Topic Eleven

Systems Analysis

Lecture Twenty Four

Cellulosic Ethanol Process Modeling

Objectives of Process Modeling

Process models are developed to

1. Visualize process
2. Model process flows
3. Perform mass and energy balances
4. Evaluate process economics
5. Evaluate emissions
6. Investigate scale up scenarios
7. Investigate effect of process modifications

Some of the commercially available process modeling software are:

1. Aspen Plus
2. *SuperPro designer*
3. Biopro designer

Economic and Emission Analysis

To develop economic evaluation, throughput analysis, and environmental impact assessment

1. Classify streams and supply stream-related cost data
2. Adjust the equipment level capital & operating cost factors (optional)
3. Adjust the operation level operating cost factors (optional)
4. Adjust the section level capital investment factors (optional), and adjust the section level operating cost factors (optional)
5. Adjust the process level economic evaluation parameters
6. Perform economic calculations and generate reports (optional)
7. View cost analysis and economic evaluation reports
8. Adjust annual production by scaling up or scaling down the process throughput
9. View throughput analysis results, environmental impact assessment and emissions reports

Ref: SuperPro Designer User Manual

Fixed Capital Cost Estimation

What is an estimate?

"An evaluation of all the costs and elements of a project or effort as defined by an agreed-upon scope. Three specific types based on the degree of definition of a process industry plant are:

1) Order of magnitude estimate
2) Budget estimate
3) Definitive Estimate"

Types of estimates (another classification):

1. Order of magnitude estimate: ±10 to 50% accuracy
2. *Study estimate (factored estimate): ±30*
3. Preliminary estimate (budget authorization estimate): ±20
4. Definitive estimate (project control estimate): ±10
5. Detailed estimate (firm or contractor's estimate): ±5

Ref: Perry's chemical engineering handbook (Chap 9)
The engineer's cost handbook: Ed. R.E. Westney.

Fixed Capital Cost Estimation

What is the use of an estimate?

1. Provides an assessment of capital cost.
2. Forms the basis of planning and control
3. Provides basic information such as hours of operations, resources, tasks that will be used to prepare schedules.
4. Provides financial input required for cash flow curves.
5. Can be used to assess productivity and risks.

What is a good estimate?

A estimate is good /adequate if another estimator independently arrives at a similar cost estimate after looking at the description of equipment and same data sources.

Ref: The engineer's cost handbook: Ed. R.E. Westney.

Fixed Capital Cost Estimation

Work Breakdown Structure (WBS)

WBS is a cascading outline of scope that organizes the estimation process.

Example: Estimates for fixed capital cost of a plant:

1. Land:
    1. Surveys
    2. Fees
    3. Property cost
2. Site development
    1. Site clearing
    2. Grading
    3. Roads. Access and ons-ite
3. …
4. Utilities
    1. Boiler plant
    2. Refrigeration unit
    3. Water wells/water intake
    4. Primary water treatment
    5. Cooling towers
    6. Waste treatment
    7. Storm sewers

Ref: Perry's Chemical Engineering handbook

The engineer's cost handbook: Ed. R.E. Westney.

Equipment Capital Costs

Often, cost information does not exist for the exact size of equipment. In such cases, the new cost can be calculated from existing information using the following approach.

$$New\ Cost = Original\ \ Cost \left(\frac{New\ Size *}{Original\ \ Size *} \right)^{exp}$$

* or characteristic linearly related to the size

Exponent ranges from 0.6 to 0.7 depending on the type of the equipment.

A similar approach is used to estimate present day costs based on historic cost data.

Sizing example:

A hammer mill with a rated grind rate of 10,000kg/hr costs $500,000 in 2004. Use a power law coefficient of 0.6 for sizing.

Ref: McAloon et al (2000)

Fixed Capital Cost Estimation

Installation costs are estimated as a factor of individual equipment cost.

Piping, insulation, and electrical facilities costs are estimated by multiplying factor with the total equipment cost (TEC).

Process Modeling in SuperPro

Following sequence of steps are followed to develop a process flow simulation model.

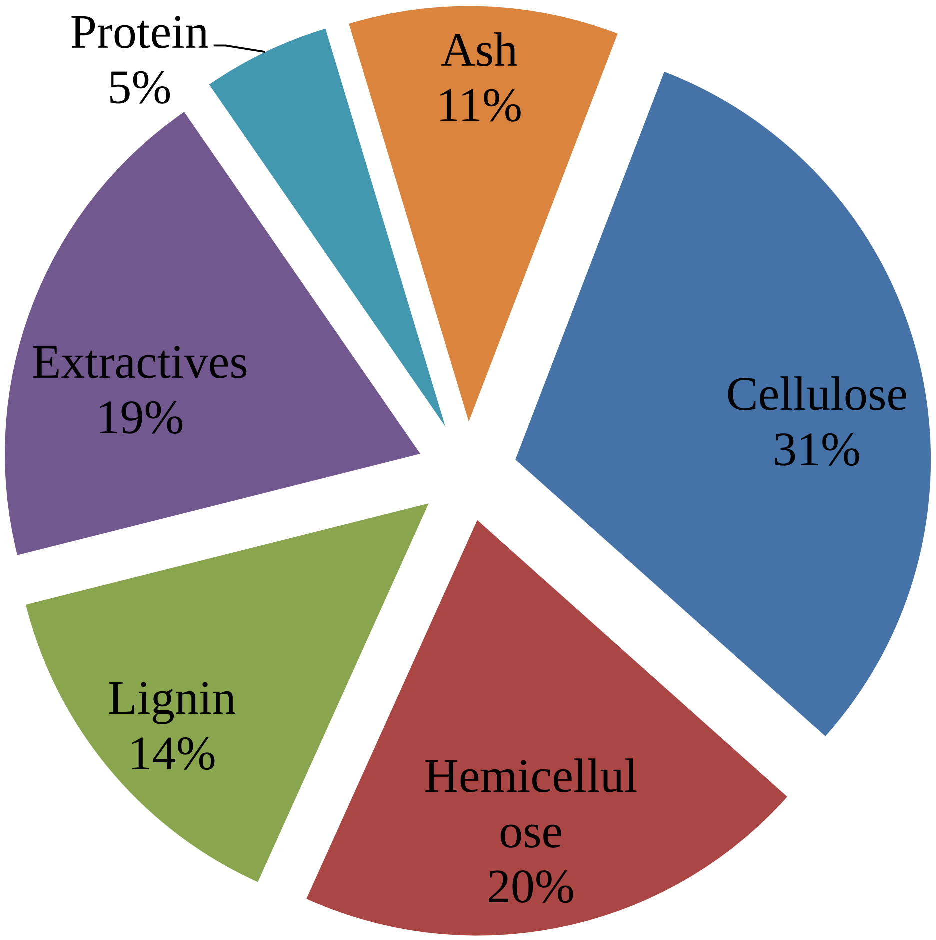
- Specify overall mode of operation
- Register pure components and mixtures
- Build flow sheet
- Initialize operations in procedures
- Initialize input streams
- Initialize scheduling
- Define process sections (optional)
- Adjust convergence parameters (optional)
- Solve mass and energy balances
- View simulation results

Ref: SuperPro Designer User Manual

Process Modeling Example

Model Feedstock: Tall Fescue (*Festuca arundinacea Schreb*)

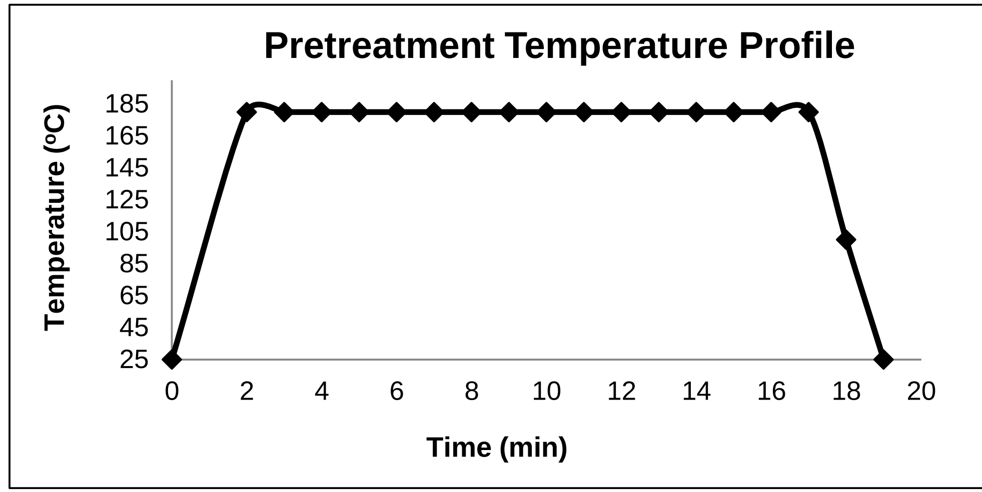
- Tall fescue grass is the largest fraction of the grass straw residues available for production of cellulosic ethanol in Oregon.



Ref: Graf and Koehler 2002, Banowetz et al 2008, Steiner et al 2006, Kumar and Murthy 2011, Juneja et al. 2011

Pretreatment of Grass Straws

- Dilute Acid *(1 % H_2SO_4, 10 % solid loading at 180°C for 15 min.)*
- Hot water *(10 % solid loading at 180°C for 15 min.)*
- Dilute Alkali *(1 % NaOH, 10 % solid loading at 180°C for 15 min.)*

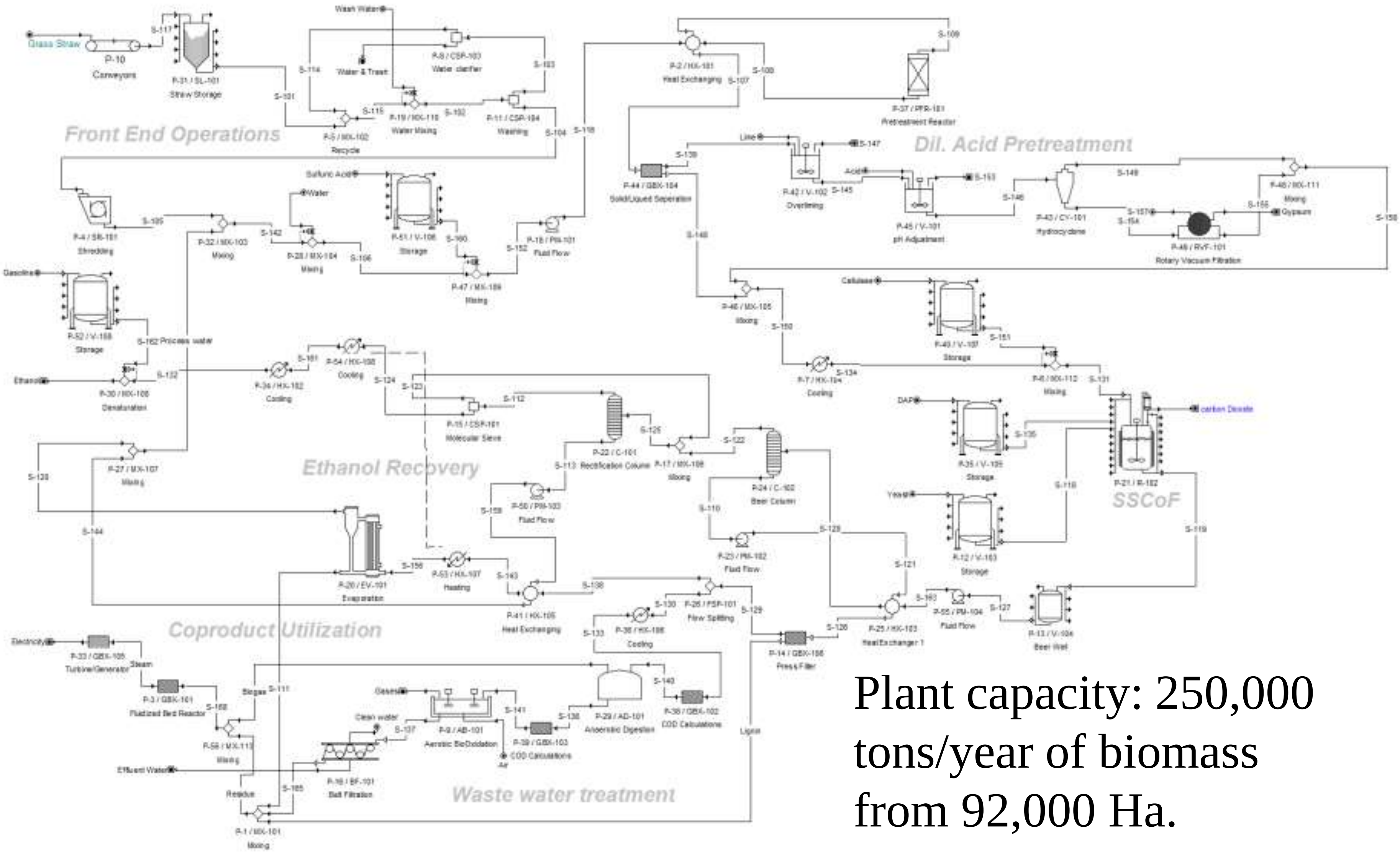


Potential Ethanol Yields

Potential Ethanol Yields from grass straws (L/ ton biomass)

Grass	Estimated C6 Fermentation Yields				Max. (C6+C5)
	Hot Water	Dil. Acid	Dil. Alkali	Max.	
TF	173.74	184.63	187.52	220.16	360.57
PR	150.15	174.96	141.67	177.22	297.87
BENT	135.92	136.80	126.93	154.05	276.74

Process Model Development: Dilute Acid Pretreatment



Plant capacity: 250,000 tons/year of biomass from 92,000 Ha.

Techno-Economic Analysis: Overall Economics

Overall economics of the ethanol production plant with 250,000 tons/yr of biomass.

