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Life Cycle Optimization: MINLP Models and Algorithms

Fengqi You

(Grossmann Group #42, PhD '09)

Northwestern University
Evanston / Chicago

http://you.mccormick.northwestern.edu

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In Honor of Professor Ignacio E. Grossmann's 65th Birthday

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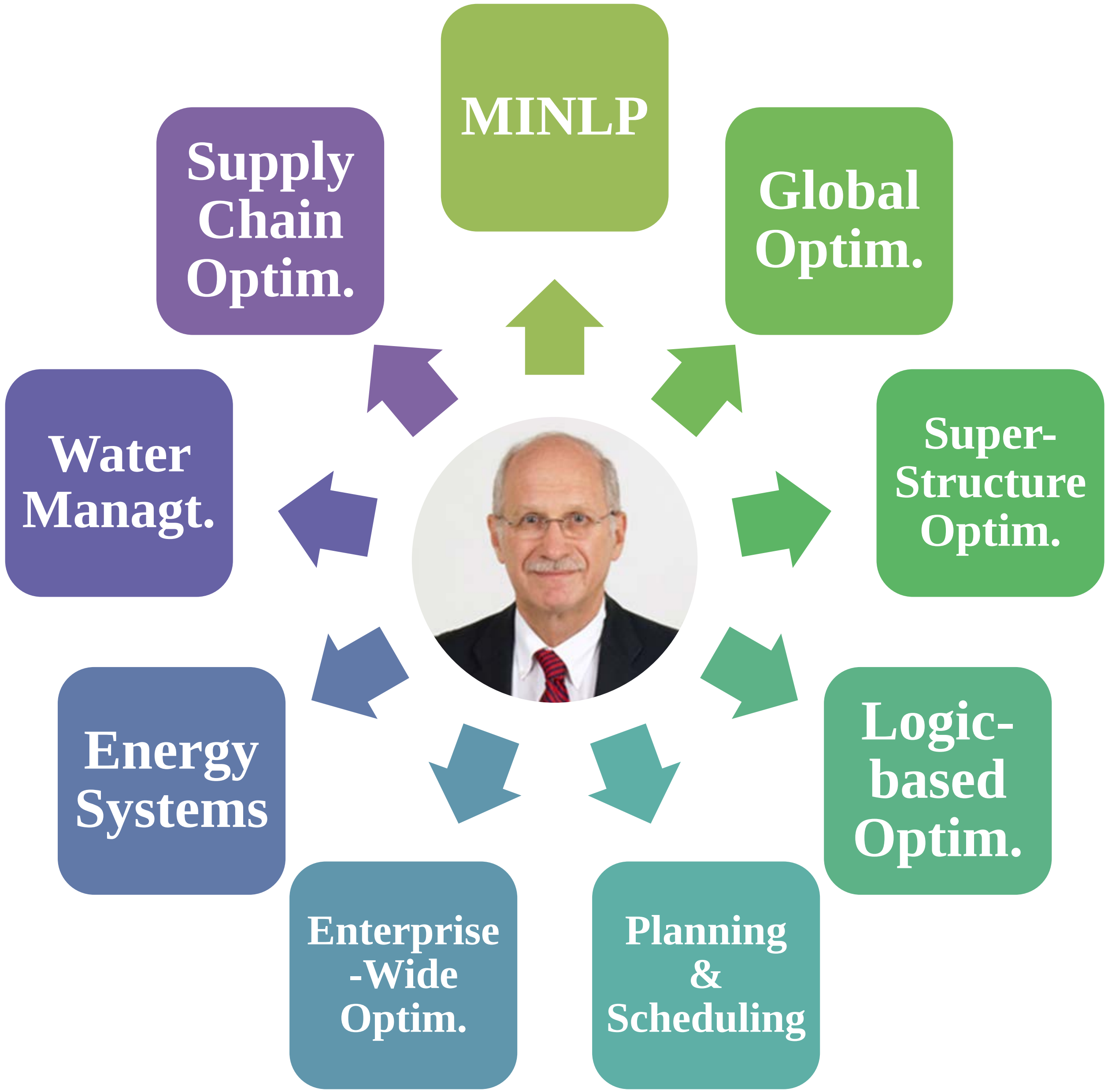
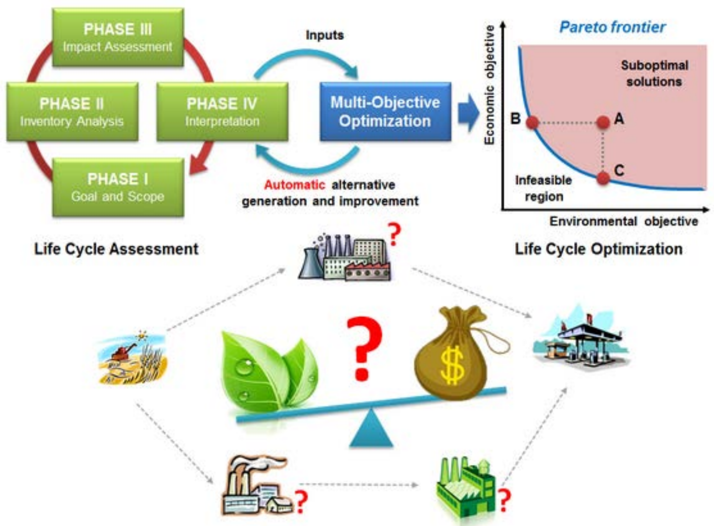
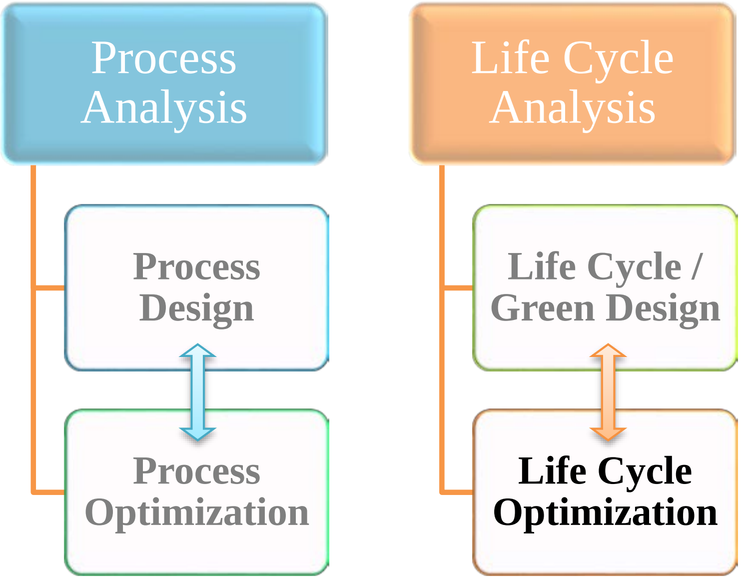
Prof. I. E. Grossmann – A PSE Research Leader



Life Cycle Optimization for Sustainability

- **Life Cycle Optimization**
  - LCA + Supply Chain Optimization (similar to process design optimization)



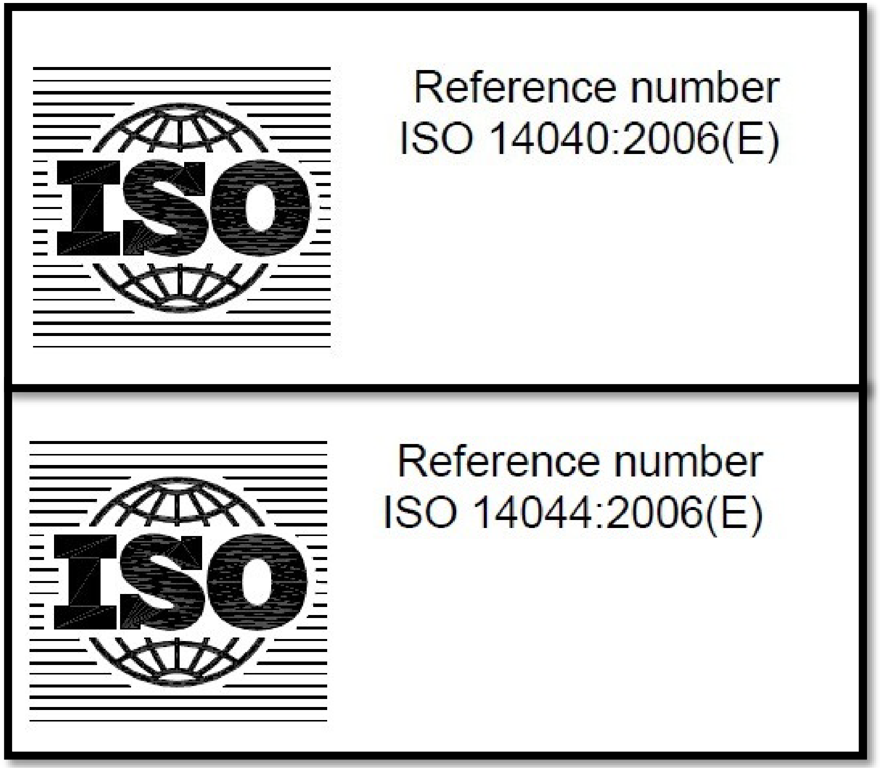


- **Challenges**
  - How to define the "optimal" systems boundary?
  - How to deal with the data quality and uncertainty?
  - How to **seamlessly** integrate LCA into process systems optimization?
  - How to effectively solve **complex, large-scale** life cycle optimization problems?

Life Cycle Optimization (LCO)

Integrating life cycle analysis approach with multi-objective optimization techniques

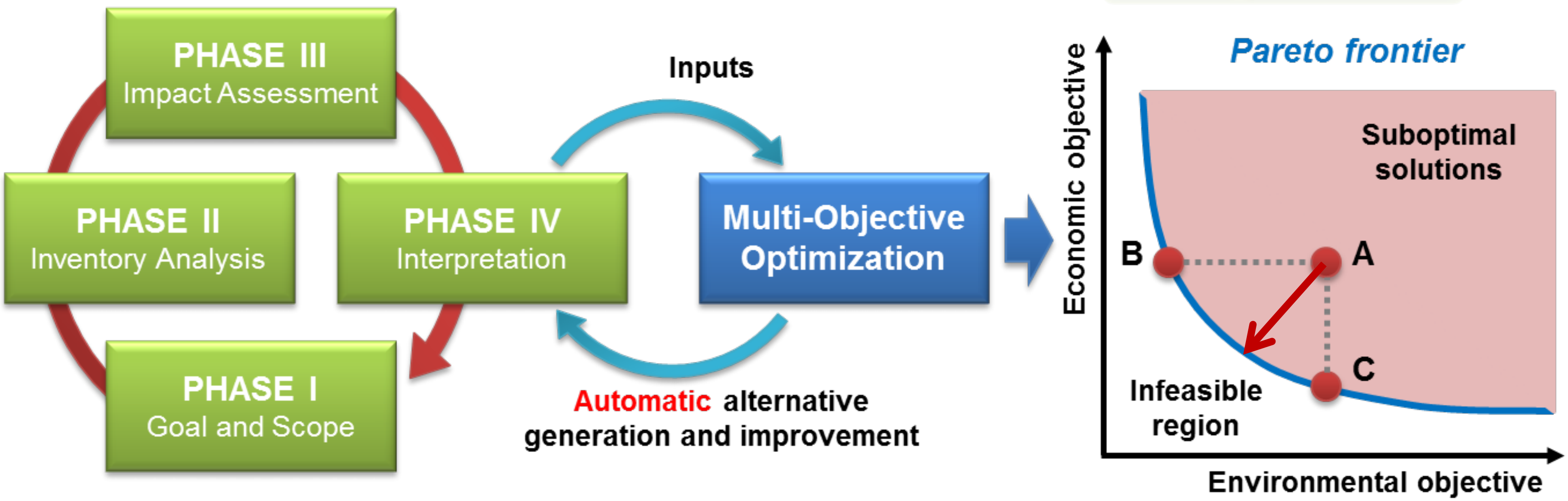
Life Cycle Assessment



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

Life Cycle Optimization (LCO)

Integrating life cycle analysis approach with multi-objective optimization techniques



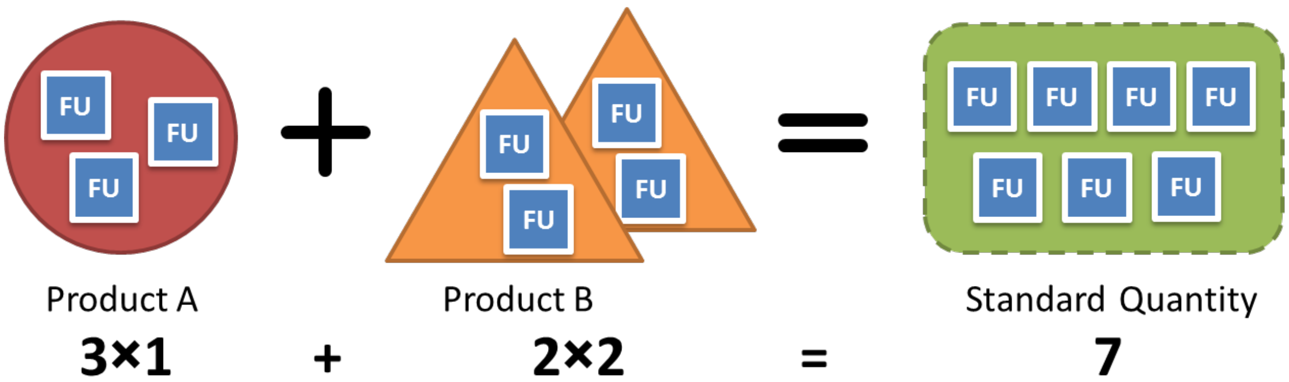
Life Cycle Assessment

Life Cycle Optimization

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

Functional Unit of Multi-Product Systems

Functional unit is a common unit that provides functions



Calculation of functional unit for multiproduct product systems

Why functional-unit-based metrics?

