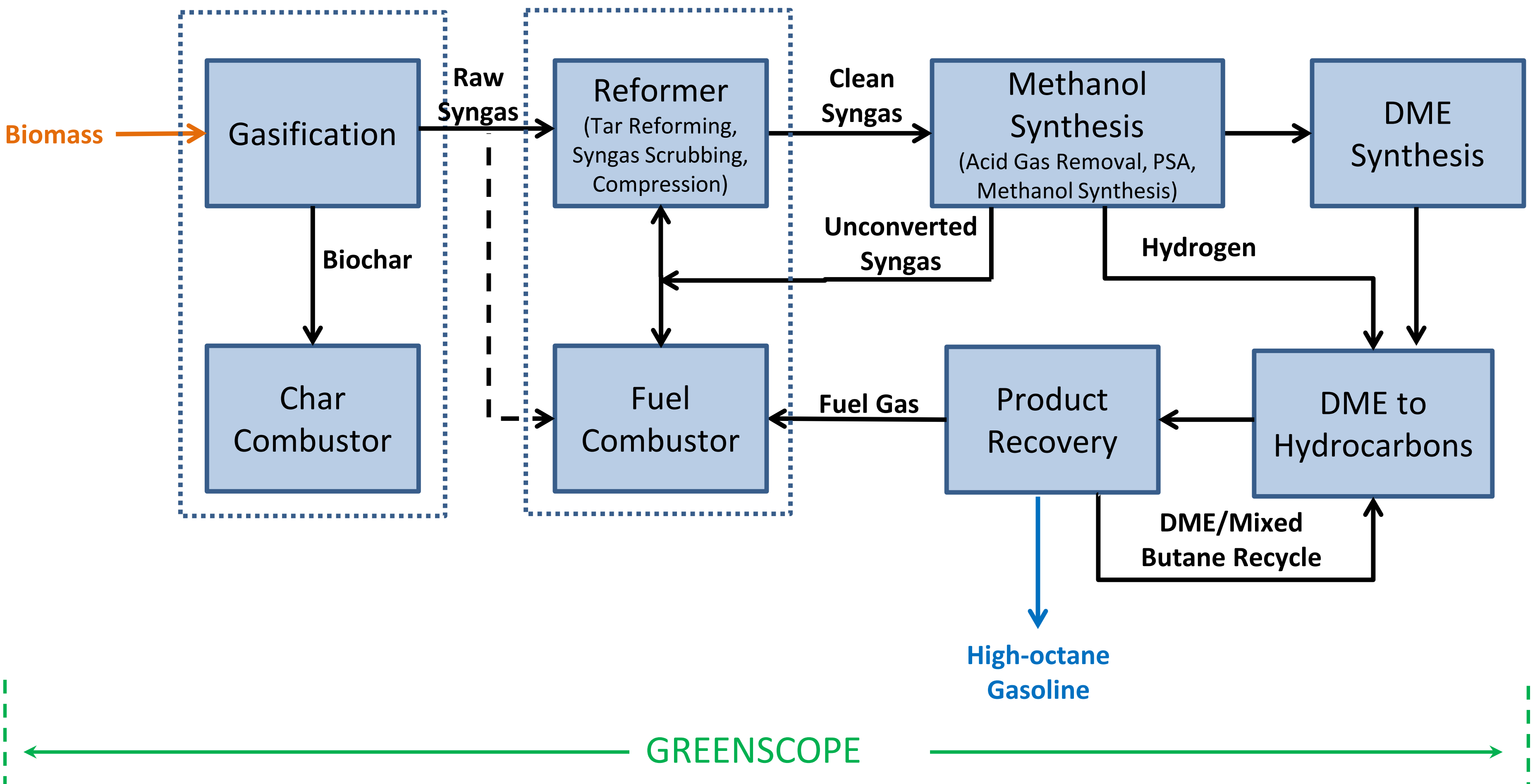

- Implementing GREENSCOPE for sustainability performance assessment of biomass-to-fuel pathways
- A sustainability tool for process evaluation and design
  - Ruiz-Mercado, et al., Ind. & Eng. Chem. Res. (2013) 52:6747-6760.
  - Ruiz-Mercado, et al., Clean Techn Environ Policy (2014) 16:703-717.
- Sustainability assessed by employing a set of indicators, categorized in 4 areas (4 E's)

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

Best: 100% sustainability; Worst: 0% sustainability

- The <u>strength/uniqueness</u> of the method was demonstrated through the definition of **best-target** and **worst-case** limits for each of the indicators (**dimensionless** scale)