	Dil. acid	Dil. Alkali	Hot Water	Steam Exp.
Total Investment (Millions $)	114.63	102.77	101.89	91.36
Operating Cost (Millions $/yr)	50.06	52.70	48.10	45.83
Ethanol Revenue (Millions $/yr)	65.41	65.21	65.07	58.64
Ethanol (Million L/yr)	59.66	59.47	59.36	53.53
Ethanol Unit Cost ($/L)	0.840	0.885	0.811	0.856

Capital and Operating Costs Vary with Pretreatment Used

250,000 tons/year capacity	Dil. Acid	Dil. Alk.	Hot Water	Steam Ex.
Ethanol Unit Cost ($/L($/gal))	0.84 (3.18)	0.89(3.35)	0.81(3.07)	0.86(3.24)
Direct Fixed Capital ($)	106.37	94.68	94.24	84.26
Equipment Cost ($/yr)	45.37	39.52	39.17	34.96
Raw Material Cost ($/yr)	22.562	27.05	22.73	22.23
Effluent Water (Kg/yr)	207.37	208.63	206.76	128.43

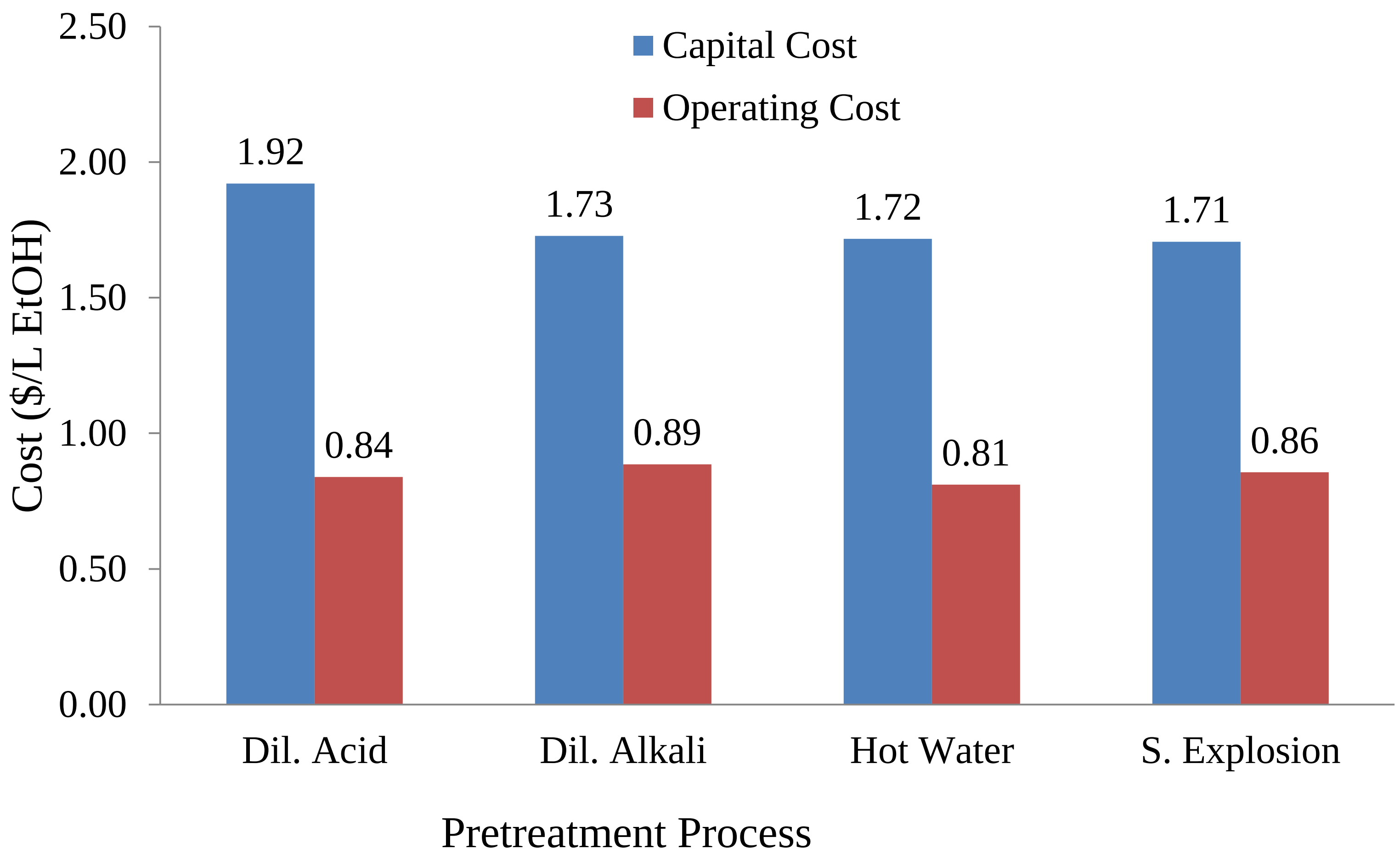
All numbers in millions.

Steam Demand and Electricity Production

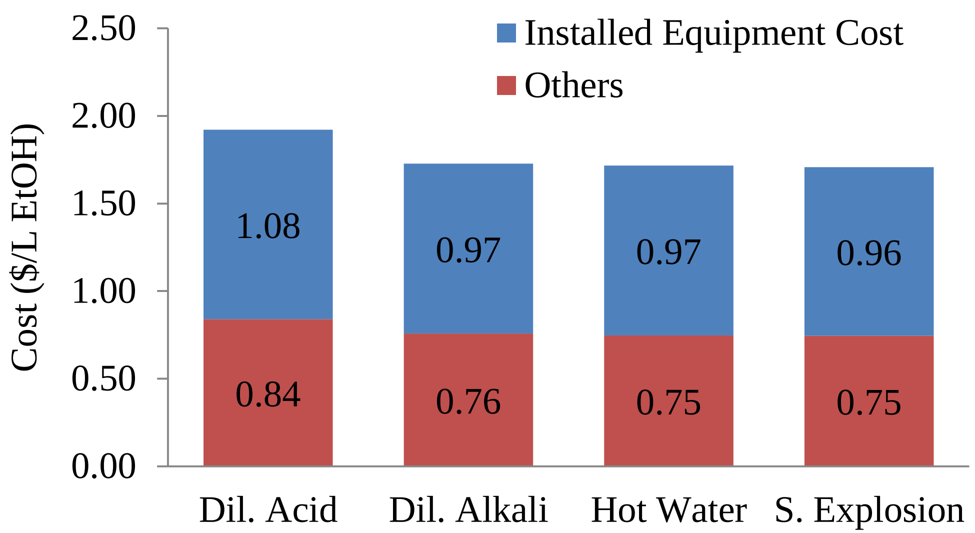
Pretreatment Process	Steam demand (kJ/L EtOH)	Lignin Energy (kJ/L EtOH)	Excess Lignin Energy (kJ/L EtOH)	Electricity Produced (kWh/L EtOH)[a]
Dil. Acid	19,010	28,232	9,223	0.769
Dil. Alkali	18,737	27,967	9,229	0.769
Hot Water	19,333	29,138	9,804	0.817
Steam Ex.	13,508	34,819	21,310	1.776