- **Important in practice** (e.g. average GPA, LCOE)
- **Necessary for multi-product systems** (product-centric view)
- **May significantly differ from optimizing total values**

min: Total Env. Impact ≠ min: Unit Env. Impact

General Model Formulation

- **Functional-Unit-Based Life Cycle Optimization**

$$\min \left\{ \frac{\text{total supply chain cost}}{\text{quantity of the function unit}}, \frac{\text{life cycle environmental impact}}{\text{quantity of the function unit}}, \ldots \right\}$$

$$\text{s.t.} \quad \boxed{A + B \cdot x + C \cdot y = 0}$$

$$x \in \mathbb{R}^n \quad \text{and} \quad \boxed{y \in \{0,1\}^m}$$

- **Discrete Variables**
  - Technology selection
  - Facility location
  - Network design
  - Discrete capacity levels
  - Discontinuous operating decisions
  - ……
- **Constraints**
  - Mass balance and energy balance
  - Cash flow and financial constraints
  - Capacity constraints
  - Logic constraints for discrete variables
  - Life cycle environmental impact
  - ……

General Model Formulation

- **Functional-Unit-Based Life Cycle Optimization**

$$\min \left\{ \frac{\text{total supply chain cost}}{\text{quantity of the function unit}}, \boxed{\frac{\text{life cycle environmental impact}}{\text{quantity of the function unit}}} \right\}$$

$$\text{s.t.} \quad A + B \cdot x + C \cdot y = 0$$

$$x \in \mathbb{R}^n \quad \text{and} \quad y \in \{0,1\}^m$$

- **Environmental Objective**
  - Typically mixed-integer linear function
    - Process-based LCA or reformulate Input-output (IO) model into LP form for IO-based or hybrid LCA
  - Mixed-integer linear fractional program
    - **Non-convex** MINLP
    - Need global optimization

$$\min \quad \frac{A_0 + A_1 \cdot x + A_2 \cdot y}{B_0 + B_1 \cdot x + B_2 \cdot y}$$

$$\text{s.t.} \quad A + B \cdot x + C \cdot y = 0$$

$$x \in \mathbb{R}^n \quad \text{and} \quad y \in \{0,1\}^m$$

Mixed-Integer Linear Fractional Program (MILFP)

General Model Formulation

- **Functional-Unit-Based Life Cycle Optimization**

$$\min \left\{ \frac{\text{total supply chain cost}}{\text{quantity of the function unit}}, \frac{\text{life cycle environmental impact}}{\text{quantity of the function unit}} \right\}$$

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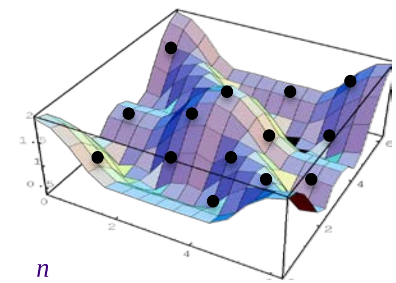


- **Economic Objective**
  - CAPEX + OPEX
  - CAPEX may include scaling factors for capital investments
  - Capital cost term = $\beta \cdot x^{\alpha}$
  - Scale factor $\alpha \approx 0.6$
  - **Non-convex MIFP**

$$\min \frac{A_0 + A_1 \cdot x + A_2 \cdot y + \sum_{i=1}^{n} \beta_i \cdot (x_i)^{\alpha_i}}{B_0 + B_1 \cdot x + B_2 \cdot y}$$

$$\text{s.t.} \quad A + B \cdot x + C \cdot y = 0$$

$$x \in \mathbb{R}^n \quad \text{and} \quad y \in \{0,1\}^m$$

MIFP with Separable Concave Terms

Parametric Approach

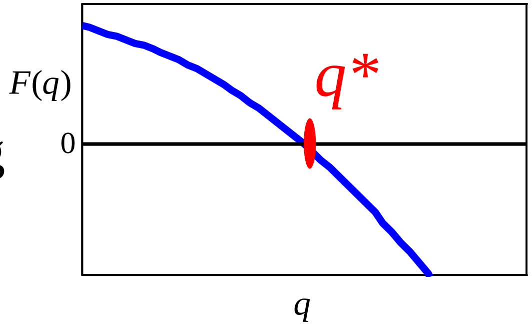
$$\min_{(x,y)\in S} \frac{N(x,y)}{D(x,y)}$$

MIFP Problem

$$F(q) = \min_{(x,y)\in S} N(x,y) - q \cdot D(x,y)$$

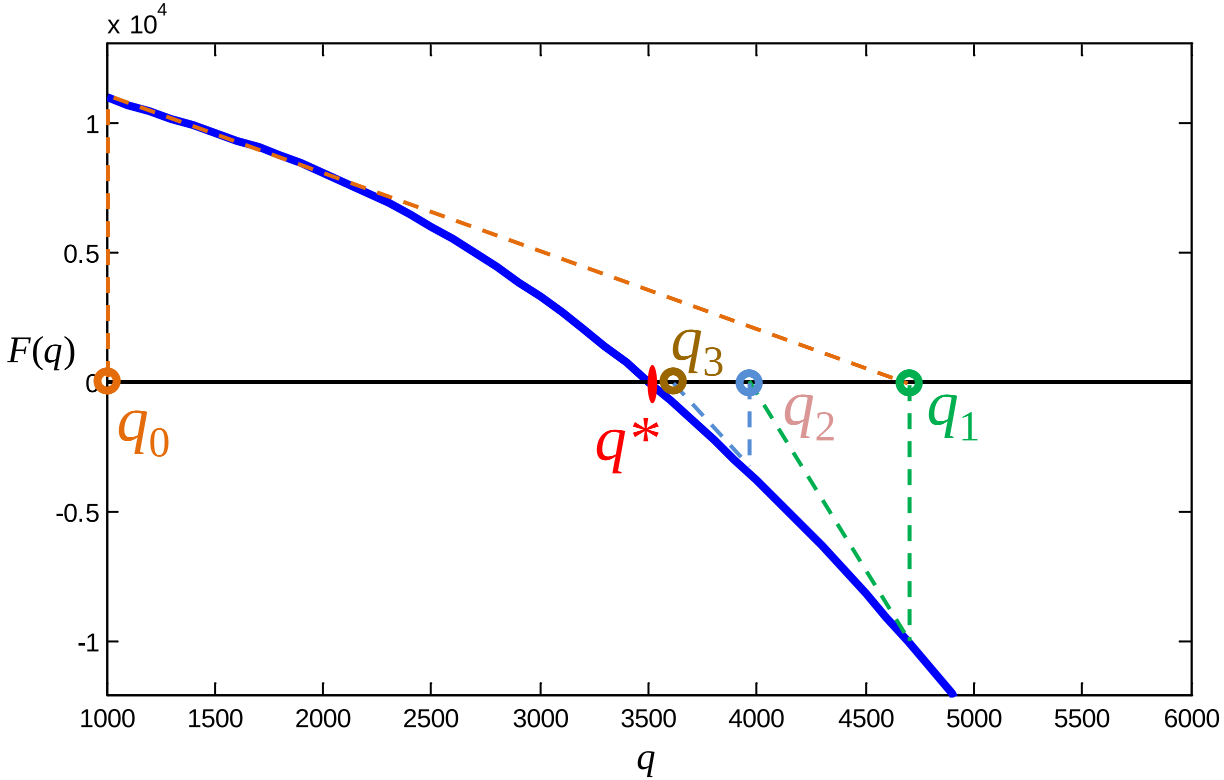
Parametric MIP Subproblem

- **Equivalence**
  - $(x, y)^*$ is the global optimal solution of the original MIFP problem if and only if $(x, y)^*$ is the global optimal solution of the parametric MIP subproblem with the parameter q^* such that $F(q^*) = 0$
  - Assumption: Positive denominator, $D(x, y) > 0$
- **Properties of $F(q)$**
  - Concave, continuous, monotonically decreasing
  - Unique solution for $F(q^*) = 0$
  - **$-D(x, y)^*$ is a subgradient of $F(q)$**

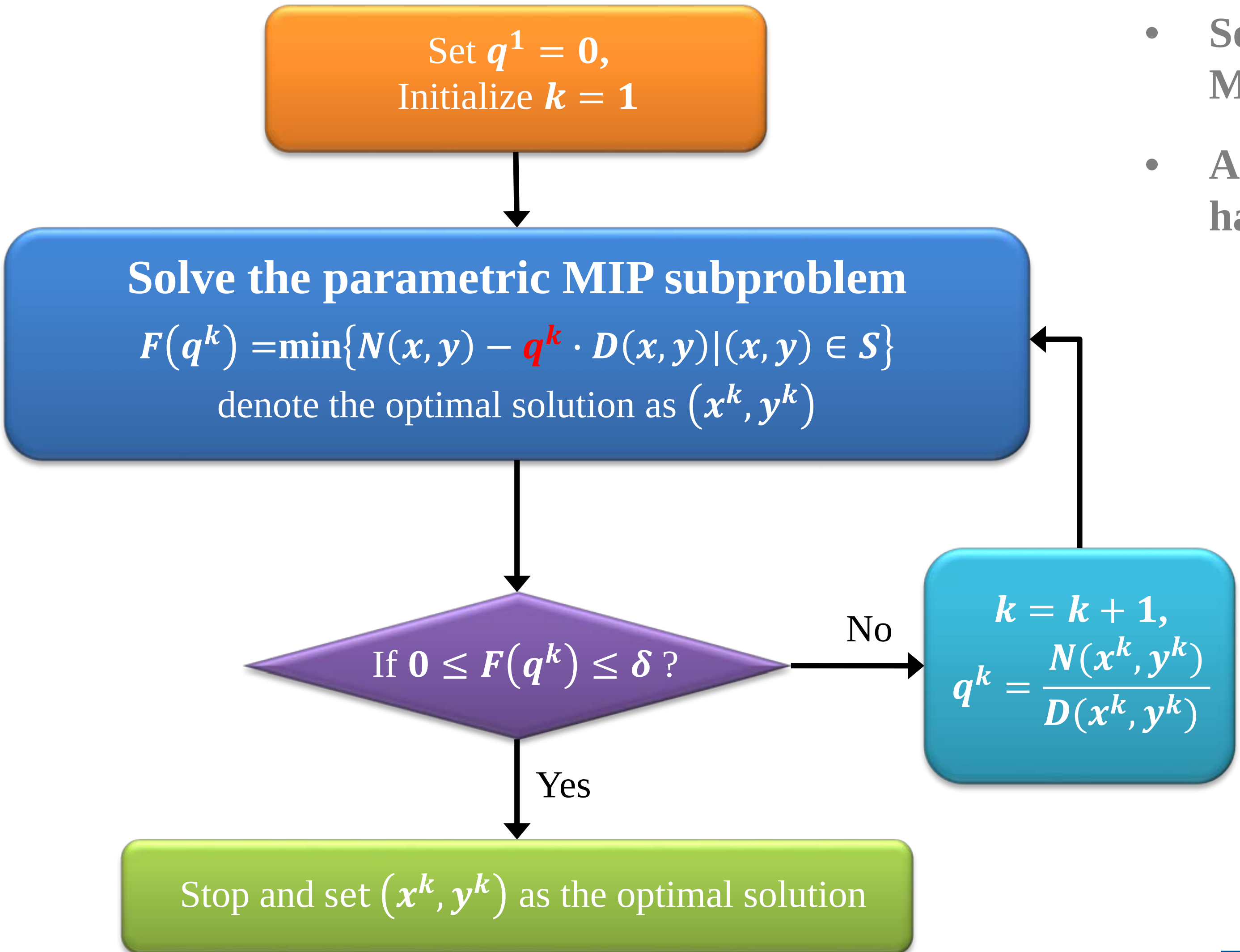


Root-Finding Method (Newton's)

- Subgradient of $F(q) \approx -D\left(x, y\right)^*$
- Upper bound sequence: $q_1 \geq q_2 \geq q_3 \geq \ldots \geq q^*$



Parametric Algorithm (Exact Newton's)

