Integrated Hybrid Life Cycle Optimization for Multi-Scale Sustainability Analytics of Energy Systems

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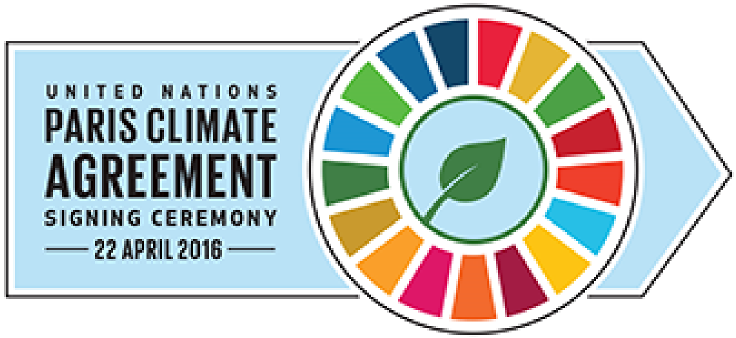
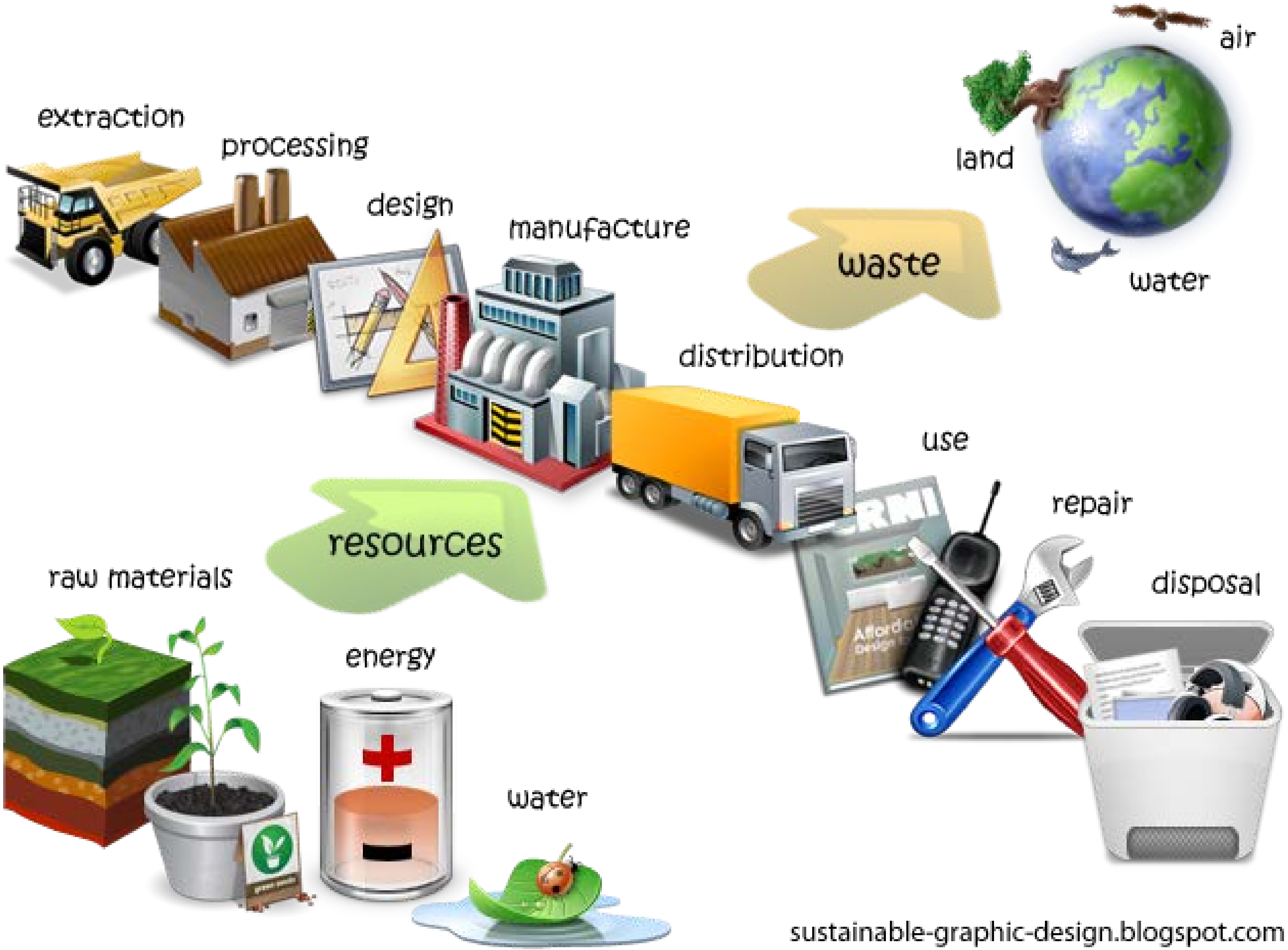
Environmental Sustainability Issues



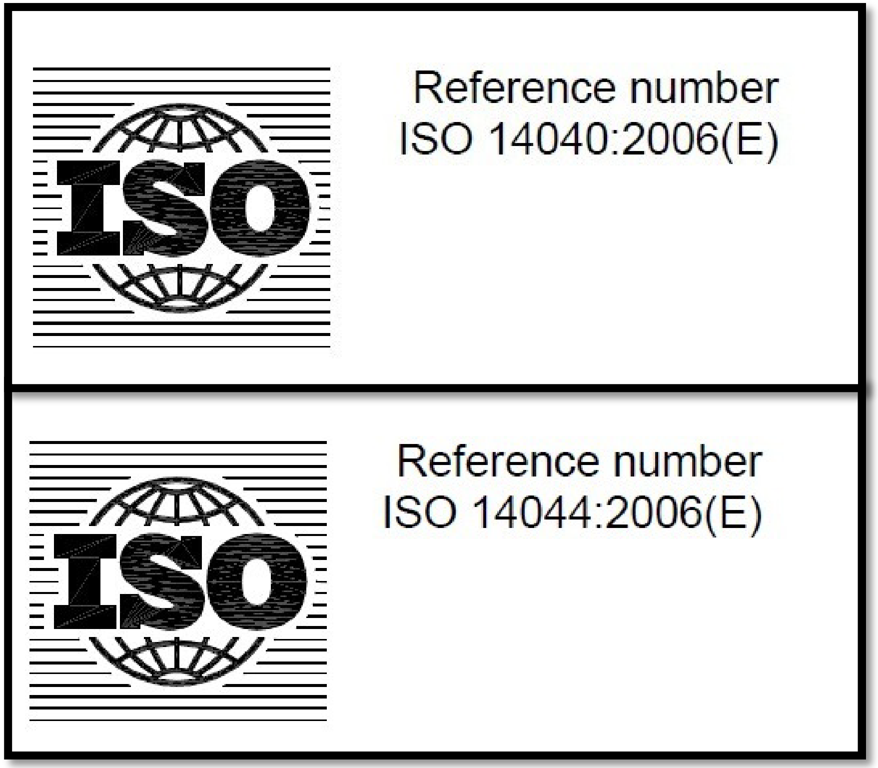
Life Cycle Analysis (LCA) – "Cradle to Grave"



Life Cycle Analysis (LCA)

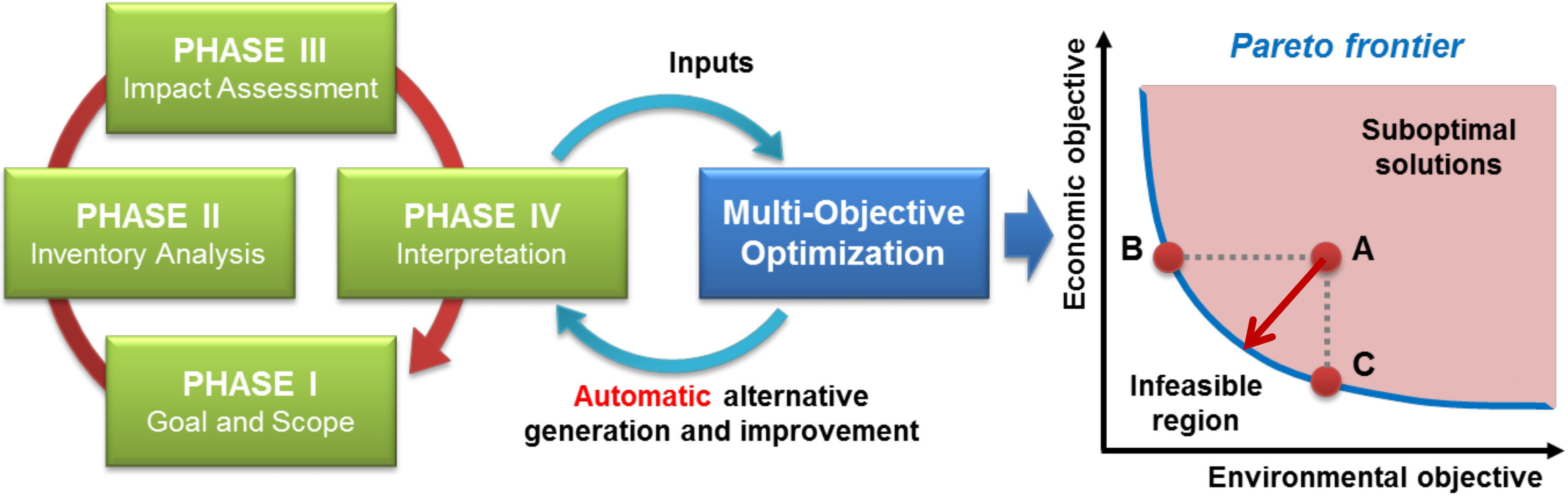
- Quantifying environmental impacts of **complex systems**
- Modeling the entire product/process **life cycle**
- Holistic view of the system

Life Cycle Analysis



Life Cycle Optimization (LCO)

Integrating life cycle analysis approach with multi-objective optimization techniques

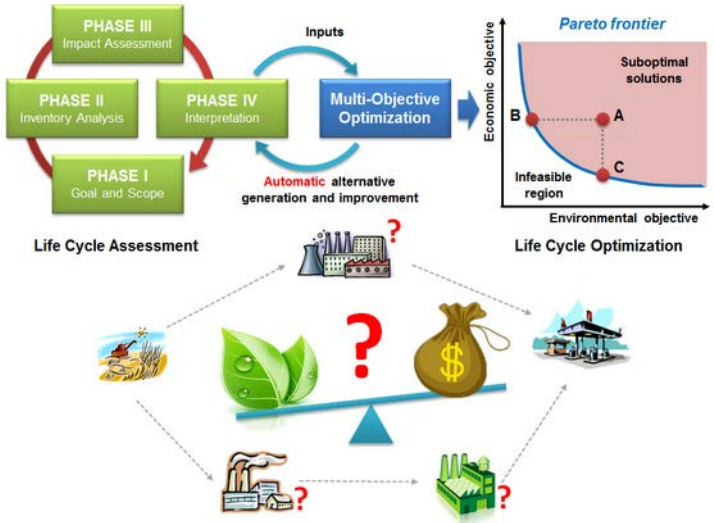


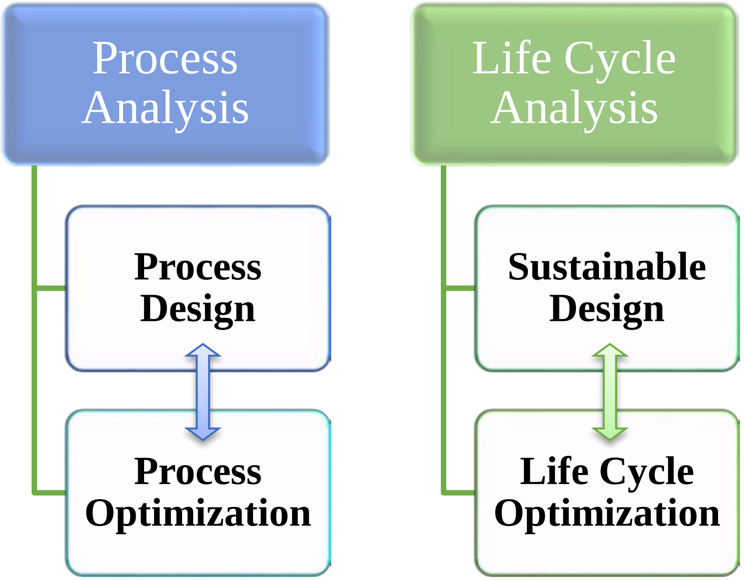
Life Cycle Analysis

Life Cycle Optimization

Life Cycle Optimization: Theory and Methods

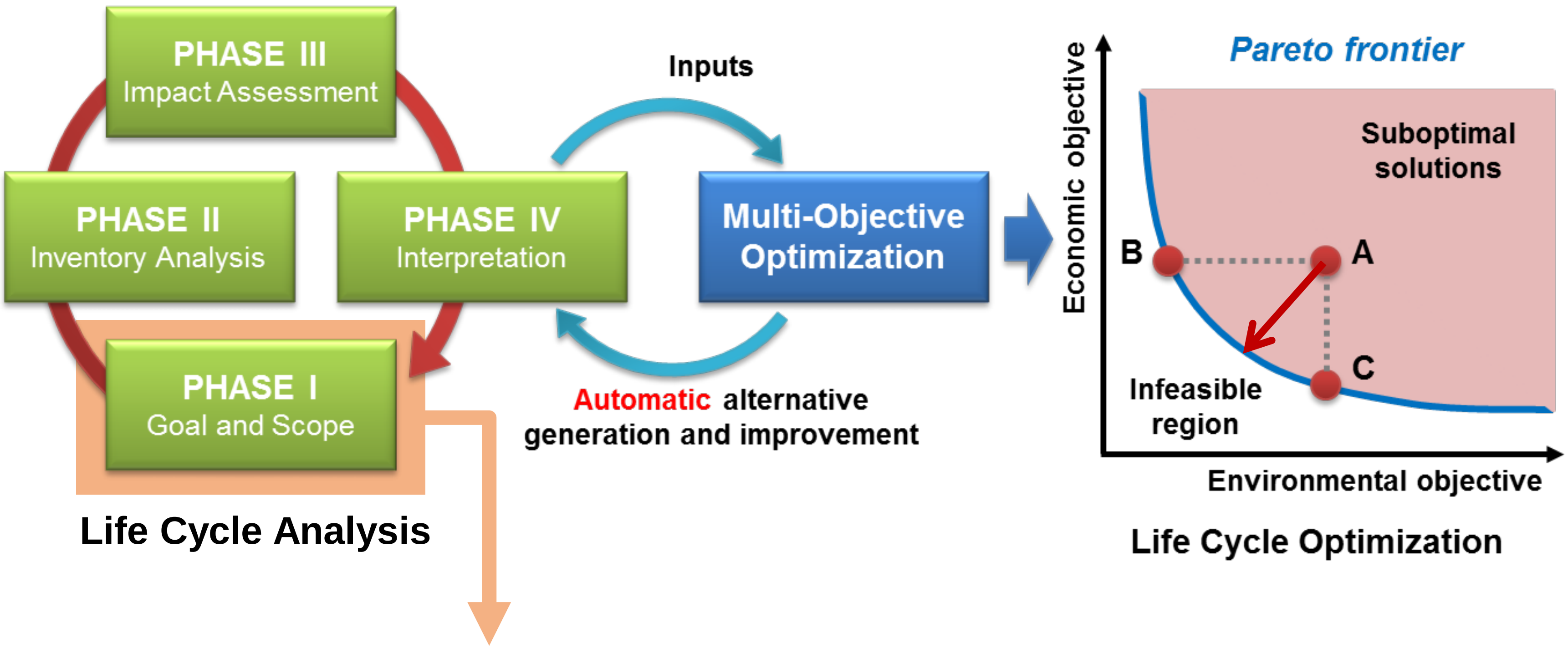
- **Life Cycle Optimization**
  - Life Cycle Analysis + Techno-economic Analysis + Design Optimization





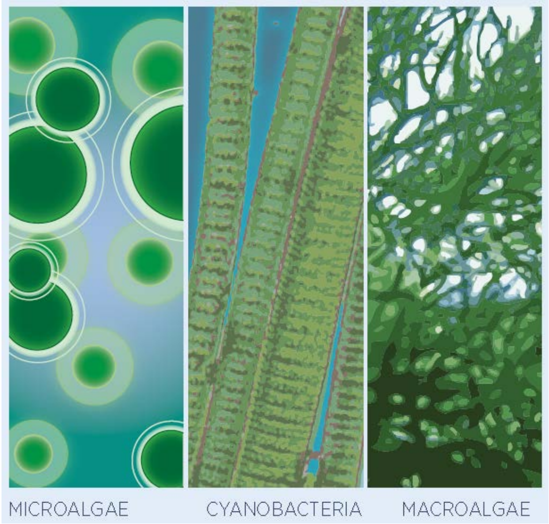
- **Research Challenges**
  - How to **seamlessly** integrate LCA into process systems optimization?
  - How to define the "optimal" systems boundary and functional unit?
  - How to incorporate state-of-the-art inventory analysis methods in LCO?
  - How to deal with uncertainty and solve large-scale LCO problems?

Process-based Life Cycle Optimization (LCO)



- **Systems boundary** must be defined in Phase I of LCA
- **Functional unit** serves as the basis for calculation and comparison

Motivation

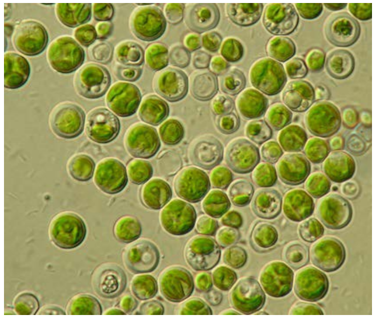


Biofuels

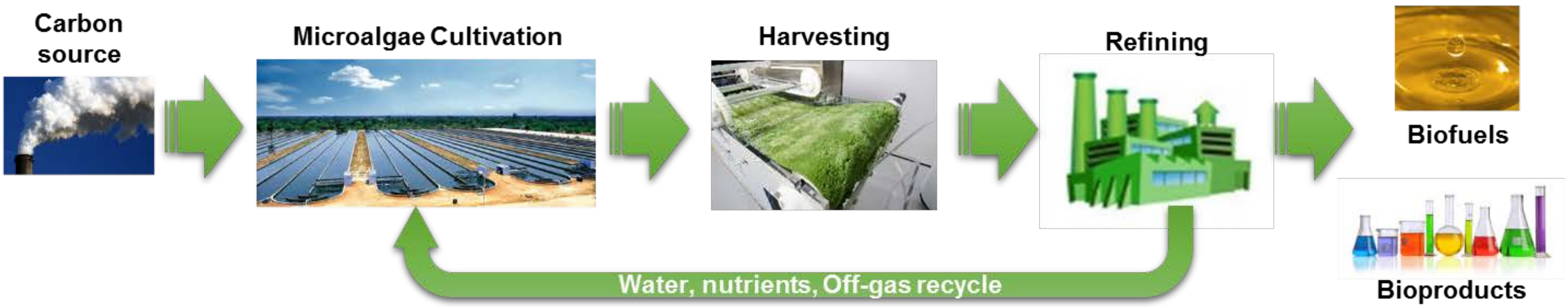
Bioproducts

- **Algae**
  - Microalgae, cyanobacteria, & macroalgae
  - Non-food; high yield; rich in oil
- **Algae-based biorefinery**
  - Consume and utilize CO_2; recycle nutrients & water
  - Produce fuels and value-added products
  - **Process economics? Environmental sustainability?**