[a]Assuming 30 % efficiency of lignin energy to electricity conversion

Techno-Economic Analysis: Cost Breakdown

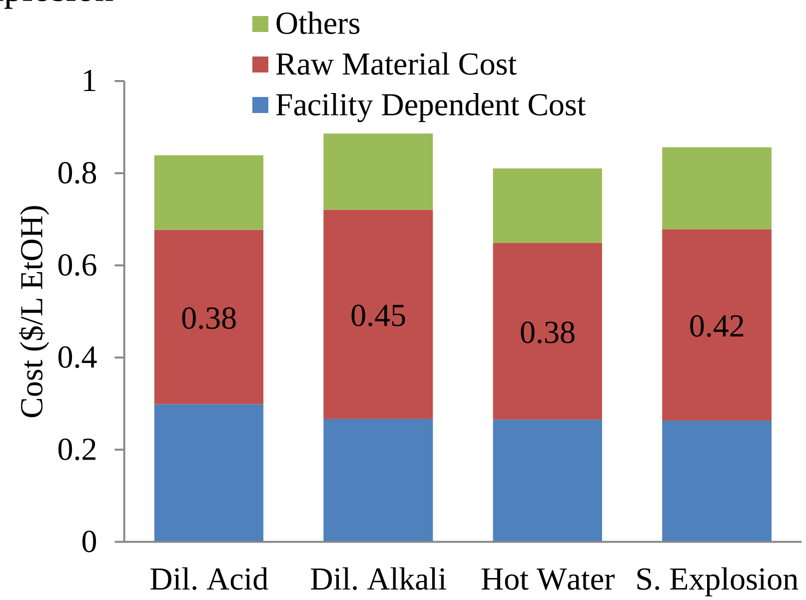


Techno-Economic Analysis: Cost Breakdown

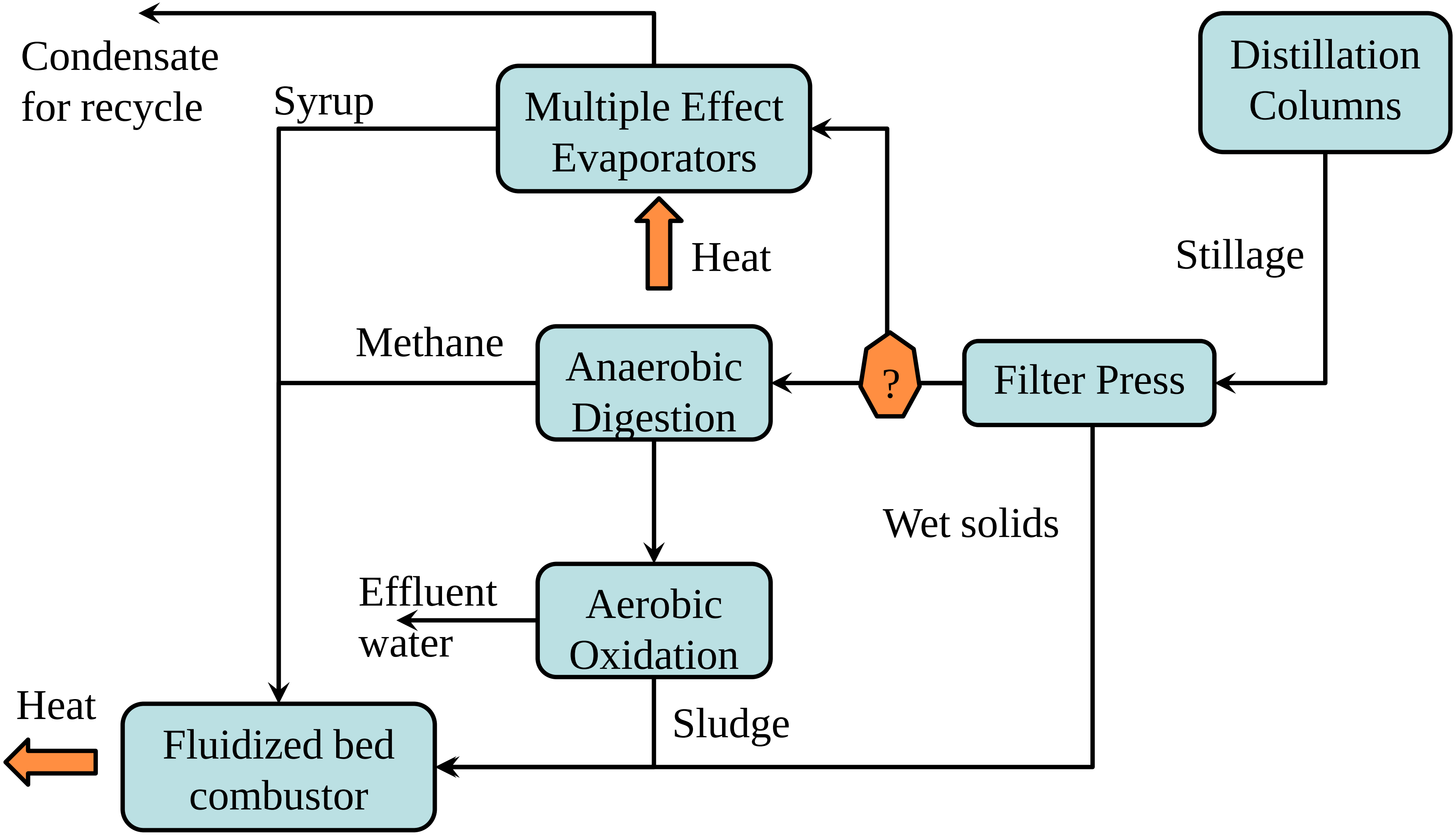


Capital Costs

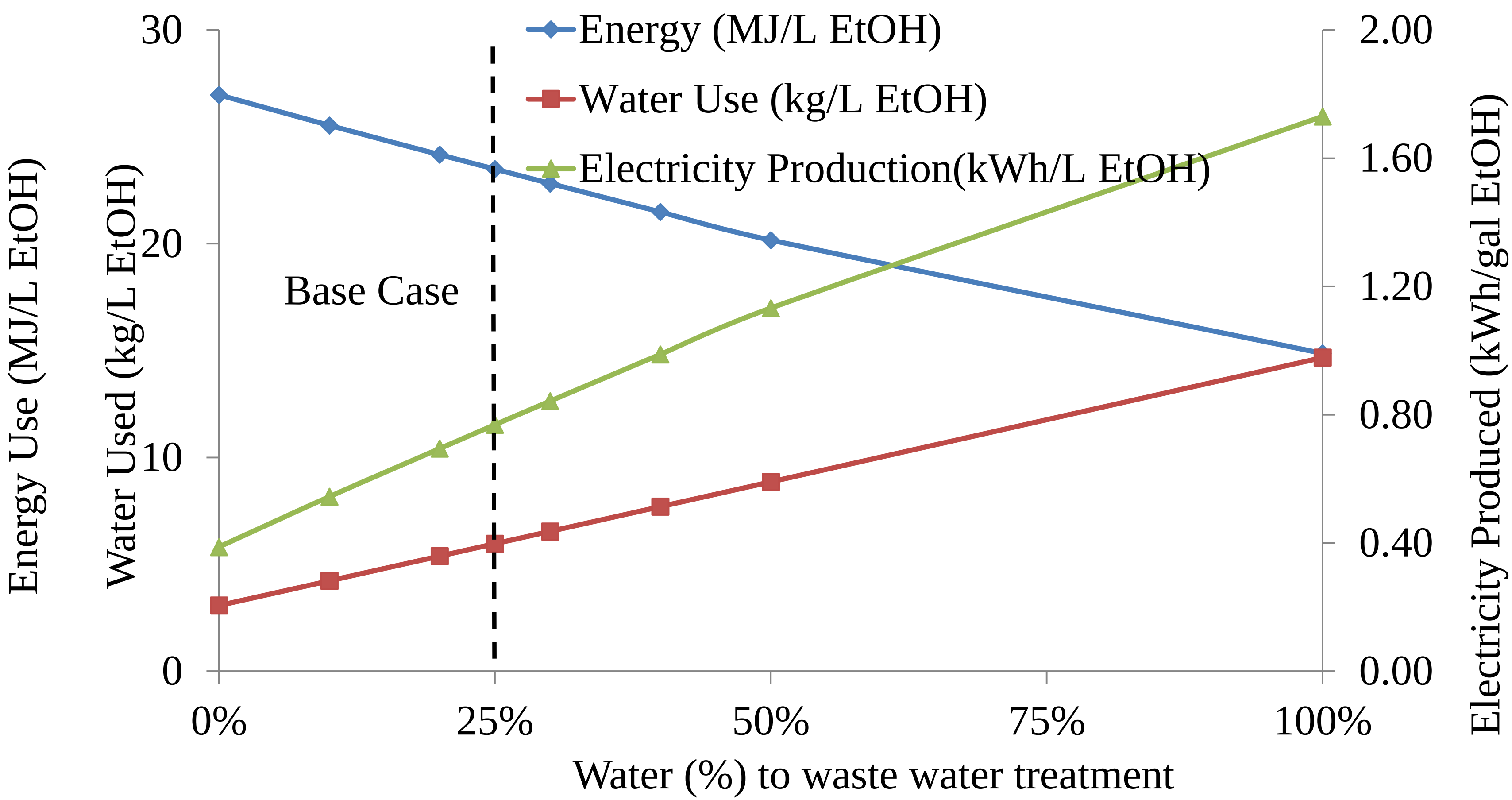
Operating Costs



Capital Costs, Energy Use and Water Recycle are Interconnected

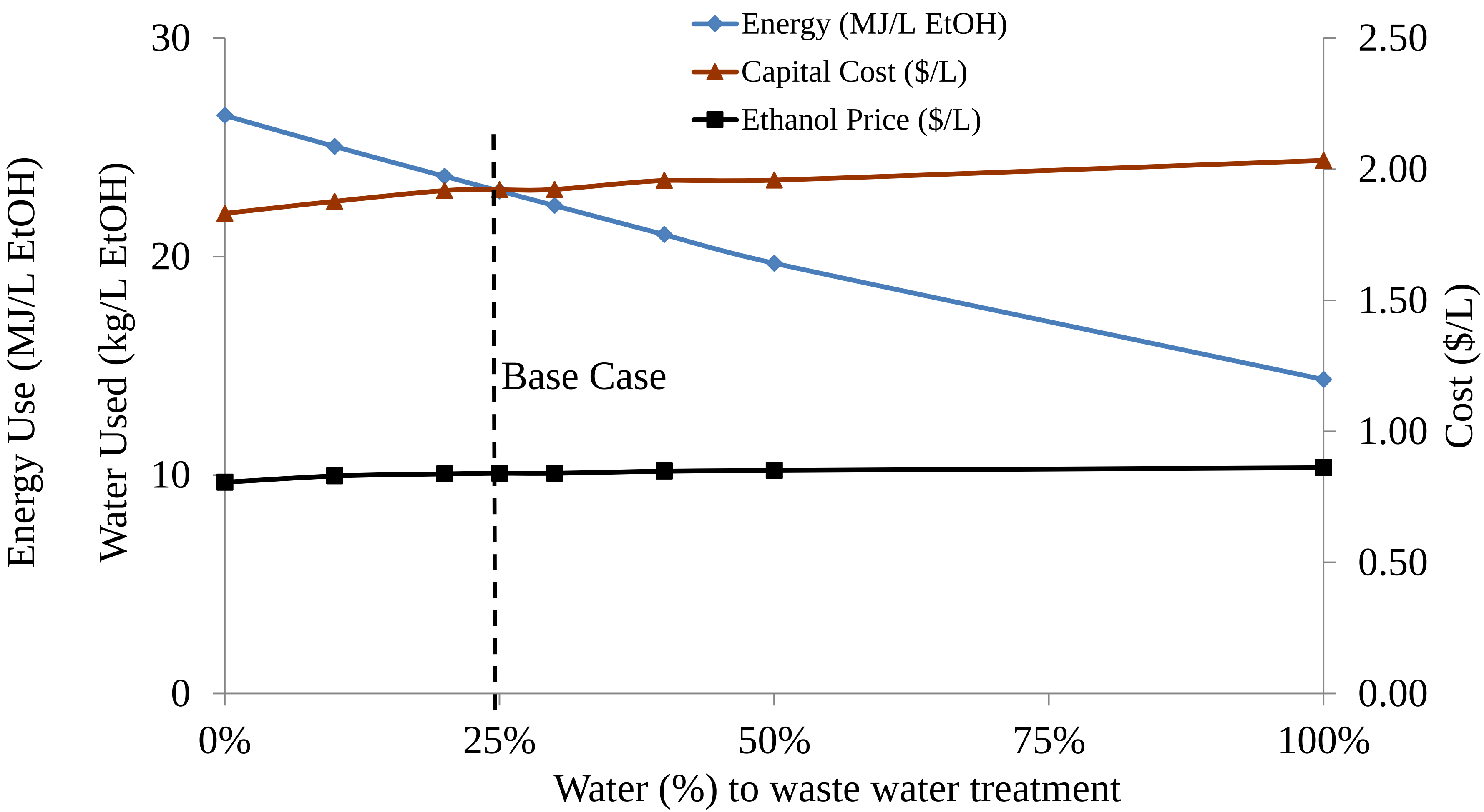


Energy Use and Water Use/Electricity Have a Strong Negative Correlation



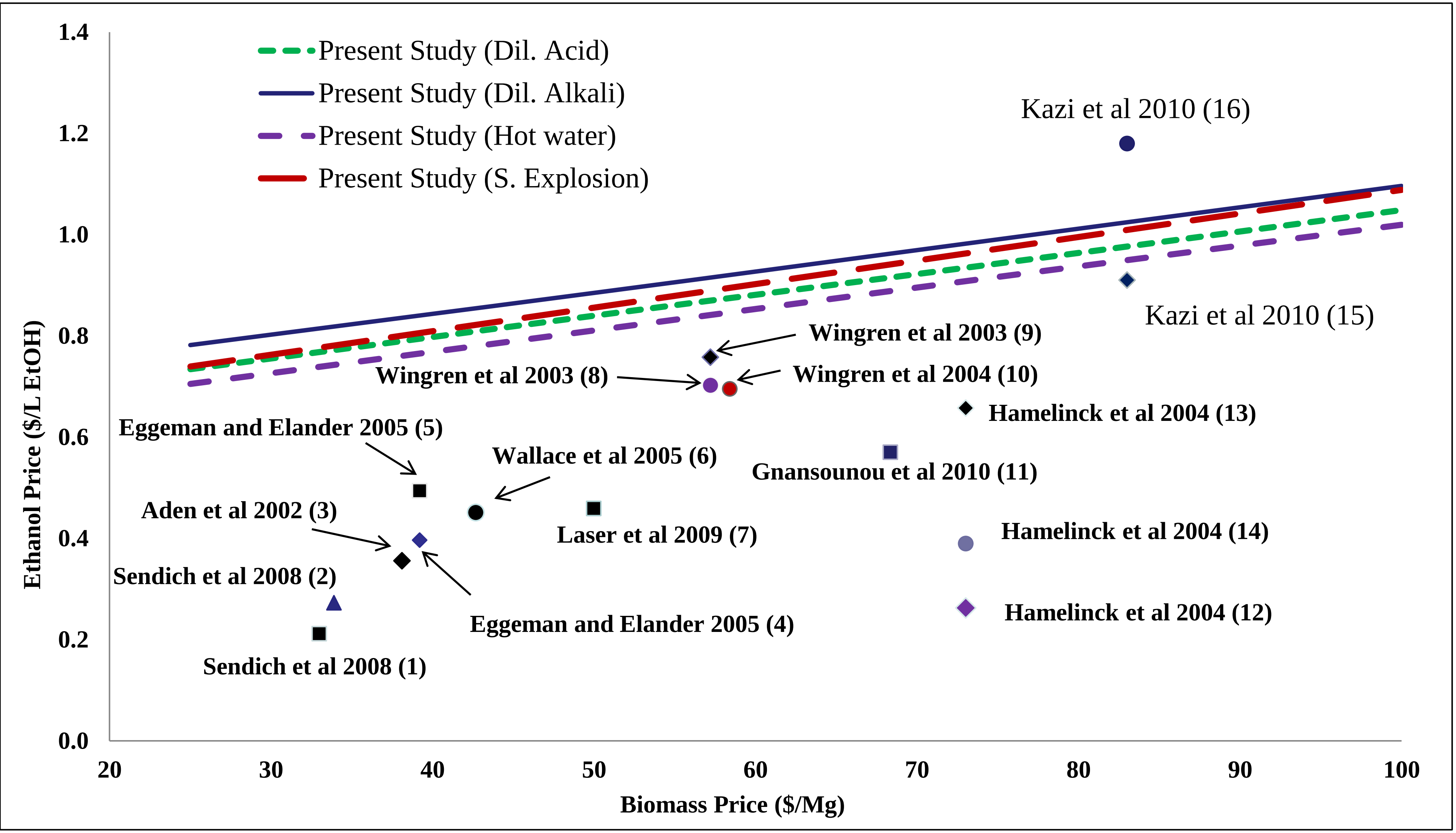
Dilute Acid Pretreatment Process Case

Energy Use and Capital/Ethanol Cost Have a Weak Negative Correlation

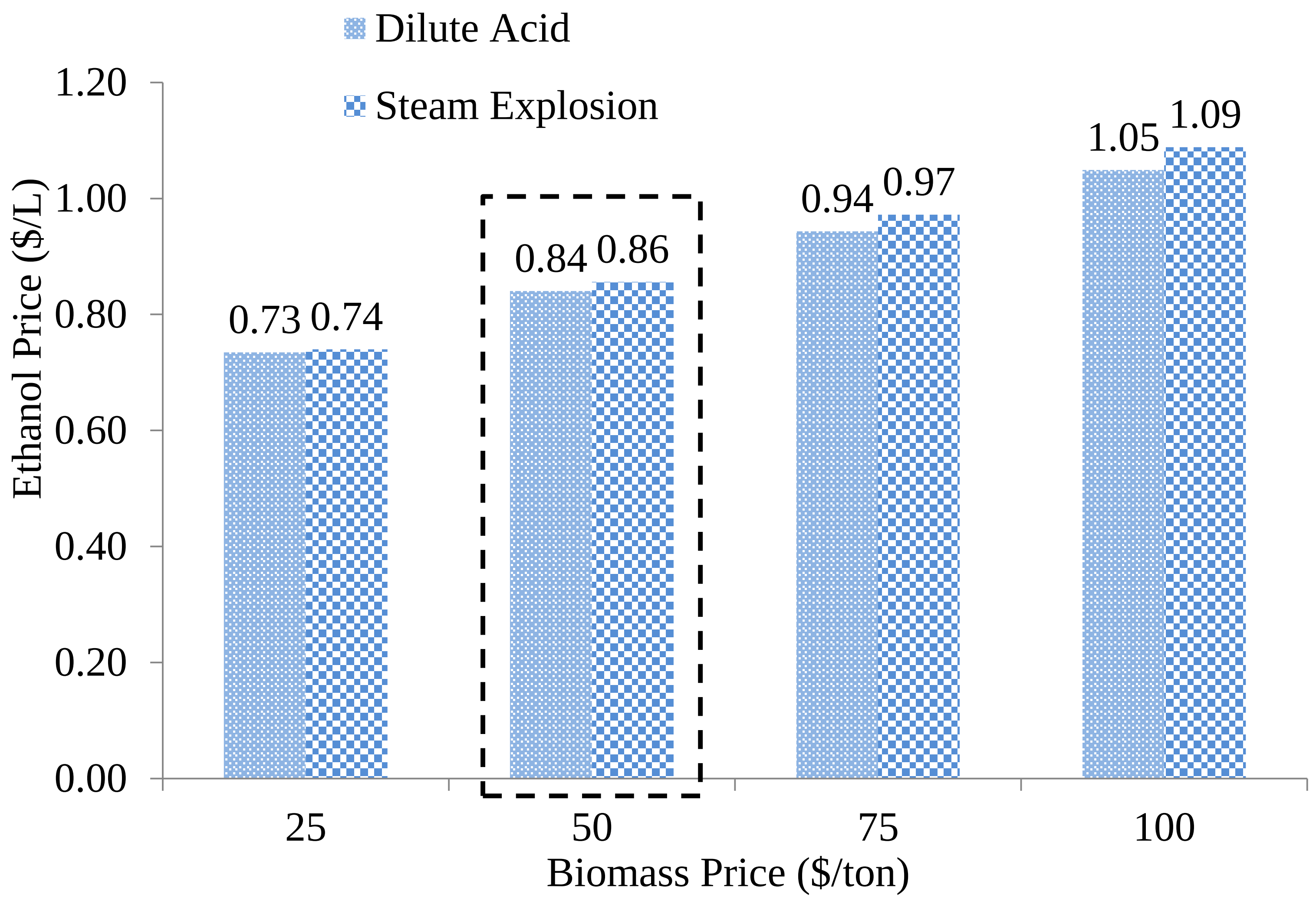


Dilute Acid Pretreatment Process Case

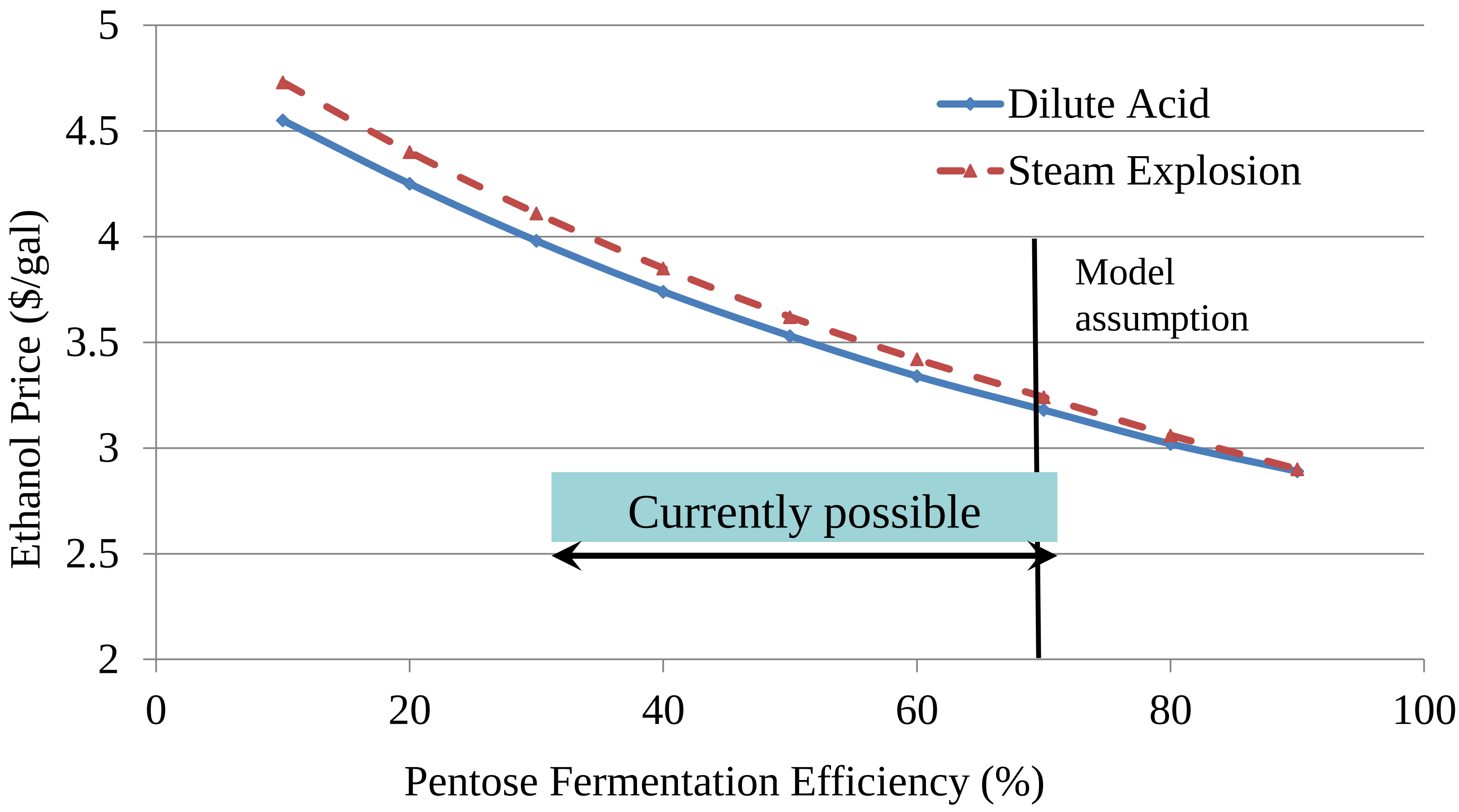
Comparison of Present Study to Extant Literature



Ethanol Price is Affected Significantly by Feedstock Price



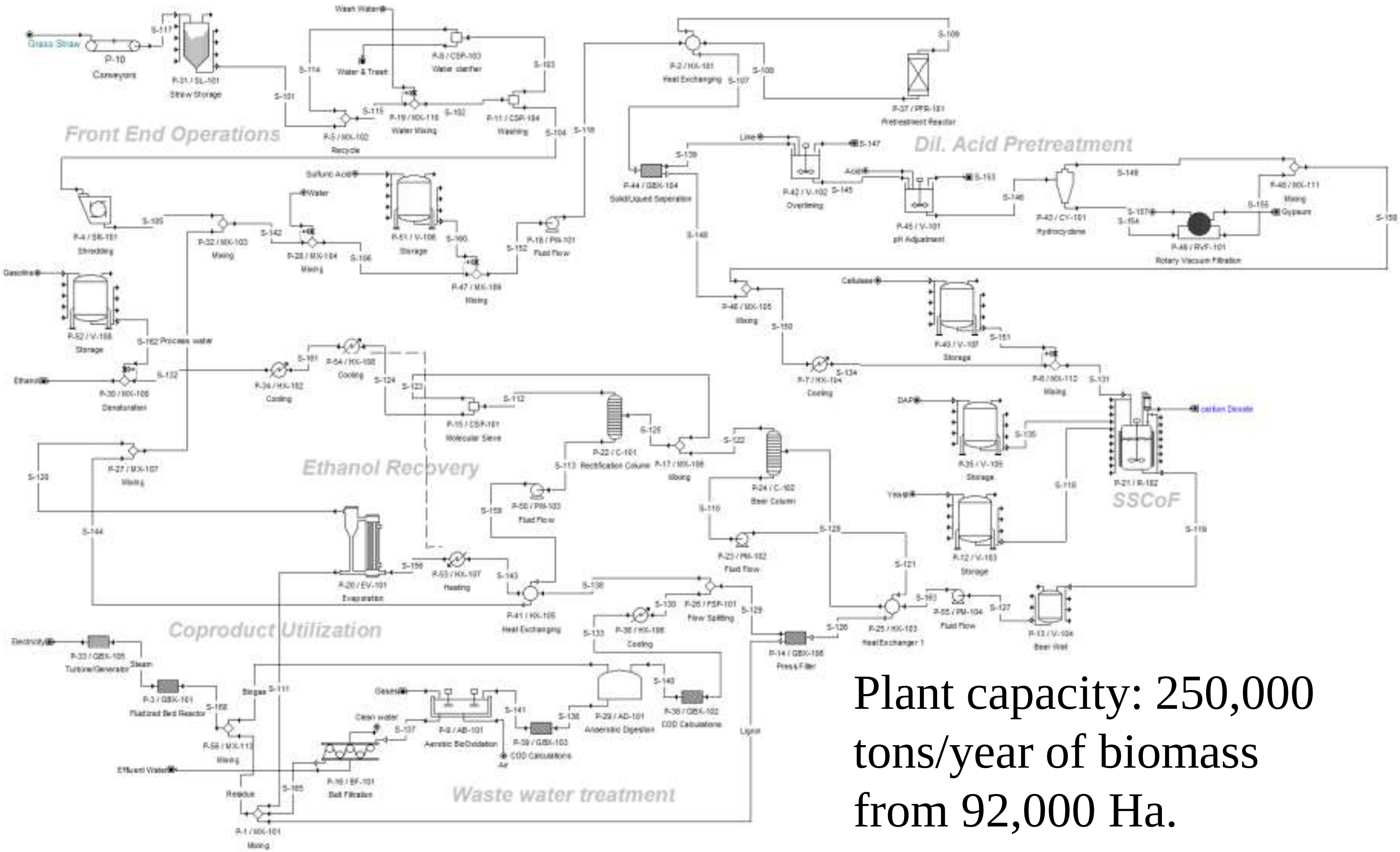
Pentose Fermentation Efficiency has a Impact on Ethanol Price



Lecture Twenty Six

Introduction to Life Cycle Analysis

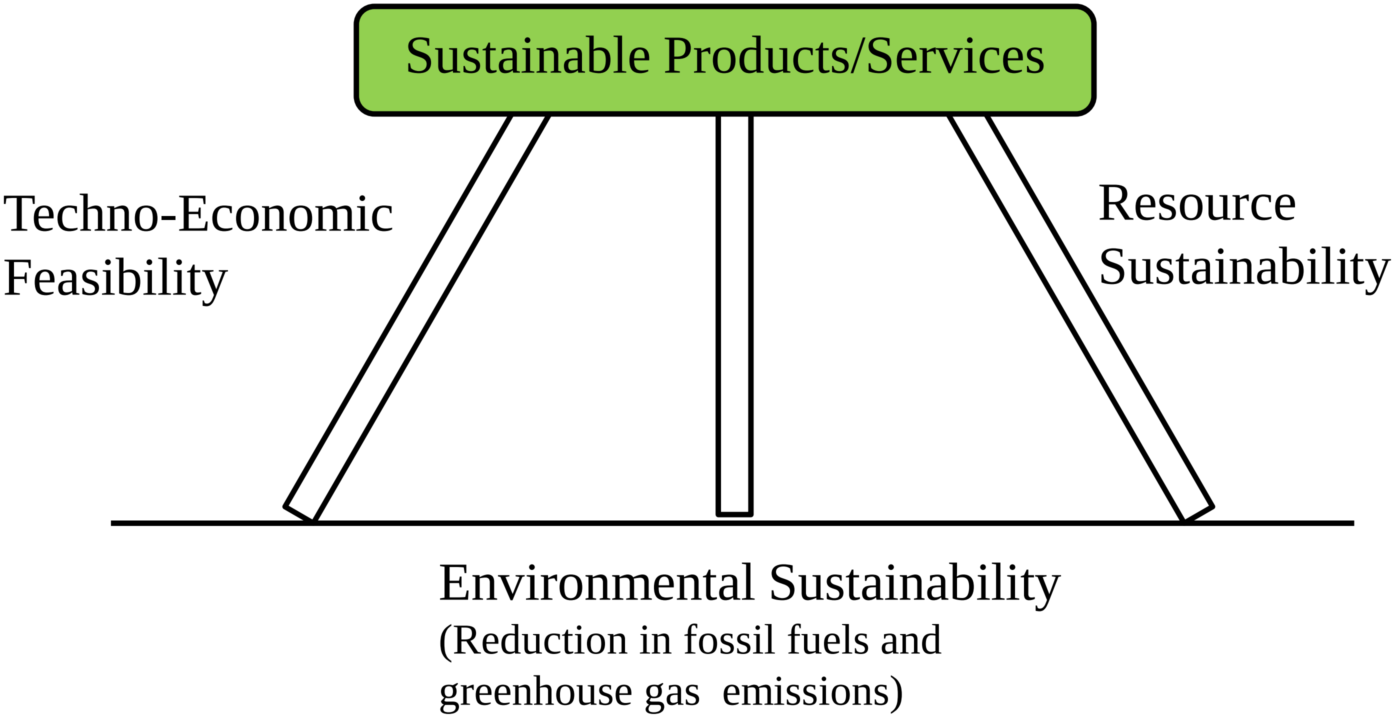
Summary of Lecture Twenty One



Plant capacity: 250,000 tons/year of biomass from 92,000 Ha.

Three Important Criteria

What are the environmental, economic and energy benefits?



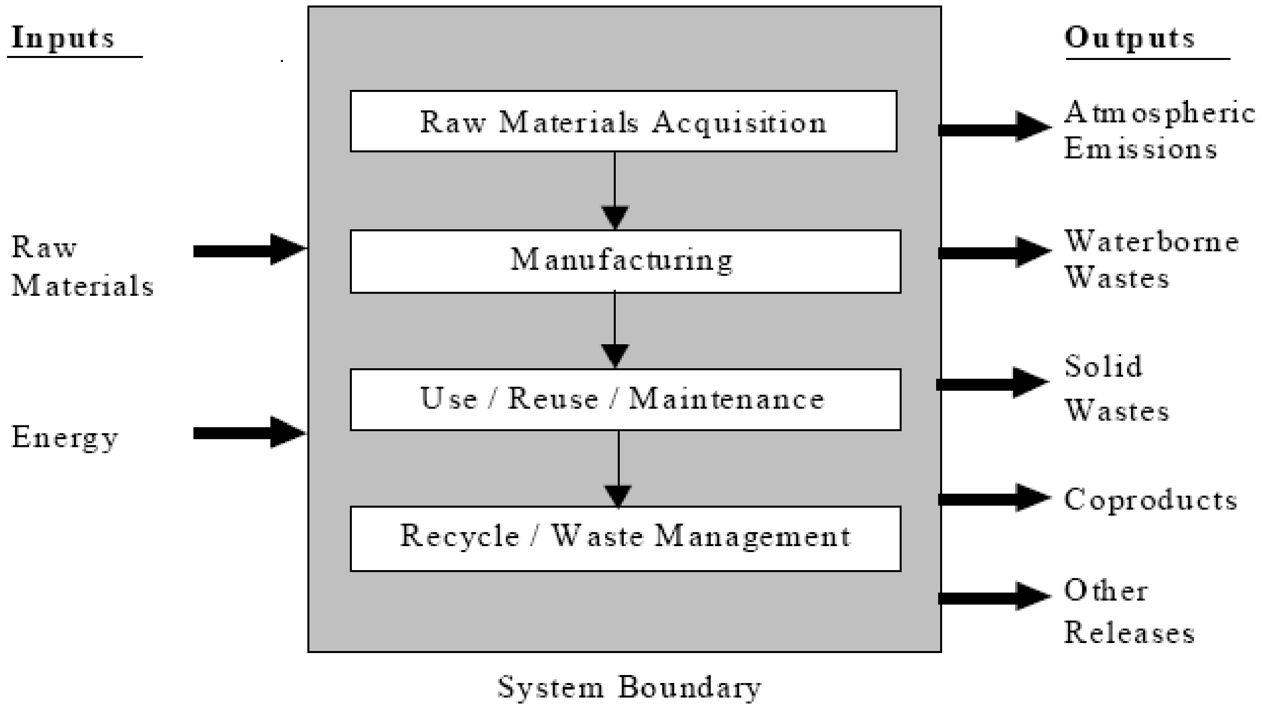
Curious case of grocery bags

Paper or Canvas or Plastic?

Image Source: http://bryoneagon.files.wordpress.com/2009/09/1244303943grocery_bag1.jpg
http://loveisdope.files.wordpress.com/2009/02/canvas-grocery-bag.jpg
http://thumb1.shutterstock.com.edgesuite.net/display_pic_with_logo/60383/60383,1222849277,1/~04625.jpg

Life Cycle Analysis

Life Cycle Analysis (LCA) is a tool to assess impact of products, processes and services on environment. All processes starting with the acquisition of raw materials, production, manufacturing and disposal are considered.



Ref: Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)

Life Cycle Analysis

What can LCA do?

- Provide a basis for comparing impact of products on environment.
- Accounts for transfer of environmental impacts from one source to another.
- Quantify environmental release of pollutants
- Develop a systematic basis for comparing products/ process /service alternatives

What LCA is not

- This is not a risk assessment
- Will not provide information on the cost/performance
- The quality of conclusions is dependent on the reliability of the data and the relevance to the scope of study.

Ref:
1. Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)
2. http://en.wikipedia.org/wiki/Life_cycle_assessment#Energy_production

Life Cycle Analysis

LCA is not Risk Assessment! LCA is not a cost/performance analysis model. LCA is a model to assess environmental impact of the products, processes and services.

Two versions: Attributional LCA and Consequential LCA.