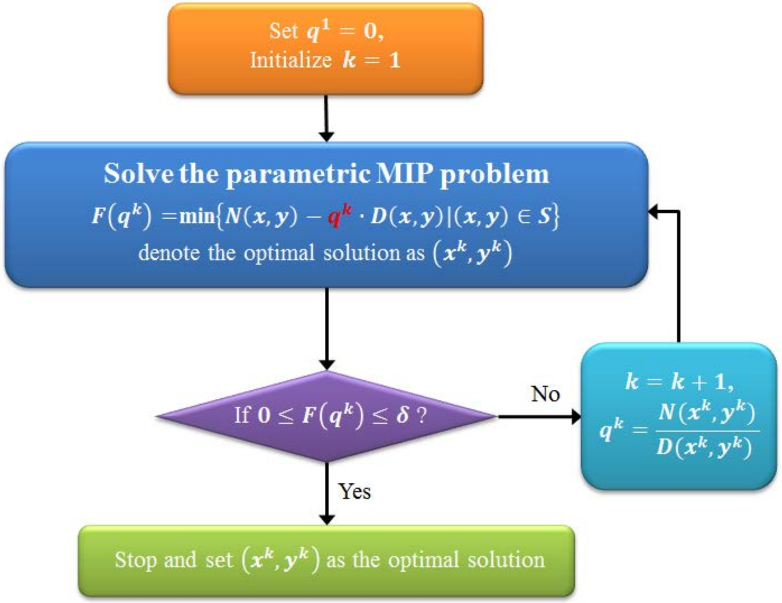


- **Solve a sequence of MIP subproblems**
- **All MIP subproblems have the same size**

Parametric Algorithm (Inexact Newton's)

- **MIP is NP-hard**
- **Globally optimization (0% gap) of all MIPs maybe challenging**

Convergence guaranteed if each (parametric) **MIP is solved to a relative optimality gap < 100%**



- Converge **superlinearly**
  - Exact Newton's: ***quadratic*** rate
- **Trade-off: more iterations v.s. shorter time per iteration** (for solving the parametric MIP subproblems)
- **Applicable to general (convex or nonconvex) MIFPs**

Zhong, Z., & You, F. (2014). Globally Convergent Exact and Inexact Parametric Algorithms for Solving Large-Scale Mixed-Integer Fractional Programs. *Computers & Chemical Engineering*, 61, 90-101.

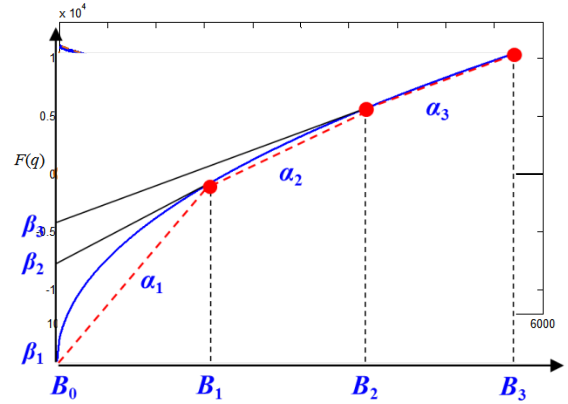
Tailored Global Optimization Algorithm

- Global optimization based on the **model structure**
  - **Inexact** parametric approach for mixed-integer fractional terms
  - Branch-and-refine method for separable concave terms

$$\min \frac{A_0 + A_1 \cdot x + A_2 \cdot y + \sum_{i=1}^{n} \beta_i \cdot (x_i)^{\alpha_i}}{B_0 + B_1 \cdot x + B_2 \cdot y}$$

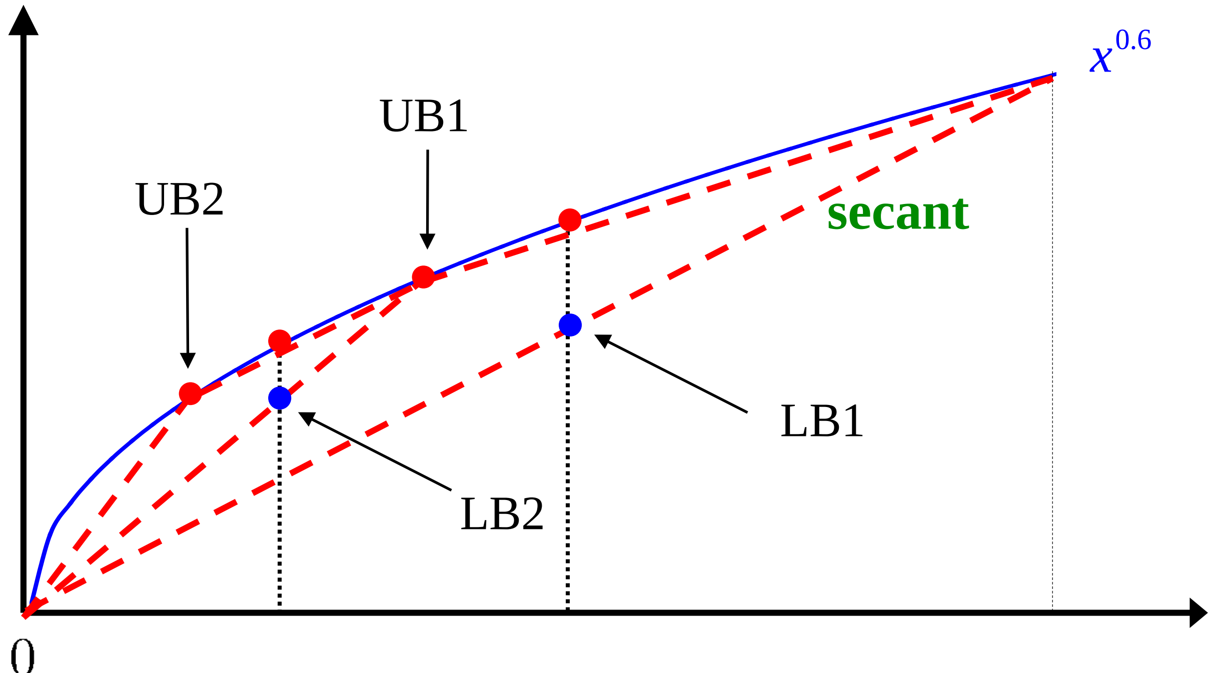
$$\min \; A_0 + A_1 \cdot x + A_2 \cdot y + \sum_{i=1}^{n} \beta_i \cdot (x_i)^{\alpha_i} - q \cdot (B_0 + B_1 \cdot x + B_2 \cdot y)$$

s.t. technology selection and network design
logic constraints for discrete variables
mass balance and capacity constraints
energy balance constraints
economic evaluation constraints
environmental life cycle analysis constraints
……

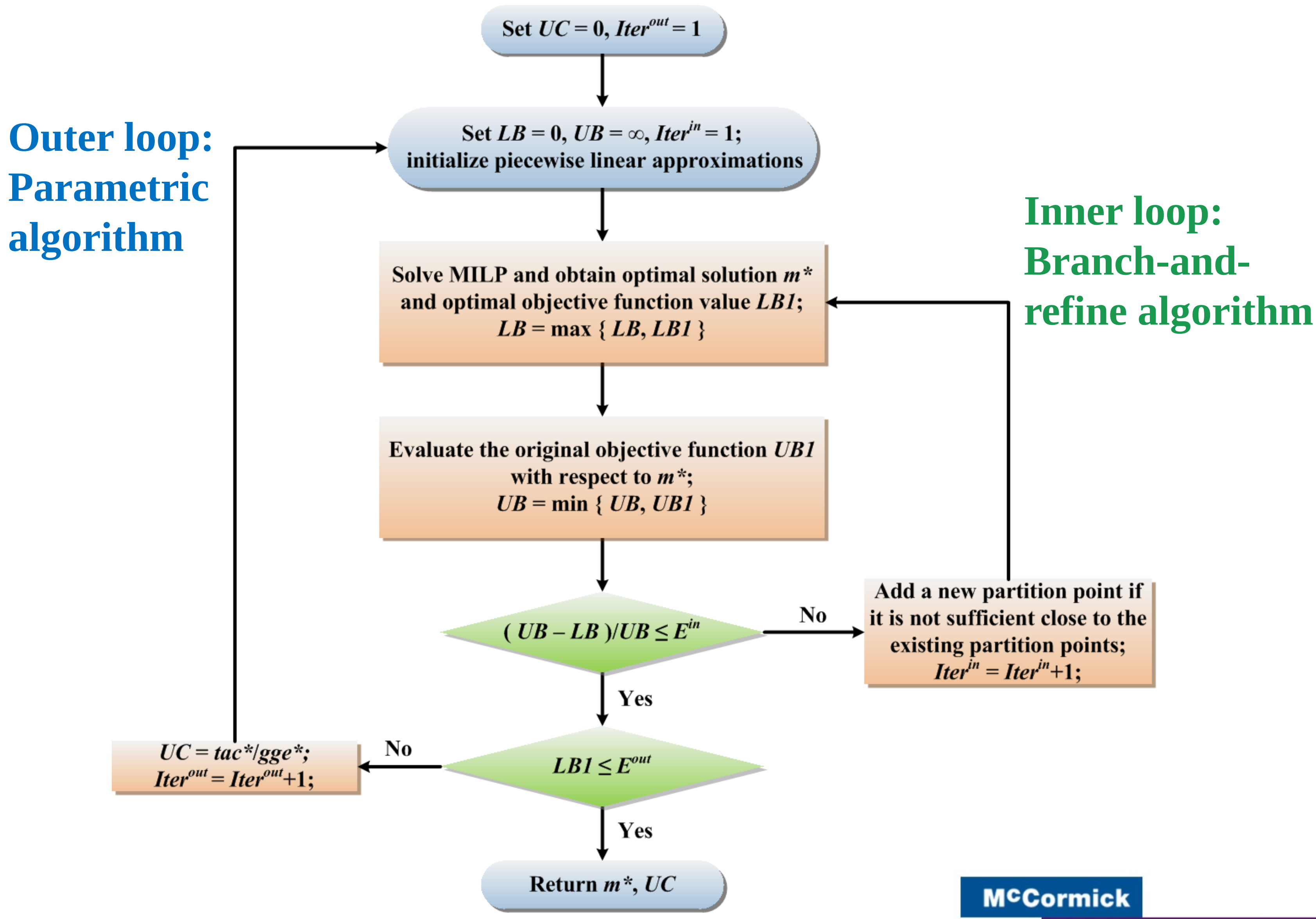


Branch-and-Refine Algorithm

- Global Optimization for MINLPs with **separable concave terms**
  - Piece-wise linear approximation (MILP) gives **global** lower bounds
  - Feasible solutions provide upper bounds – solving a reduced MINLP
  - Increasing the number of pieces as iteration number increases



Solution Algorithm



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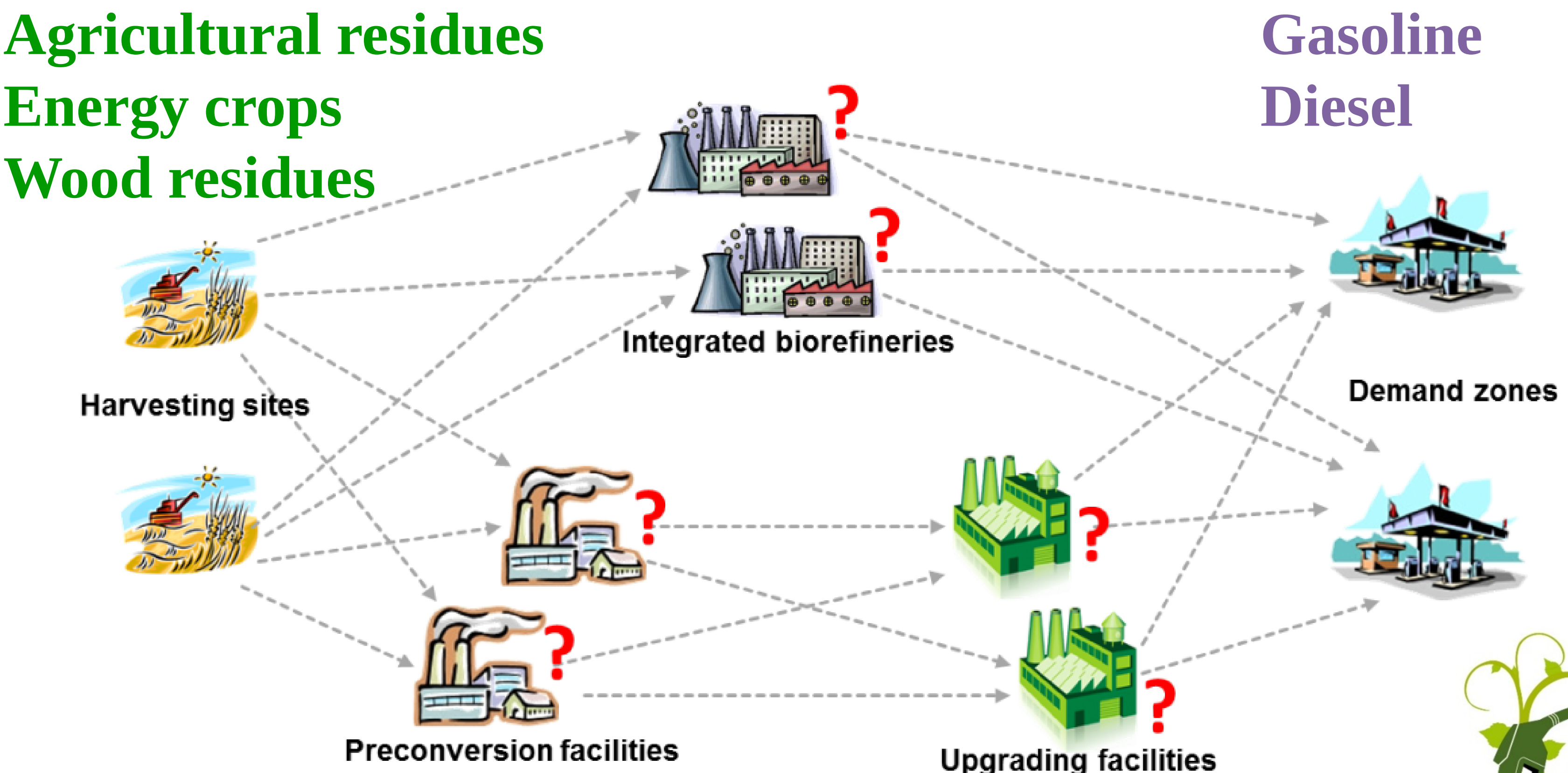
Application on Hydrocarbon Biofuels



Hydrocarbon Biofuel Supply Chain

Biomass Acquisition	Biofuels Production	Transportation & Distribution	Biofuels End-Use
			

Cellulosic biomass:
residual, non-edible parts of food crops as well as other non-food crops

Agricultural residues

Residues of corn, wheat, cotton, soybean, etc.