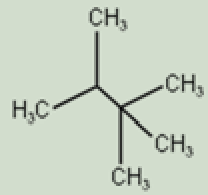
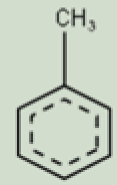
# **Case Study:** Conversion of biomass to high-octane gasoline blendstock via indirect liquefaction and methanol / dimethyl ether intermediates




Tan, et al. NREL Technical Report: http://www.nrel.gov/docs/fy15osti/62402.pdf

Tan, et al., Biofuels, Bioprod. Bioref. **10**:17-35 (2016): https://onlinelibrary.wiley.com/doi/epdf/10.1002/bbb.1611

# High-Octane Gasoline Pathway vs. MTG

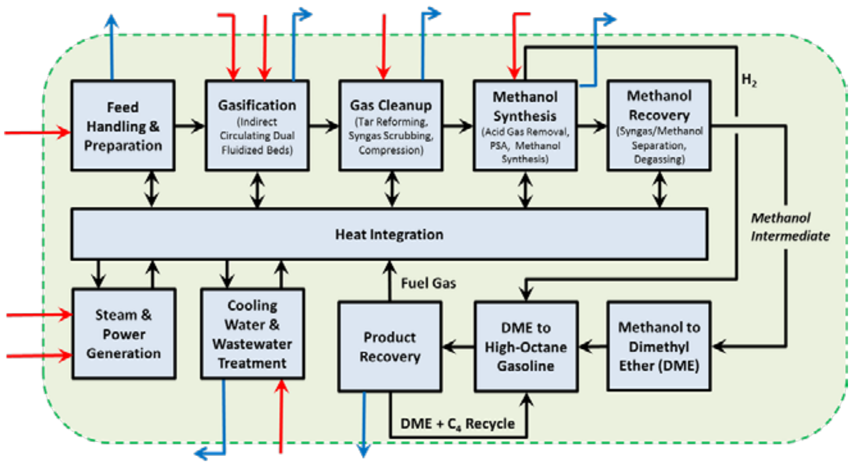
| Process Attribute | High-Octane Gasoline Pathway Target | Methanol to Gasoline (MTG) Pathway | Impact on Techno-Economic Analysis |
|---|---|---|---|
| Molecular structures favored in synthesis reactions | Branched paraffins<br> | Aromatics<br> | High octane product rich in branched paraffins, similar to a refinery alkylate. H-saturation decreases density, increasing product volume. |
| Example Compound<br>Specific Gravity | Triptane<br>0.70 | Toluene<br>0.87 | |
| Hydrocarbon synthesis catalyst | Beta-Zeolite<br>(12-membered rings) | ZSM-5<br>(10-membered rings) | Different pore sizes and structures result in different compound selectivities. |
| Octane number of gasoline-range product | RON: 95+<br>MON: 90+ | RON: 92<br>MON: 83 | Octane number increases value of product as a finished fuel blendstock. |
| Selectivity of $C_5$+product | $C_5$+ product only<br>(~65 Gal / Ton) | ~ 85% $C_5$+<br>(~55 Gal / Ton) | High selectivity to primary (premium quality) product maximizes overall product value. |
| Severity of synthesis operating conditions | 350 – 450 Deg. F<br>130 PSIA | 650 – 950 Deg. F<br>315 PSIA | The lower severity operating conditions result in lower capital and operating costs relative to MTG. |
| Coke formation | Coke formation is minimized by hydrogen addition and selectivity to branched paraffins rather than aromatics. | High propensity for coke formation due to aromatic coke pre-cursors. | Minimizing coke formation helps to maximize product yield / carbon efficiency and maximizes catalyst regeneration and replacement cycles. |

# Material and Energy Flows (per annum)

Capacity: 2,000 dry tonne/day

| Releases | | |
|---|---|---|
| Sand and ash purge | 9593 | ton |
| Tar reformer catalyst | 35 | ton |
| Scrubber solids | 37 | ton |
| Wastewater | 44677 | ton |
| Flue gas | 1206071 | ton |

| Raw Materials | | |
|---|---|---|
| Blended woody biomass (dry) | 724218 | ton |
| Magnesium oxide (MgO) | 27 | ton |
| Fresh olivine | 2141 | ton |
| Tar reformer catalyst | 35 | ton |
| Methanol synthesis catalyst | 21 | ton |
| DME catalyst | 26 | ton |
| Beta zeolite catalyst | 124 | ton |
| Zinc oxide catalyst | 10 | ton |
| Cooling tower water makeup | 7812 | ton |
| Boiler feed water makeup | 322214 | ton |
| Dimethyl Disulfide (DMDS) | 8 | ton |
| Amine (MDEA) makeup | 15 | ton |
| LO-CAT chemicals | 467 | ton |
| Boiler feed water chemicals | 11 | ton |
| Cooling tower chemicals | 2 | ton |
| No. 2 diesel fuel | 273 | ton |