Chlorella Vulgaris

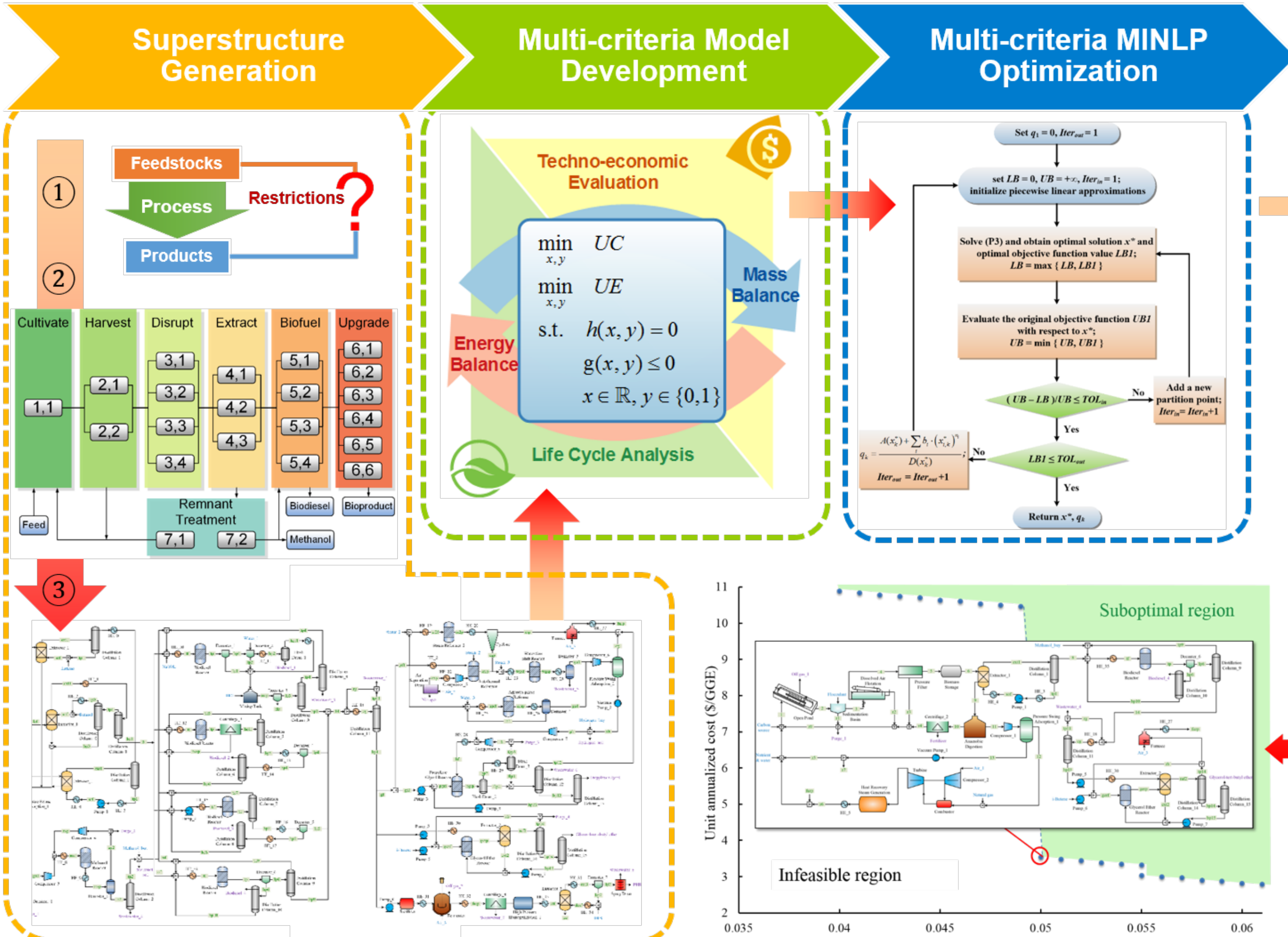


Algal Biorefinery Process Design and Optimization



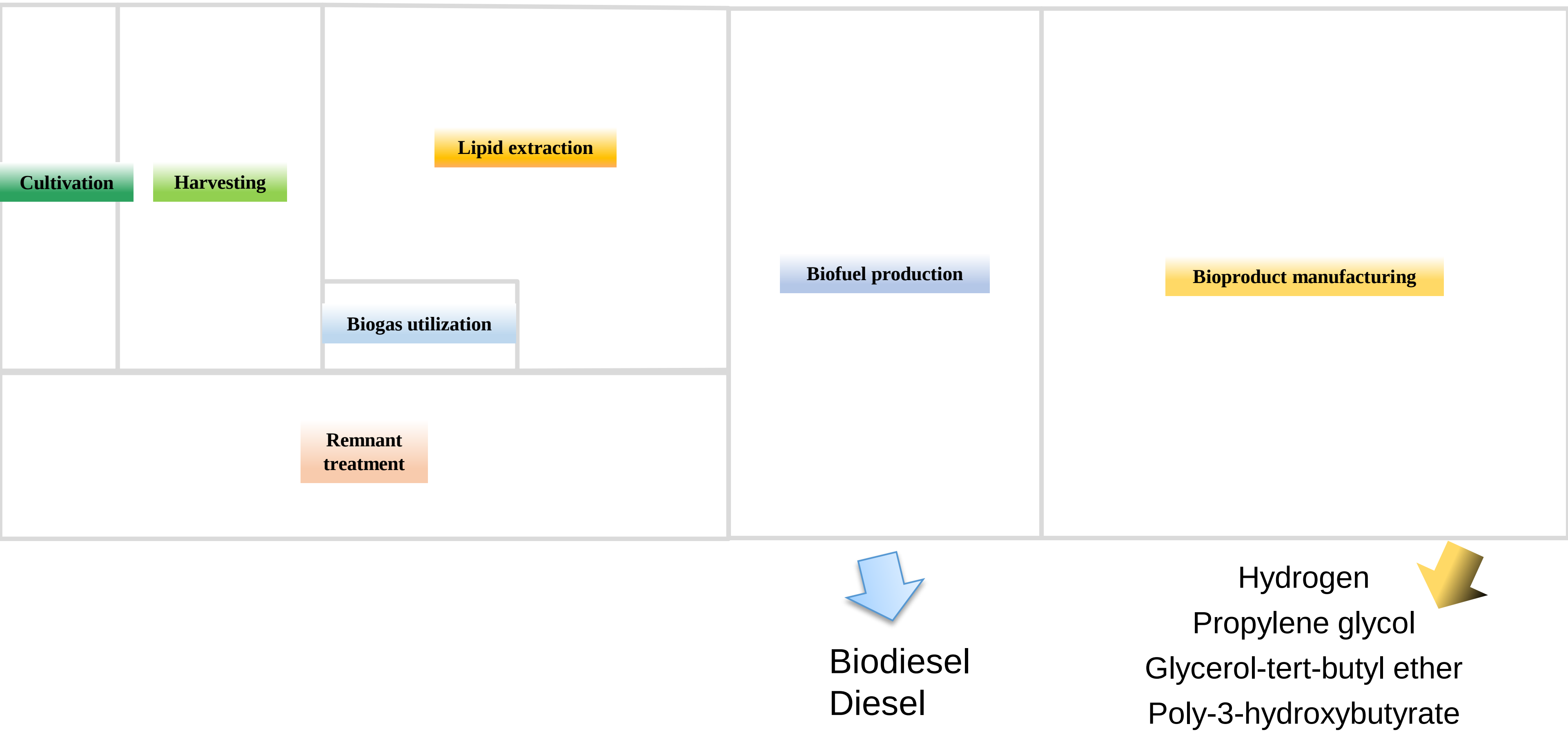
- **Optimal design and synthesis of algal biorefinery**
  - Selection of technology, pathway, and processing methods
  - Determination of product portfolio under the given feed
  - Recycling nutrients, water and carbon dioxide
  - Mass balance, capacity, and equipment sizing
  - Energy and utility consumption
  - Process economics ? → **Techno-econmic analysis**
  - Environmental sustainability ? → **Life cycle analysis**
  - Cost-effective & sustainable design

LCO for Sustainable Design of Energy Systems

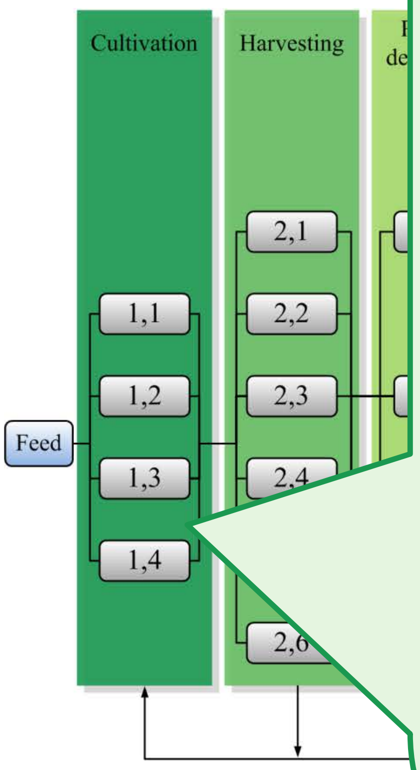


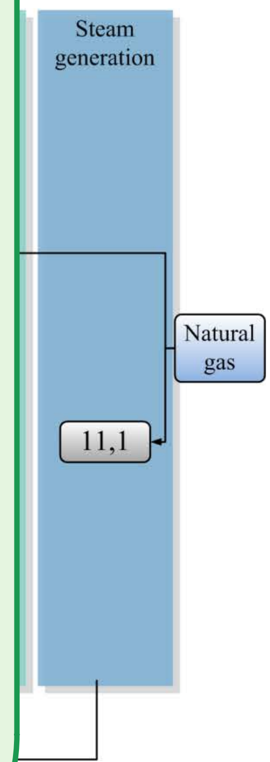
Gong & You (2015). *Current Opinion in Chemical Engineering*, 10, 77-86.

Superstructure of Algae Process



Superstructure of Algae Process





<1,2> Flat plate photobioreator

<1,3> Bubble column photobioreator

<1,4> Tubular photobioreator

7,800+ processing pathways

Optimization Model: Constraints for ONE Unit

Mass and material balance
Process network design specifications
Technology and pathway selection
Equipment sizing and capacity

Techno-economic analysis

Energy balance
Utility consumption

Life cycle environmental impact analysis

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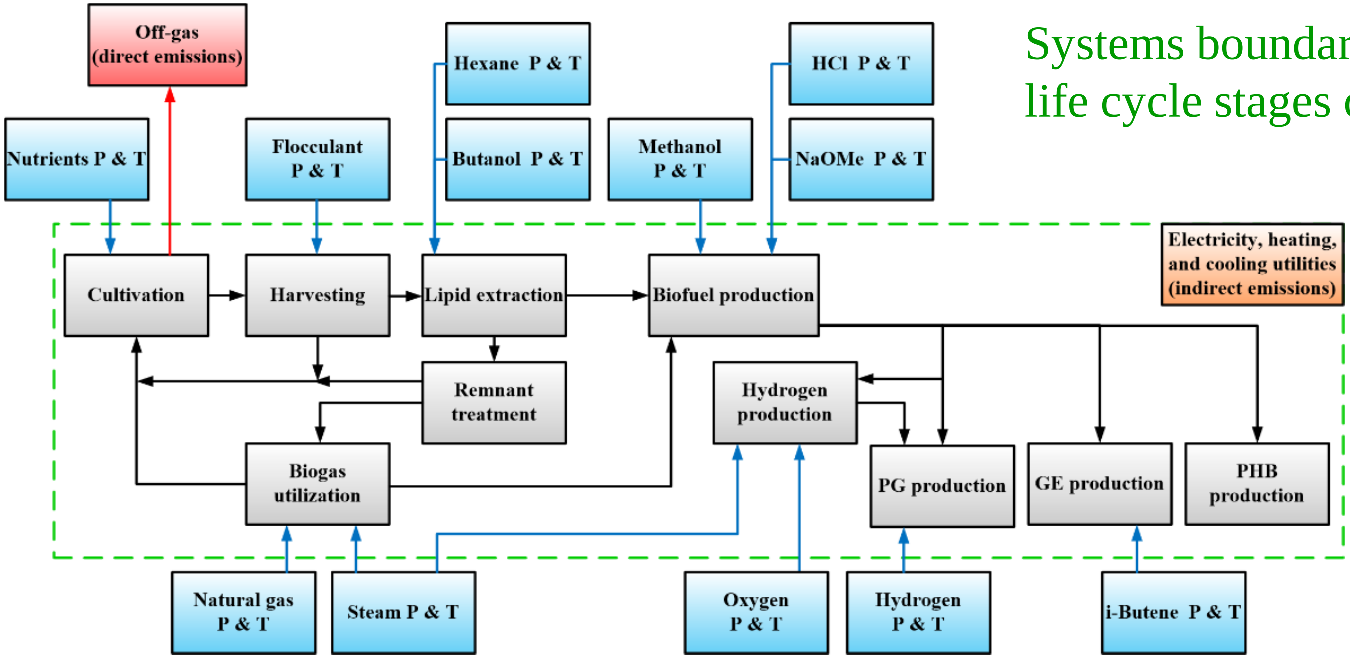
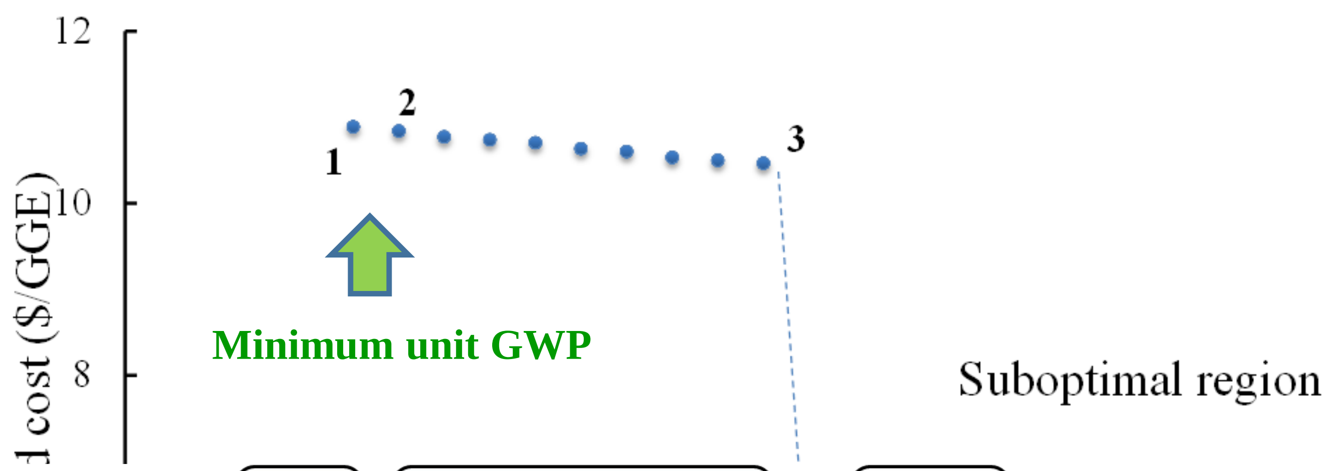
Optimization Model: Objectives

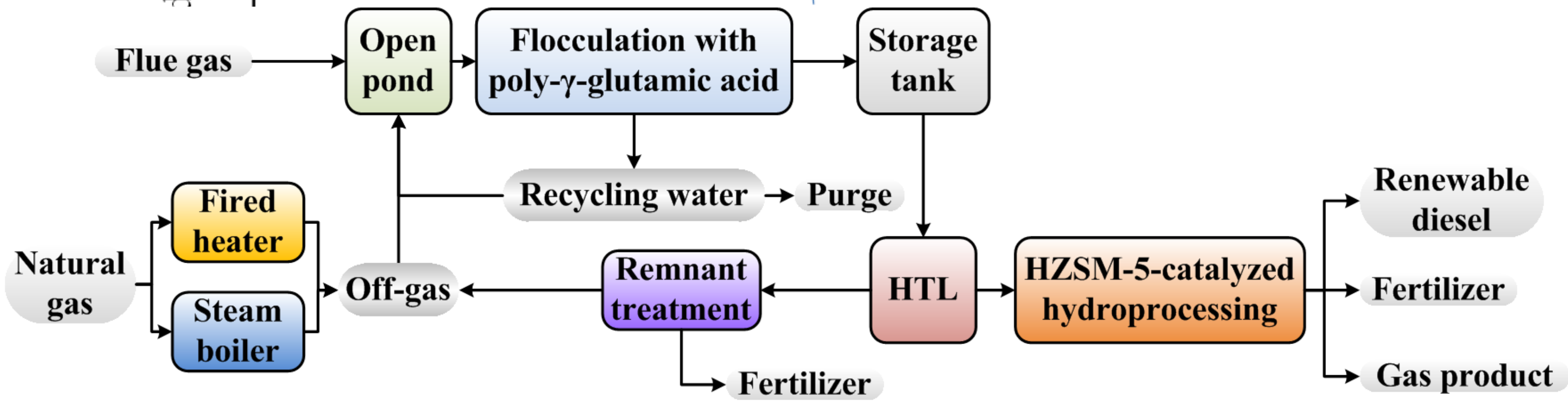
- **Objectives:**
  - Minimize: Unit cost of fuel product **(techno-economic analysis)**
    - CAPEX + OPEX
    - Credit from selling by-products (glycerol, fertilizer, biogas, …)
  - Minimize: Unit life cycle GHG emission **(life cycle analysis)**
    - Direct emissions: Cultivation, remnant treatment, & utility generation
    - Indirect emissions: External utility, e.g. electricity and steam, …



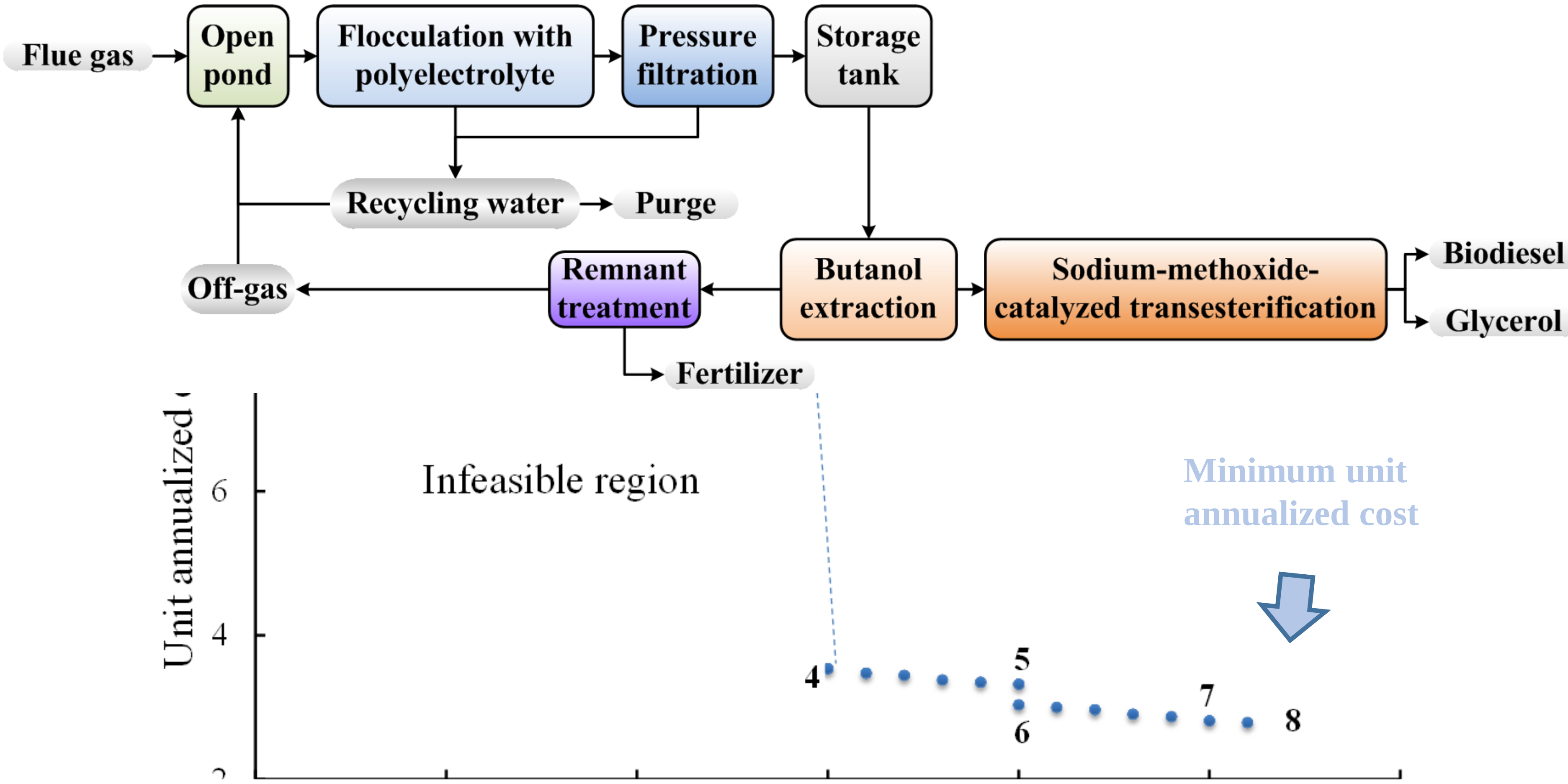
Systems boundary and life cycle stages of LCA