Energy crops

Switchgrass

Wood residues

Forest residues and primary mills, secondary mills, urban wood residues

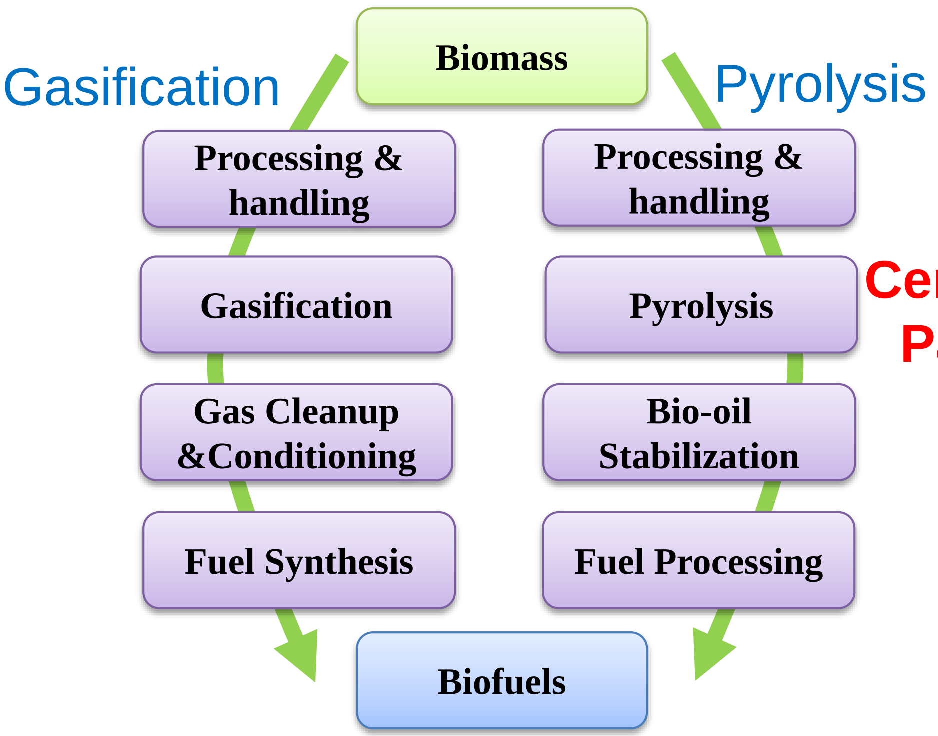
Hydrocarbon Biofuel Supply Chain

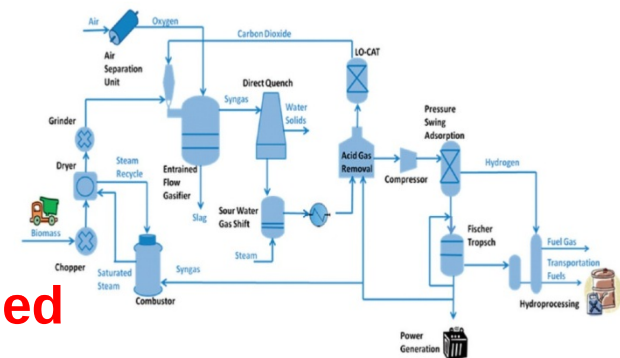
Biomass Acquisition

Biofuels Production

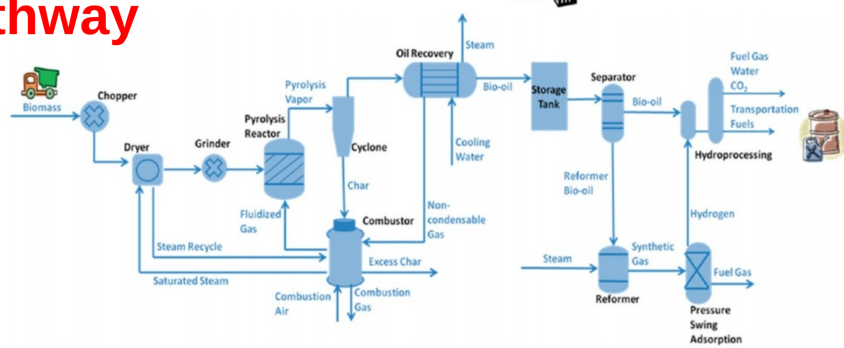
Transportation & Distribution

Biofuels End-Use





Centralized Pathway



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Hydrocarbon Biofuel Supply Chain

Biomass Acquisition

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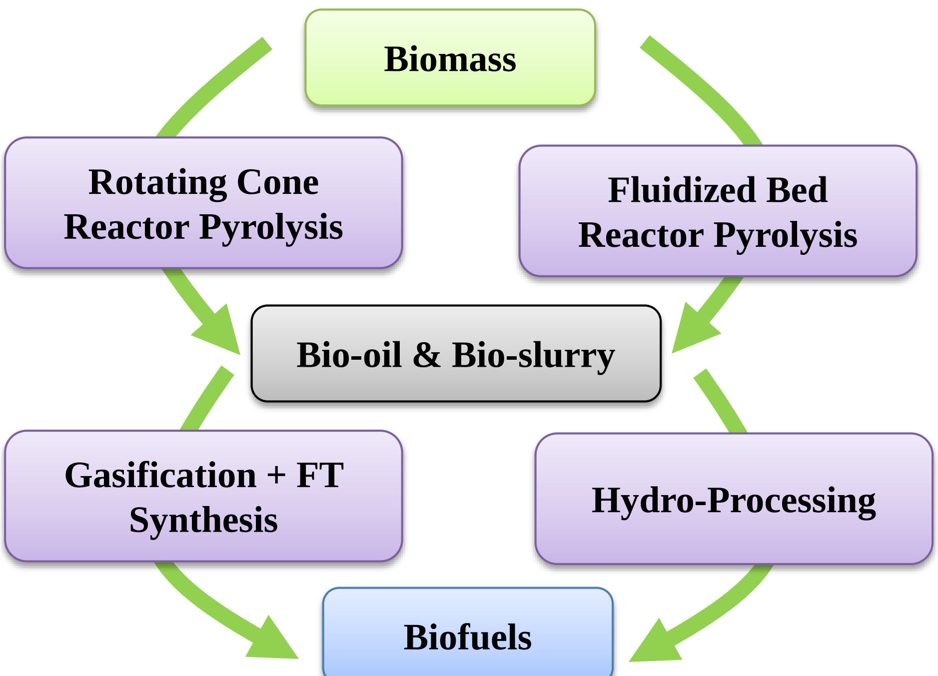
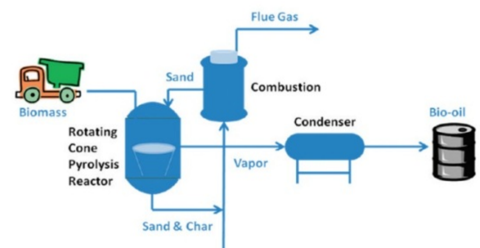
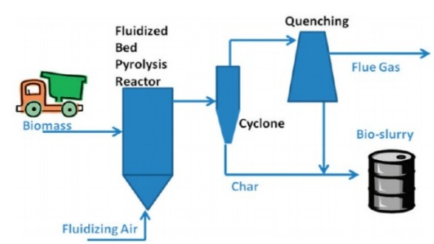




Distributed Pathway



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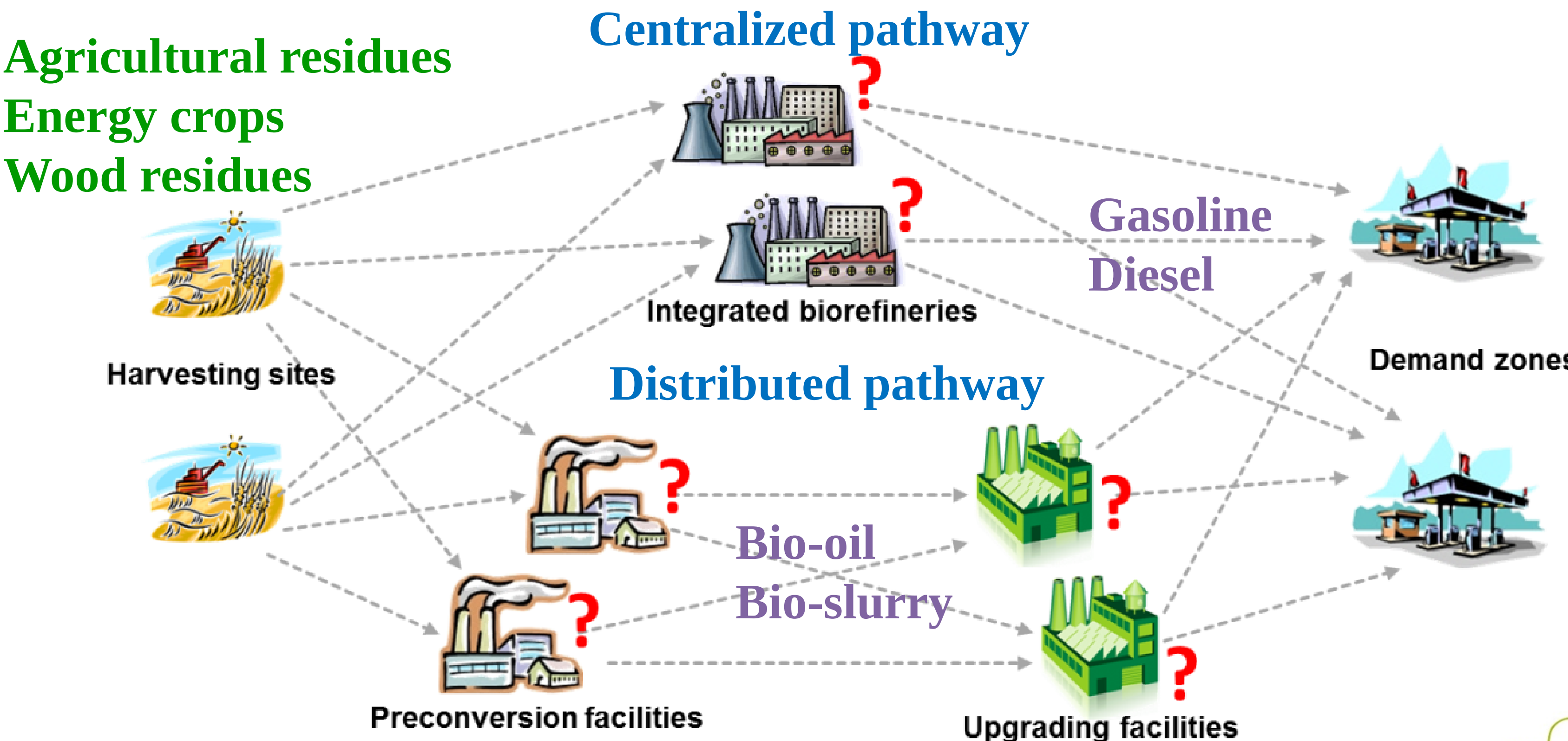
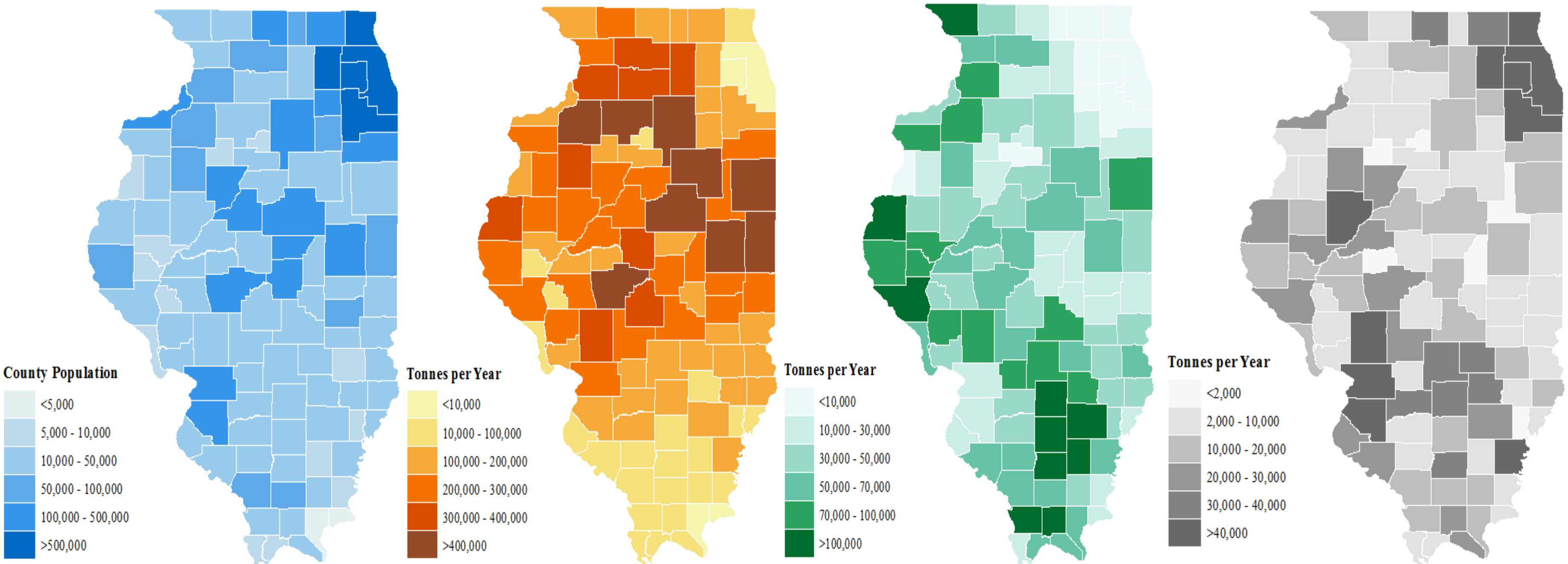