Other variants:

- Cradle to grave: Involves LCA for production, manufacturing, use and disposal
- Cradle to cradle: Involves recycle in addition to all the phases mentioned above.
- Cradle to gate: This is a partial LCA assessing impact from cradle to factory gate. Used to declare environmental friendliness of process.
- Well to wheel: A specific LCA for transportation sector.

Ref:

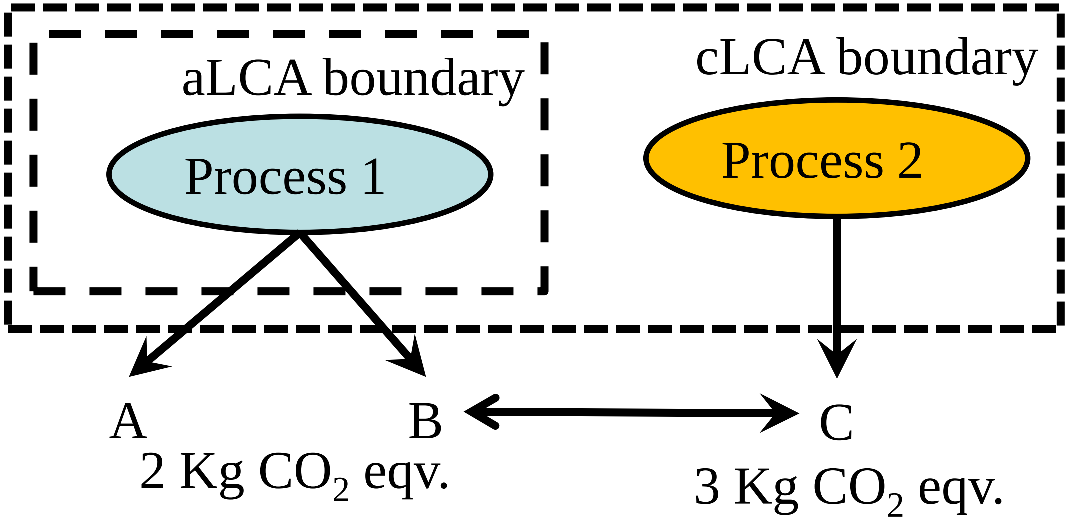
1. Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)
2. http://en.wikipedia.org/wiki/Life_cycle_assessment#Energy_production

Variants of LCA

The two types of Life Cycle Assessments which answer different questions:

• Attributional Life Cycle Assessment (aLCA): What are the ***total*** emissions from the process during the life cycle of the product?

• Consequential Life Cycle Assessment (cLCA): What is the ***change*** in total emissions from the process during the life cycle of the product?



B replaces C

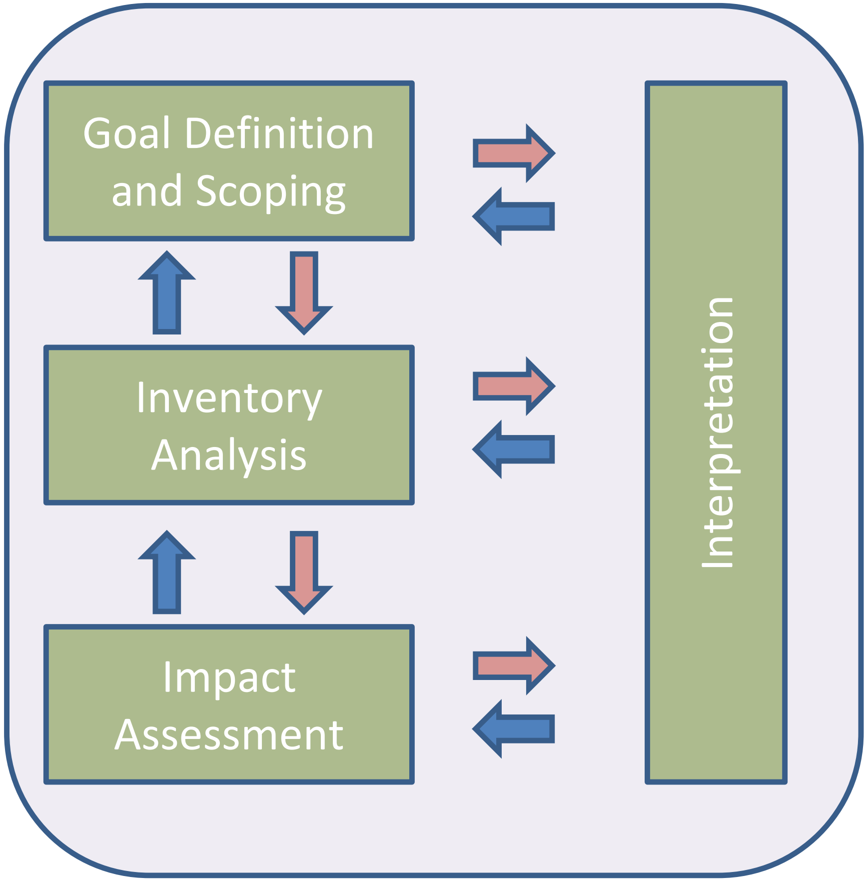
aLCA: 2 = 2 Kg CO2 eq.

cLCA: 2-3= -1 Kg CO2 eq.

Life Cycle Analysis

LCA is divided into four distinct stages:

1. Goal Definition and Scoping
2. Life Cycle Inventory
3. Life Cycle Impact Assessment
4. Life Cycle Interpretation



Ref: Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)

Life Cycle Analysis: Goal Definition and Scoping

Formulation of goals and the scope of study is the most critical part of LCA. The object of the study is defined in terms of "functional unit".

- Description of the products, processes, and the system boundaries.
- Clear and quantifiable goals will help in arriving at more objective interpretation
- Setting clearly identifiable the boundaries of the system is critical

Factors to be considered

- What is the required specificity?
- What are the resources available for the study?
- What type of information is needed?
- How should the results be displayed?

Ref:

- http://en.wikipedia.org/wiki/Life_cycle_assessment#Energy_production
- Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)

Life Cycle Analysis: Inventory

Life Cycle Inventory : A process to quantify the energy, material flows and emissions during the entire life cycle of the product/process/service.

Key steps in LCI

- Develop a flow diagram of the process
- Develop a data collection plan
- Collect Data
- Evaluate and report results

Factors to be considered

- What are the resources available for the study?
- What type of information is needed?
- Data sources, quality goals and quality measures.

Ref: Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)

Life Cycle Analysis: Impact Assessment

Life Cycle Impact Assessment : The information gathered in LCI is used to determine the impact of the products and processes on the environment. This is used to distinguish between different options by comparing the environmental impact of options

Key steps in LCIA

- Selection and definition of impact categories
- Classification
- Characterization
- Normalization
- Grouping
- Weighting
- Evaluating and Reporting LCIA results

Ref: Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)

Life Cycle Analysis: Interpretation

Life Cycle Interpretation: "It is a systematic technique to identify, quantify, check and evaluate information from the results of LCI and LCIA and communicate them effectively."

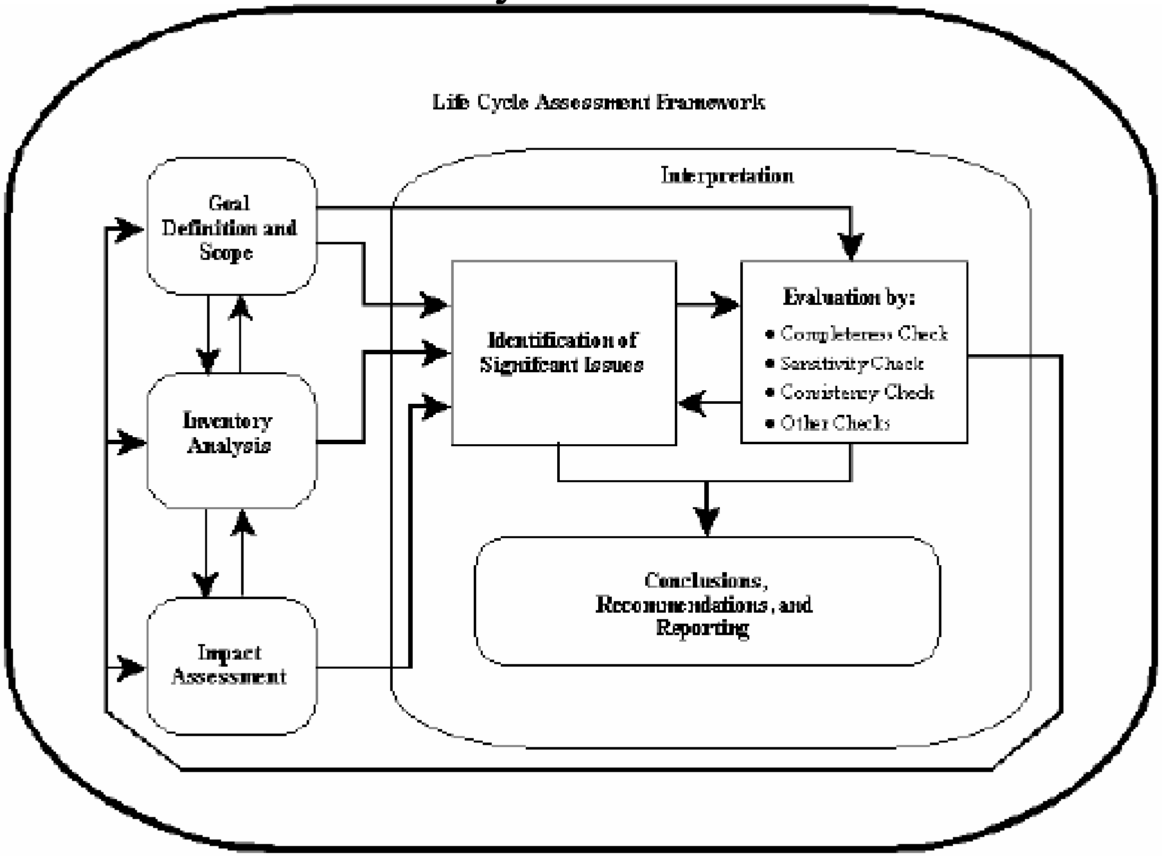
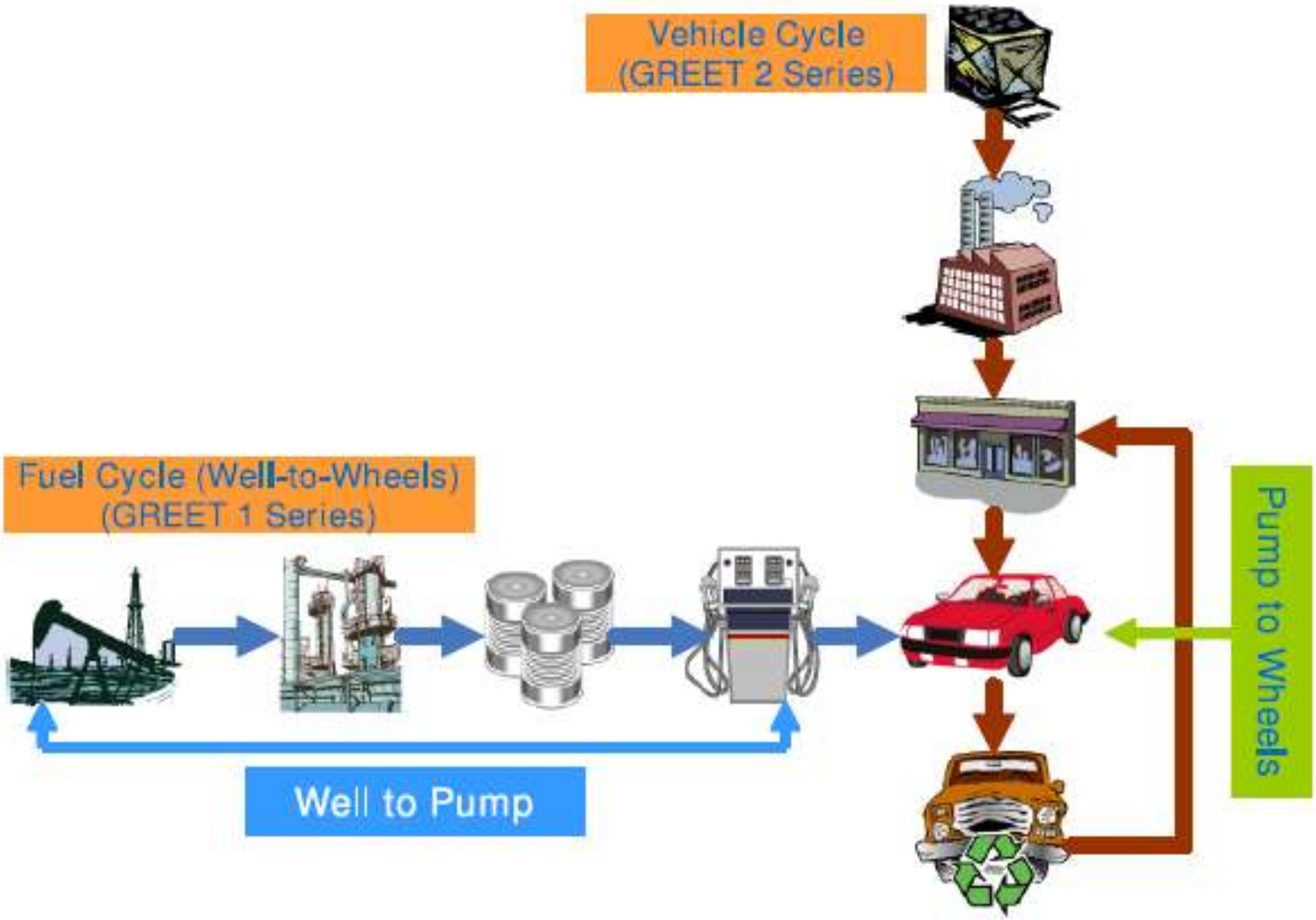


Exhibit 5-1. Relationship of Interpretation Steps with other Phases of LCA (Source: ISO, 1998b)