Pareto Optimal Curve

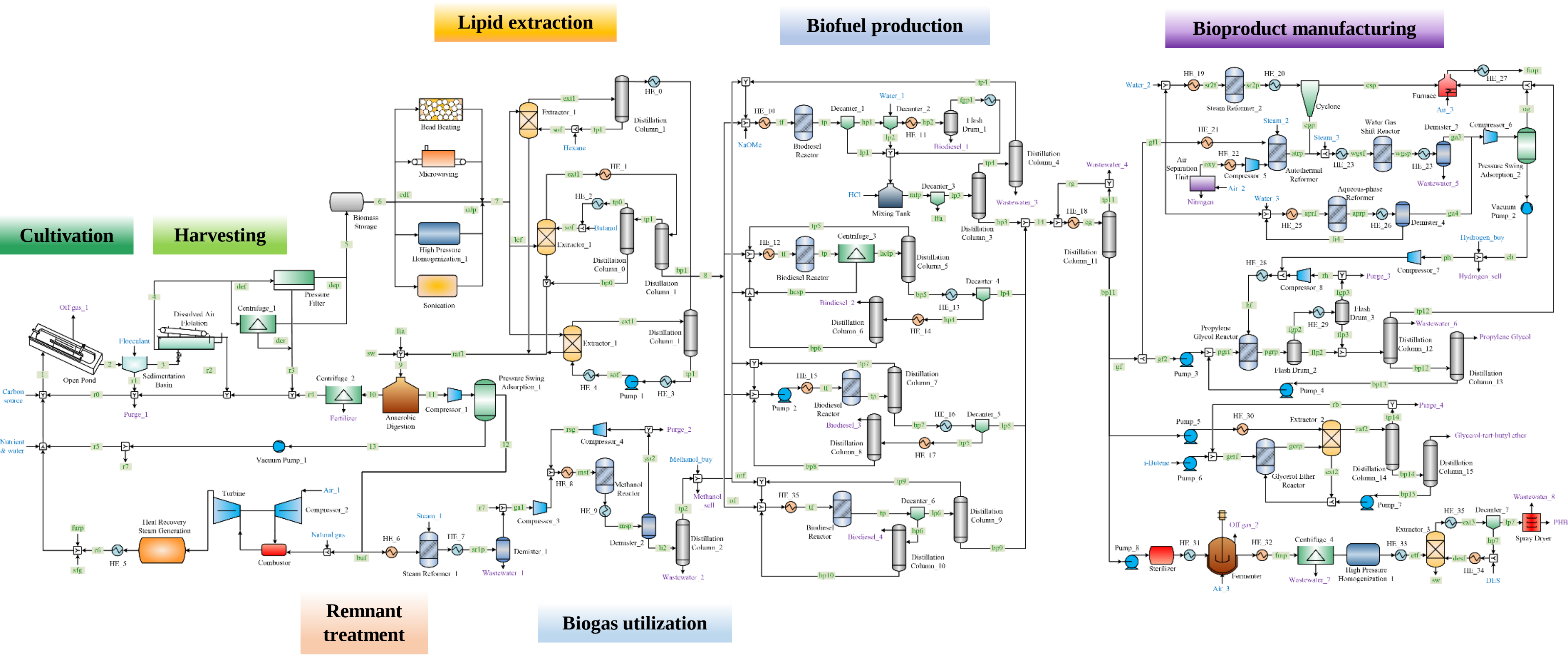




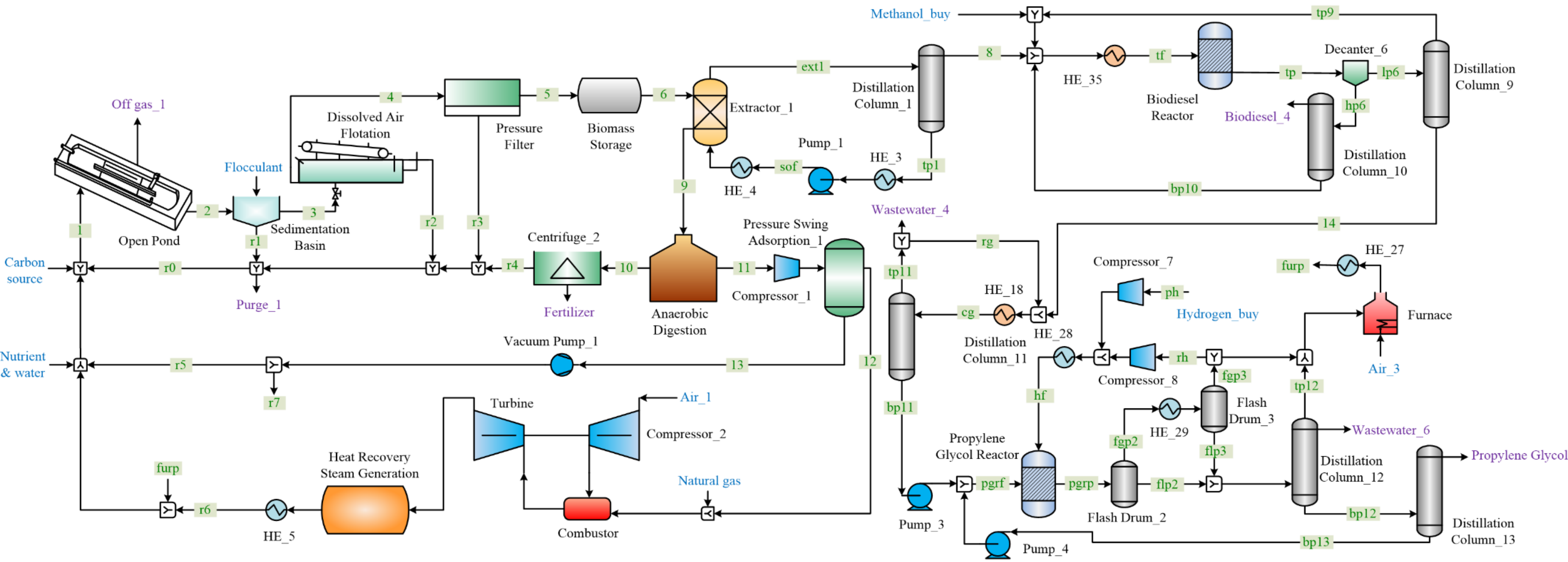
Pareto Optimal Curve



Superstructure of Algae Process



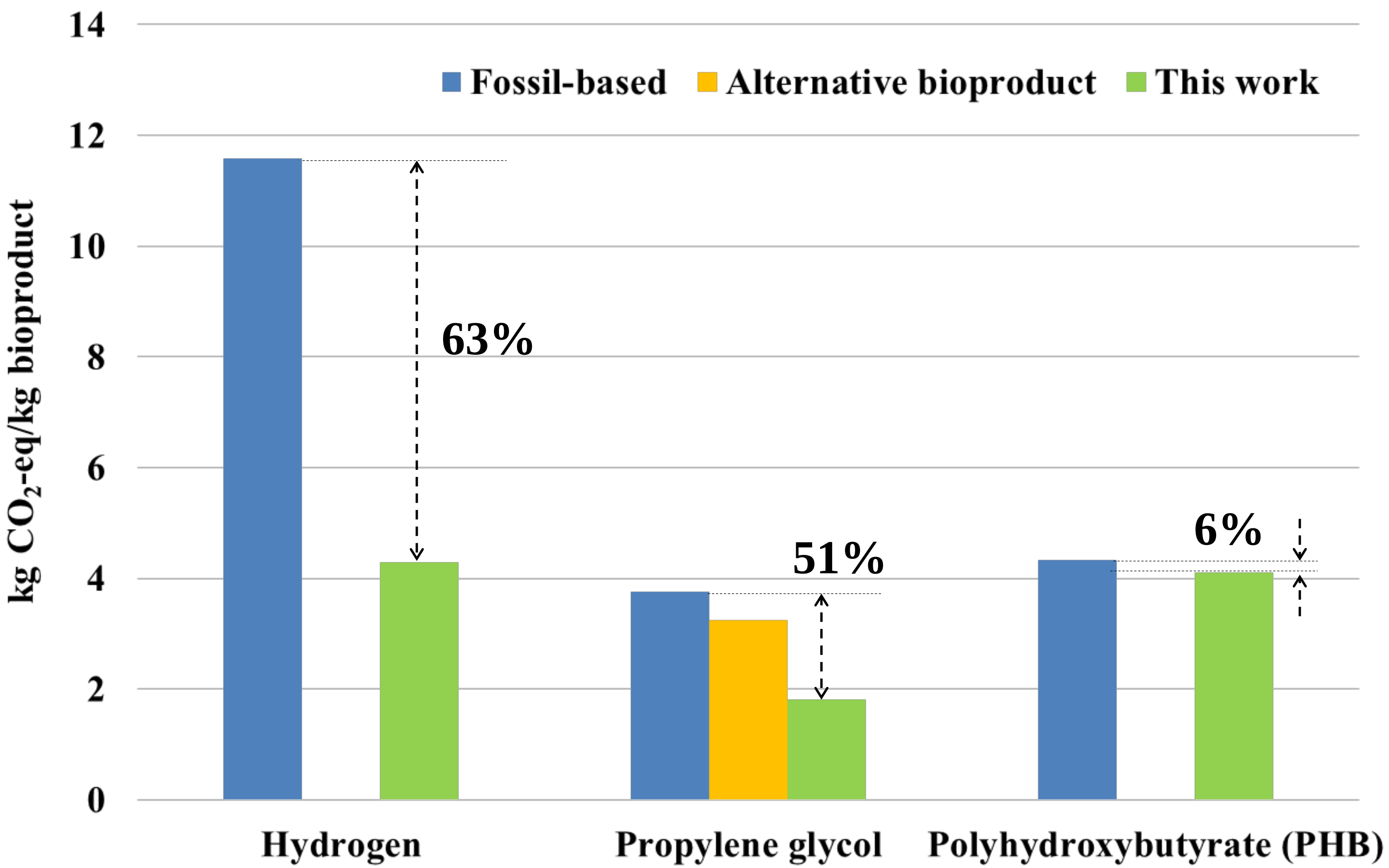
Optimal Design of Minimum Unit Biofuel Cost



Unit cost of biofuel ($/GEG)	Unit GHG emissions (kg CO_2-eq/GEG)	Biodiesel Throughput (million GGE)	Bioproduct
2.79	**7.21**	47	Propylene glycol

2.71 – 3.78	14.43	Petroleum-derived diesel

GWP of Algae-based H_2, PHB, Propylene Glycol



Alternative bio-based propylene glycol is derived from soybean by ADM(R).

ACS Sustainable Chem. Eng. 2015, *3*, pp 82−96

ACS Sustainable Chemistry & Engineering

Research Article

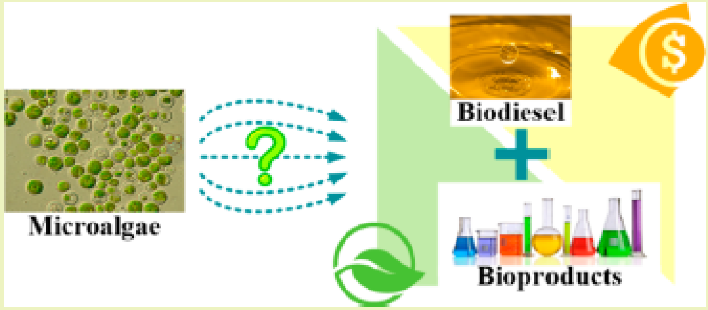
pubs.acs.org/journal/ascecg

Value-Added Chemicals from Microalgae: Greener, More Economical, or Both?

Jian Gong and Fengqi You*

Department of Chemical and Biological Engineering, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, United States

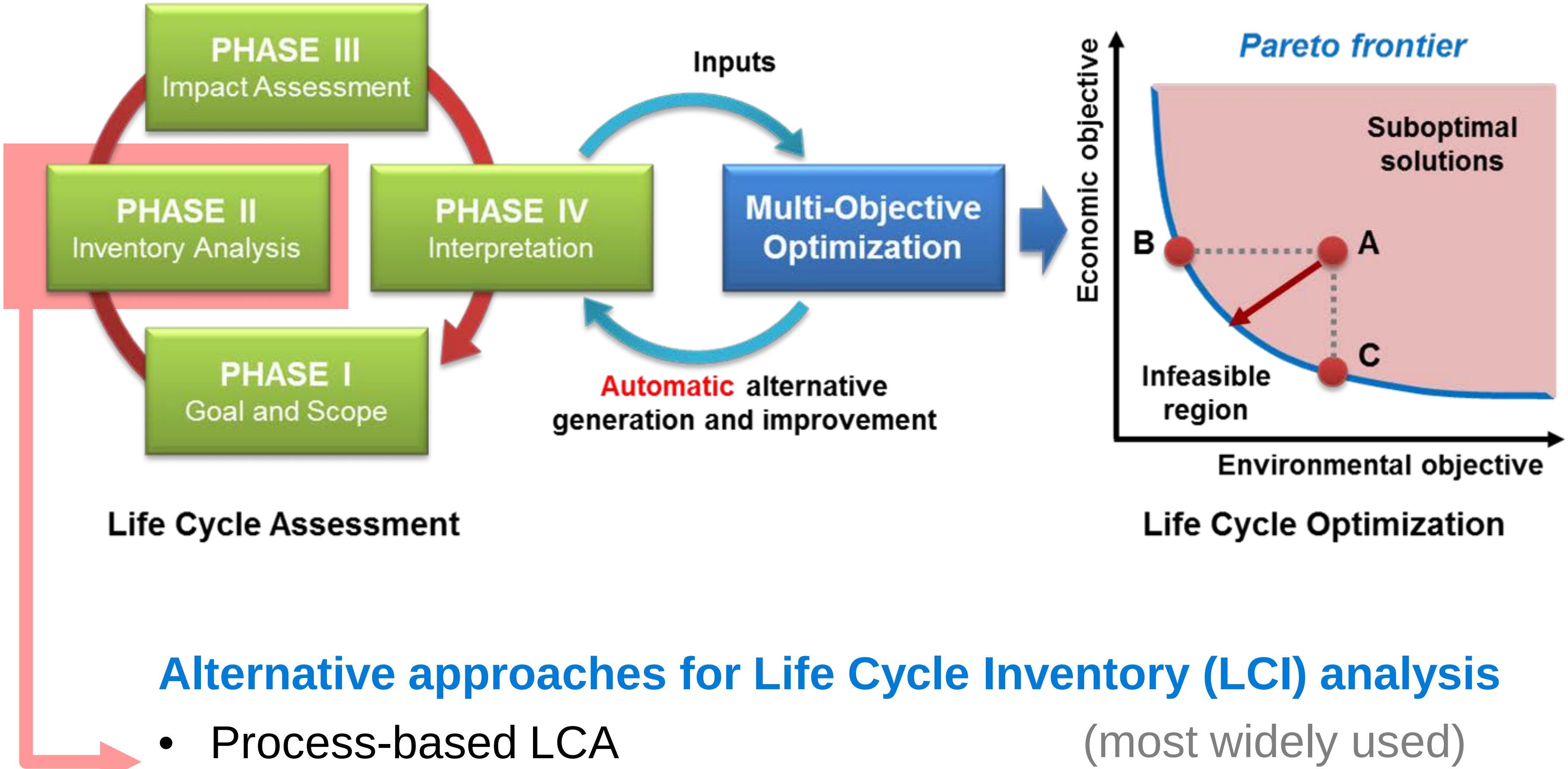
Supporting Information



ABSTRACT: This paper addresses the sustainable design and synthesis of manufacturing processes for making algal bioproducts. We propose by far the most comprehensive superstructure capable of producing biodiesel, hydrogen, propylene glycol, glycerol-*tert*-butyl ether, and poly-3-hydroxybutyrate from microalgae. The major processing sections include cultivation, harvesting, lipid extraction, remnant treatment, biogas utilization, biofuel proneduction, and bioproduct manufacturing. On the basis of the superstructure, we integrate a cradle-to-gate life cycle analysis and techno-economic analysis with multiobjective optimization to simultaneously optimize the environmental and economic performance. We also apply a tailored global optimization algorithm to efficiently solve the problem in reasonable computation times. Results show that the most environmentally sustainable processes reduce life cycle greenhouse gas emissions per kilogram of the algal bioproducts by 5% to 63%, compared with petrochemical counterparts. In addition, the coproduction of value-added bioproducts in the algal glycerol process helps reduce the biodiesel production cost to as low as \$2.79 per gasoline-gallon-equivalent.

KEYWORDS: *Life cycle analysis, glycerol, bioproduct, algal biofuels, global optimization*

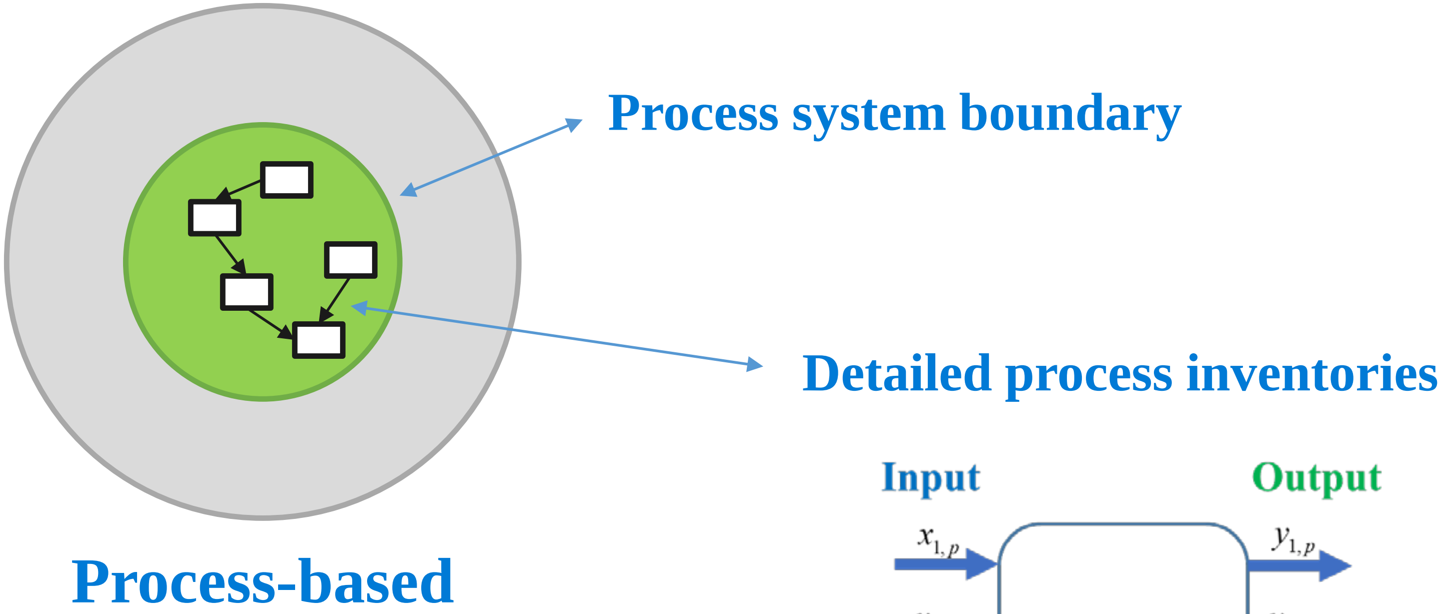
Hybrid Life Cycle Optimization (h-LCO)

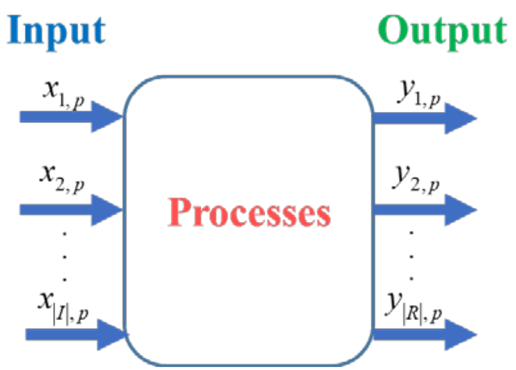


Alternative approaches for Life Cycle Inventory (LCI) analysis

- Process-based LCA (most widely used)
- Economic Input-Output (EIO)-based LCA (for macroscopic analysis)
- **Hybrid LCA** (state of the art)

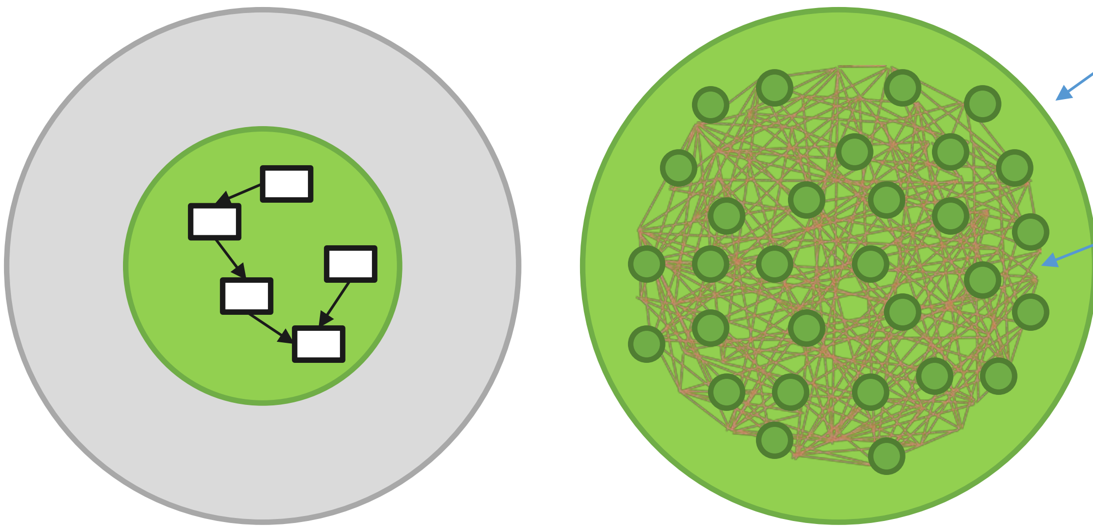
Process-based LCA





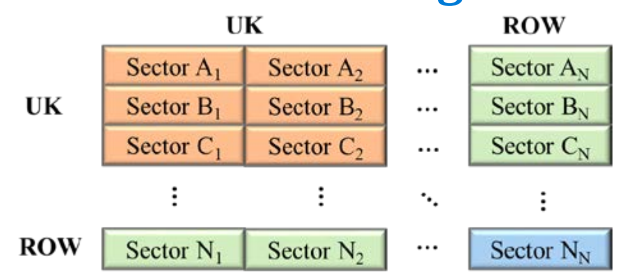
Resolution	Process
Construction	Bottom Up
Scope	Selected Processes

EIO-based LCA



Entire macroeconomy

Transactions among sectors



Process-based

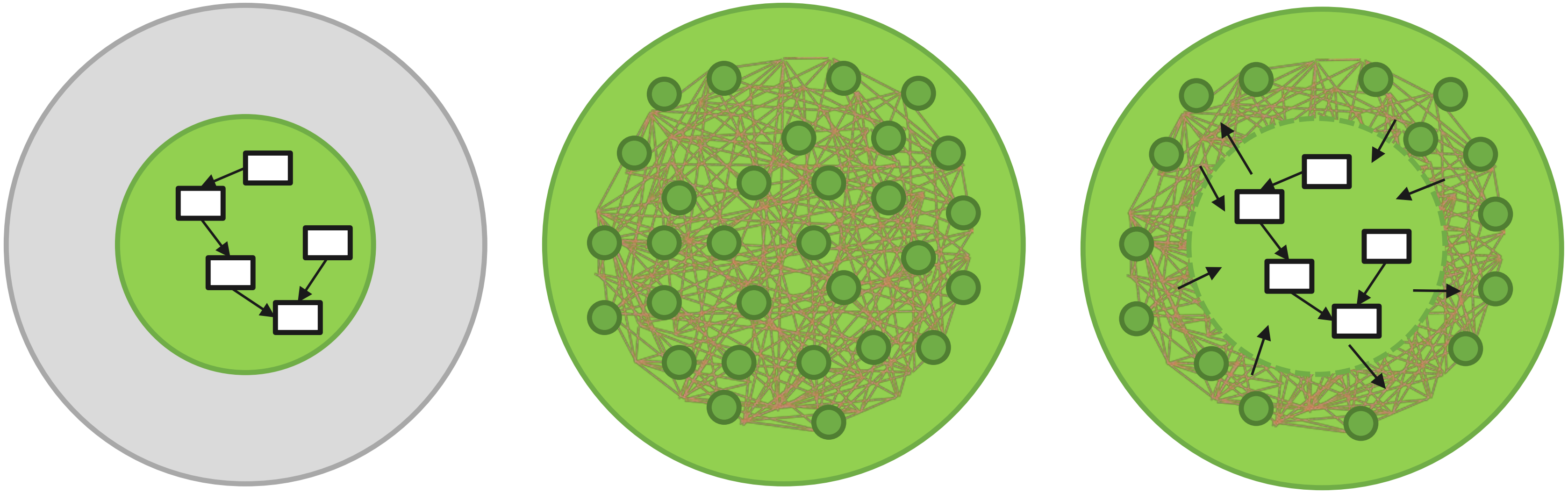
EIO-based

Resolution	Process	Sector
Construction	Bottom Up	Top Down
Scope	Selected Processes	Entire Economy

Sectors:

Agriculture, mining, construction, manufacturing, wholesale trade, retail trade, transportation, etc.