Functional Unit: Gasoline-Equivalent Gallon (GEG)

- 1 GEG = 114,000 BTU per gallon
- 1 gallon of diesel = 1.1363636 GEG
- 1 gallon of gasoline = 1 GEG

GIS Data for Illinois



a) Population distribution of Illinois
b) Spatial distribution of agricultural residues in Illinois
c) Spatial distribution of energy crops in Illinois
d) Spatial distribution of wood residues in Illinois

Computational Result (a Pareto optimal solution)

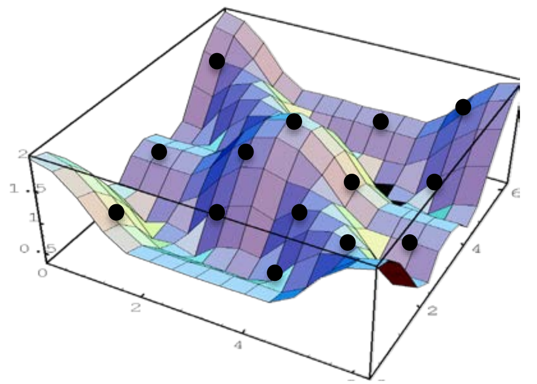
- **Functional-Unit-Based Life Cycle Optimization**

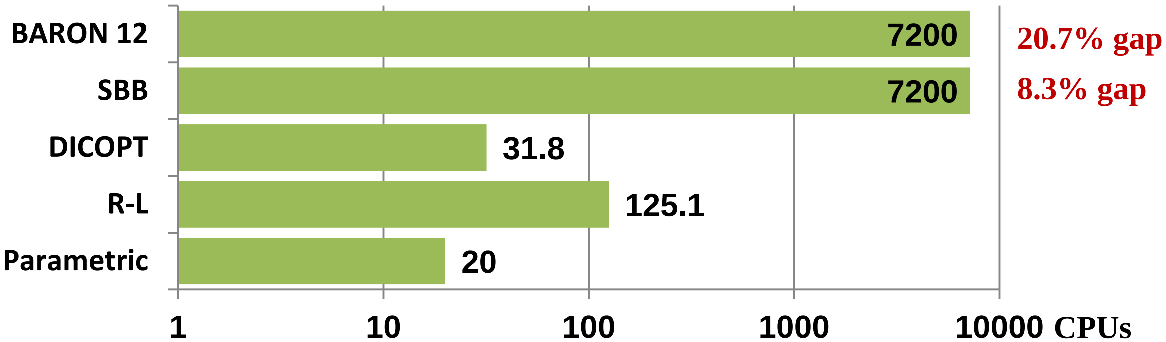
$$\min \left\{ \frac{\text{total supply chain cost}}{\text{quantity of the function unit}}, \frac{\text{life cycle environmental impacts}}{\text{quantity of the function unit}} \right\}$$

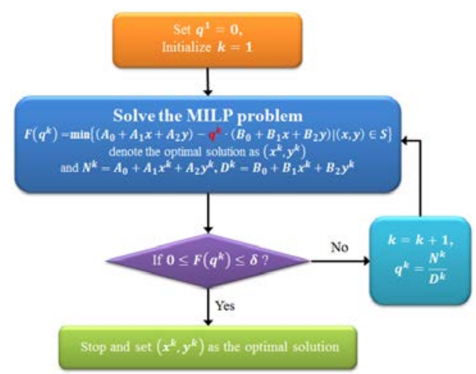
$$\text{s.t.} \quad A + B \cdot x + C \cdot y = 0$$

$$x \in \mathbb{R}^n \quad \text{and} \quad y \in \{0,1\}^m$$

- **Mixed-Integer Linear Fractional Programming**
  - 224 discrete variables
  - 131,351 continuous variables
  - 30,826 constraints







Yue, D., Kim, M., & You, F. (2013). Design of Sustainable Product Systems and Supply Chains with Life Cycle Optimization Based on Functional Unit. *ACS Sustainable Chemistry & Engineering*, 1, 1003–1014.

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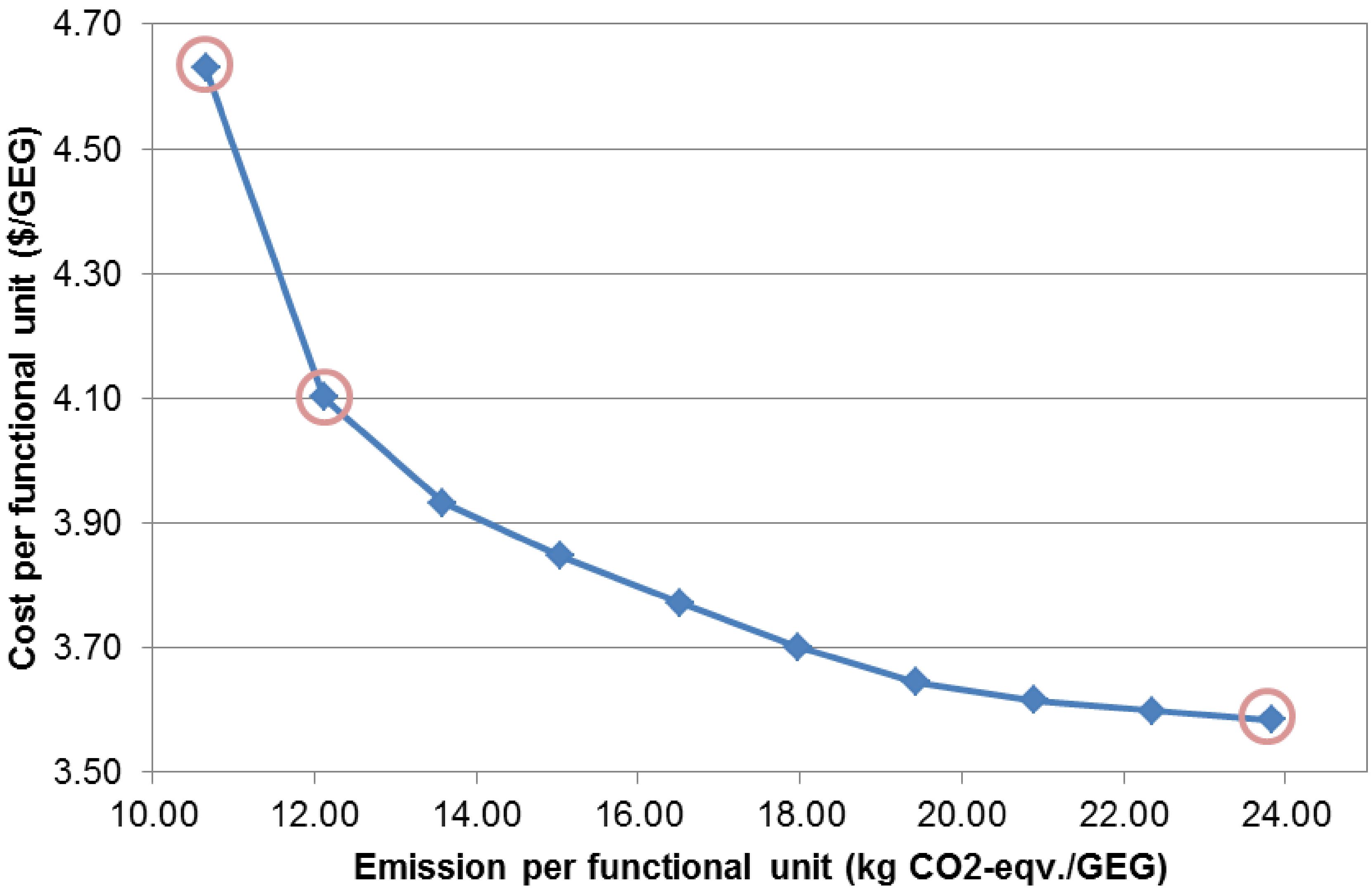
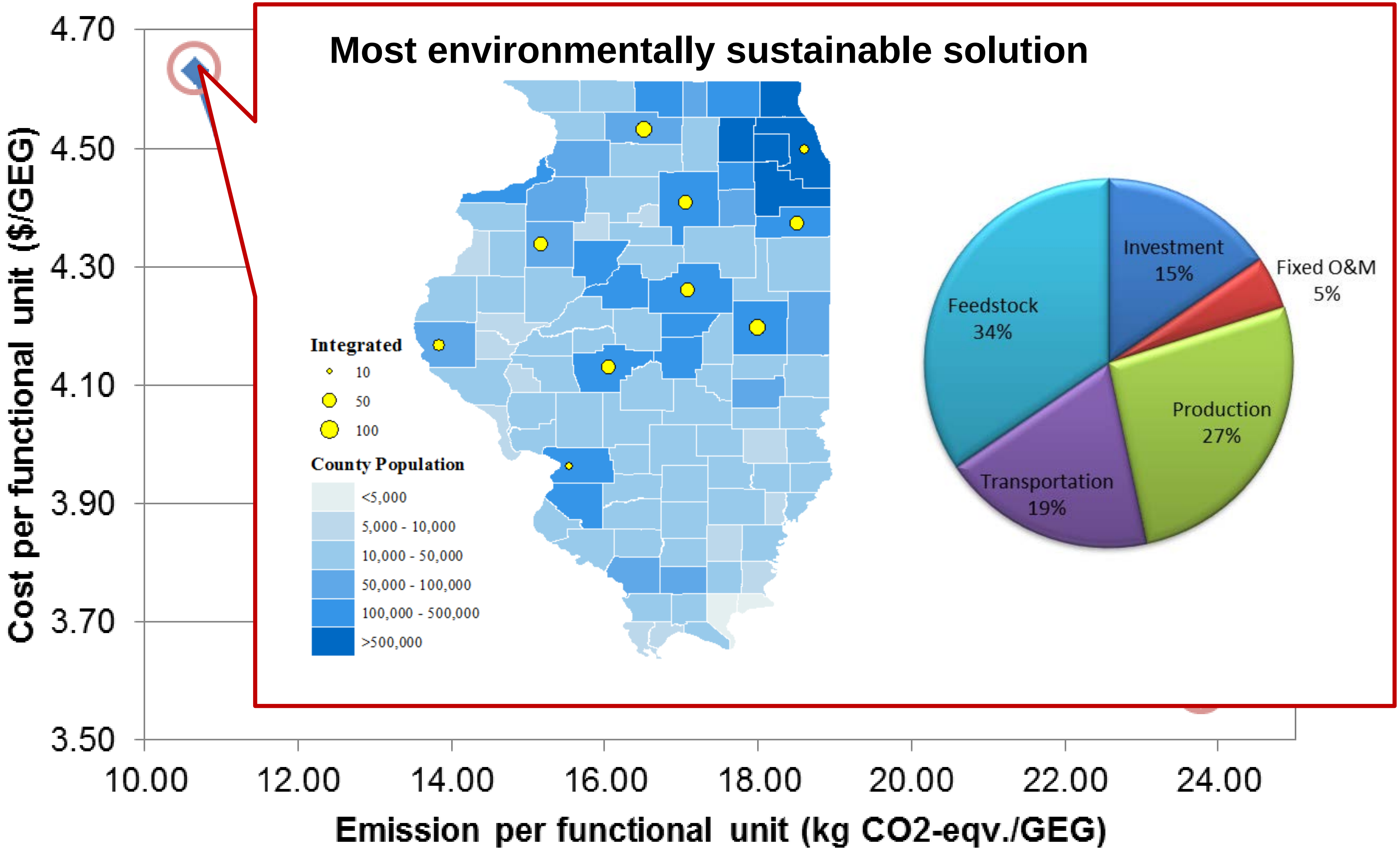
Pareto Curve