**Data for GREENSCOPE**

Classification list, energy conversion factors, potency factors

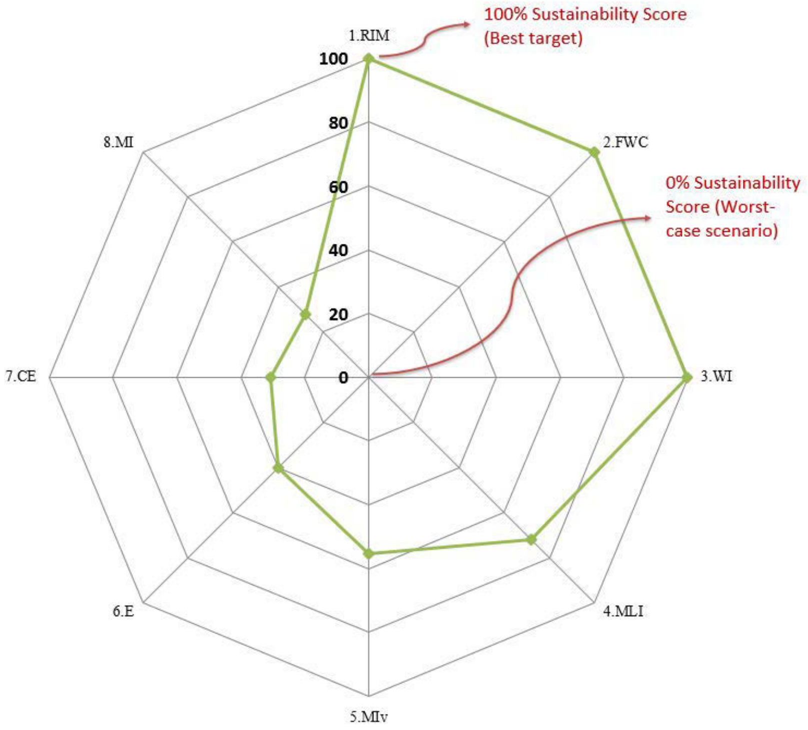
Physicochemical, thermodynamics, and toxicological properties

Equipment, raw material, utility, product costs, annual salary, etc.

| Products | | |
|---|---|---|
| High octane gasoline | 129700 | ton |
| Sulfur | 469 | ton |

| Economic | |
|---|---|
| Cost year / on-stream factor | 2014 / 90% |
| Total Installed Equipment Cost (TIC) | $247.1 MM |
| Total Capital Investment (TCI) | $430.4 MM |
| Total Annual Sales | $155.8 MM |
| Annual Manufacturing Cost (Average) | $95.4 MM |

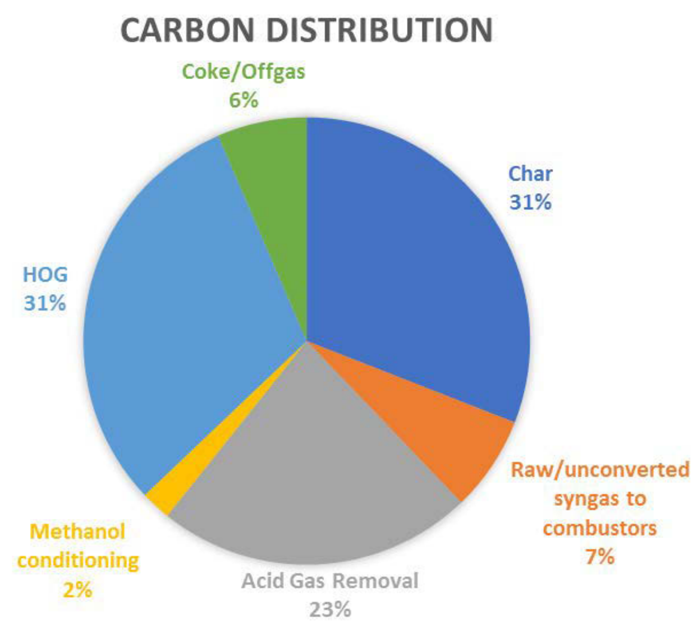
# GREENSCOPE Material Efficiency Indicators