Integrated Hybrid LCA



Process-based | **EIO-based** | **Integrated Hybrid**

Resolution	Process	Sector	Process (foreground) Sector (background)
Construction	Bottom Up	Top Down	Hybrid
Scope	Selected Processes	Entire Economy	Entire Economy

Insights into Different LCA Approaches

Process-based LCA

Drawbacks:

- System boundary truncation
- Underestimation of the true impact

Advantage:

- Specificity of process analysis

EIO-based LCA

Drawbacks:

- Loss of precision at process level

Advantage:

- Completeness of life cycle boundary

Integrated Hybrid LCA

Integrates process- and IO-based LCA

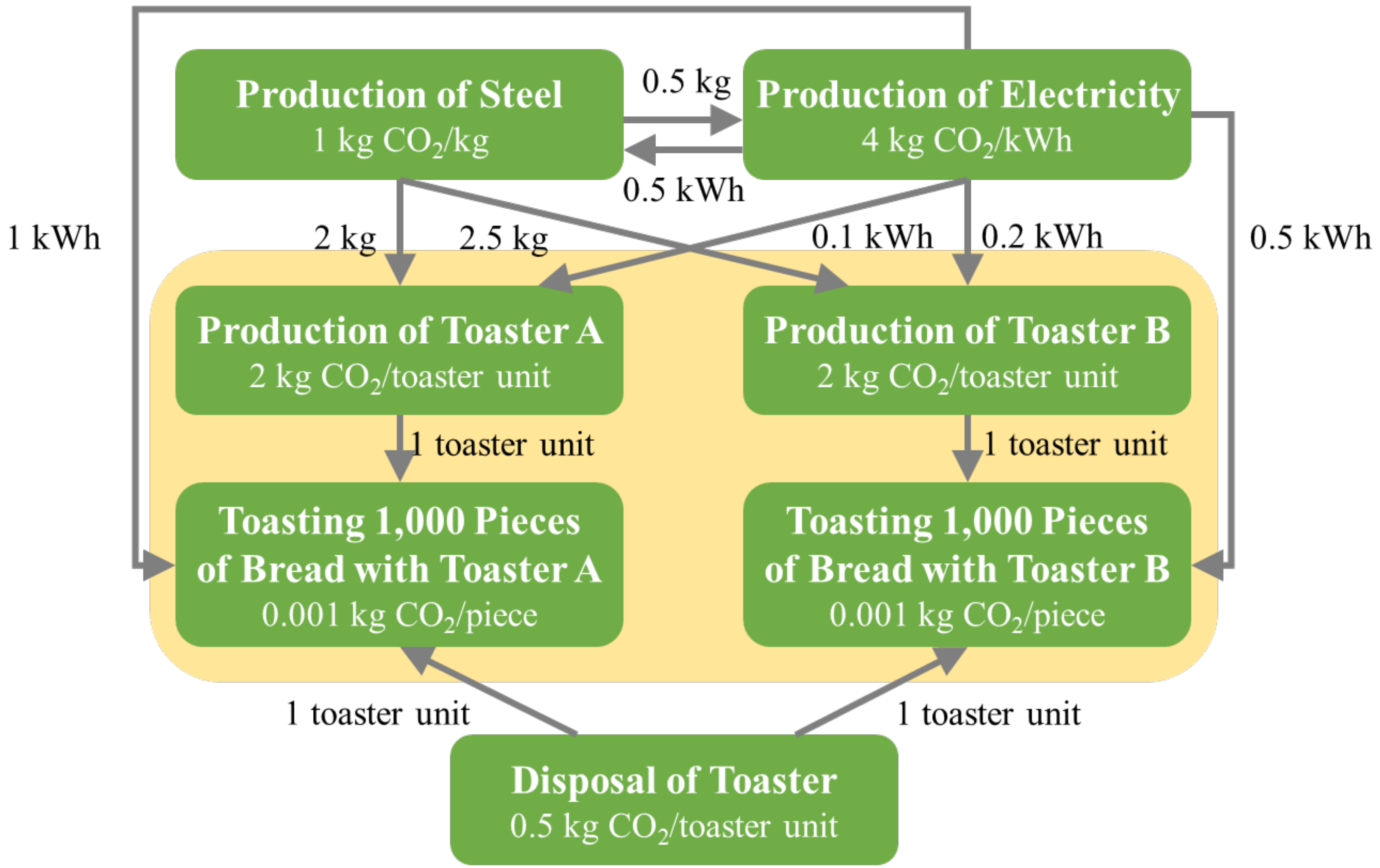
Advantages:

- Completeness of life cycle boundary
- Specificity of foreground processes

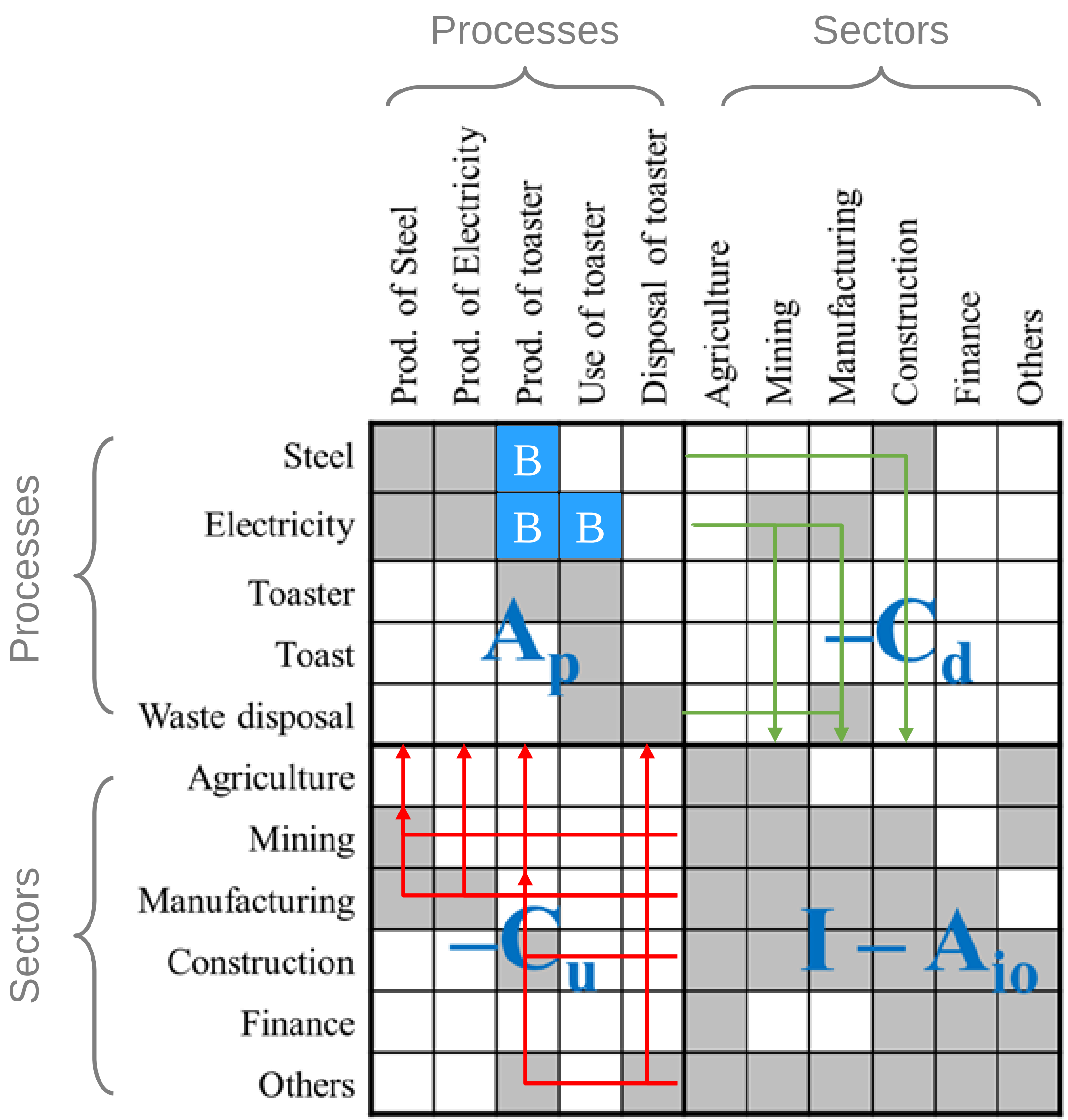
Toaster Example

Comparing two toasters

(Functional unit: produce **1,000** pieces of bread)

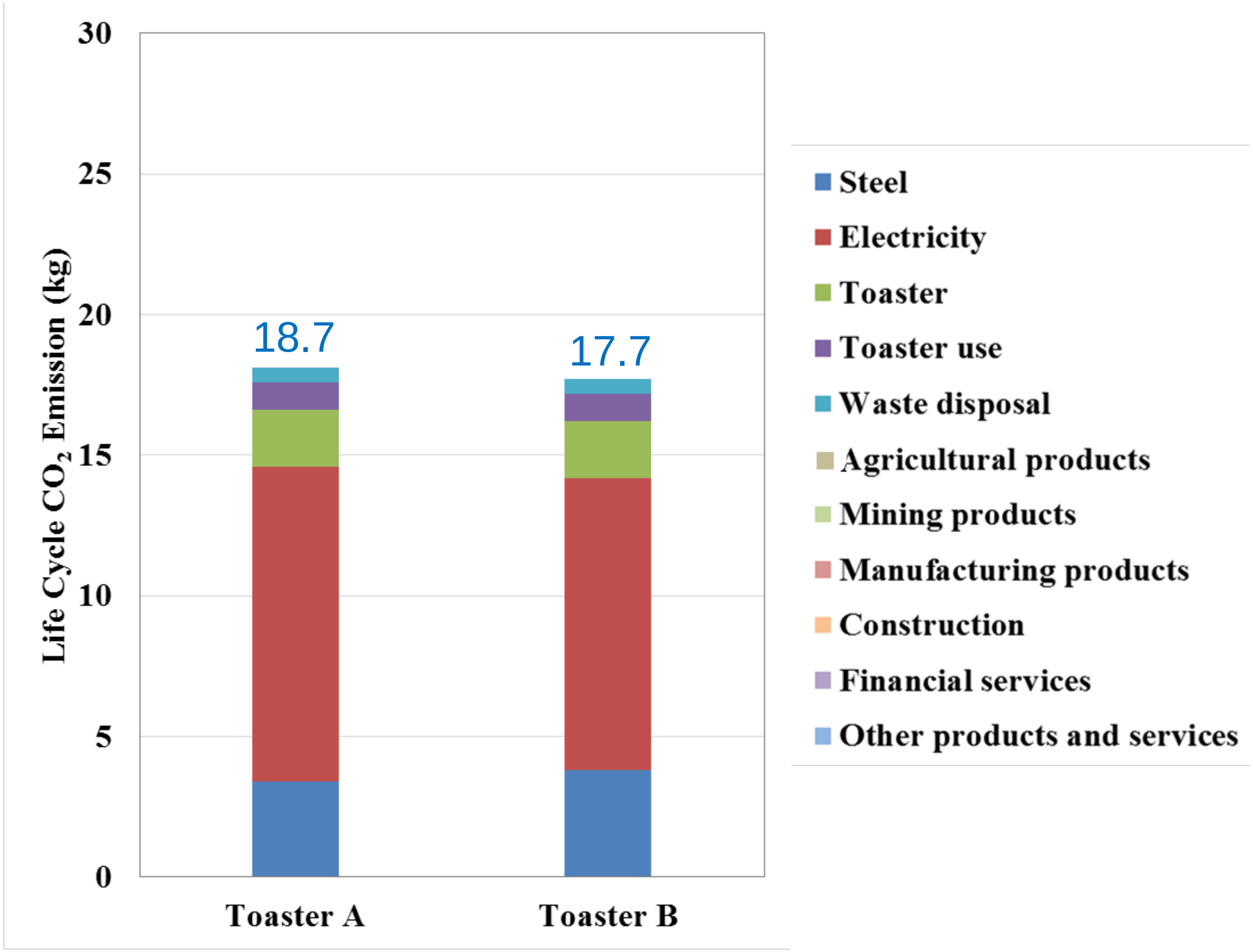


Toaster Example



Toaster Example

Direct emission
(process system)

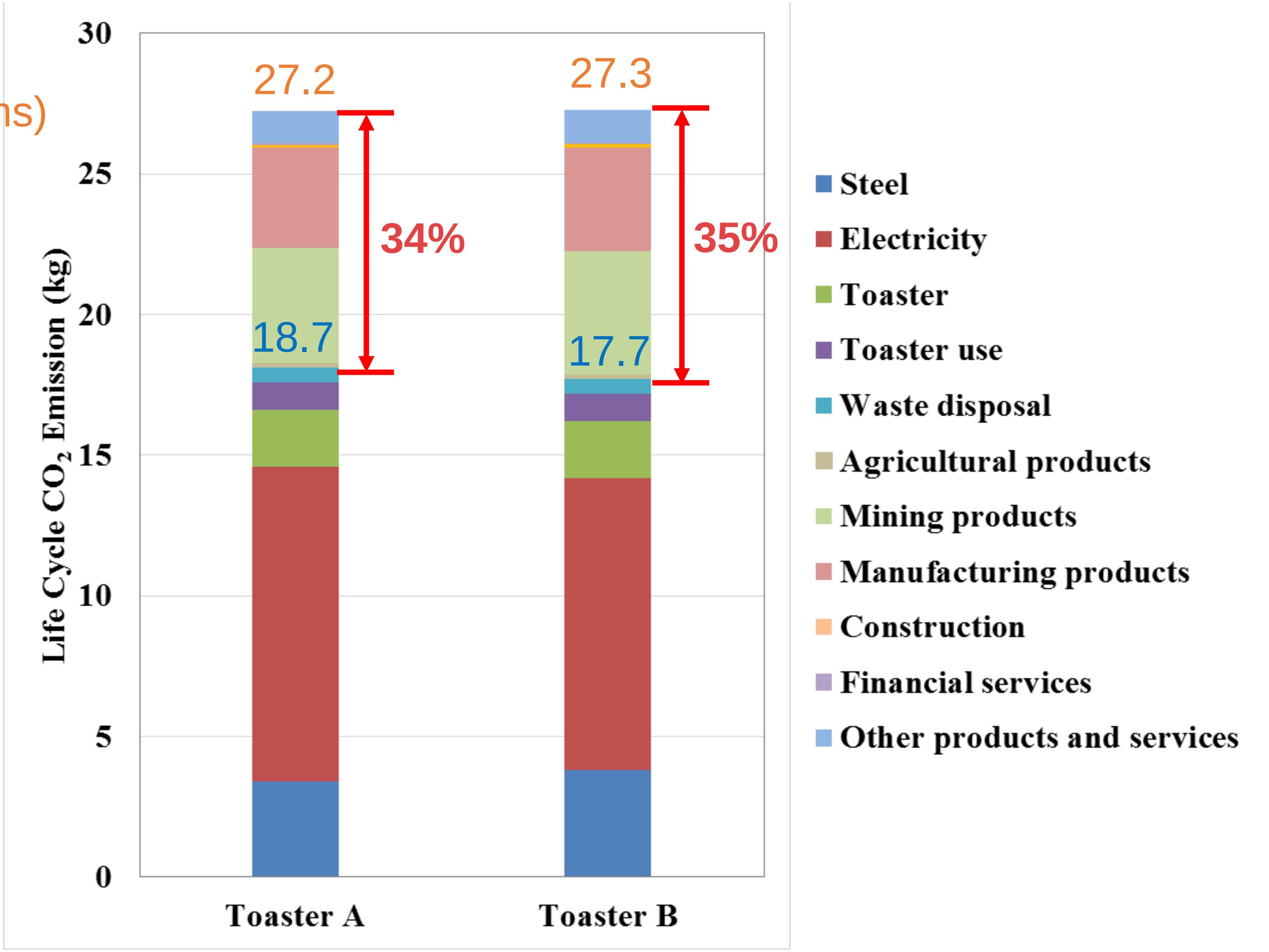


Toaster Example

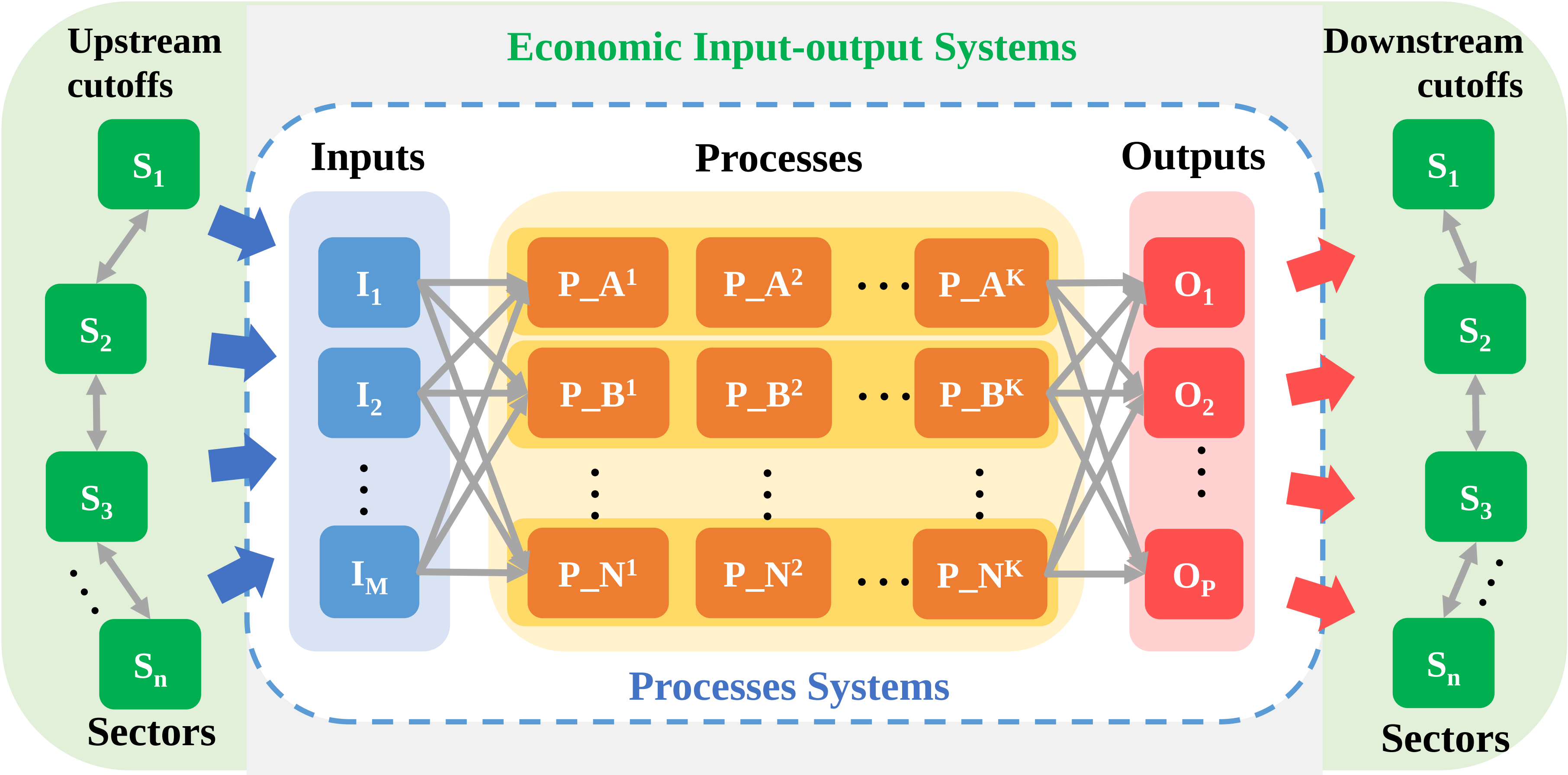
Full emission
(process + IO systems)

Neglected
indirect emission
(IO system)

Direct emission
(process system)



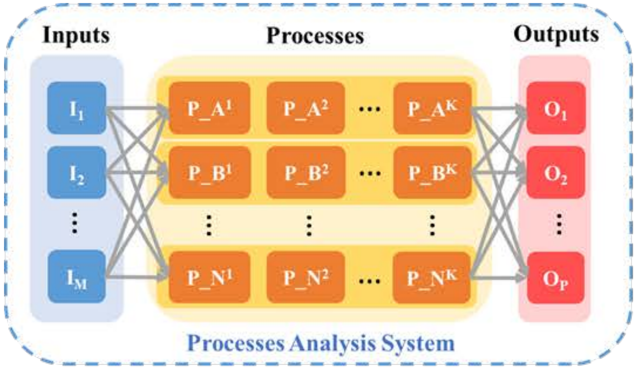
Integrated Hybrid LCA

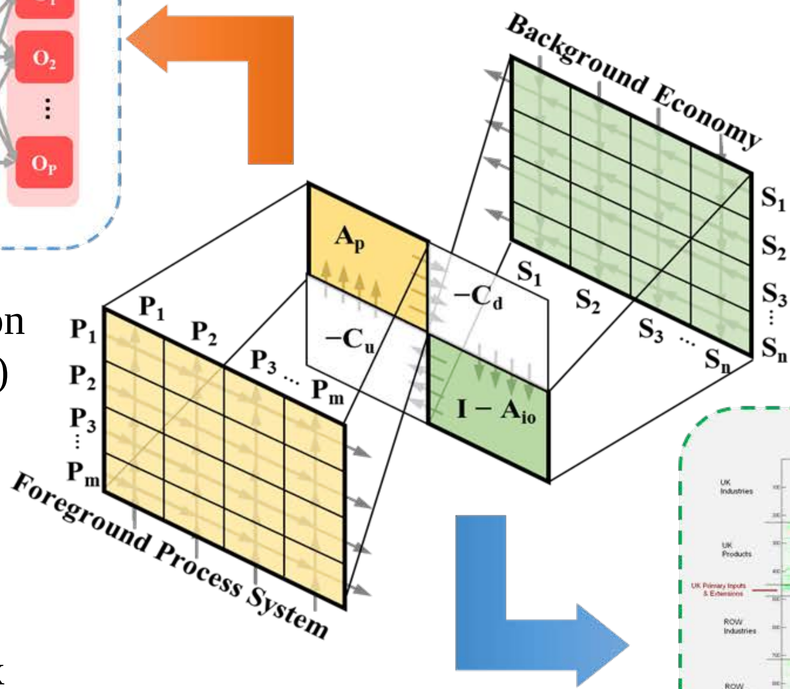


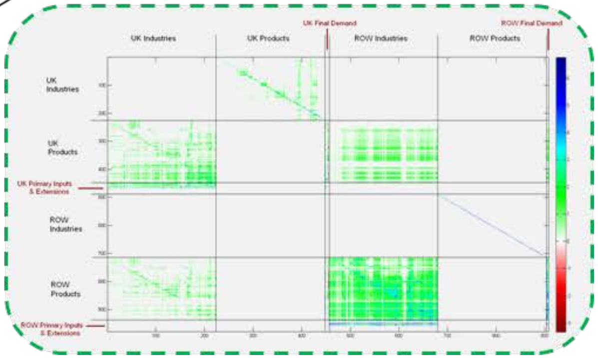
Integrated Hybrid LCA:

- Explicit process analysis – foreground process systems (precision of analysis)
- EIO analysis – background macroeconomic systems (complement the truncated system boundary)

Mathematical Foundation







E_{io} Environmental extension factor (EIO systems)

A_{io} Direct requirements matrix

C_d Downstream cutoff matrix

E_p Environmental extension factor (process systems)

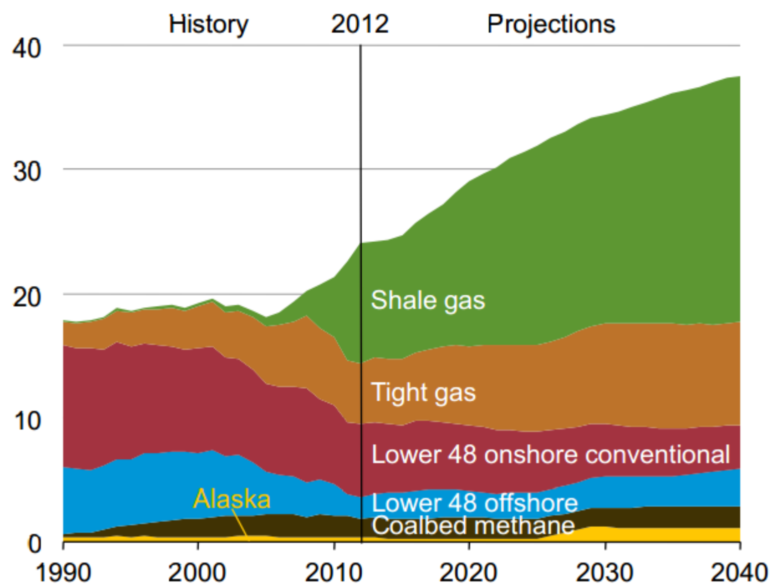
A_p Process matrix

C_u Upstream cutoff matrix

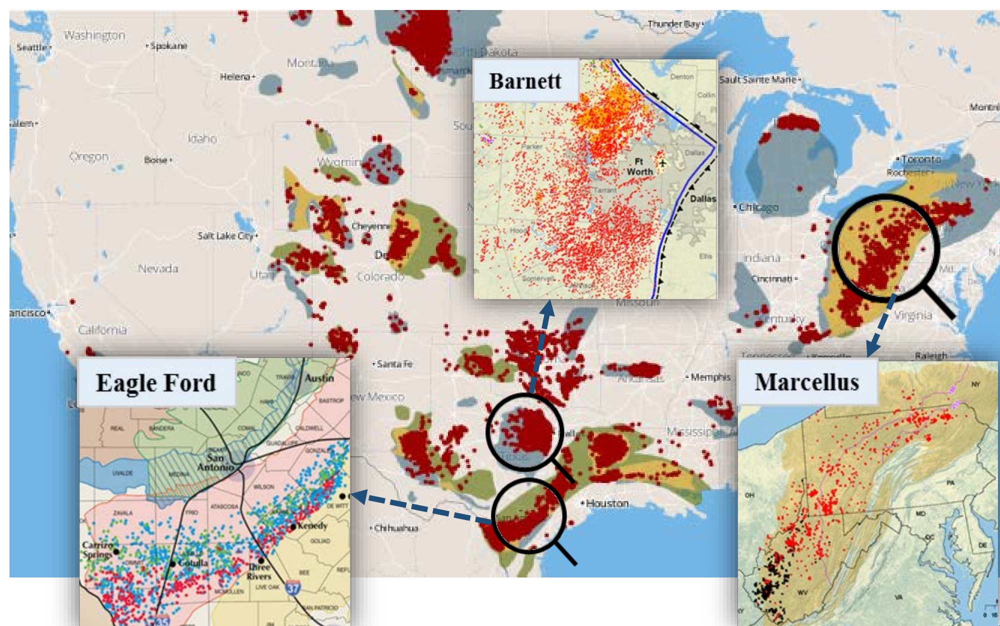
$$\text{Total environmental impact} = \begin{bmatrix} E_p & E_{io} \end{bmatrix} \begin{bmatrix} A_p & -C_d \\ -C_u & I - A_{io} \end{bmatrix}^{-1} \begin{bmatrix} y \\ 0 \end{bmatrix}$$

Application to Shale Gas

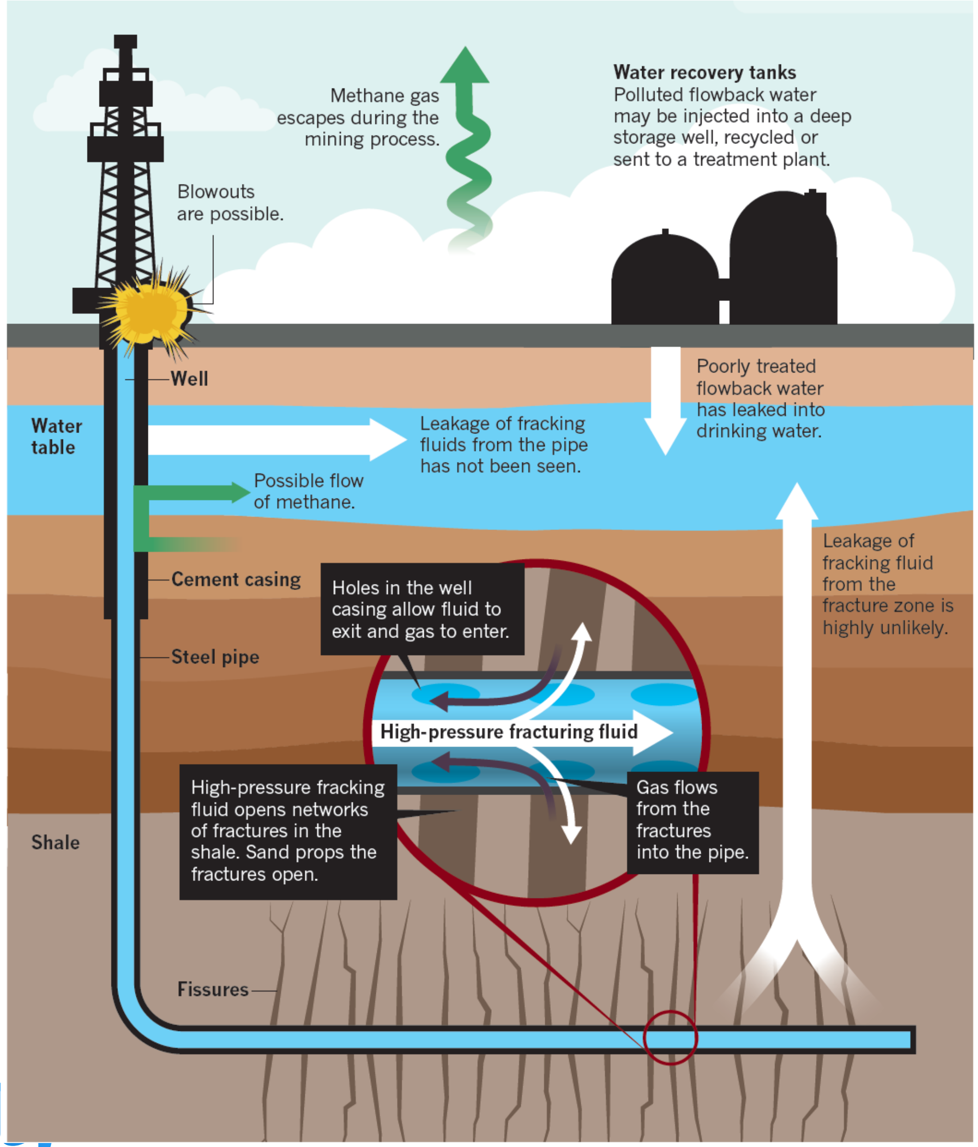
- Unconventional natural gas from shale rocks
- Large-scale production due to hydraulic fracturing and horizontal drilling
- Half of the NG production in the U.S.
- Over 63,000 shale wells in the U.S.



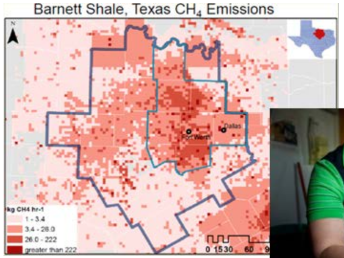
U.S. natural gas production



Hybrid LCA of Shale Gas

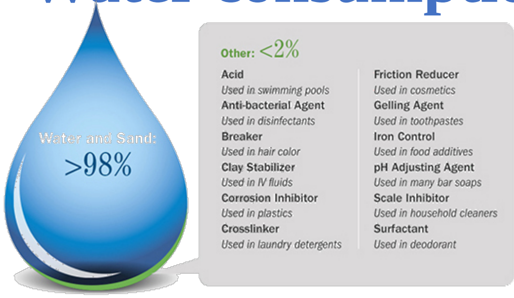


- **Climate change**



Lyon et al, 2015.

- **Water consumption**



- **Energy consumption**

LCA of Shale Gas

Goal and scope

- **UK** shale gas
- System boundary: **well-to-wire**
- Functional unit: **1 MWh electricity** generation from shale gas

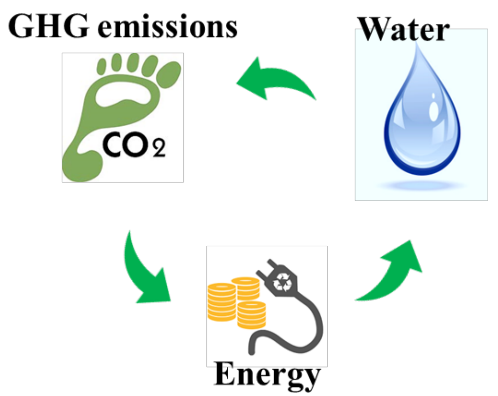
Shale gas

Life cycle inventory

- **40** basic processes in the process systems
- Two-region IO model (UK-ROW) with **224** industrial sectors
- Three cases from literature: **best, balance, and worst** cases corresponding to the **lowest, the medium, and the highest** environmental impacts

Impact assessment

- **GHG** emissions (100-year GWP factors; CO_2, CH_4, N_2O, HFCs, PFCs, and SF_6)
- **Water** consumption
- **Energy** consumption



Process Systems – *40 Basic Processes*

Process ID	Description	Process ID	Description
m_1	Steel production, converter, chromium steel 18/8	m_{21}	Soda ash, dense, to generic market for neutralizing agent
m_2	Concrete production, for civil engineering, with cement CEM I	m_{22}	Sodium persulfate production
m_3	Tap water production, direct filtration treatment	m_{23}	Sodium borates production
m_4	Diesel production, low-sulfur	m_{24}	Citric acid production
m_5	Diesel, burned in building machine	m_{25}	Pesticide production, unspecified
m_6	Diesel, burned in diesel-electric generating set, 18.5kW	m_{26}	N, N-dimethylformamide production
m_7	Barite production	m_{27}	UK electricity generation, with mixed energy inputs
m_8	Bentonite quarry operation	m_{28}	Transport, freight, lorry, all sizes, EURO3 to generic market for transport, freight, lorry, unspecified
m_9	Chemical production, inorganic	m_{29}	Injection in disposal well
m_{10}	Chemical production, organic	m_{30}	Wastewater treatment by CWT
m11	Lignite mine operation	m_{31}	Onsite treatment with MSF
m12	Treatment of inert waste, inert material landfill	m_{32}	Onsite treatment with MED
m13	Treatment of drilling waste, landfarming	m_{33}	Onsite treatment- with RO
m14	Silica sand production	m_{34}	Steam production, in chemical industry
m15	Petroleum refinery operation	m_{35}	Tap water production, direct filtration treatment
m16	Isopropanol production	m_{36}	Transporting gas through pipelines
m17	Hydrochloric acid production, from the reaction of hydrogen with chlorine	m_{37}	Ethanolamine production
m18	Ethylene glycol production	m_{38}	Ethylene glycol production
m19	Potassium chloride production	m_{39}	Fugitive emissions of CO_2
m20	Carboxymethyl cellulose production, powder	m_{40}	Fugitive emissions of CH_4

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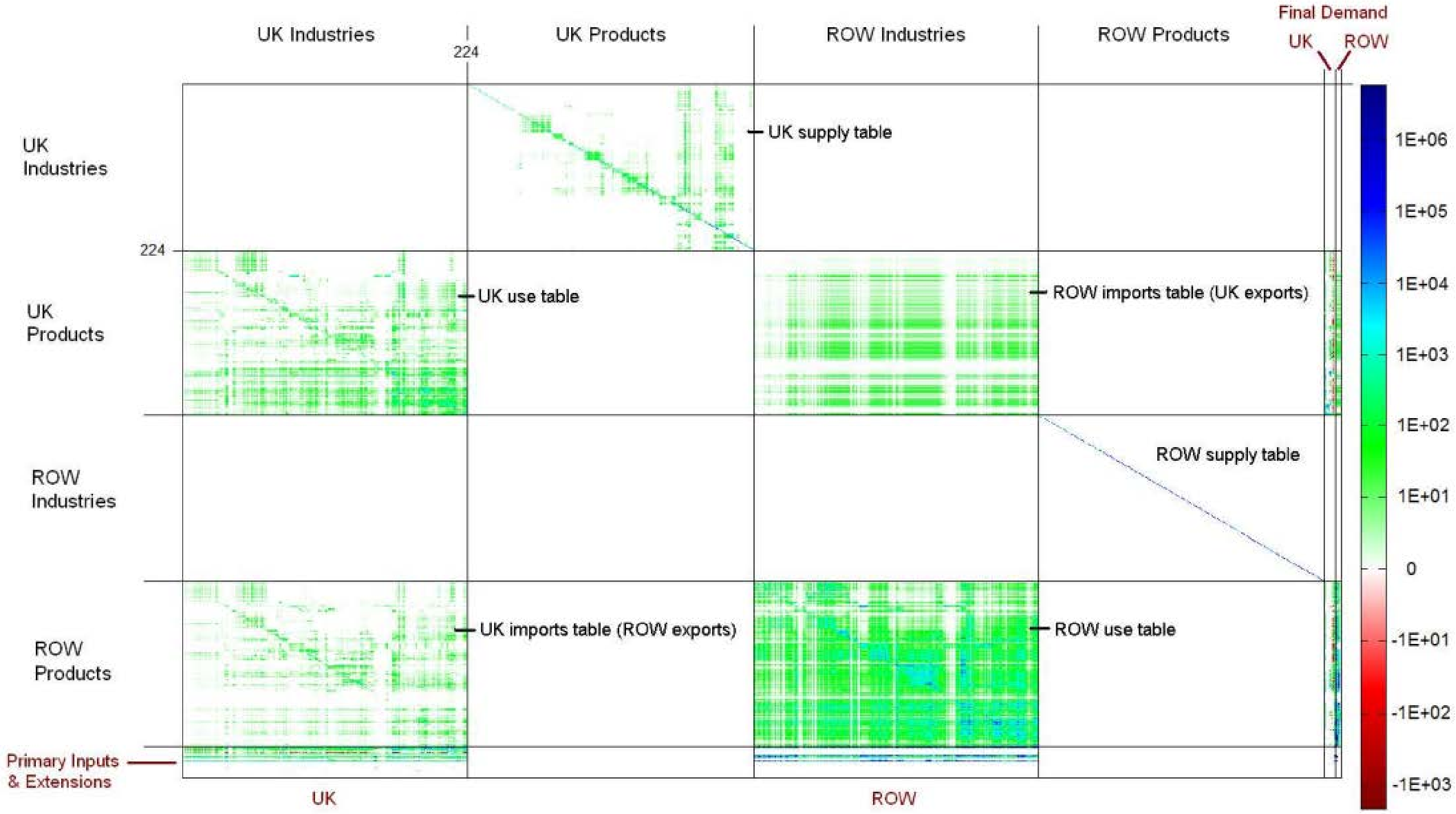
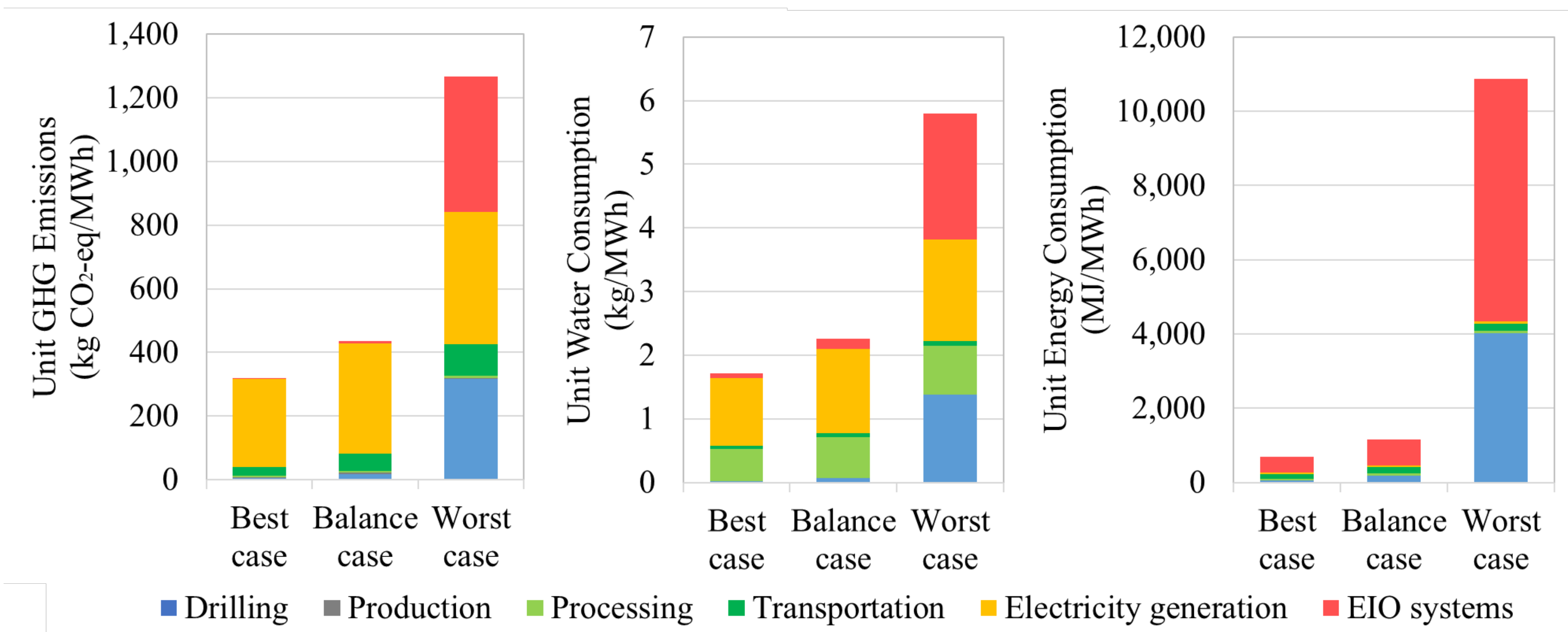
Hybrid LCI Data Structure

IO System (896 × 896 matrix)

- Multi-region: UK and ROW (rest of world)
- Supply-Use Table (SUT): each containing 224 industrial sectors/products