Pareto Curve



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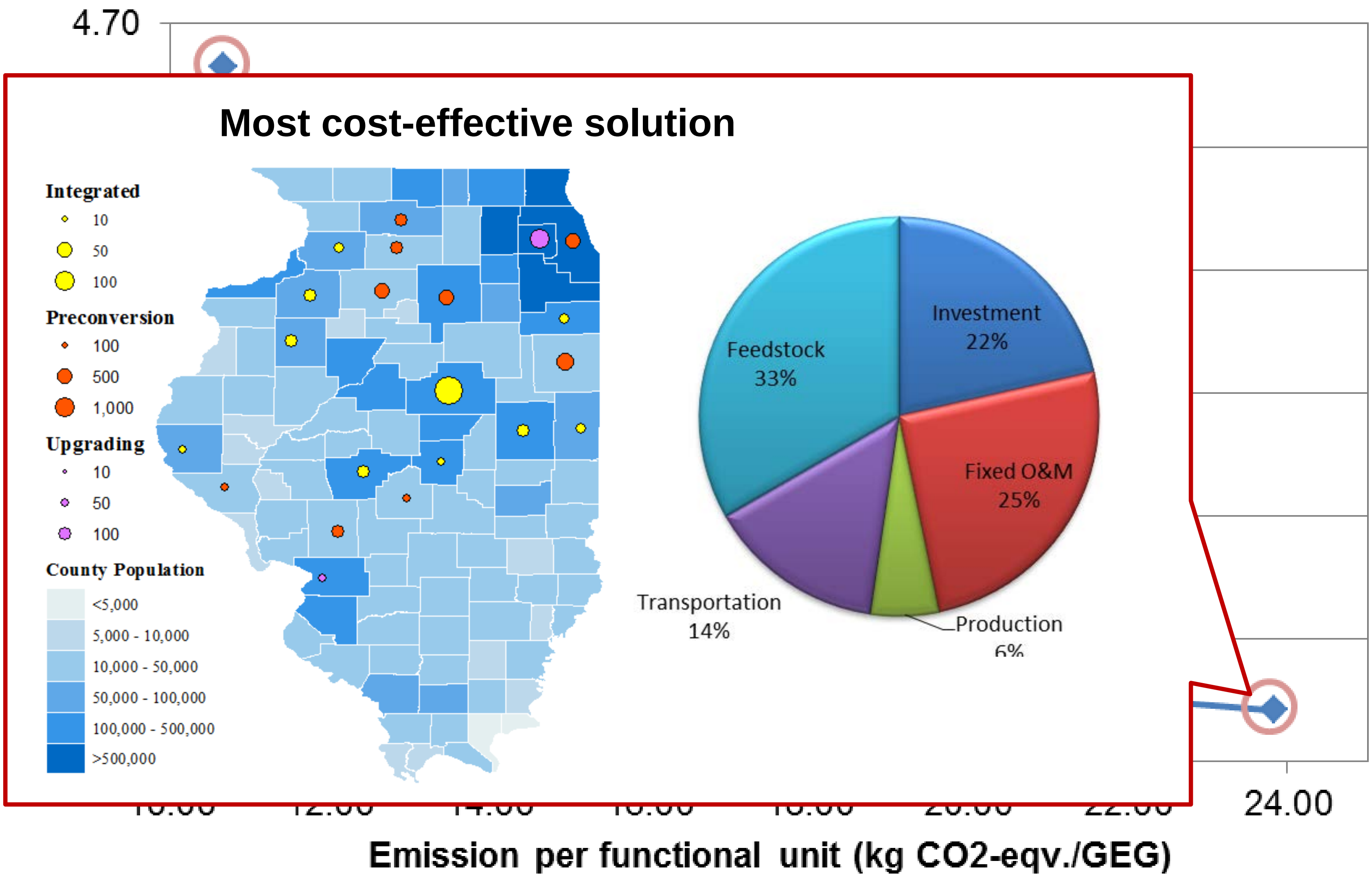

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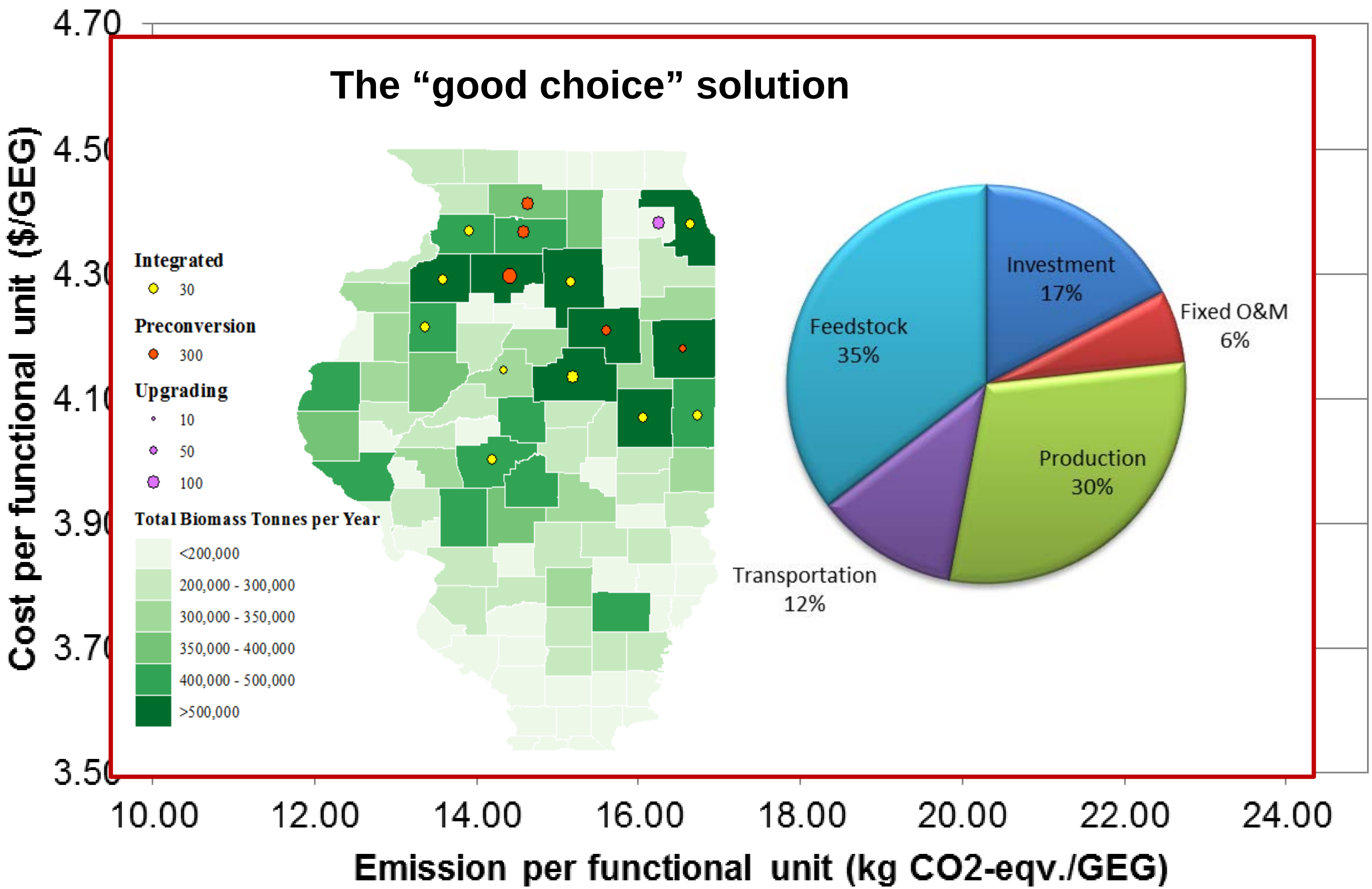
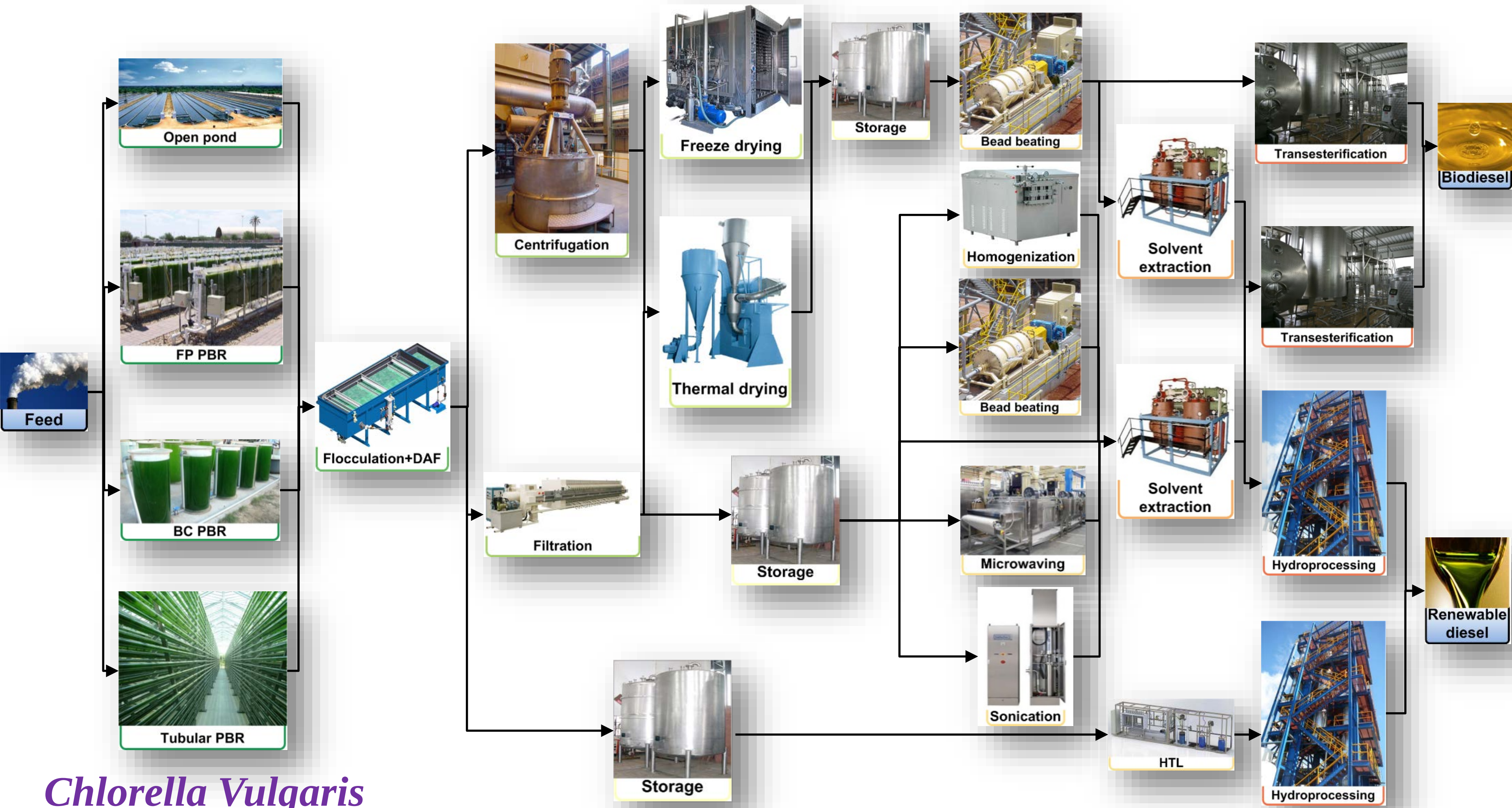
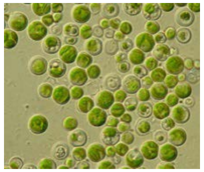
Pareto Curve