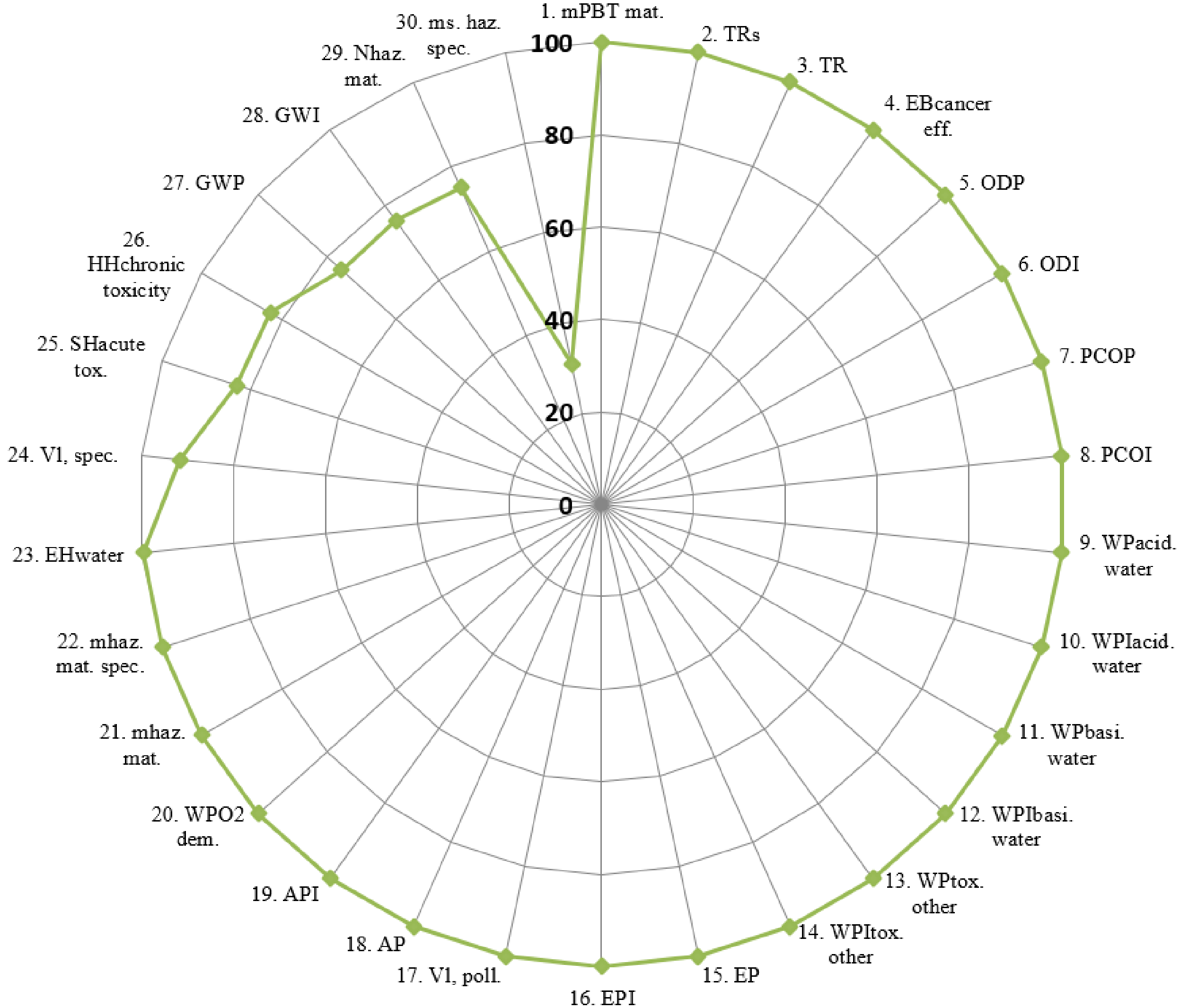

| Indicator | Description |
|---|---|
| 1. $RI_M$ | Renewability-Material Index |
| 2. FWC | Fractional water consumption |
| 3. WI | Water intensity |
| 4. MLI | Mass Loss Index |
| 5. $MI_v$ | Value mass intensity |
| 6. *E* | Environmental Factor |
| 7. CE | Carbon Efficiency |
| 8. MI | Mass intensity |