LCA Results

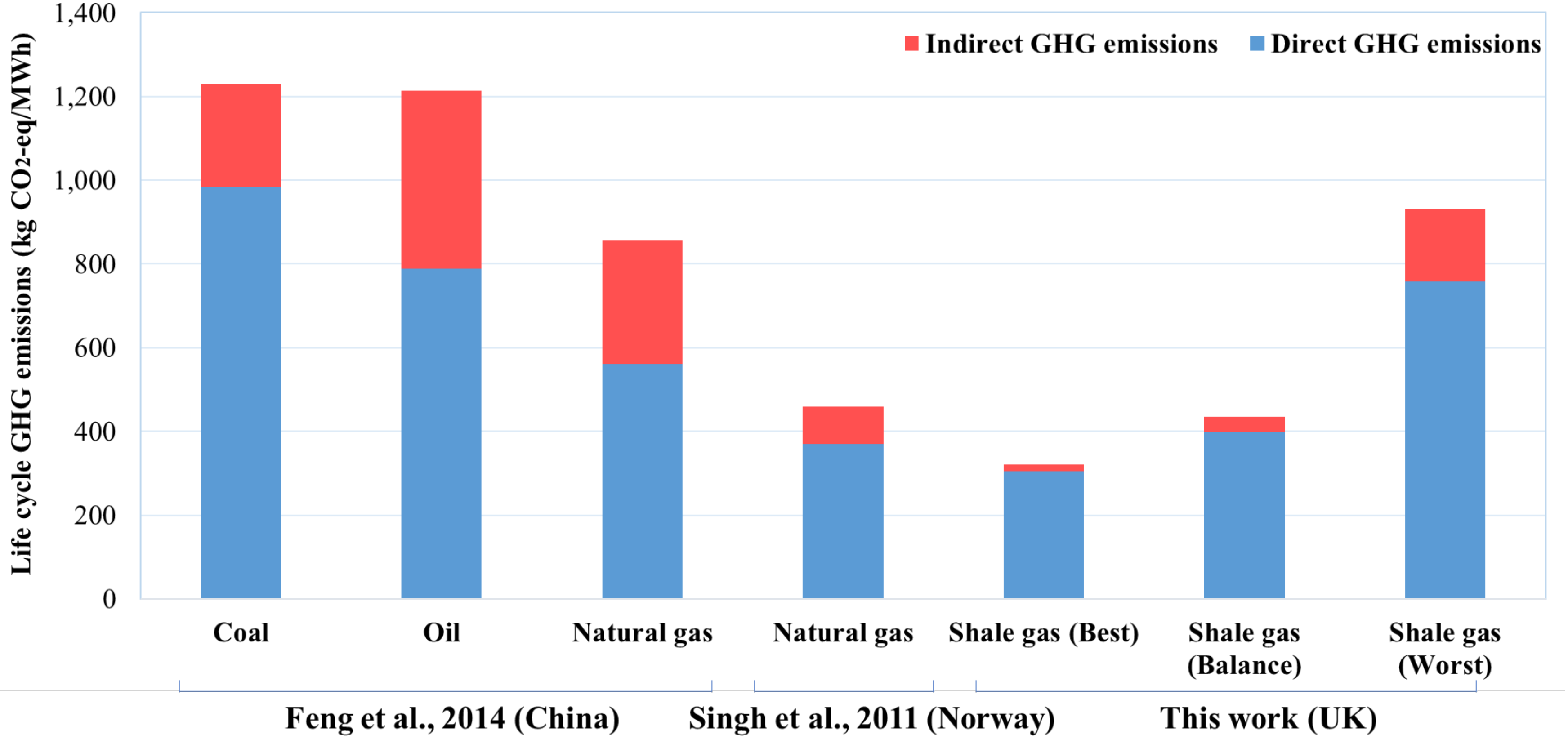


- Electricity generation
- Transportation

- Electricity generation
- Processing

- Drilling
- EIO system

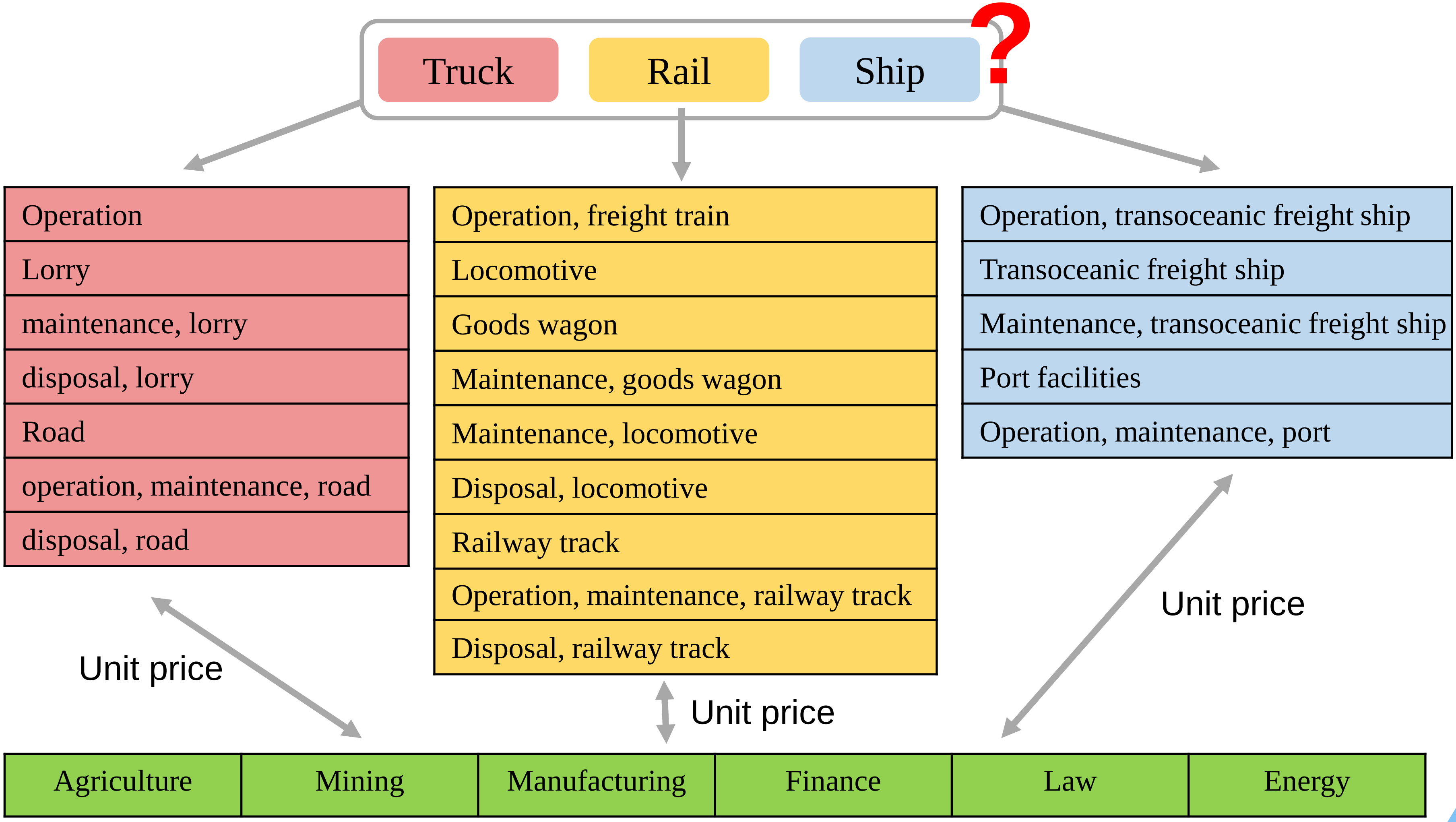
Comparison with Existing Hybrid LCA Studies



- GHG emissions of shale gas are comparable to those of natural gas
- Less GHG emissions than Coal and Oil

Activity – Linking SC Decisions with h-LCO

Definition: *Activity* is a flexible process that involves decision making.



Yue, Pandya, & You (2016). *Environmental Science & Technology*, 50, 1501–1509.

Hybrid LCO Model for Shale Gas

Economic objective:

$$\min \ LCOE = \frac{TC^{cap} + \sum_{t \in T} \frac{TC^{oper}}{(1+dr)^t}}{TGE}$$

Environmental objective:

$$\min \ UE = \frac{TE^{pro} + TE^{IO}}{TGE}$$

Nonlinear term:

$$C_{proc}^{cap} = \sum_{p \in P_n} pri \cdot \left(\frac{PC_p}{prc}\right)^{sfp} \cdot \left(\frac{pci}{rpci}\right)$$

s.t. Economic Constraints

Environmental Constraints

Mass Balance Constraints

Capacity Constraints

Composition Constraints

Bounding Constraints

Logic Constraints

Total GHG emissions :

$$TE^{pro} = e_m^{pro} Q_m \qquad TE^{IO} = e_{ns}^{IO} P_{ns}$$

Total output of each industrial sector P_{ns}

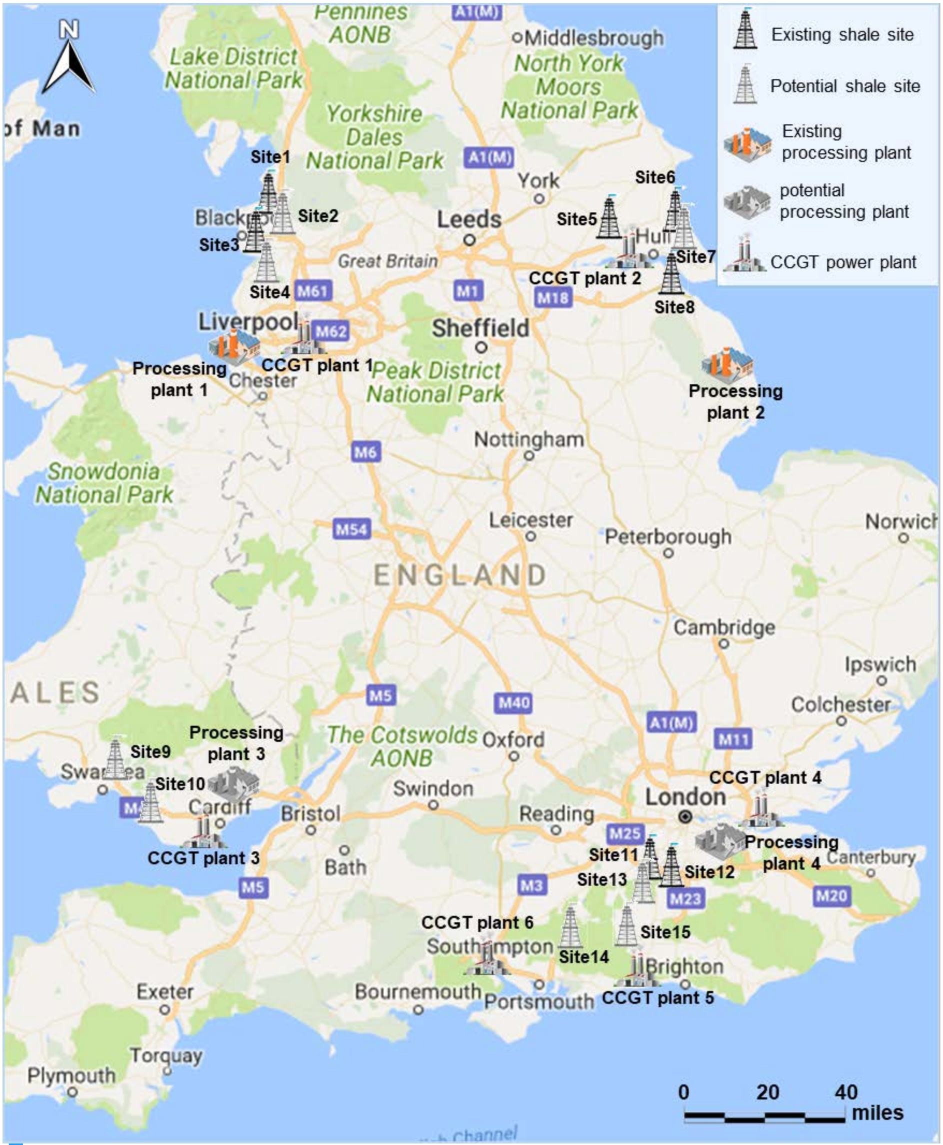
$$P_{ns} - \sum_{ns' \in NS} aio_{ns,ns'} \cdot P_{ns} \geq UP_{ns}$$

Upstream input from industry sector *ns* to process systems

$$UP_{ns} = \sum_{m \in M} c_{ns,m} \cdot price_m \cdot Q_m$$

Mixed-Integer Nonlinear Fractional Program

Case Study of UK Shale Gas Supply Chain



- **15 Shale sites**

(7 existing, 8 potential ones)

- **4 processing plants**

(2 existing, 2 potential)

- **6 CCGT power plants**

- **10-year planning horizon**

(40 time periods)

MINLP problem:

- 414 integer variables
- 11,797 continuous variables
- 15,370 constraints

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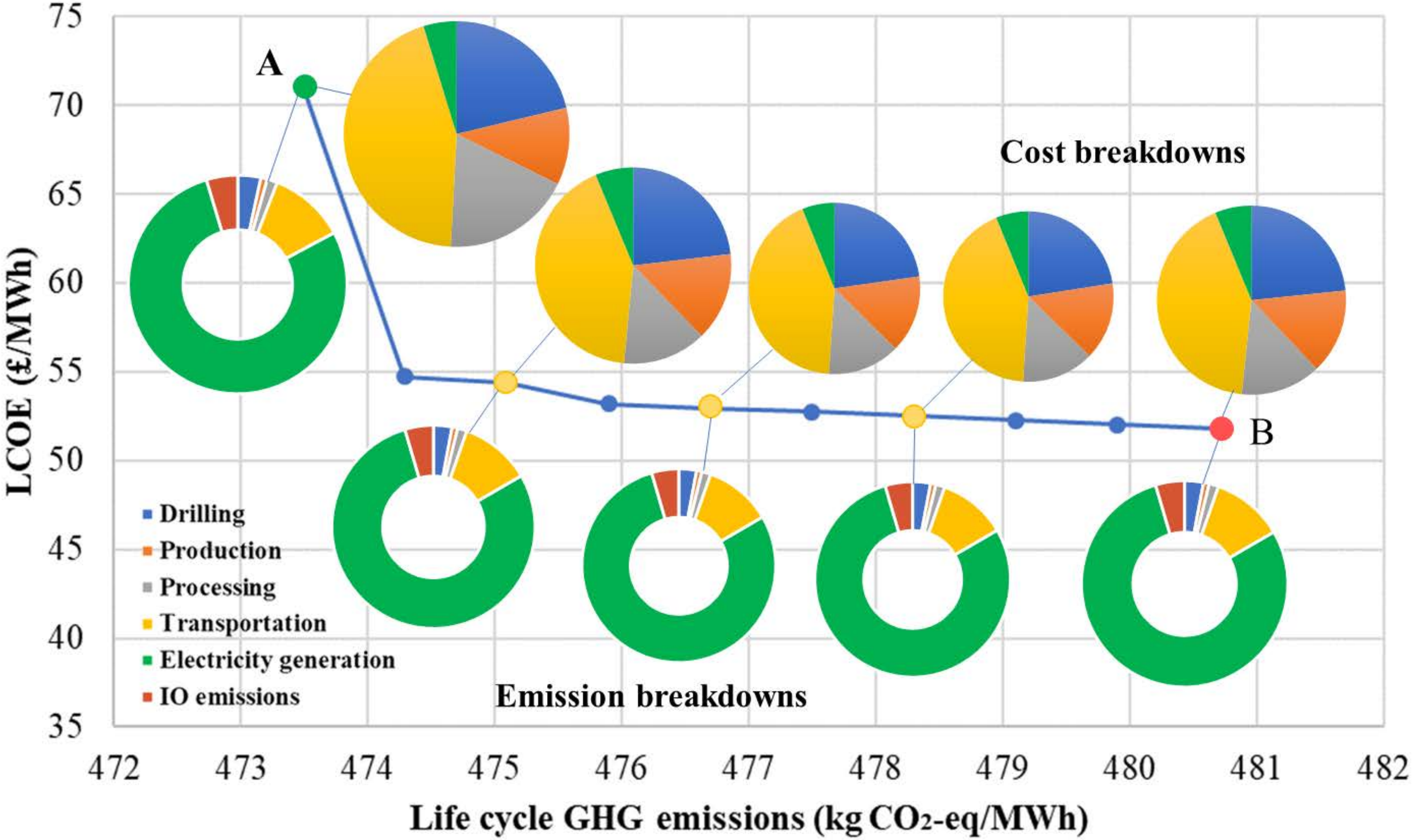
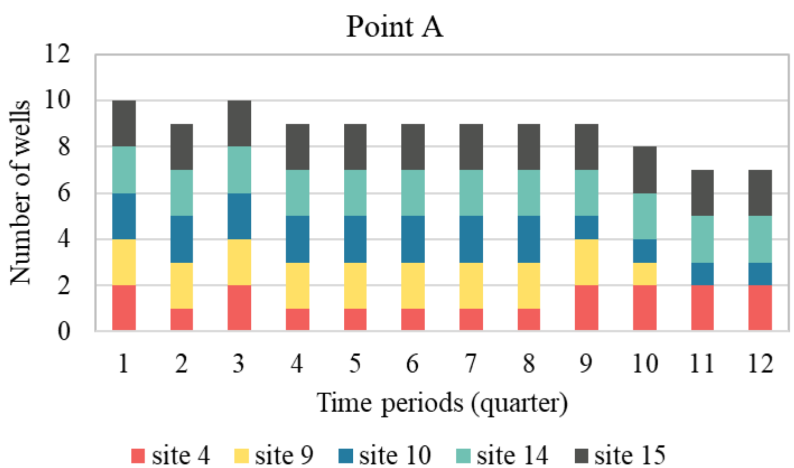
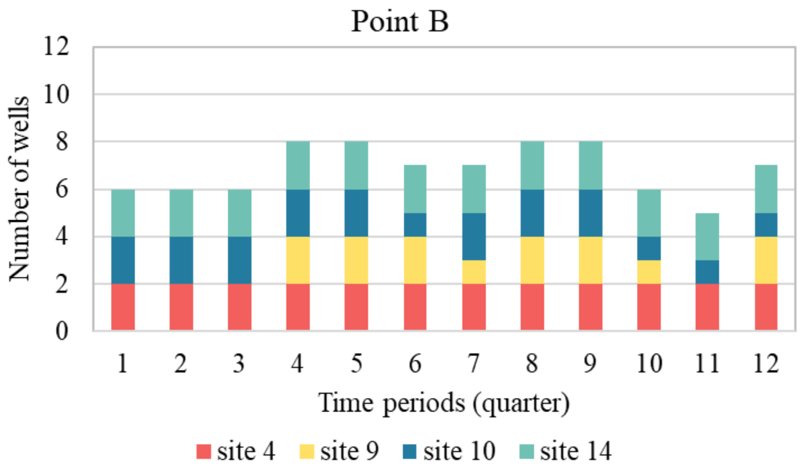
Pareto-optimal Curve



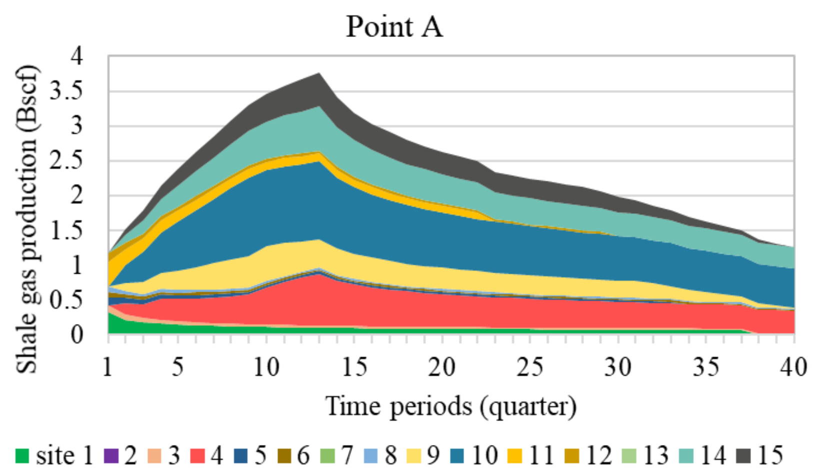
Drilling Schedules and Production Profiles