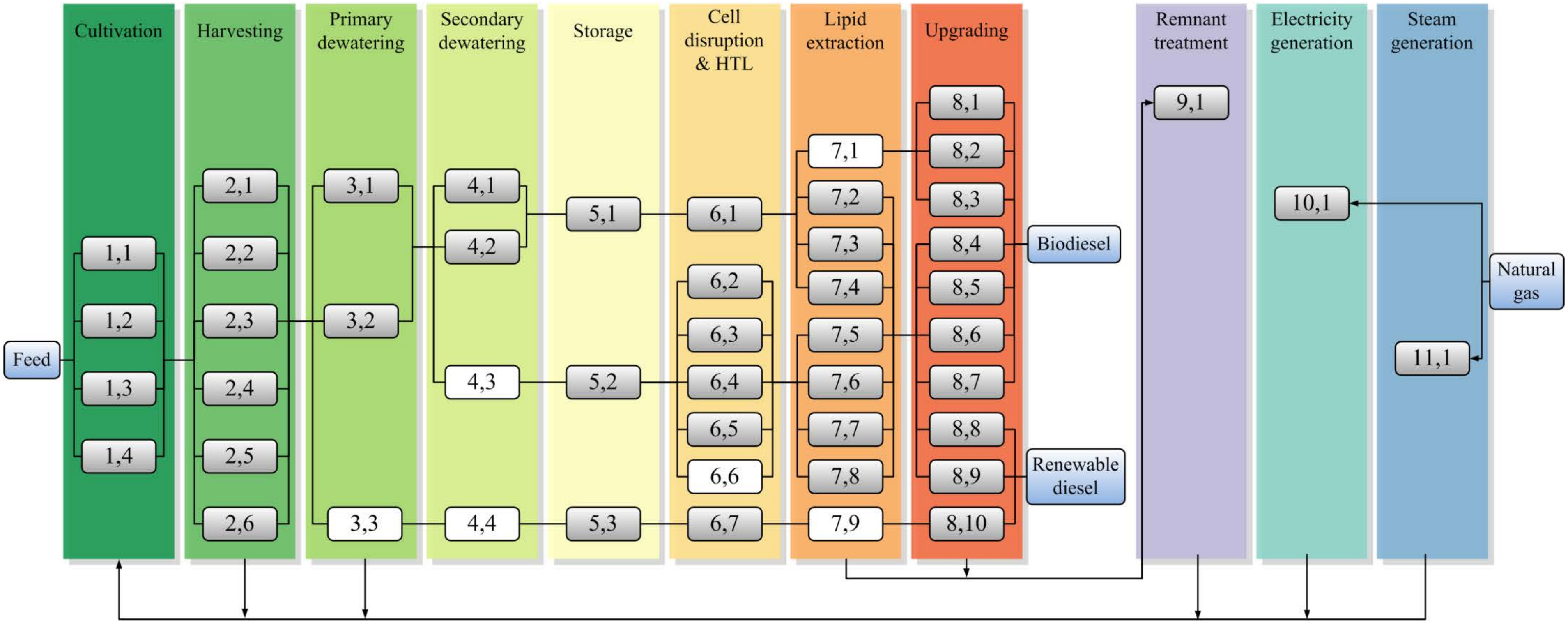
Application on Algae Processing Network



Chlorella Vulgaris

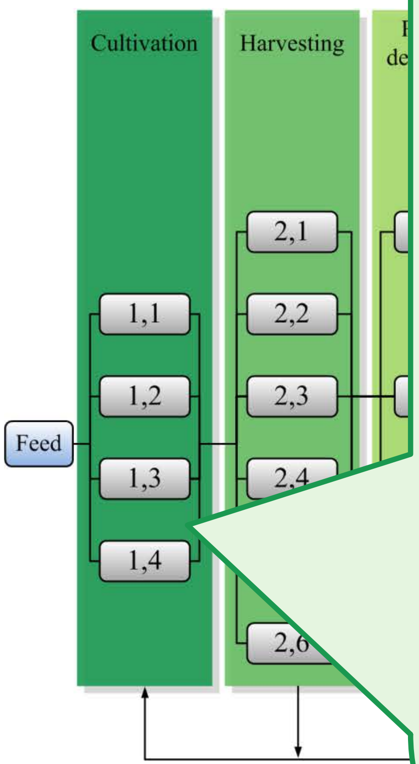


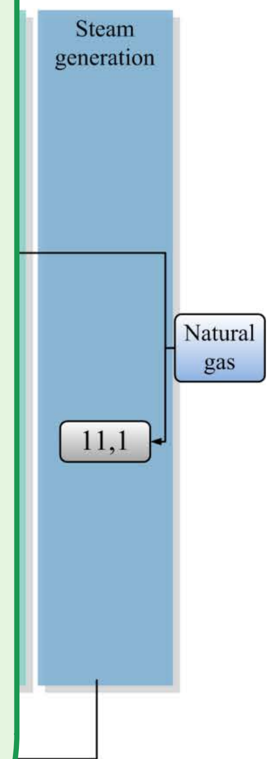
Algae Processing Network Superstructure



7,800+ processing routes

Algae Processing Network Superstructure





<1,2> Flat plate photobioreactor

<1,3> Bubble column photobioreactor

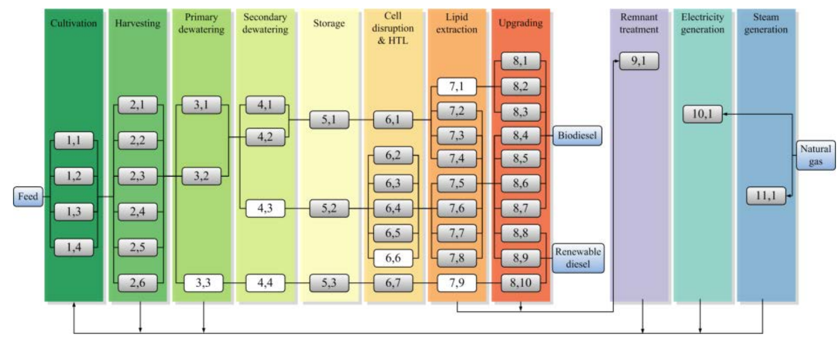
<1,4> Tubular photobioreactor

7,800+ processing routes

Algae Process Design and Optimization

- **Optimal design and operations of algal biorefinery**
  - Selection of technology, pathway, and processing methods
  - Determination of product portfolio under the given feed
  - Mass balance, capacity, and equipment sizing
  - Energy and utility consumption
  - **Process Economics**
  - **Environmental Sustainability**

Chlorella Vulgaris



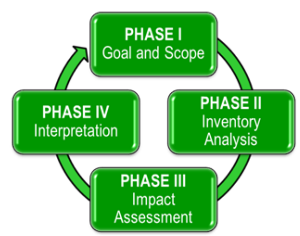
- **Life cycle optimization w/ FU**
  - Recycle water and nutrients
  - **Direct** and **indirect** GHG emissions
  - Multiple fuel/chemical products
  - Cost-effective & sustainable design

Process / SC Superstructure → **MINLP Optimization Model** → **Optimal Design**

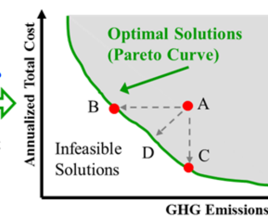
$$\min_{x,y} \left[f_1(x,y), f_2(x,y) \right]^T$$
$$s.t. \quad h(x,y) = 0$$
$$g(x,y) \le 0$$
$$x \in R^n, \ y \in \{0,1\}^m$$

Multiobjective MINLP

Automatically search alternatives for improvement



Life Cycle Assessment



Life Cycle Optimization

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Model Formulation

- **Mixed-Integer Nonconvex Fractional Programming**
- **Objectives:** **Choose Discrete (0-1), continuous variables**
  - Minimize: Life cycle GHG emission **per GGE** (life cycle analysis)
    - Direct emissions: Cultivation, remnant treatment, & utility generation
    - Indirect emissions: External utility, e.g. electricity and steam
  - Minimize: Cost **per GGE** (techno-economic analysis)
    - Credit from selling by-products (glycerol, fertilizer, and biogas)
    - Annualized capital cost (cc)
    - Operating cost
- **Constraints:**
  - Process network design specifications
  - Technology and pathway selection
  - Mass and material balance
  - Production planning, and capacity limits
  - Energy balance and utility consumption

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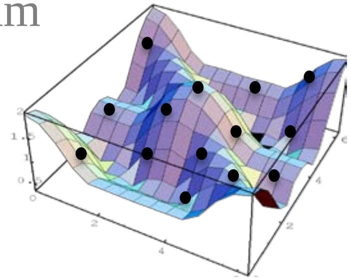


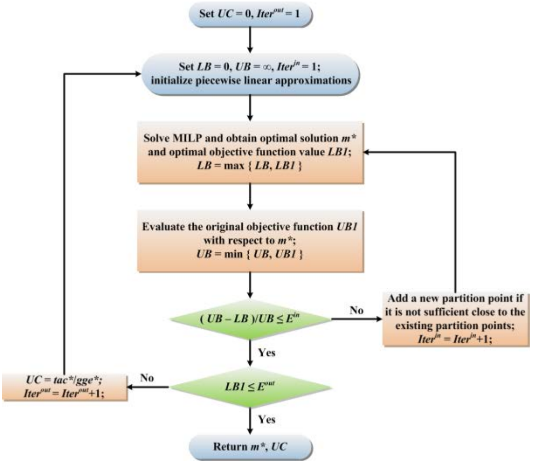
$$\min \frac{\sum_{i,j} A_{i,j} \cdot x_{i,j}^{cc} + \sum_{i,j} \beta_{i,j} \cdot \left(x_{i,j}^{cc}\right)^{\alpha_{i,j}}}{gge}$$

$$cc = \beta \cdot x^{\alpha}, \ \alpha \approx 0.6$$

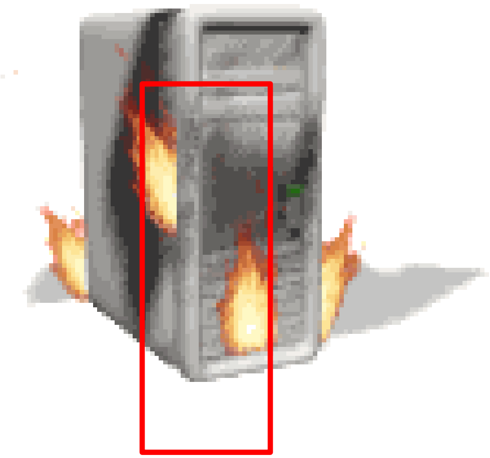
- **Constraints:**
  - Process network design specifications
  - Technology and pathway selection
  - Mass and material balance
  - Production planning, and capacity limits
  - Energy balance and utility consumption

Computational Results

- **Problem size** (MIFP with concave terms):
  - Discrete 0-1 variables: 49
  - Continuous variables: 32,958
  - Constraints: 56,274
  - Non zero elements: 145,383



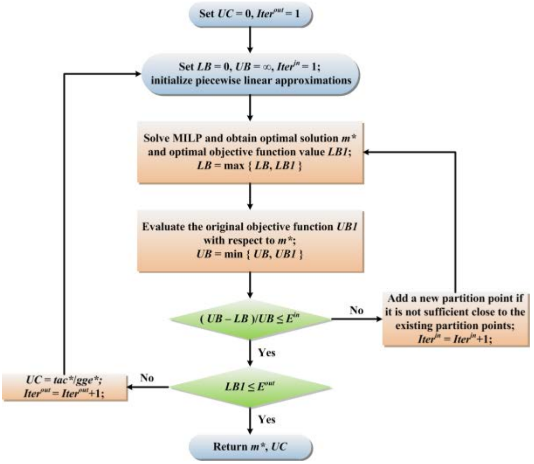
	SCIP		Bonmin		SBB	
	$/GGE	CPU(s)	$/GGE	CPU(s)	$/GGE	CPU(s)
A	---	72,000	Infeas.	72,000	Infeas.	72,000
B	---	72,000	Infeas.	72,000	Infeas.	72,000
C	---	72,000	Infeas.	72,000	Infeas.	72,000
D	---	72,000	Infeas.	72,000	Infeas.	72,000



Gong, J., & You, F. (2014). Global Optimization for Sustainable Design and Synthesis of Algae Processing Network for CO_2 Mitigation and Biofuel Production using Life Cycle Optimization. *AIChE Journal*, 60, 3195–3210.