Carbon efficiency :
Percentage of carbon in the reactants remaining in the final product.
Best target = 1
Worst-case = 0

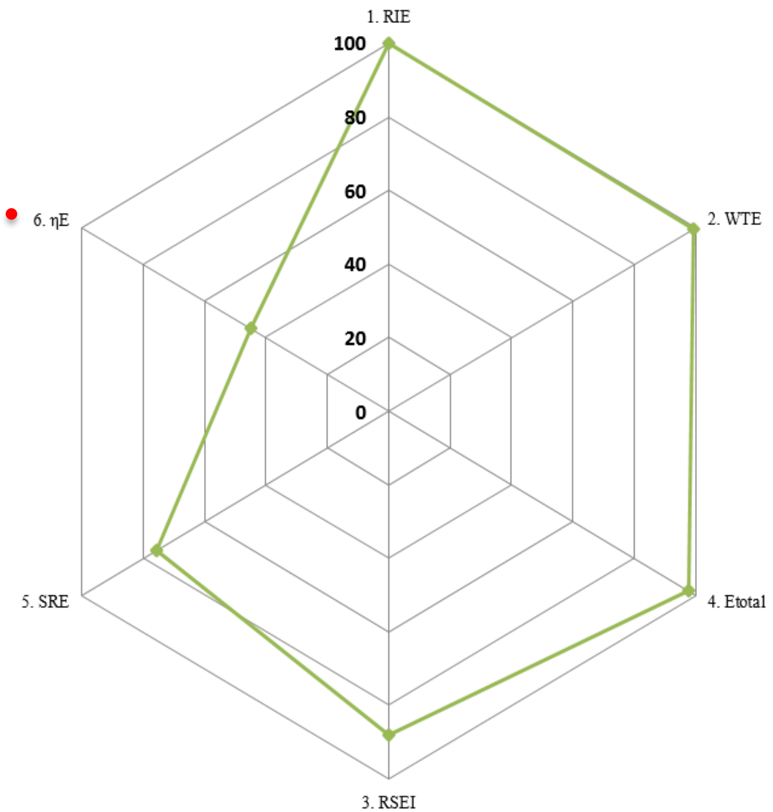
Recycle CO2 from AGR to reformer for dry reforming
Reactivate CO2 from AGR in HC synthesis reactor