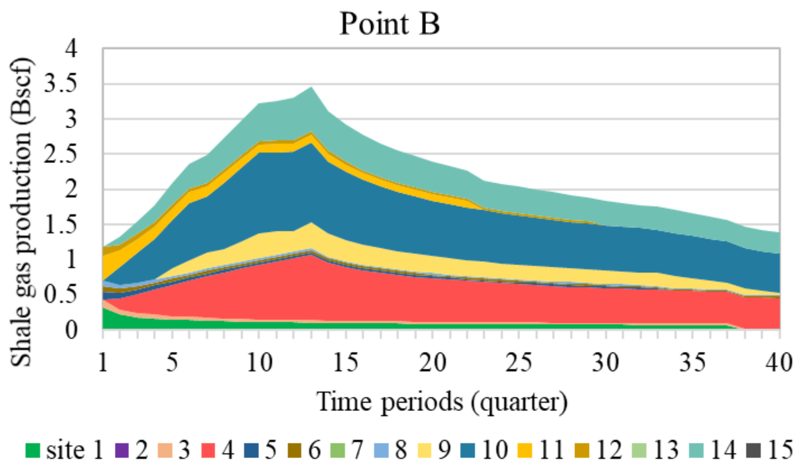
Drilling Schedules



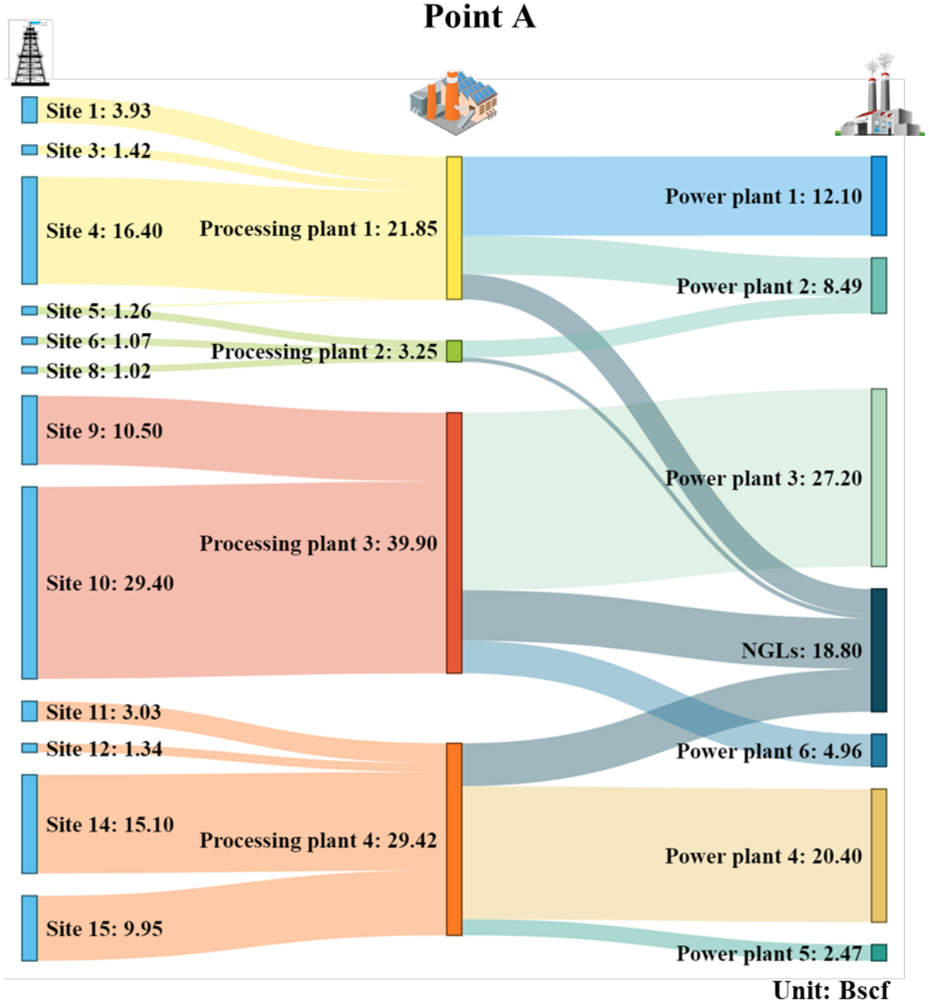


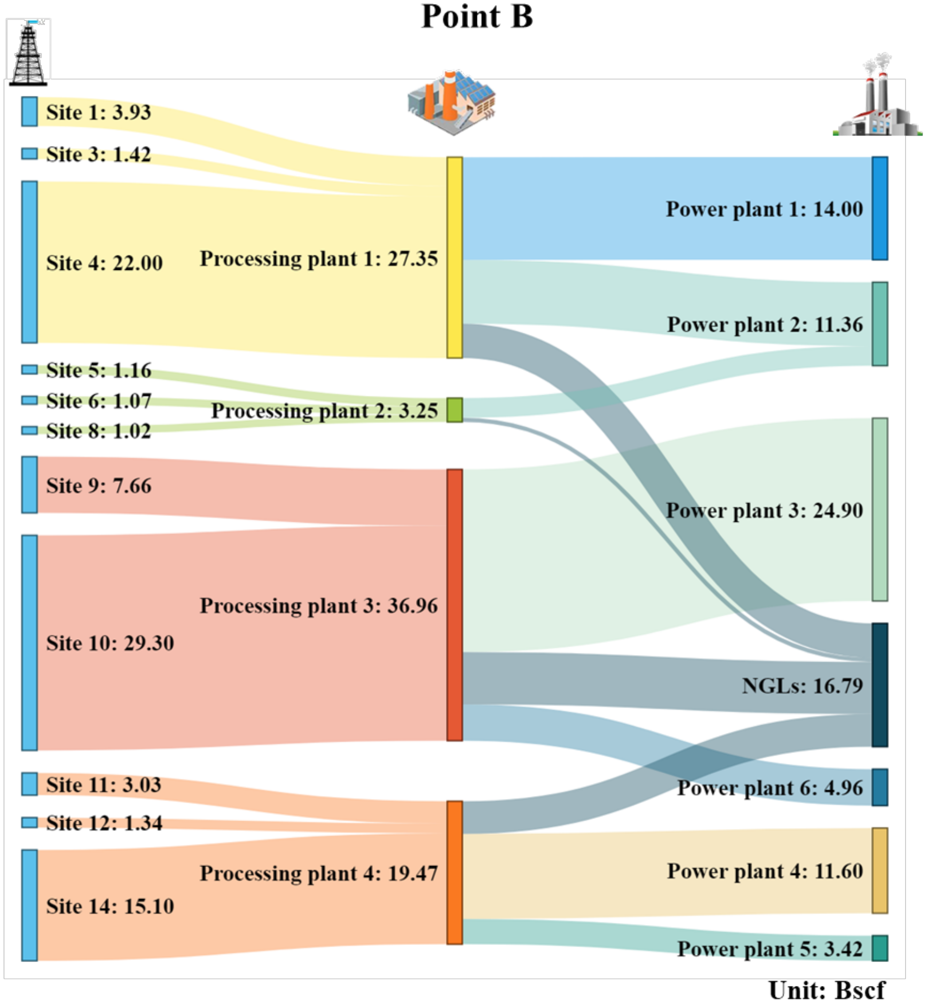
Production Profiles





Supply Chain Design and Flow Information





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Research Article

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Integrated Hybrid Life Cycle Assessment and Optimization of Shale Gas

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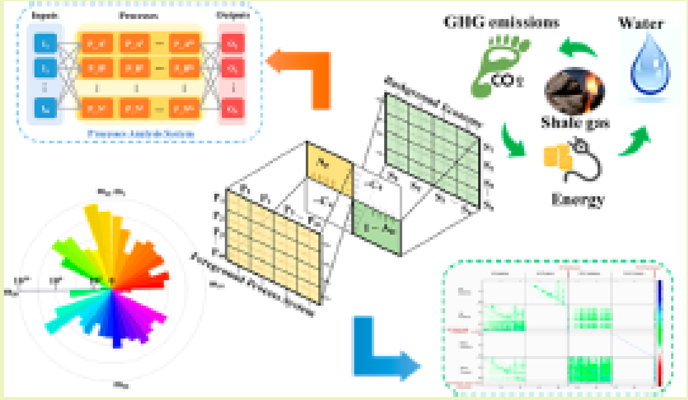

ABSTRACT: This paper analyzes the life cycle environmental impacts of shale gas by using an integrated hybrid life cycle analysis (LCA) and optimization approach. Unlike the process-based LCA that suffers system truncation, the integrated hybrid LCA supplements the truncated system with a comprehensive economic input-output system. Compared with the economic input−output-based LCA that loses accuracy from process aggregation, the integrated hybrid LCA retains the precision in modeling major unit processes within the well-to-wire system boundary. Three environmental categories, namely, life cycle greenhouse gas emissions, water consumption, and energy consumption, are considered. Based on this integrated hybrid LCA framework, we further developed an integrated hybrid life cycle optimization model, which enables automatic identification of sustainable alternatives in the design and operations of shale gas supply chains. We applied the model to a well-to-wire shale gas supply chain in the UK to illustrate the applicability. According to the optimization results, the lowest levelized cost of electricity generated from shale gas is £51.8/MWh, and the optimal life cycle GHG emissions, water consumption, and energy consumption are 473.5 kg CO_2-eq/MWh, 2263 kg/MWh, and 1009 MJ/MWh, respectively.

KEYWORDS: *Hybrid life cycle assessment, Hybrid life cycle optimization, Shale gas, Supply chain*

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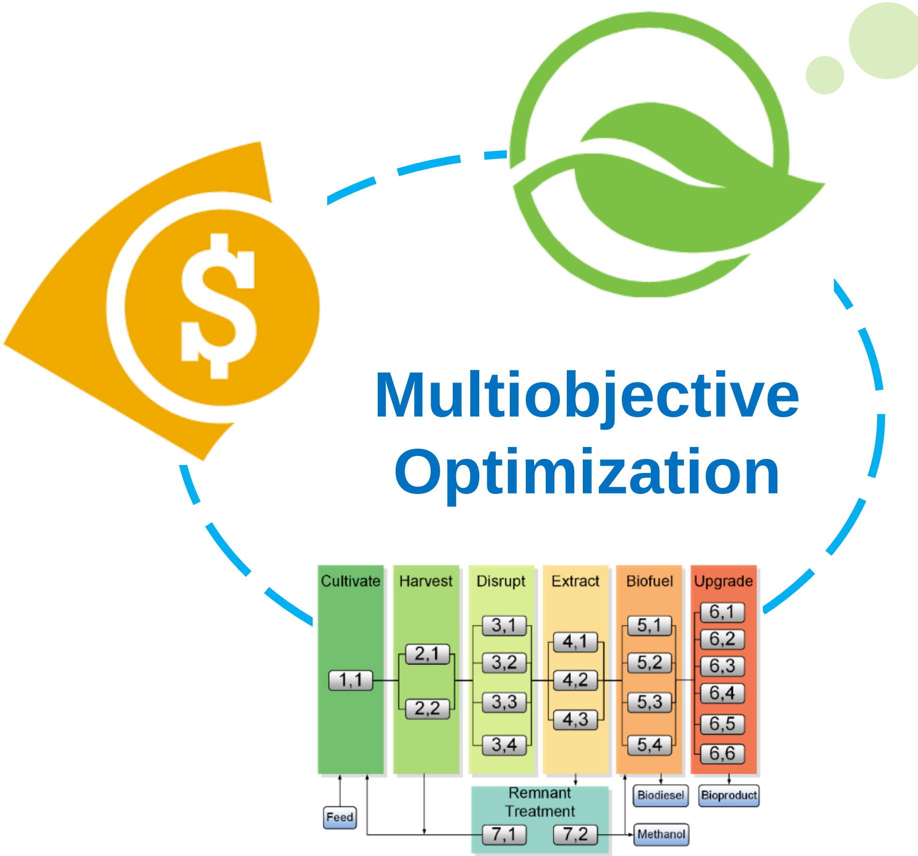
LCO: Attributional v.s. Consequential



Automatic generation of system design decisions

Life Cycle Assessment

- Goal and Scope Definition
- Life Cycle Inventory Analysis
- Life Cycle Impact Assessment
- Interpretation

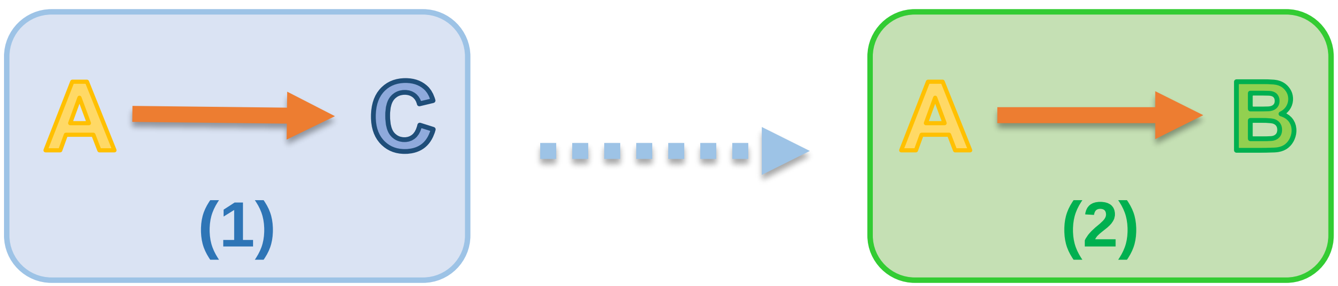
- **Attributional LCA**
- **Consequential LCA**

Motivating Example

Attributional LCA: static and fact-based

Environmental Impacts of producing A + Environmental Impacts of the conversion + Environmental Impacts of end of life of B

Consequential LCA: dynamic and change-driven

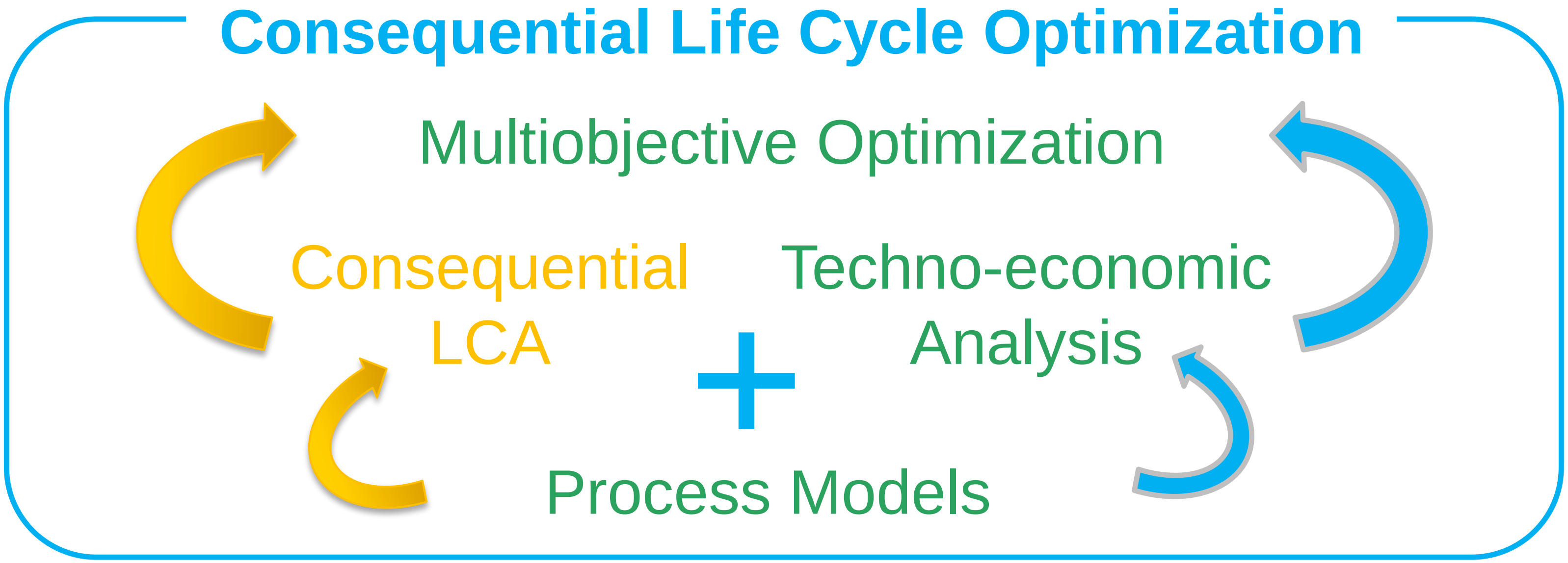


Environmental Impacts of the new system - Environmental Impacts of the original system

Or

Environmental Impacts of conversion (2) + Environmental Impacts of end of life of B - Environmental Impacts of conversion (1) - Environmental Impacts of end of life of C

Consequential Life Cycle Optimization



How does it work?

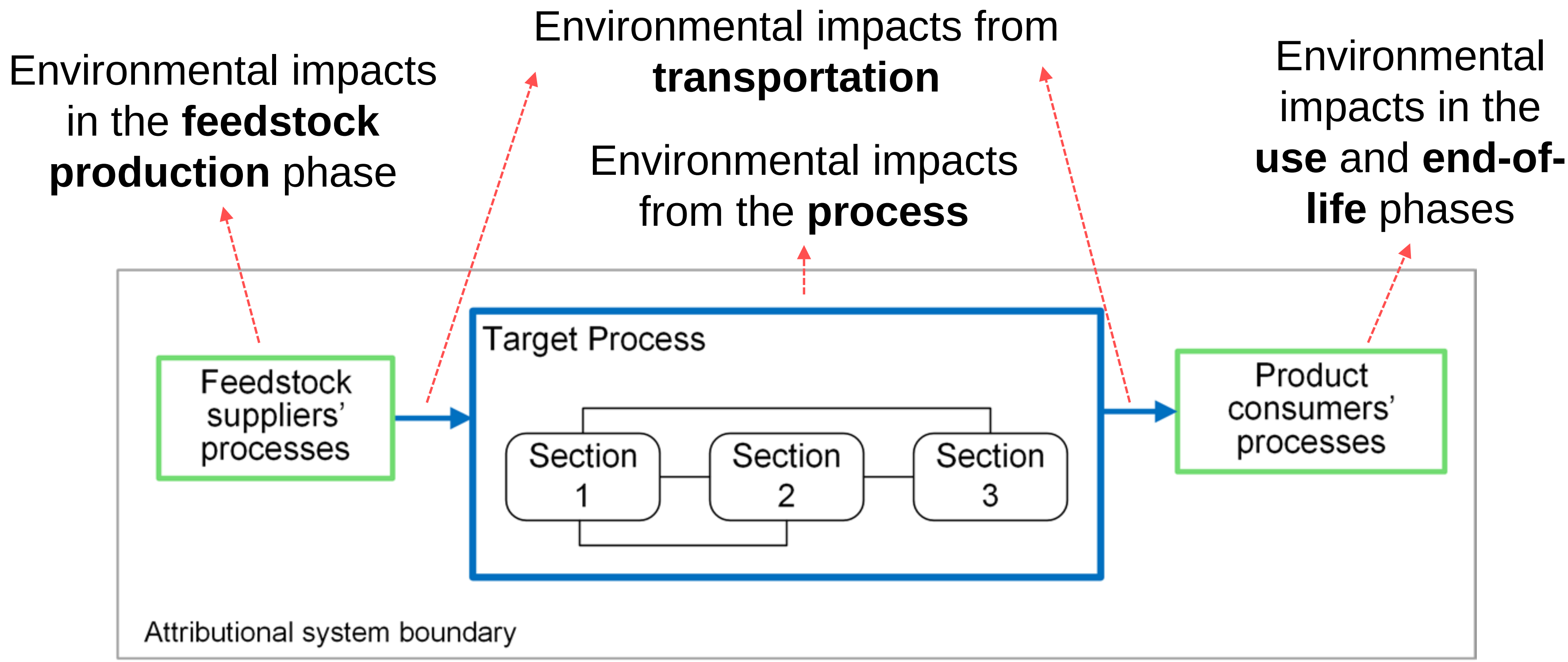
- What upstream and downstream processes are influenced by the target process?
- How does the target process influence the upstream and downstream processes?

An Analogy – Spot the Difference

Before

After

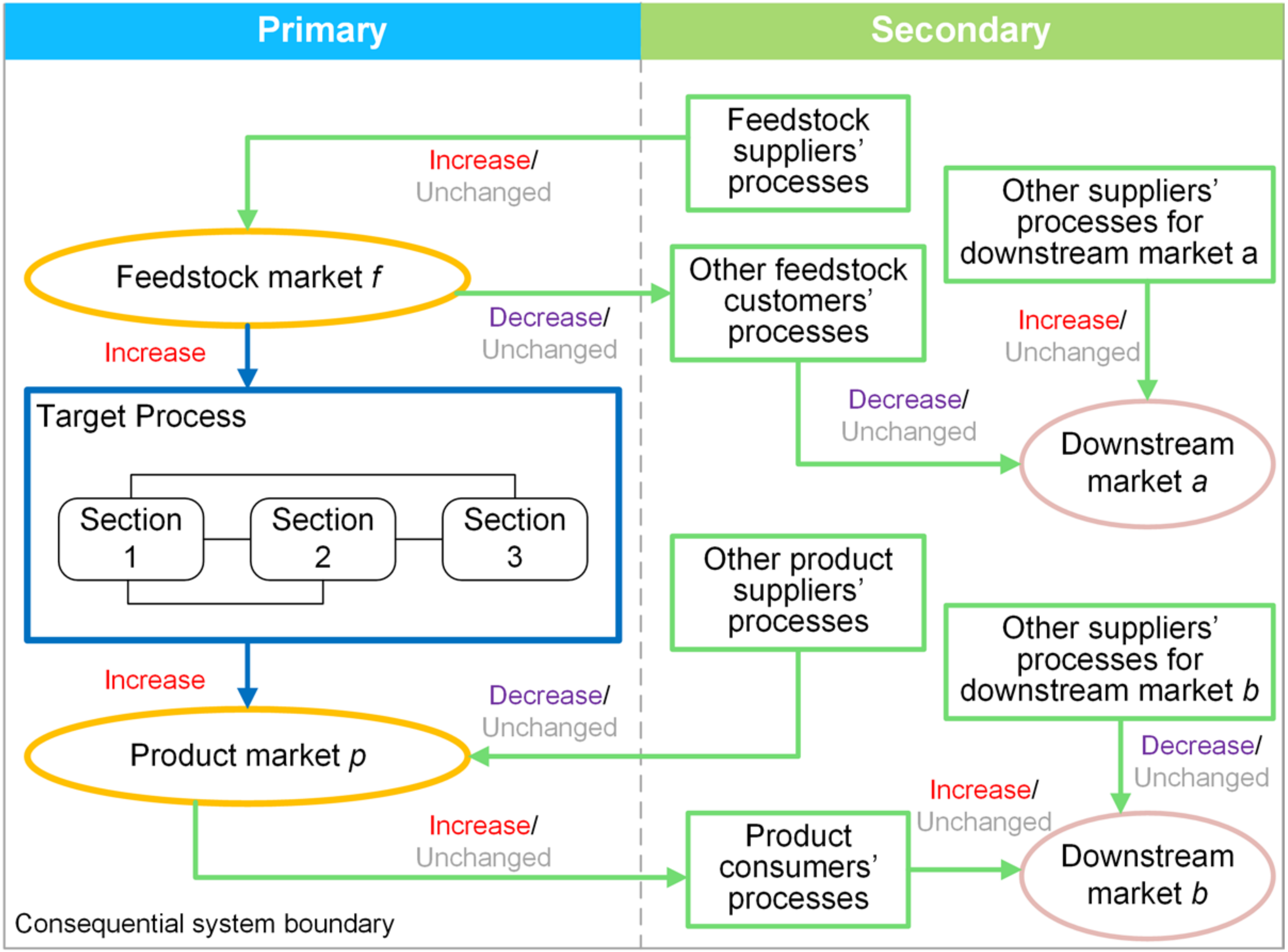
Attributional LCA for Process Design Problems



- Applicable to existing systems

- Not suitable for new systems
- Overlook the power of markets and influences in other processes

System Boundary of the Consequential LCO



Partial Equilibrium Model

Supply

$$as0_l = ad0_l, \quad \forall l$$

Demand

Aggregate supply function

$$AS_l = \sum_{p \in PPC_l} \left(asc_{l,p} \cdot XS_{l,p} + bsc_{l,p} \cdot YS_{l,p} \right) + PS_l, \quad \forall l$$

$$asc_{l,p} = \frac{ns_{l,p} - ns_{l,p-1}}{ms_{l,p} - ms_{l,p-1}}, \quad \forall l,p$$

$$bsc_{l,p} = ns_{l,p} - asc_{l,p} \cdot ms_{l,p}, \quad \forall l,p$$

$$\sum_{p \in PPC_l} YS_{l,p} = 1, \quad \forall l$$

$$\sum_{p \in PPC_l} XS_{l,p} = PR_l, \quad \forall l$$

$$ms_{l,p} \cdot YS_{l,p-1} \le XS_{l,p} \le ms_{l,p} \cdot YS_{l,p}, \quad \forall l,p$$

Price elasticity of demand

$$AD_l = \frac{ed_l \cdot \alpha_l}{\beta_l} \cdot PR_l + \alpha_l \cdot (1 - ed_l) + PD_l, \quad \forall l$$