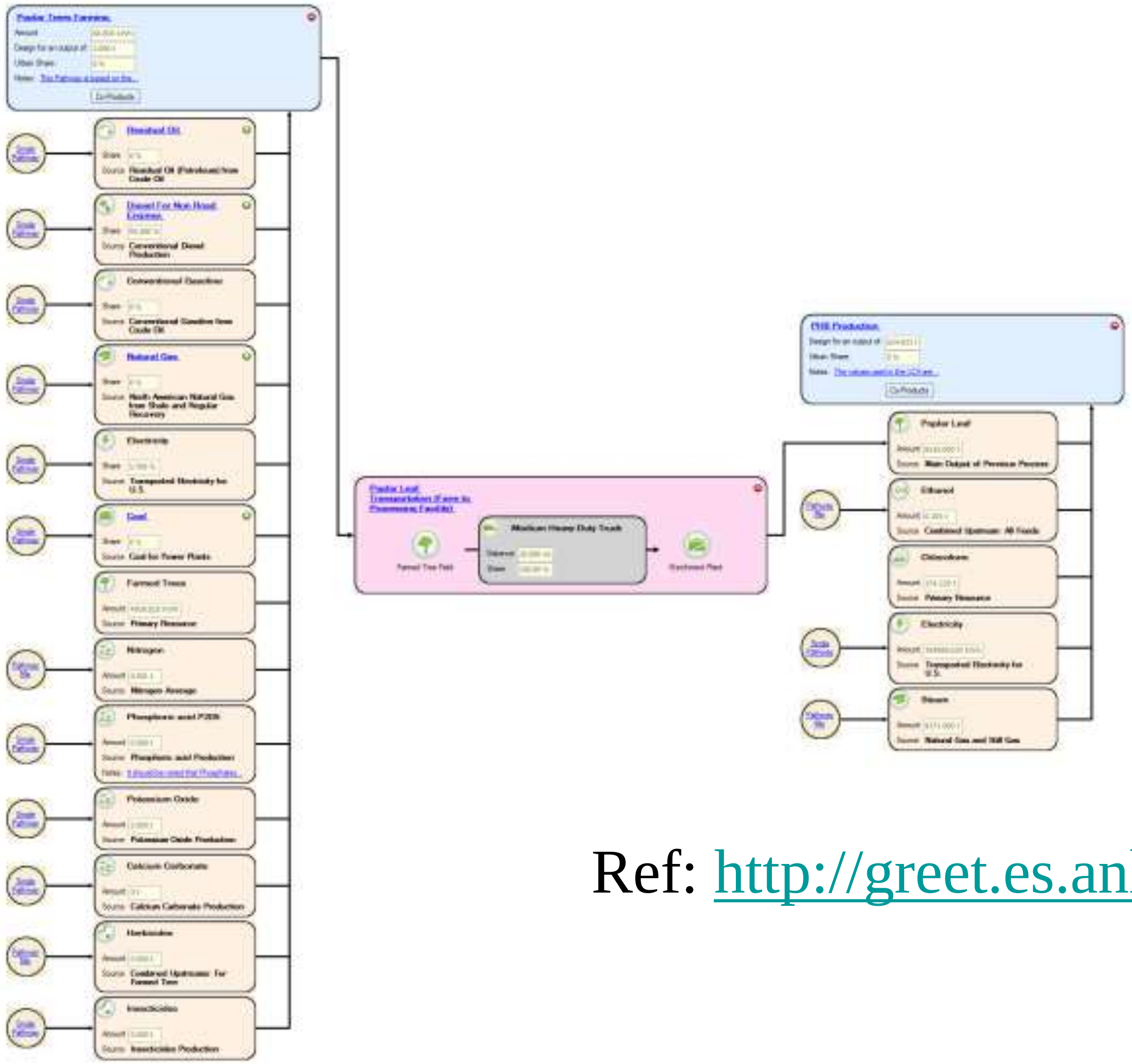
Ref: Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)

GREET Model



Ref: Wang, M., Wu, M., and Huo H. 2007. Life-cycle energy and greenhouse gas emission impacts of different corn ethanol plant types. Environ. Res. Lett. doi:10.1088/1748-9326/2/2/024001

New GREET Model



Ref: http://greet.es.anl.gov/

Well to Wheel LCA

GREET (Greenhouse gases, Regulated Emissions, and Energy in Transportation) is a life cycle analysis model for transportation fuels.

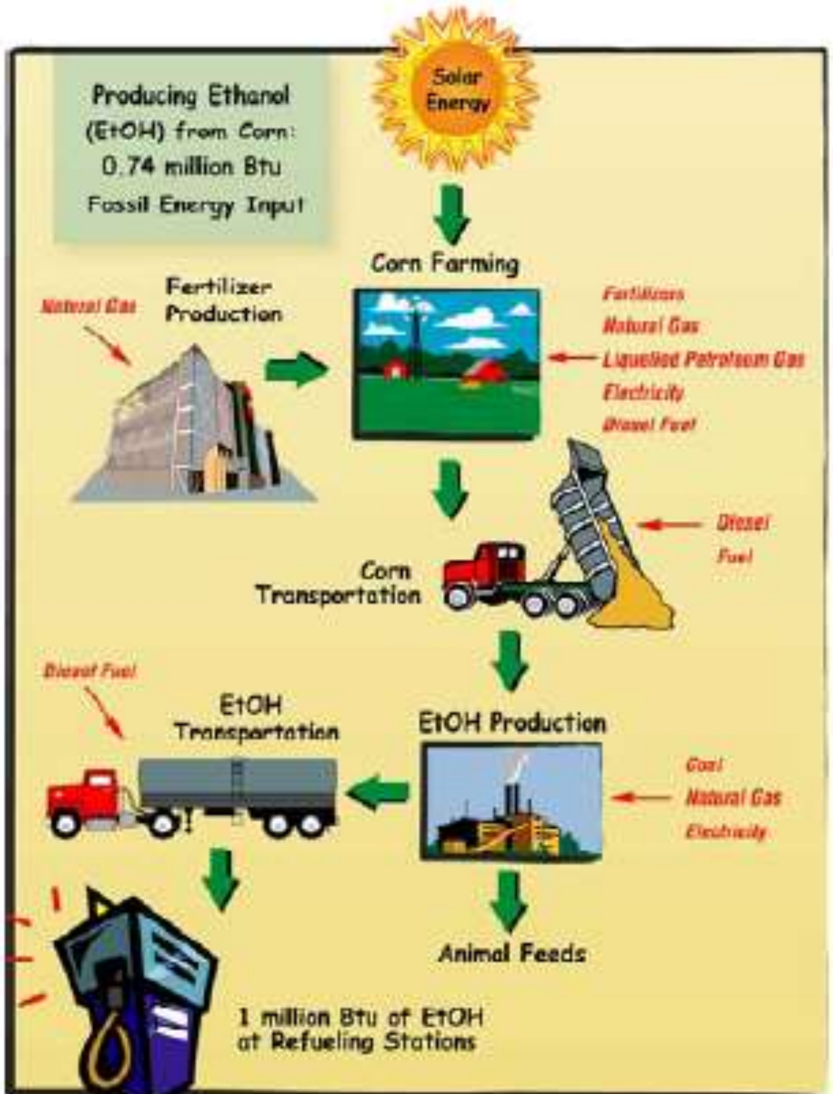
1. Developed at Argonne National Lab in 1995.
2. More than 85 transportation fuel pathways.
3. www. transportation.anl.gov/software/GREET

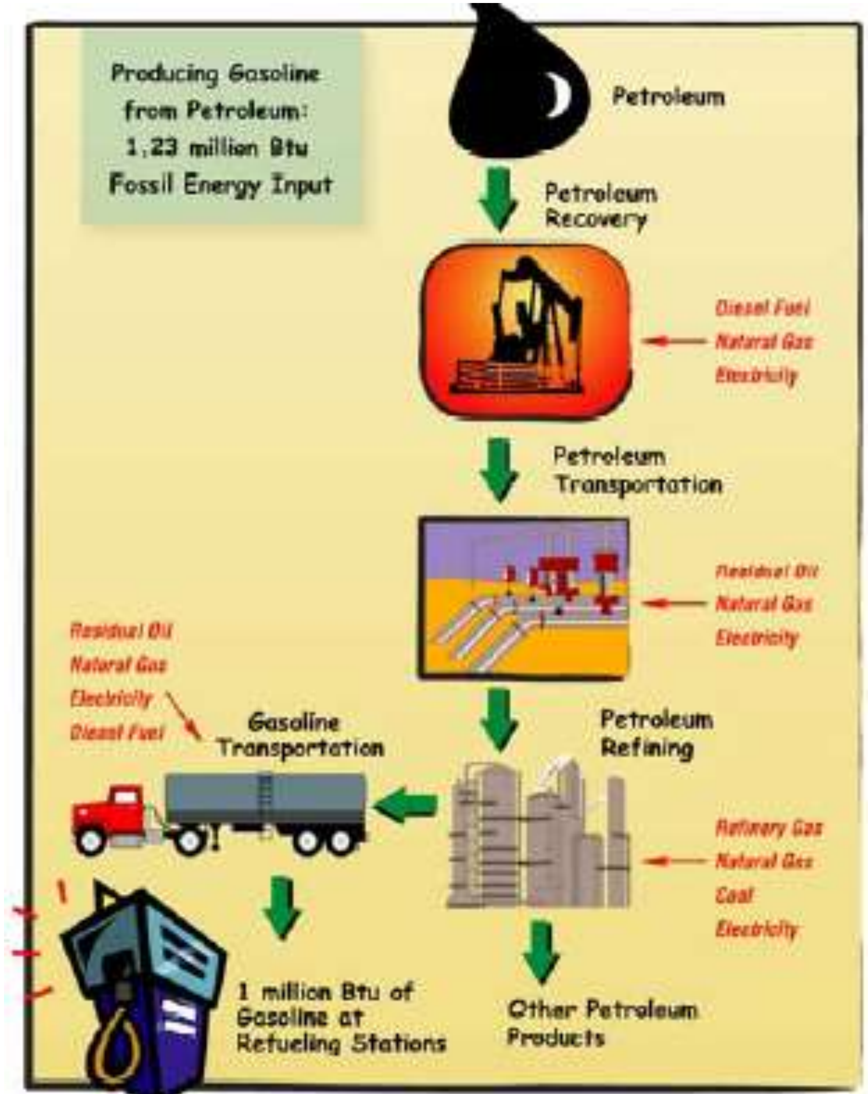
Net Energy

Net energy is the amount of energy in a product minus fossil energy used to produce the energy product. It does not include energy from renewable sources such as sun, wind, hydropower and nuclear energy.

Ref: Wang, M. 2005. Updated energy and greenhouse gas emission results of fuel ethanol. Intl. Sympo. Alcohol Fuels.

Case Study 1: Corn Ethanol Well to Pump LCA

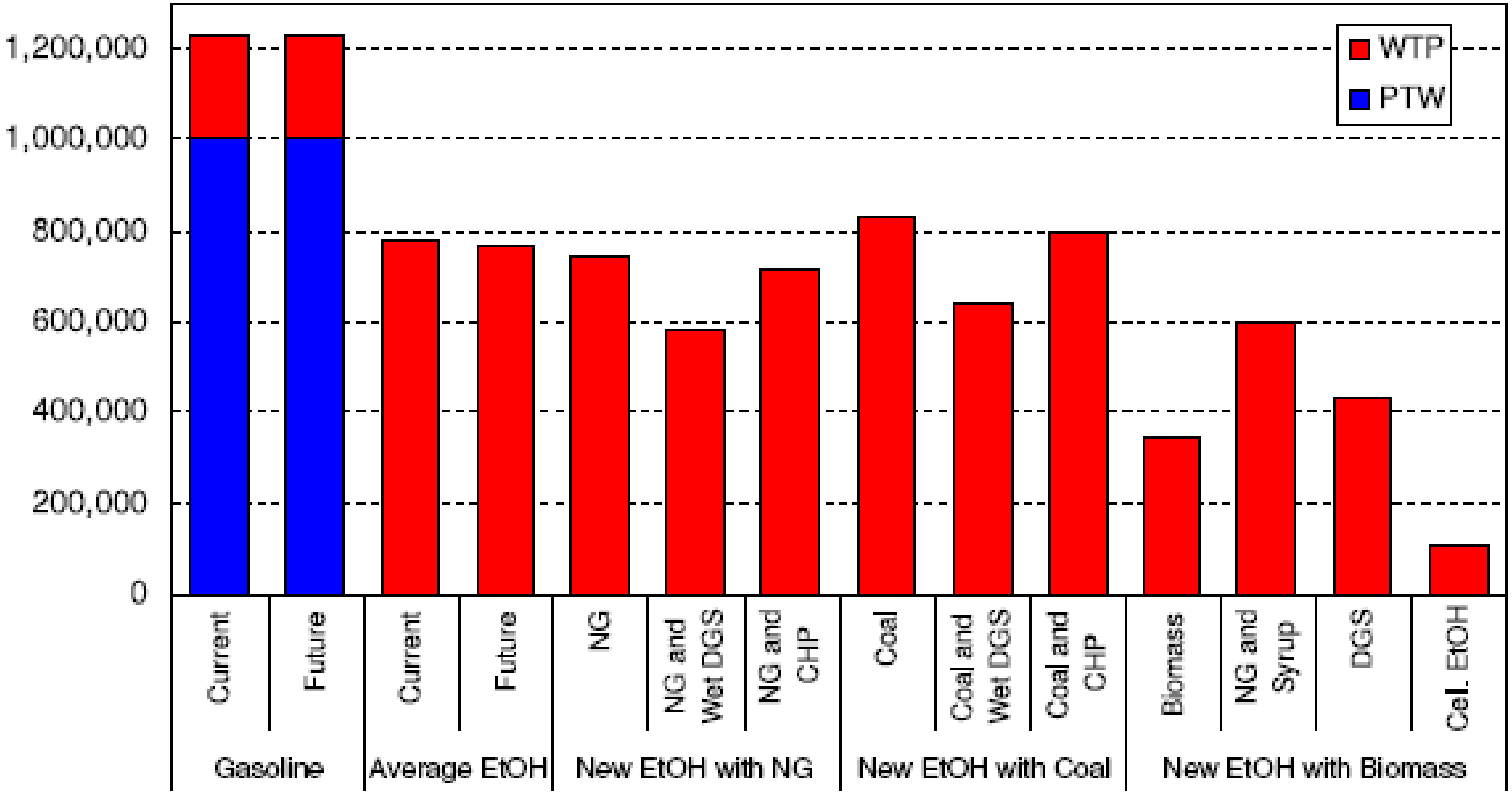




Ref: Wang, M. 2005. Updated energy and greenhouse gas emission results of fuel ethanol. Intl. Sympo. Alcohol Fuels.

