Integration of Industrial Scale Processes using Biomass Feedstock in the Petrochemical Complex of the Lower Mississippi River Corridor

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Introduction

- Introduction to Sustainable Development
- Research Vision
- Biomass conversion processes, Aspen HYSYS 2006® designs, Aspen ICARUS Process Evaluator 2006® cost estimations
- Integration of biotechnology in existing plant complex
- Conclusions

Sustainability

Sustainability refers to integrating development in three aspects

- Economic
- Environmental
- Societal

There are numerous approaches to attempt an integration of these aspects by world organizations, countries and industries.

MONSANTO

DOW

USDA

UNIDO

BASF
The Chemical Company

DUPONT
The miracles of science

ExxonMobil
Taking on the world's toughest energy challenges.

EASTMAN

UNEP

AIChE Total Cost Assessment Methodology

- A methodology was developed by an industry group working through the AIChE to assess the total cost in a project and they issued a detailed report on total cost assessment (Constable et al., TCA Report 1999).

- Project Team

  AD Little (Collab. & Researcher)
  DOE
  Eastman Chemical
  Georgia Pacific
  Merck
  Owens Corning
  SmithKline Beecham (Lead)
  Bristol-Myers Squibb
  Dow
  Eastman Kodak
  IPPC of Business Round Table
  Monsanto
  Rohm and Haas
  Sylvatica (TCAce Dev.)

- TCA Users Group created in May 2009. Work is ongoing to update the costs identified in the report.
  - Type I: Direct
  - Type II: Indirect
  - Type III: Contingent Liability
  - Type IV: Intangibles
  - Type V: External

Constable, D. et al., “Total Cost Assessment Methodology; Internal Managerial Decision Making Tool”, AIChE, ISBN 0-8169-0807-9, July ,1999.

Corporate Sustainability

- A company’s success depends on maximizing the profit as expressed below.

$$\text{Profit} = \Sigma \ \text{Product Sales} - \Sigma \ \text{Raw Material Costs} - \Sigma \ \text{Energy Costs}$$

- The profit equation above can be expanded to meet the “Triple Bottomline” criteria of sustainability.
- This will incorporate the economic costs expanded to environmental costs and societal costs (also referred to as the sustainable or sustainability costs)

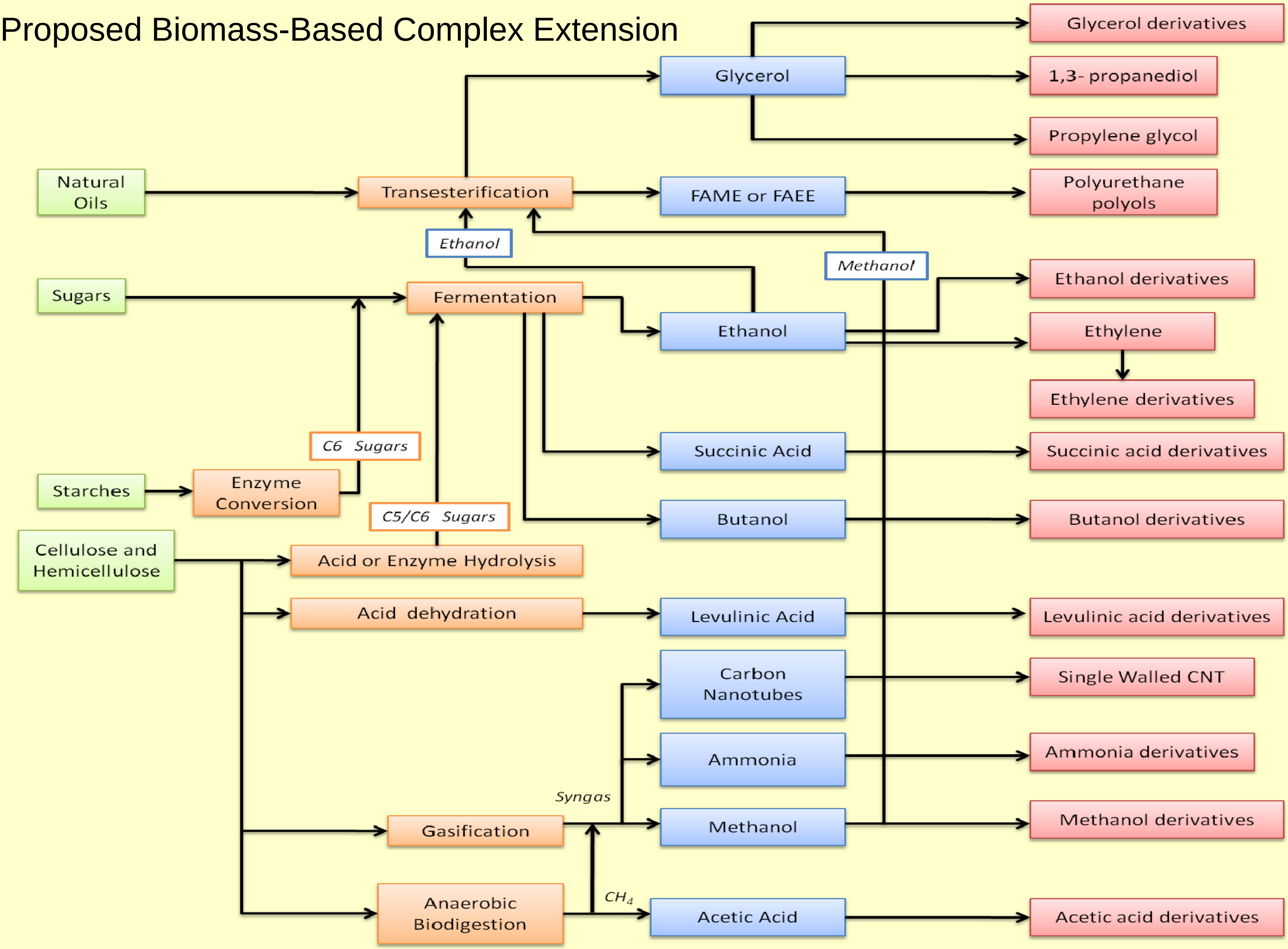
$$\begin{aligned}\text{Triple Bottom Line} = {} & \Sigma \ \text{Product Sales} && + \Sigma \ \text{Sustainable Credits}\\ & - \Sigma \ \text{Raw Material Costs} && - \Sigma \ \text{Energy Costs}\\ & - \Sigma \ \text{Environmental Costs} && - \Sigma \ \text{Sustainable Costs}\end{aligned}$$