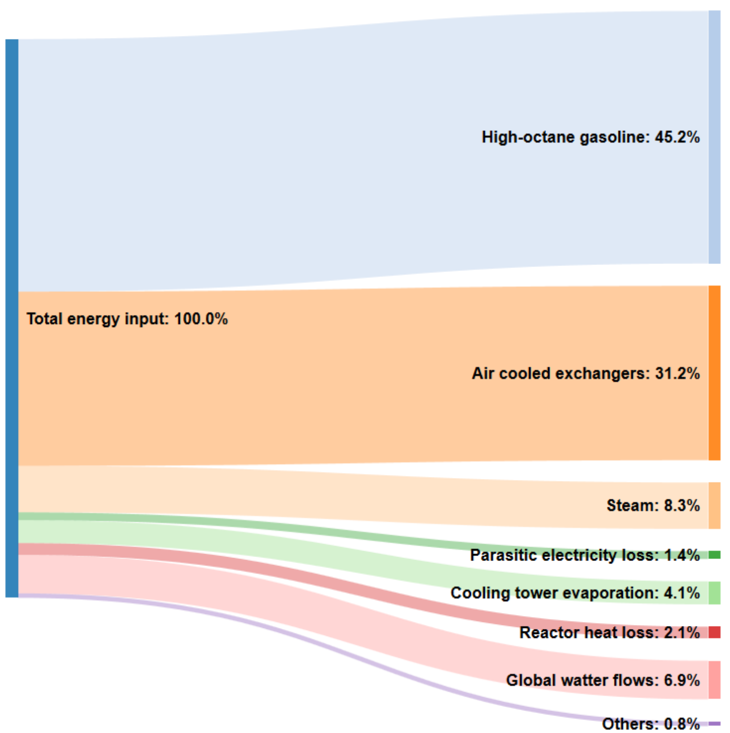
# GREENSCOPE Environmental Indicators



# GREENSCOPE Energy Indicators

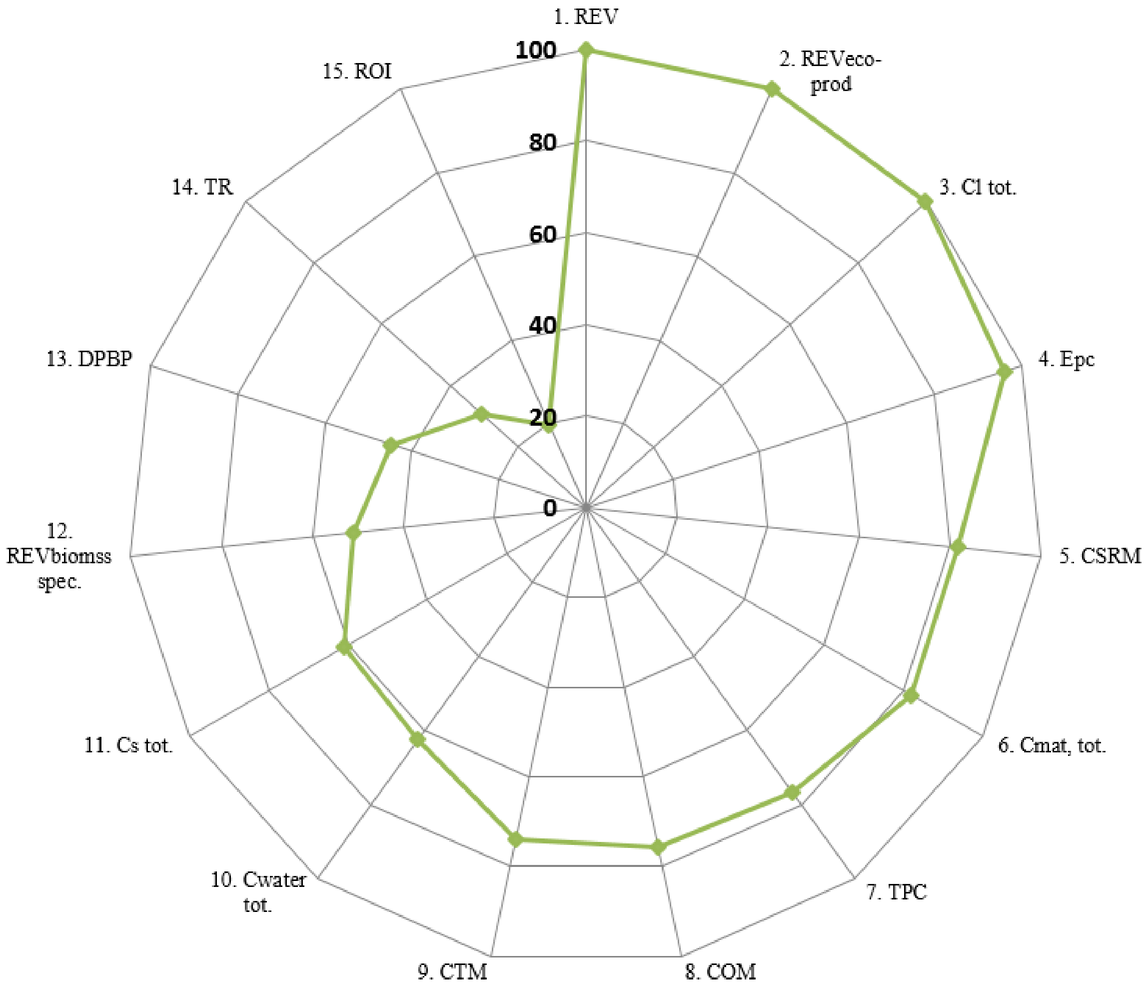



| Indicator | Description | Sustainability % Score |
|---|---|---|
| 1. RIE | Renewability-energy index | 100 |
| 2. WTE | Waste treatment energy | 99.2 |
| 3. RSEI | Specific energy intensity | 97.9 |
| 4. Etotal | Total energy consumption | 88.1 |
| 5. SRE | Solvent recovery energy | 75.6 |
| 6. $\eta E$ | Resource-energy efficiency | 45.0 |




Resource-energy efficiency :
The ratio between the energy content of the products to the total energy content of the feedstocks
Best target = 1
Worst-case = 0
Increasing HOG yield (catalyst productivity) and better heat integration for achieving improved process sustainability