Well to Pump LCA

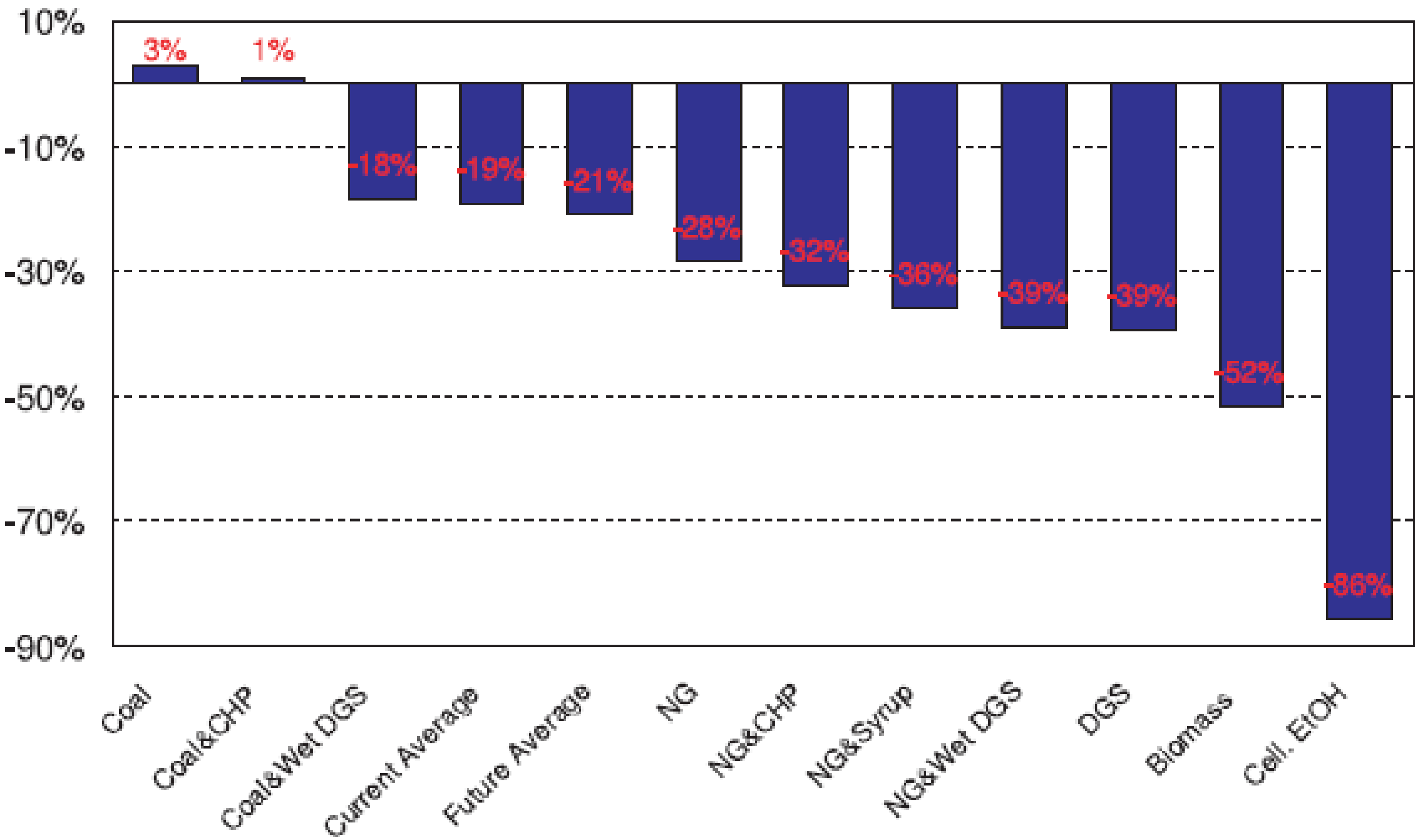
WTW fossil energy use to produce one million BTU of energy.



Ref: Wang, M., Wu, M., and Huo H. 2007. Life-cycle energy and greenhouse gas emission impacts of different corn ethanol plant types. Environ. Res. Lett. doi:10.1088/1748-9326/2/2/024001

Well to Pump LCA

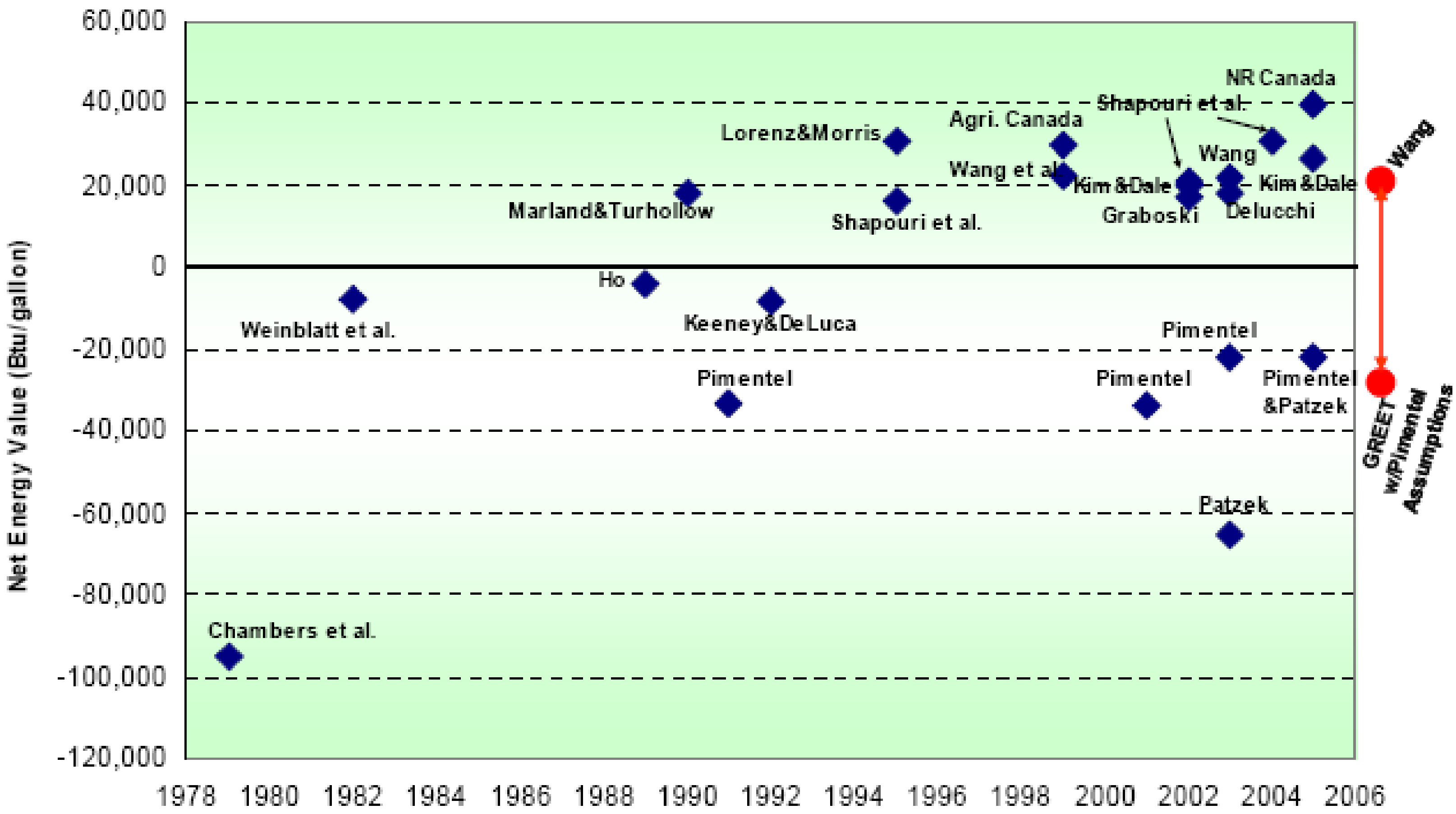
WTW greenhouse gas emission changes for fuel ethanol relative to gasoline



Ref: Wang, M., Wu, M., and Huo H. 2007. Life-cycle energy and greenhouse gas emission impacts of different corn ethanol plant types. Environ. Res. Lett. doi:10.1088/1748-9326/2/2/024001

Results From Few Well to Pump LCA Studies for Corn Ethanol

Comparison of Fuel Ethanol Energy Balance from various studies



Ref: Wang, M. 2005. Updated energy and greenhouse gas emission results of fuel ethanol. Intl. Sympo. Alcohol Fuels.

Why are the results from various LCA analyses so different?

- *System boundaries*
- *Data quality, accuracy*
  - *Age of data, sources of data, geographical context*
- *Allocation of coproducts*
  - *Mass, energy and displacement methods*
- *Nitrous oxide emissions*
  - *Varying fertilizer use for different crops*
- *Indirect land use change (ILUC)*
  - *Variation in ILUC among first, second and third generation fuels.*
- *Reported units*
  - *GHG emissions/MJ of fuel or GHG emissions/Ha of land?*

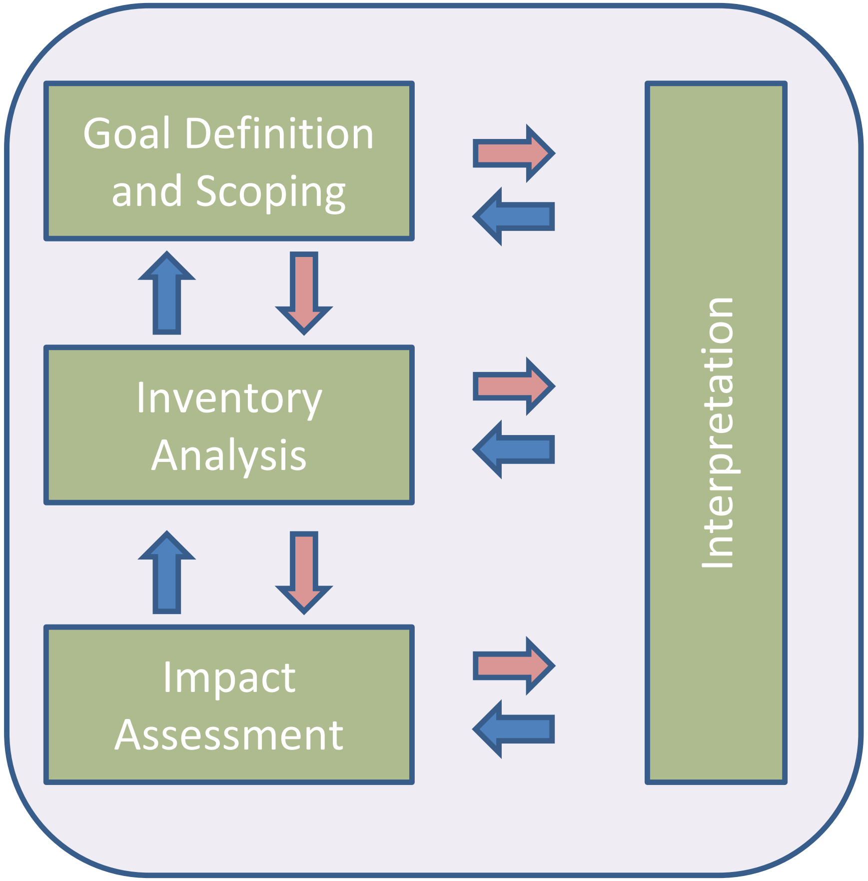
LCA results depend on coproduct allocation strategy

Method	*Dry Milling Plant*	*Wet Milling Plant*
Weight-based	51%	52%
Energy content-based	39%	43%
Market value-based	24%	30%
Energy use of individual processes	41%	36%
Displacement	20%	16%

Life Cycle Analysis: Summary of Process Steps

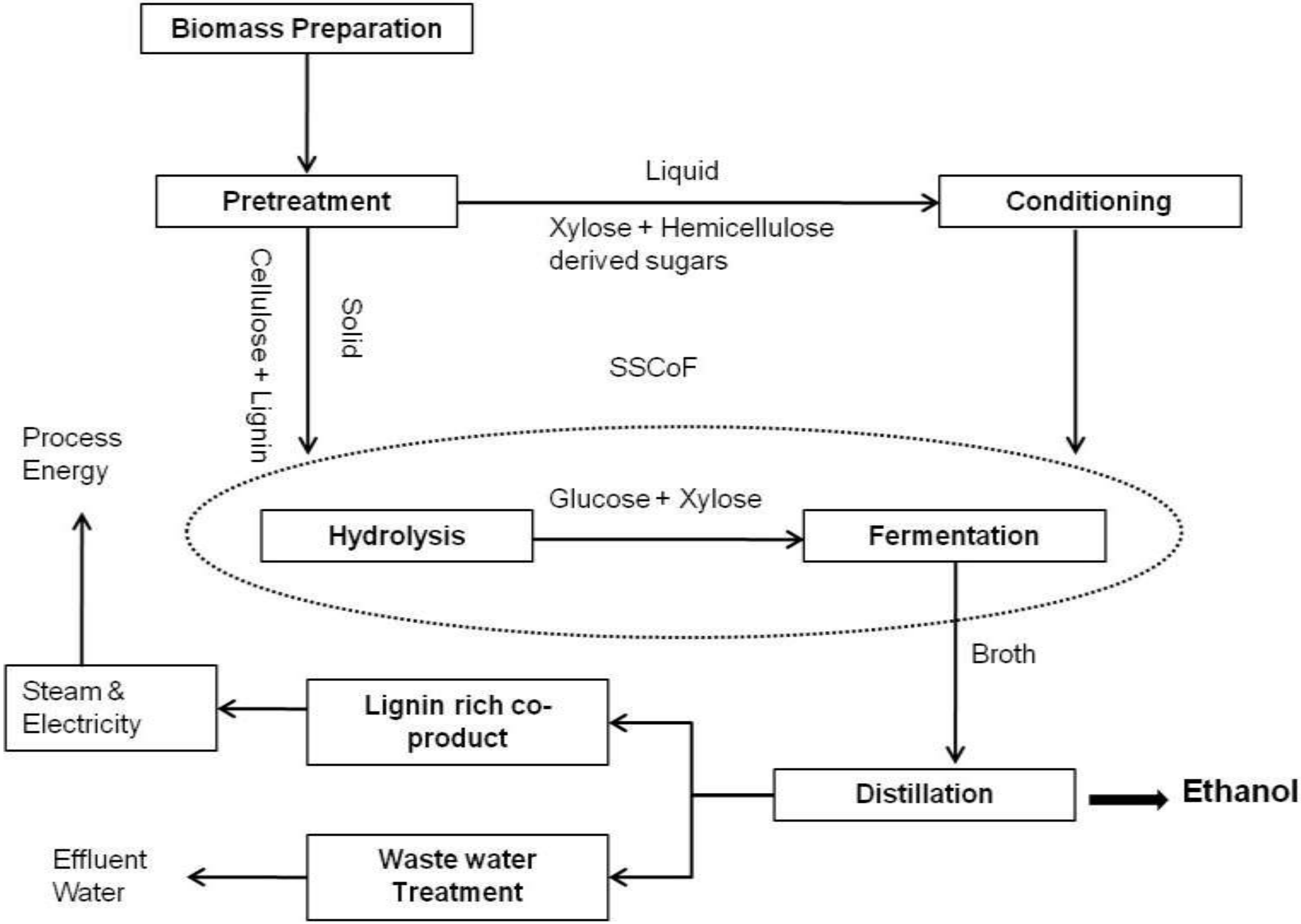
LCA is divided into four distinct stages:

1. Goal Definition and Scoping
2. Life Cycle Inventory
3. Life Cycle Impact Assessment
4. Life Cycle Interpretation



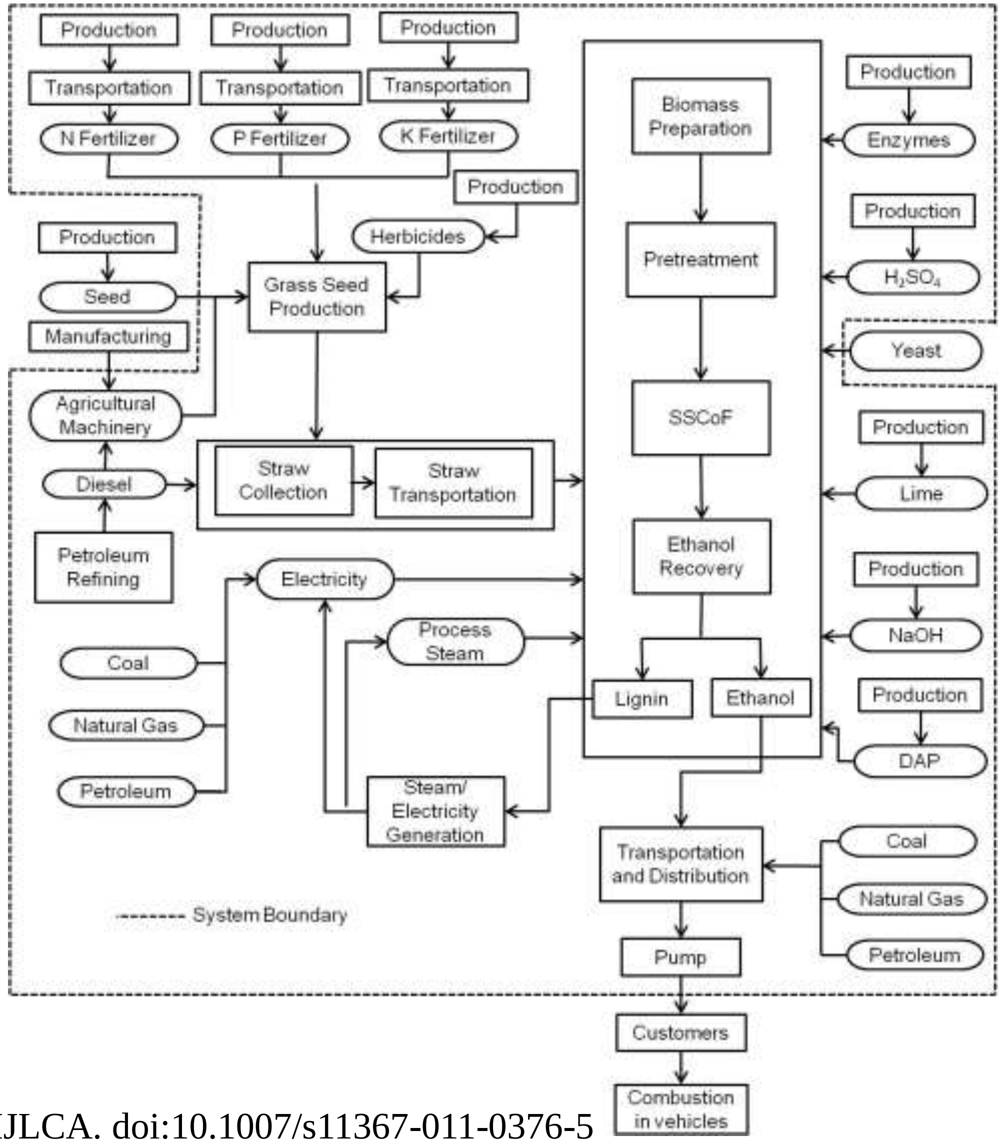
Ref: Life Cycle Analysis: Principles and Practice. EPA/600/R-06/060 (2006)

Case Study 2: Life Cycle Assessment of Cellulosic Ethanol



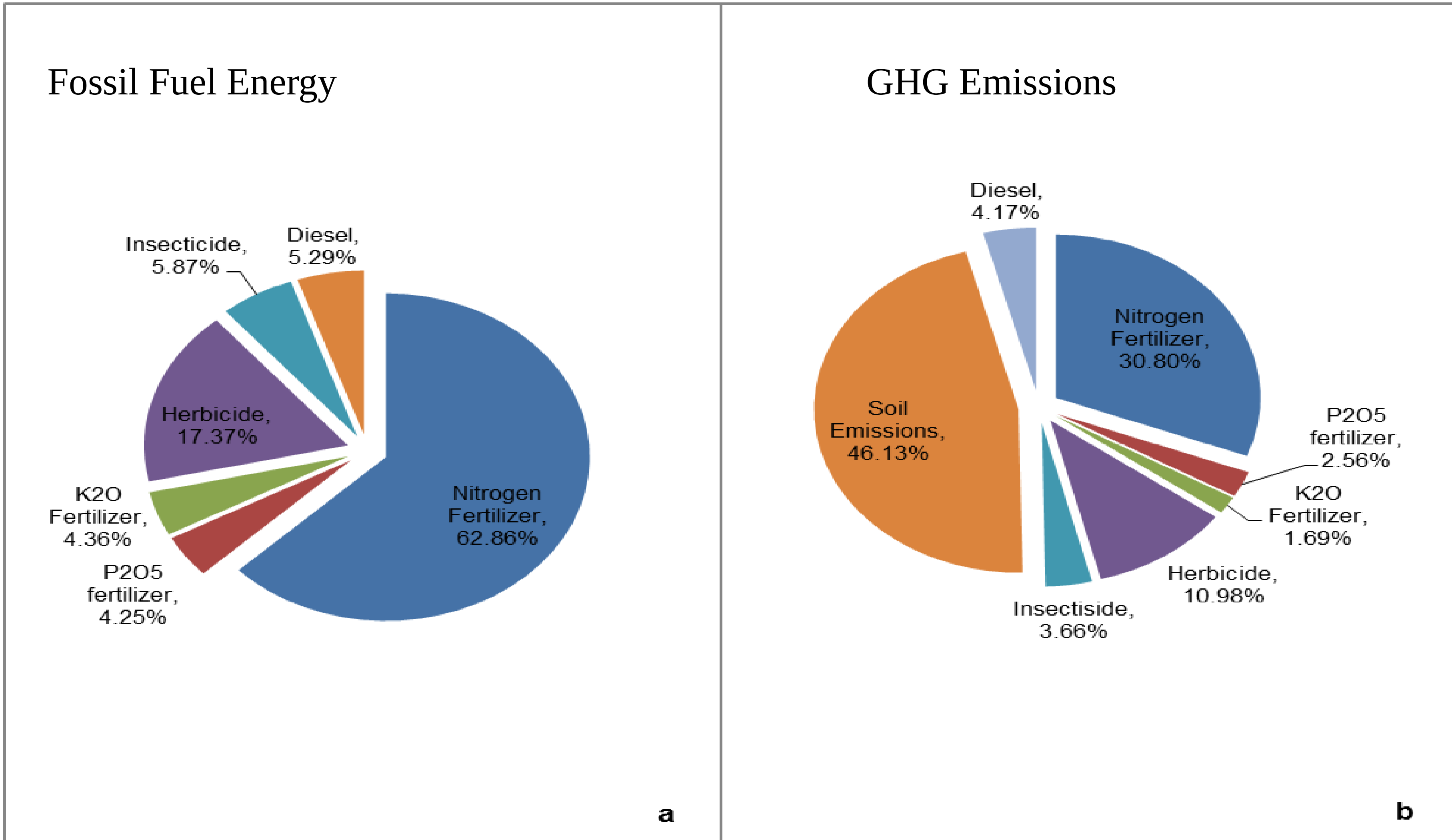
Ref: Kumar and Murthy, 2012. IJLCA. doi:10.1007/s11367-011-0376-5

Case study 2: System Boundary



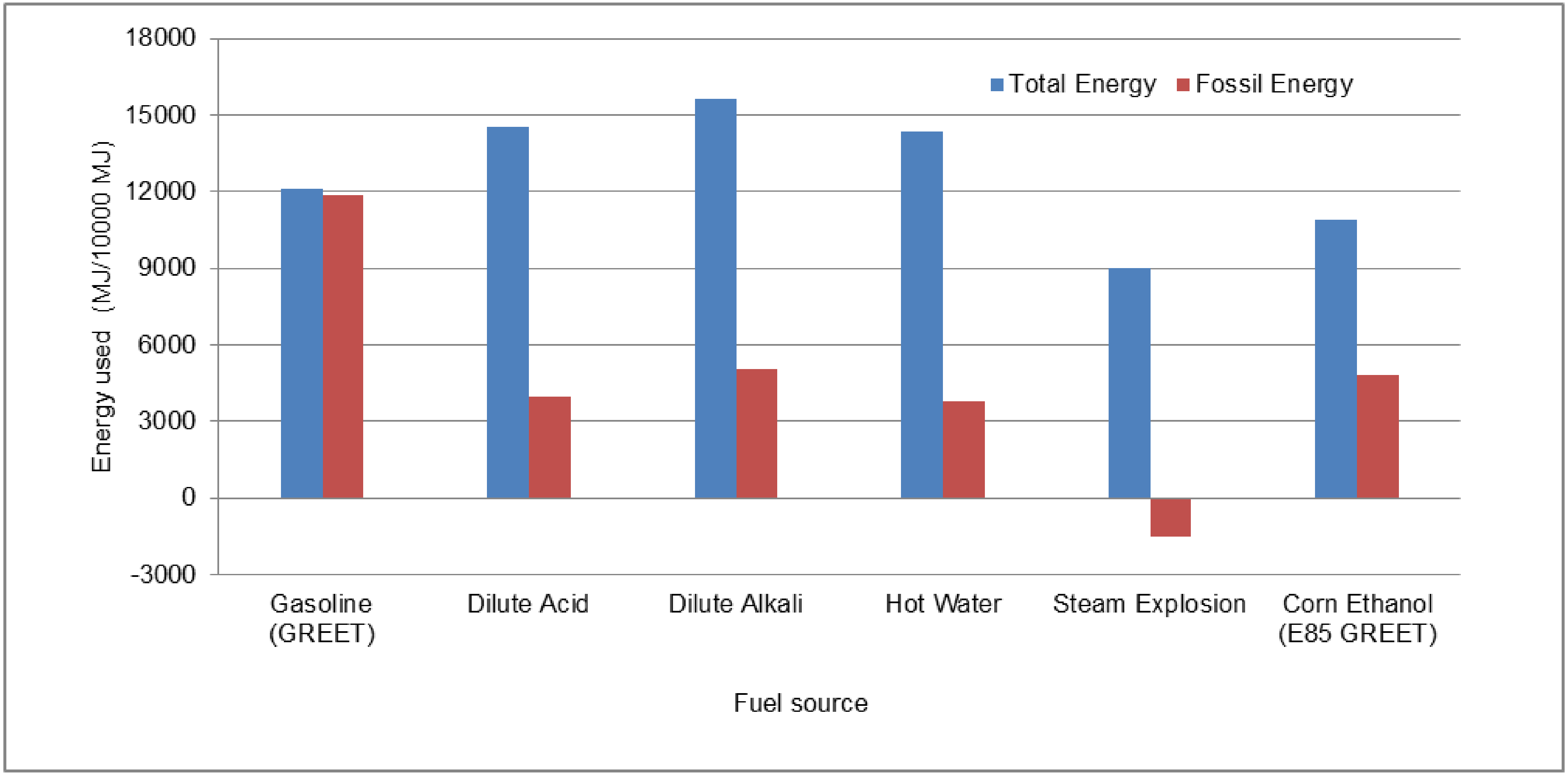
Ref: Kumar and Murthy, 2012. IJLCA. doi:10.1007/s11367-011-0376-5

Case study 2: Life Cycle Assessment Results



Ref: Kumar and Murthy, 2012. IJLCA. doi:10.1007/s11367-011-0376-5

Case study 2: Life Cycle Assessment Results



Ref: Kumar and Murthy, 2012. IJLCA. doi:10.1007/s11367-011-0376-5

Curious case of grocery bags

Paper or Canvas or Plastic?

Image Source: http://bryoneagon.files.wordpress.com/2009/09/1244303943grocery_bag1.jpg
http://loveisdope.files.wordpress.com/2009/02/canvas-grocery-bag.jpg
http://thumb1.shutterstock.com.edgesuite.net/display_pic_with_logo/60383/60383,1222849277,1/~04625.jpg

Databases and Software for Performing Sustainability Analysis

Software

- GREET: http://greet.es.anl.gov/
- EIO-LCA: http://www.eiolca.net/index.html
- Eco-LCA: http://resilience.eng.ohio-state.edu/eco-lca/index.htm
- SPIonExcel: http://spionexcel.tugraz.at/

Databases

- US LCI Database: http://www.nrel.gov/lci/
- NAICS Sectors: http://www.census.gov/cgi-bin/sssd/naics/naicsrch?chart=2002
- SPI Database: http://spionexcel.tugraz.at/

Thank you

Ganti S. Murthy

Biological and Ecological Engineering Department

Oregon State University

murthy@engr.orst.edu

541-737-6291

Thank you