$$\text{Triple Bottom Line} = \Sigma \ \text{Profit} - \Sigma \ \text{Environmental Costs} + \Sigma \ \text{Sustainable} \ (\text{Credits} - \text{Costs})$$

Research Vision

- Propose **biomass based processes** integrated into the chemical production complex in the Gulf Coast Region and other chemical complexes of the world.
- Utilize **carbon dioxide** from processes in the complex to make chemicals and produce algae for biomass feedstock.
- Assign costs to the **Triple Bottomline Equation** components.
- Propose a **Mixed Integer Non-Linear Programming** problem to maximize the Triple Bottomline based on constraints: multiplant material and energy balances, product demand, raw material availability, and plant capacities
- Use **Chemical Complex Analysis System** to obtain Pareto optimal solutions to the MINLP problem
- Use Monte Carlo simulations to determine **sensitivity** of optimal solution

Proposed Biomass-Based Complex Extension



Biomass Processes

The following biomass conversion processes are considered for integration into the chemical complex superstructure:

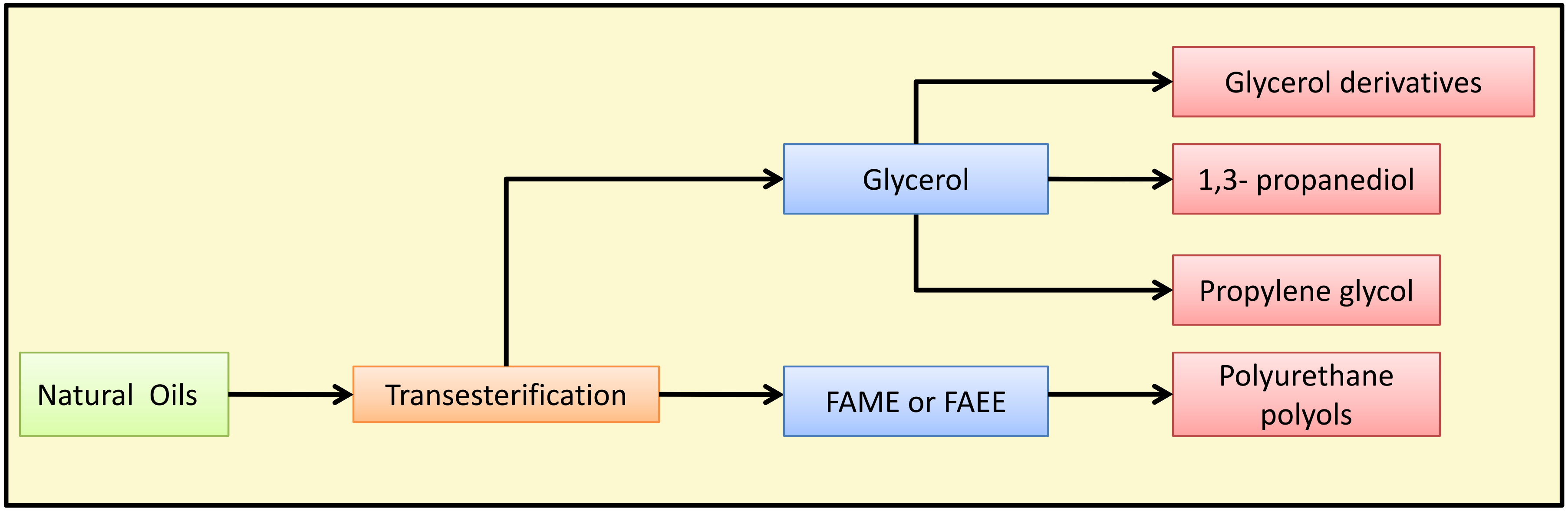
- Fermentation
- Anaerobic digestion
- Transesterification
- Gasification

Pretreatment of biomass is necessary before any of the biomass conversion processes.