# GREENSCOPE Economic Indicators

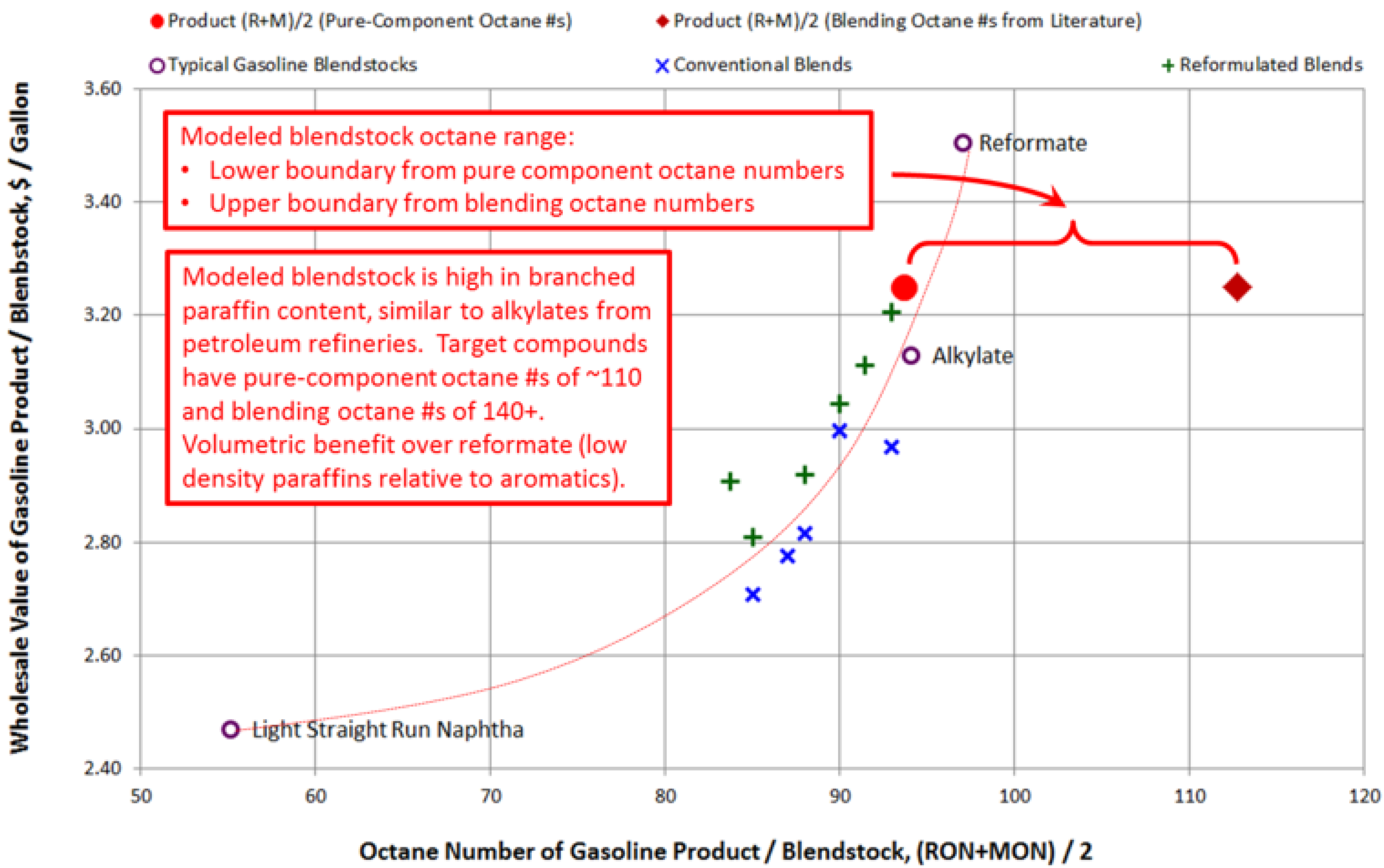



Opportunities potentially can improve sustainability indicator scores for

- Discounted payback period (DPBP)
- Turnover ratio (TR)
- Rate of return on investment (ROI)