Quantities by the target process

Equilibrium

$$AS_l = AD_l, \quad \forall l$$

Life Cycle Inventory

$$LCI_l^{Supplier} = (AS_l - PS)_l - as0_l, \quad \forall l$$

$$LCI_l^{customer} = (AD_l - PD_l) - ad0_l, \quad \forall l$$

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Consequential LCO framework

$$\max \sum_{k,l} h_{k,l}\left(P_l, Q_l, X_k, YC_k\right)$$

Economic Objective
e.g. maximize net present value

$$\min \sum_{l,r,s}\left[c_{l,r,s} \cdot v_{l,r,s}\left(Q_l, AS_l, AD_l\right)\right]$$

Environmental Objective
e.g. minimizing ReCiPe points

$$\text{s.t.} \quad Q_l = \sum_k f_{k,l}\left(X_k, YP_k\right), \quad \forall l$$

Process Model
Integer variables for technology selection;
Mass and energy balance

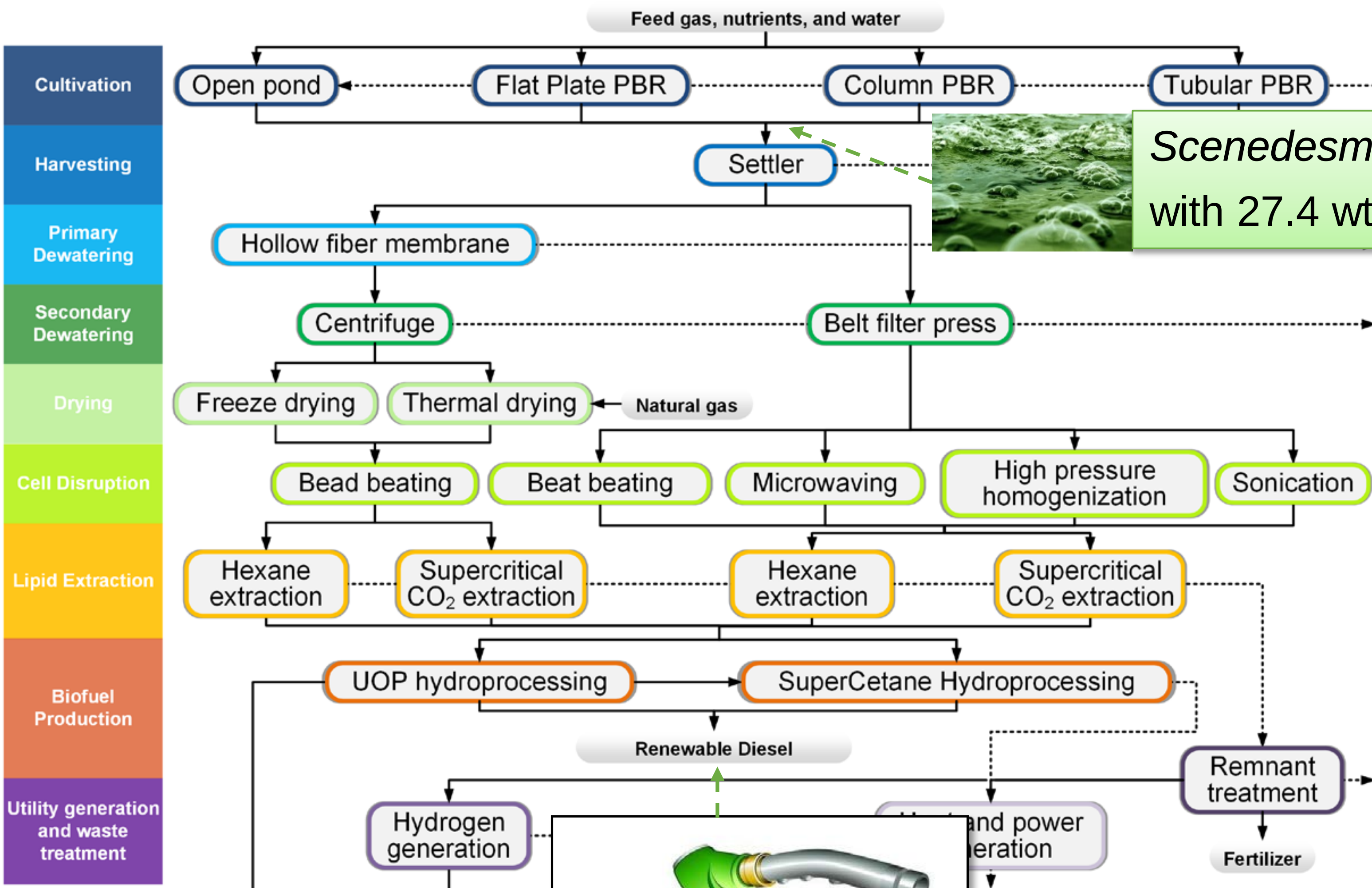
$$AS_l = m_l\left(Q_l, P_l, YS_l\right), \quad \forall l$$

$$AD_l = n_l\left(Q_l, P_l, YD_l\right), \quad \forall l$$

$$AS_l = AD_l, \quad \forall l$$

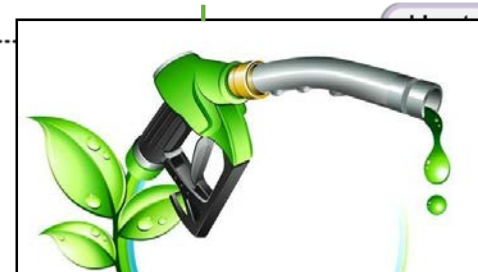
Market Model
Partial equilibrium models

Application to Algae-based Biofuel Production



Scenedesmus sp.

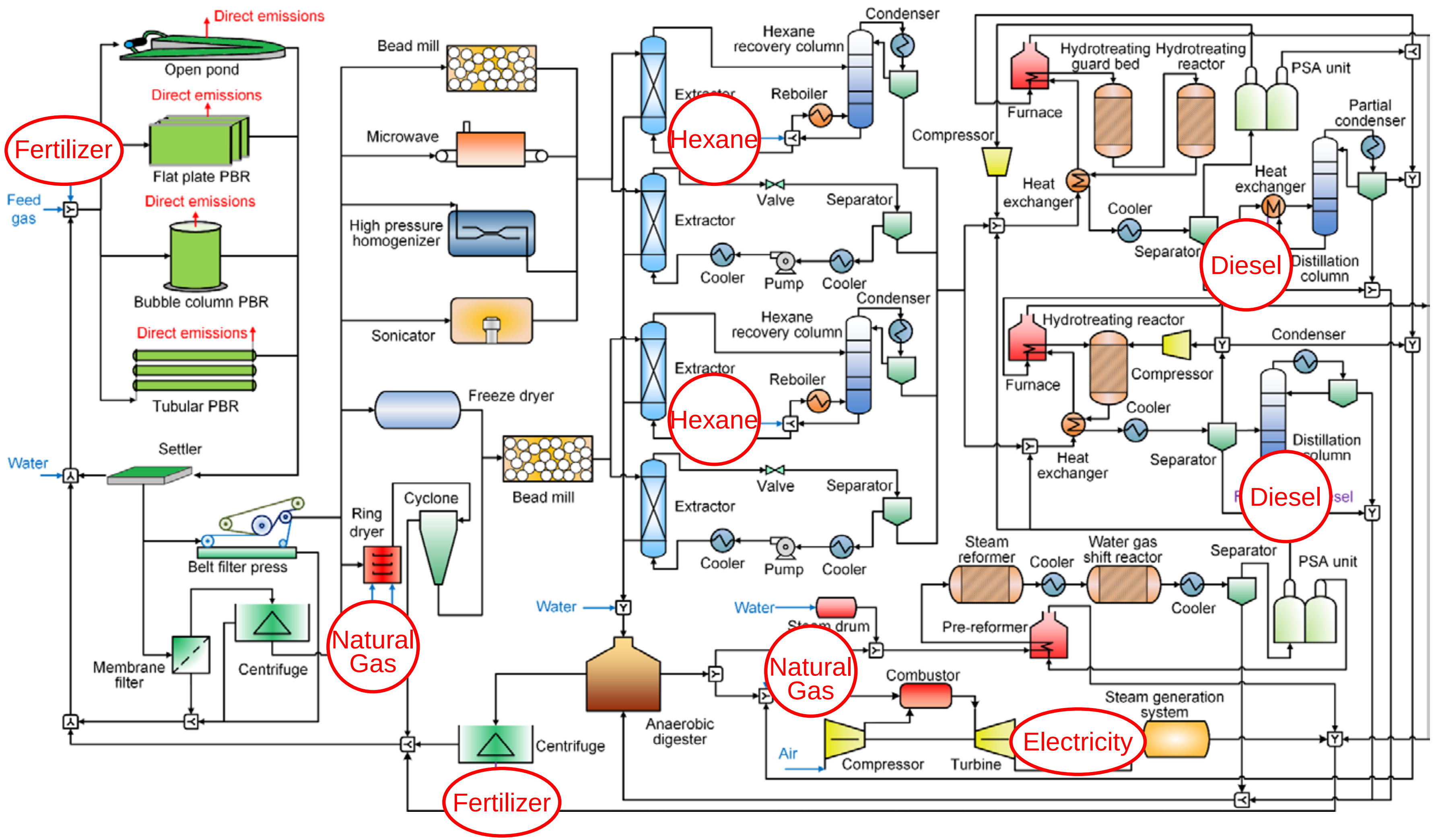
with 27.4 wt % lipid



Renewable diesel

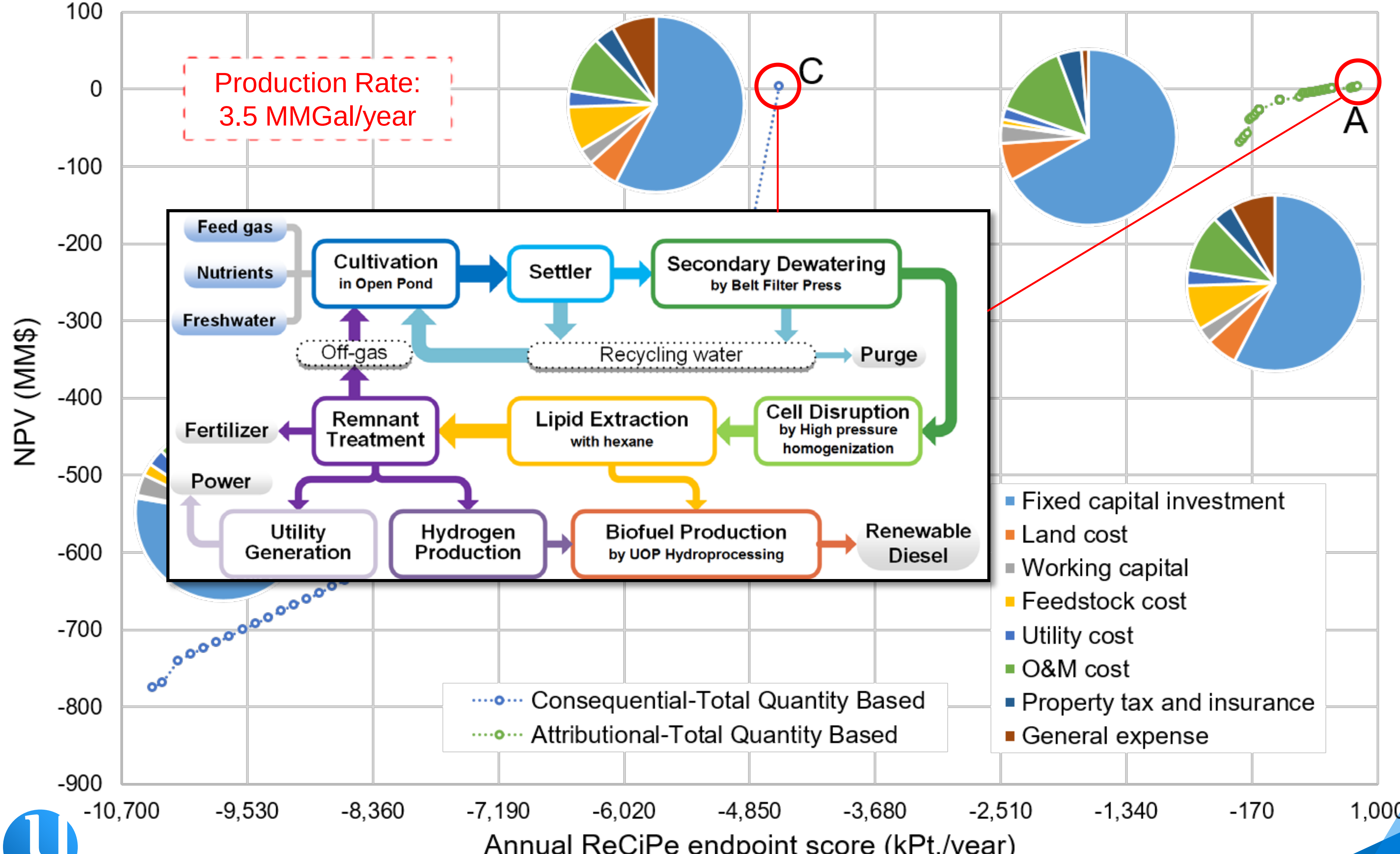
Functional Unit:
1 GJ of renewable diesel

Detailed superstructure

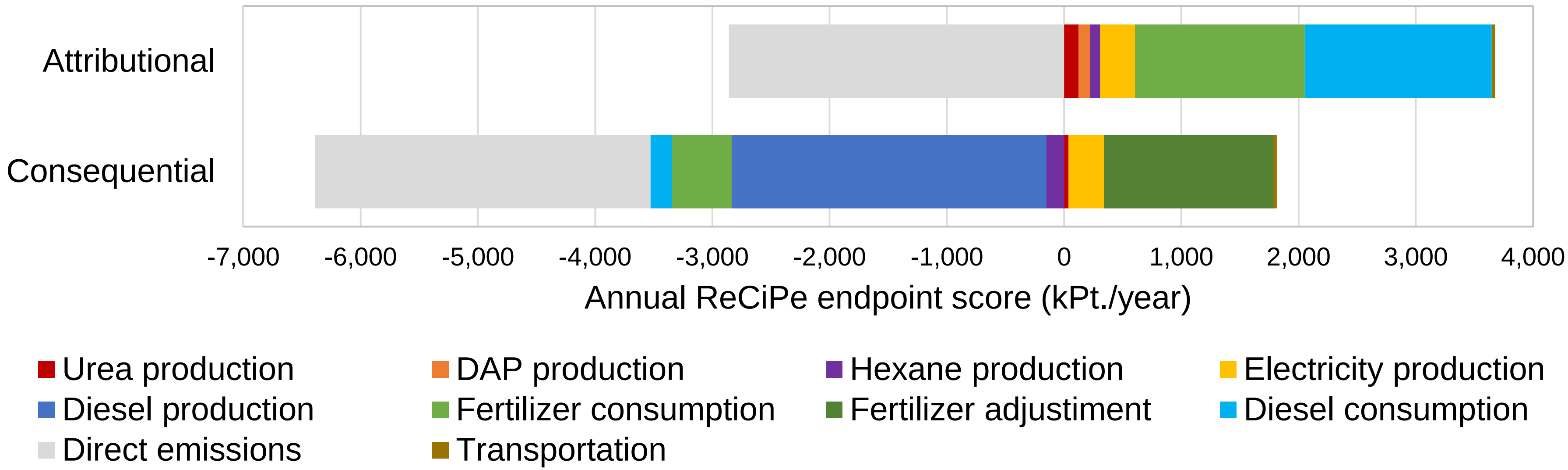


6 markets in the U.S.

Optimization Results for ReCiPe



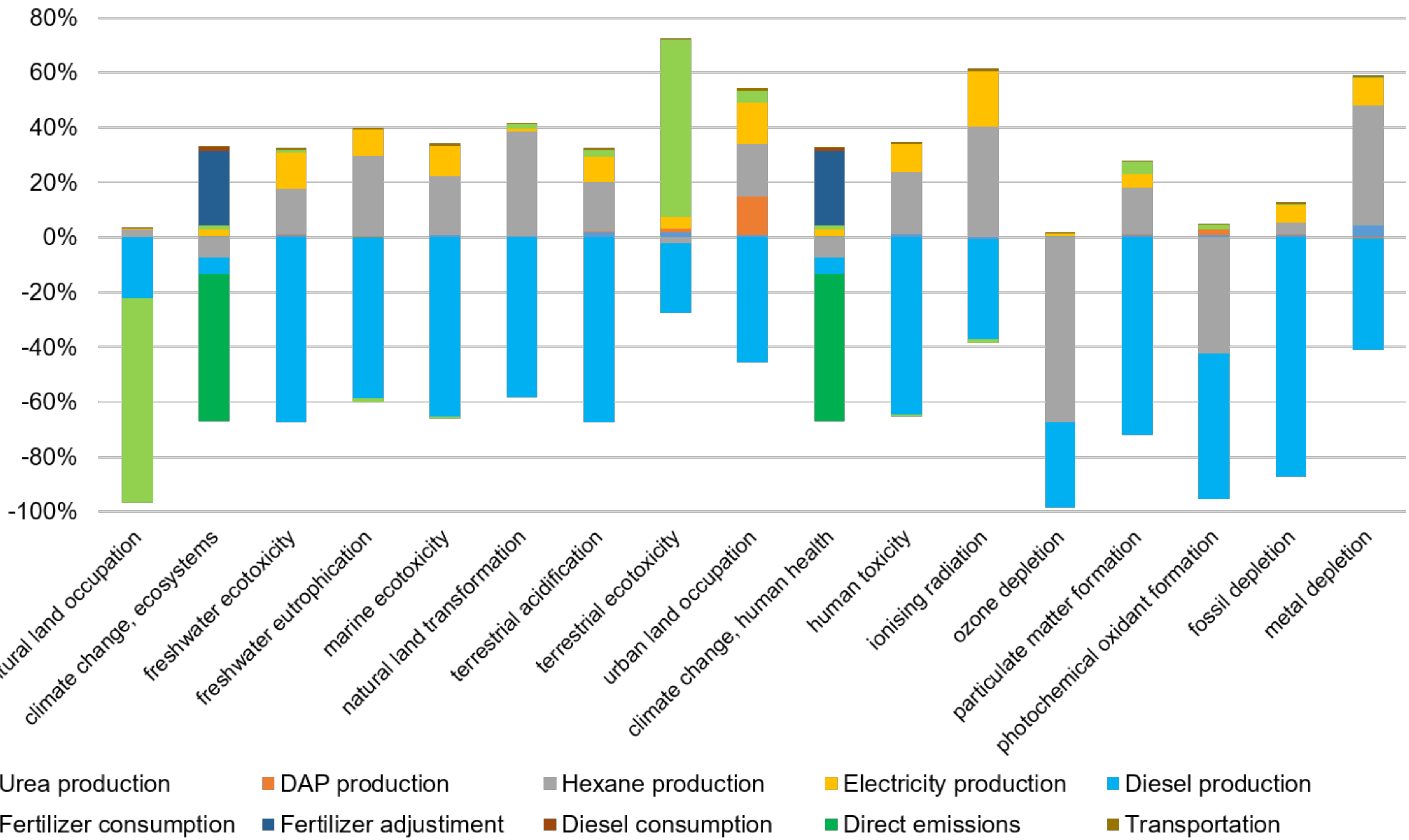
Environmental Impact Breakdown



Primary Markets	Attributional	Consequential
Fertilizers	Increase fertilizer production	(1) Increase but not as much; (2) Crops market (foreign ↑; domestic ↓)
Hexane	Positive characterization factors*	Negative characterization factors*
Diesel	Combustion in end of life	(1) Displace fossil diesel; (2) Transportation market (diesel ↑; gasoline ↓)

*Data for “rest of the world” from Ecoinvent 3.3

Consequential Environmental Profile



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Consequential Life Cycle Optimization: General Conceptual Framework and Application to Algal Renewable Diesel Production

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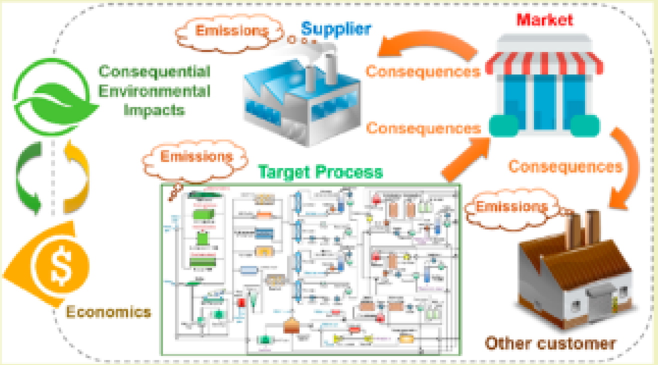
Supporting Information

ABSTRACT: Life cycle optimization (LCO) enables static life cycle analysis (LCA) and techno-economic analysis to be performed dynamically for automatic generation and optimization of process alternatives. Existing LCO models are developed following an attributional LCA approach, which overlooks the environmental consequences in response to the changes in the market. In this study, we develop a consequential LCO framework that simultaneously optimizes consequential environmental impacts and economic performance. We propose a general system boundary that encloses processes linked by markets. On the basis of the general system boundary, we develop a multiobjective optimization model, which integrates process models and market models with the tenets of consequential LCA and techno-economic analysis methodologies. To efficiently solve the resulting nonconvex mixed-integer nonlinear programming problem, a global optimization algorithm is proposed to integrate the inexact parametric algorithm and the branch-and-refine algorithm. The application of the proposed framework is illustrated through a case study of producing renewable diesel from microalgae. We conduct detailed market analysis to identify the consequences associated with the renewable diesel production process. The environmental impacts of the optimal process designs based on the proposed consequential LCO framework are significantly lower than those based on the existing attributional LCO framework.



KEYWORDS: *Life cycle optimization, Consequential life cycle analysis, Superstructure optimization, Sustainability, Algal biofuel*

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Conclusion

- **Life cycle analysis and life cycle optimization**
  - Process-level LCA and life cycle design/optimization
    - Systems boundary
    - Functional unit
  - **Integrated hybrid** LCA and LCO
    - Process systems to supply chain, and to macroeconomics scales
  - **Consequential** LCA and LCO
    - Dynamic and change-driven
    - Suitable for new product systems to account for influences of other processes through the market

- **Applications to energy systems**
  - Algal biorefinery
  - Shale gas
  - ……

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Thank you for your attention

Questions?