Computational Results

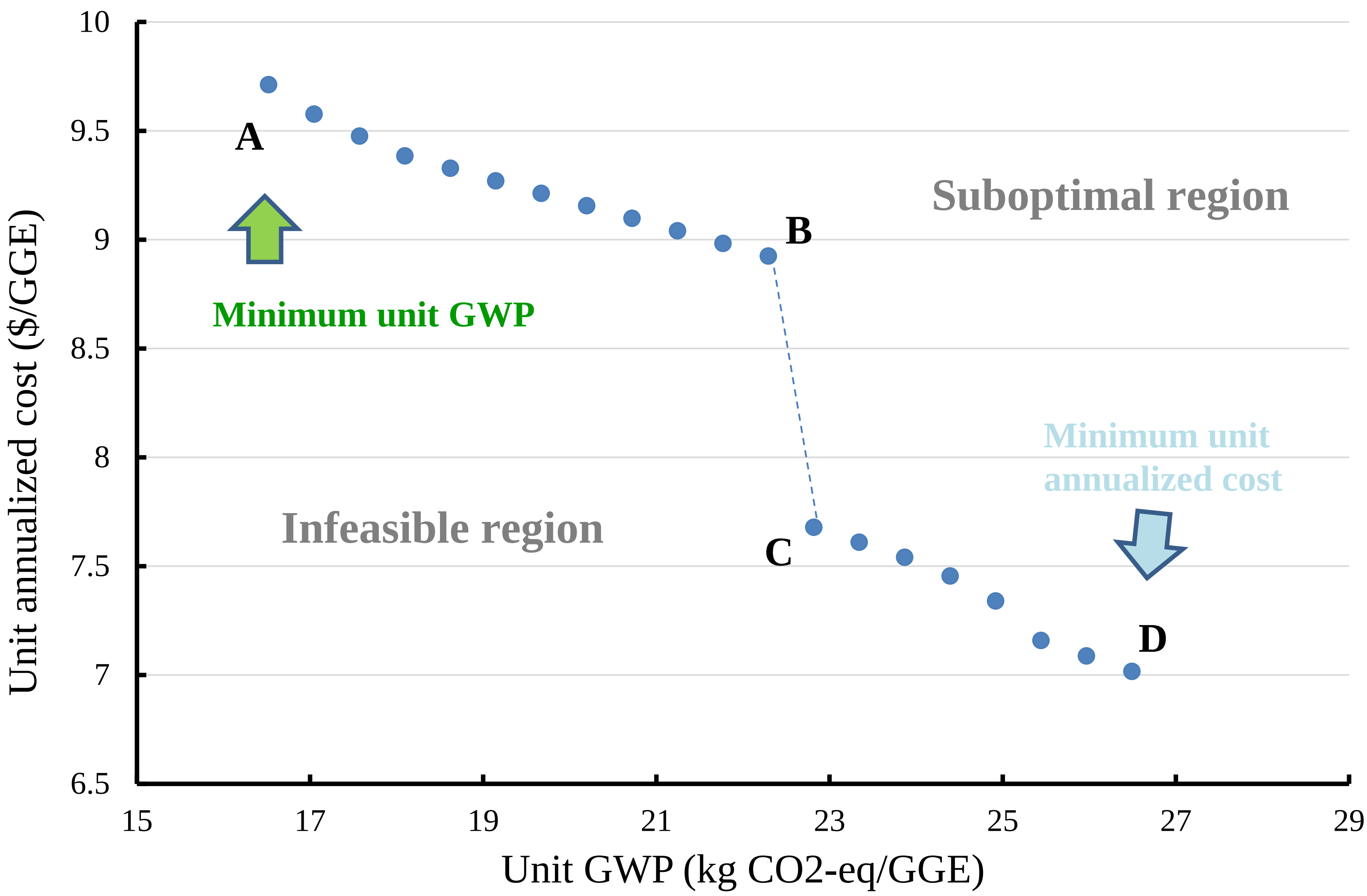
- **Problem size** (MIFP with concave terms):
  - Discrete 0-1 variables: 49
  - Continuous variables: 32,958
  - Constraints: 56,274
  - Non zero elements: 145,383



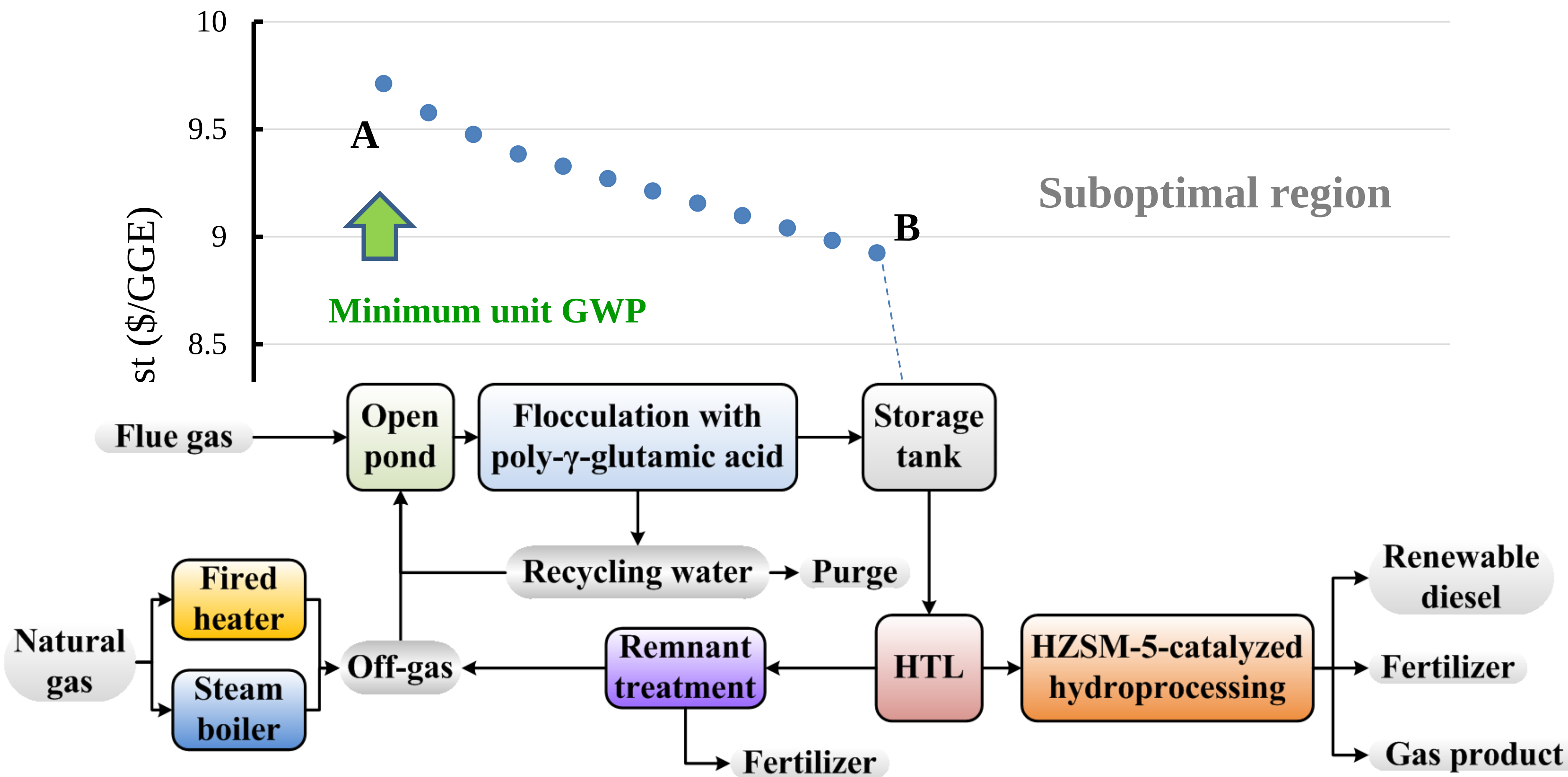
	SCIP		Bonmin		SBB		Proposed algorithm		
	$/GGE	CPU(s)	$/GGE	CPU(s)	$/GGE	CPU(s)	$/GGE	CPU(s)	Iter.
A	---	72,000	Infeas.	72,000	Infeas.	72,000	9.712	9	10
B	---	72,000	Infeas.	72,000	Infeas.	72,000	8.925	3	6
C	---	72,000	Infeas.	72,000	Infeas.	72,000	7.679	3	6
D	---	72,000	Infeas.	72,000	Infeas.	72,000	7.017	3	6

Gong, J., & You, F. (2014). Global Optimization for Sustainable Design and Synthesis of Algae Processing Network for CO_2 Mitigation and Biofuel Production using Life Cycle Optimization. *AIChE Journal*, 60, 3195–3210.

Pareto Optimal Curve



Pareto Optimal Curve



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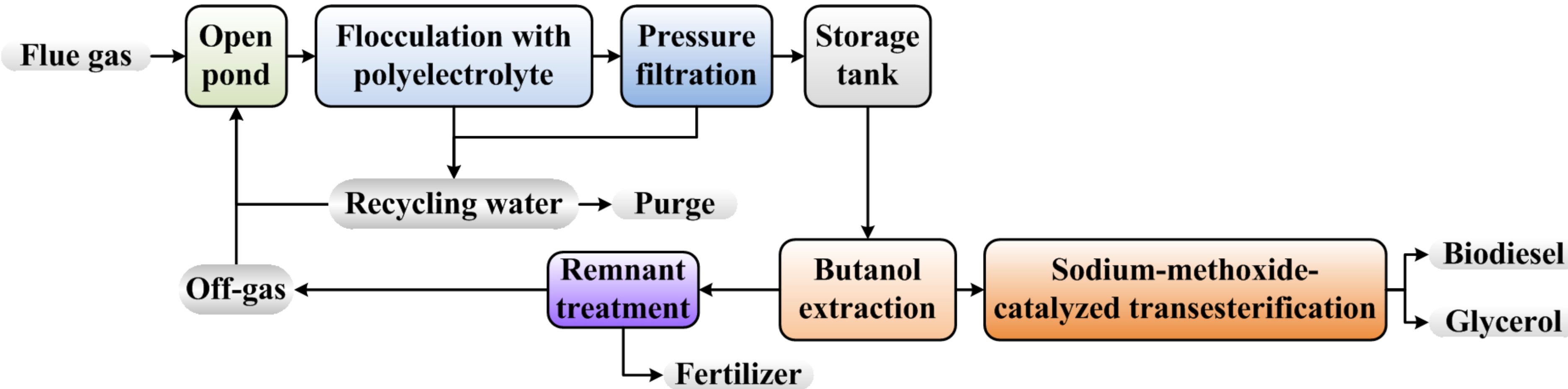
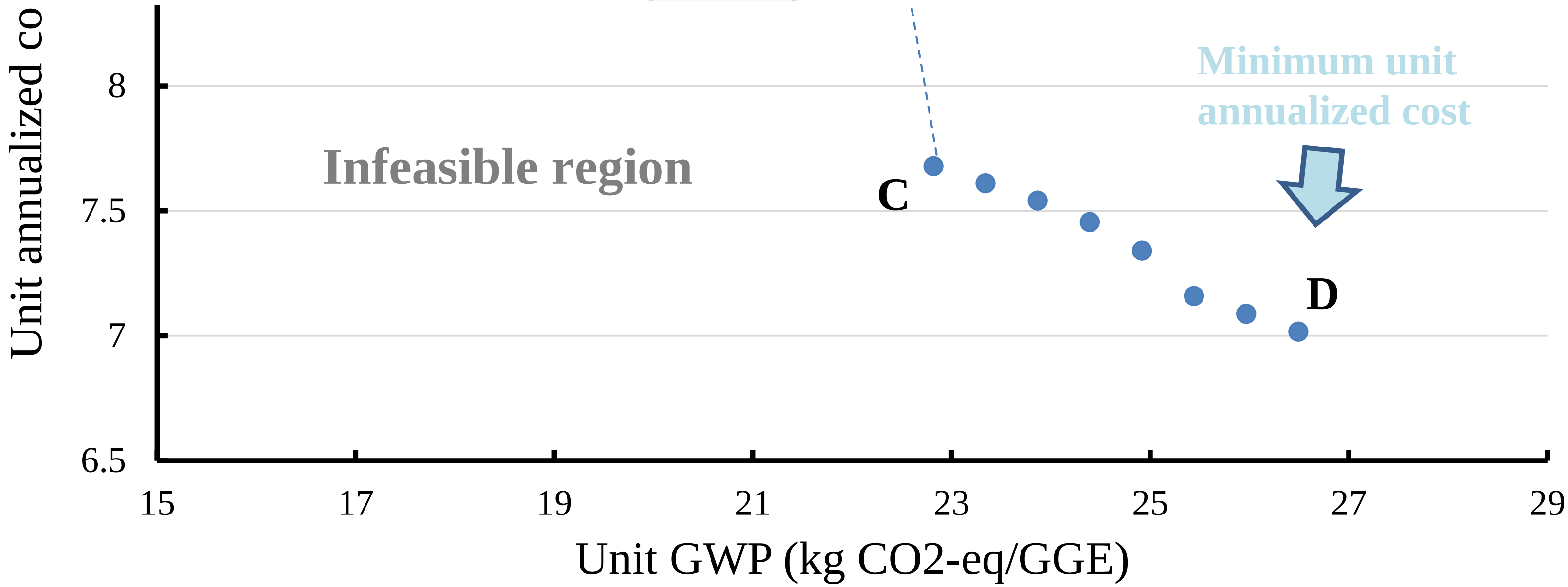
Pareto Optimal Curve





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Conclusion

- Research challenges for life cycle optimization
  - How to define the “optimal” systems boundary?
  - How to deal with the data quality and uncertainty?
  - How to **seamlessly** integrate LCA into process systems optimization?
  - How to effectively solve **complex, large-scale** LCO problems?

- MINLP methods provide powerful tools for sustainability analysis, especially on life cycle optimization

- The need of more computationally efficient algorithms for **previously intractable** MINLP problems

Congratulations on your 65th Birthday, Ignacio!

Happy 65th Birthday to my academic father,

Professor Ignacio E. Grossmann

Thank you so much for your guidance and support, and for your many contributions to PSE and to the broader scientific and engineering community!