Increase sales revenues and decrease capital costs

# "Premium" product value can improve sales/revenue/income

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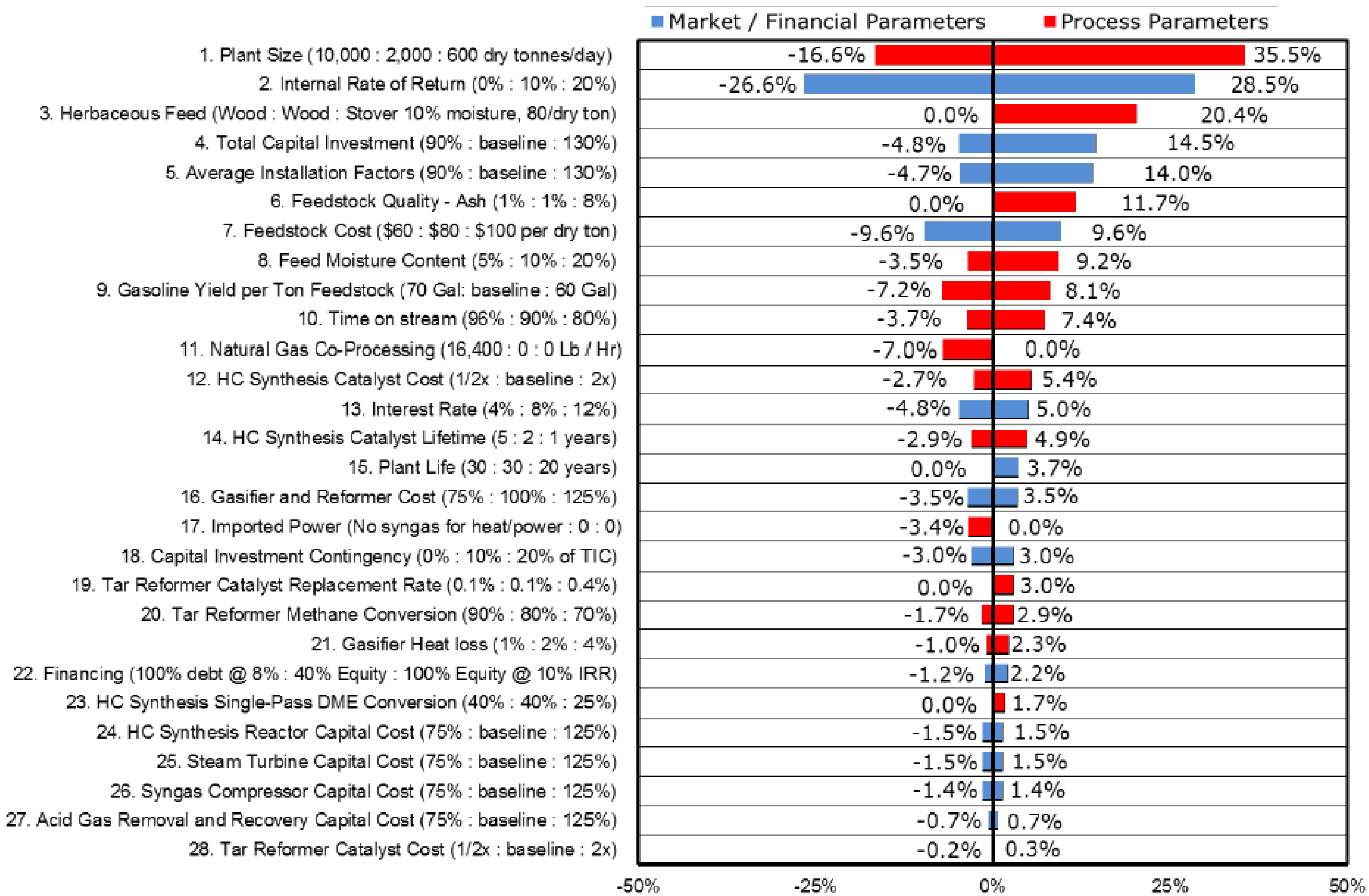
# Key parameters that can impact economic indicators

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# Summary

- Integrating sustainability in process design should be considered a worthy practice in biorefinery design. It should also be done in early stages of development and not something to wait to do until the end.

- Considering multiple metrics for evaluation when comparing technologies and design modifications can help make more informed decisions by looking at the design more holistically.

- GREENSCOPE can be an effective tool for biomass-to-fuels/chemicals process sustainability evaluation and design.

- The successful implementation and use of GREENSCOPE for a sustainability performance assessment for the production of high-octane gasoline from biomass has been demonstrated.

- The conceptual process exhibits high sustainability in every aspect of the sustainability areas. Results from the current sustainability evaluation help answer the following questions:
  - What process areas are in need of sustainability improvement?
  - What are the challenges and opportunities for achieving the best possible sustainability targets?
  - Where to allocate the resources?

# Acknowledgements

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