Aspen HYSYS® - Process simulation

Aspen ICARUS Process Evaluator® - Cost Estimation

Transesterification



Natural Oils

Transesterification

Glycerol

FAME or FAEE

Glycerol derivatives

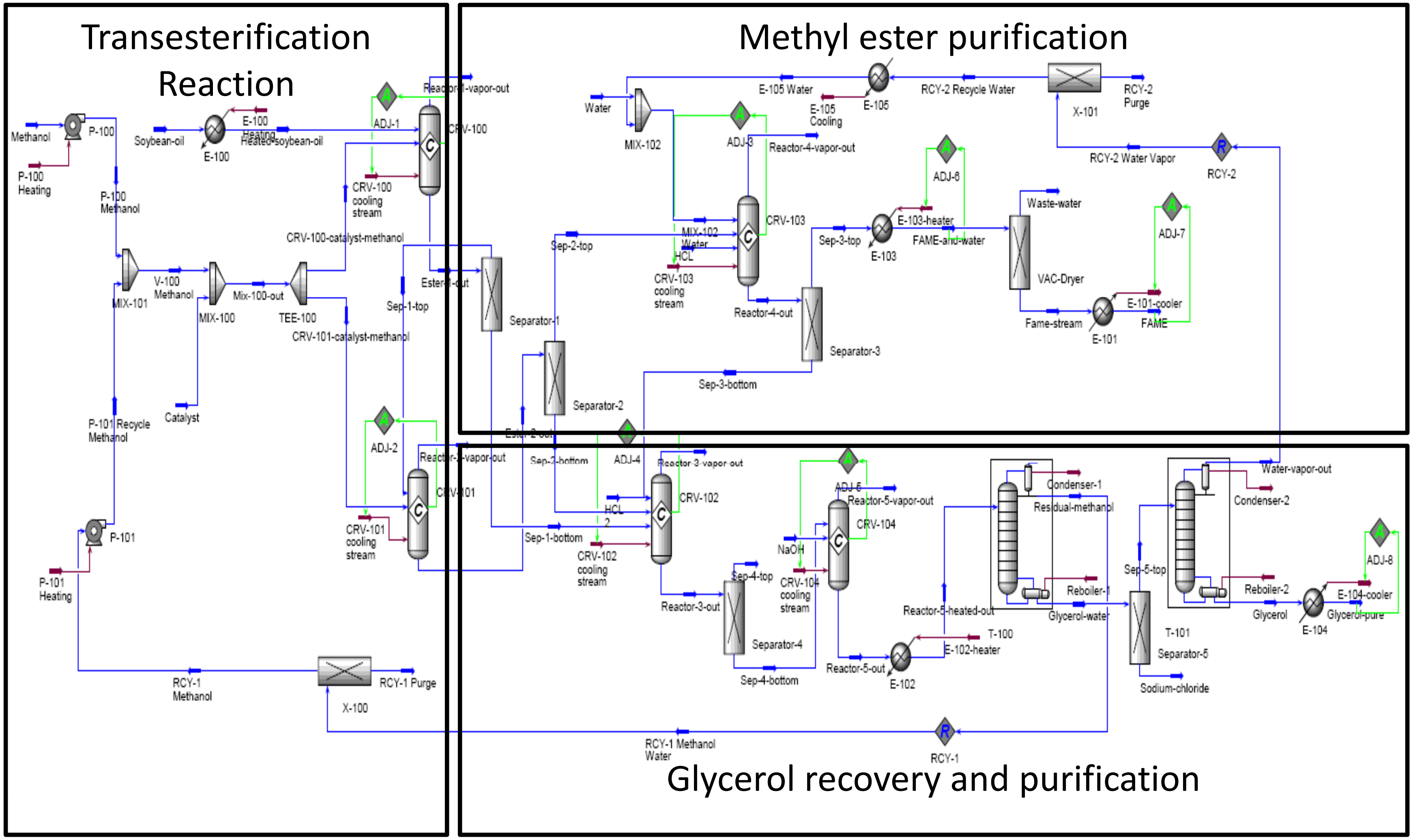
1,3- propanediol

Propylene glycol

Polyurethane polyols

- Transesterification process is the treatment of natural oils with an alcohol and a catalyst to produce esters and glycerol.
- Methanol or ethanol is used as alcohol for fatty acid methyl or ethyl esters (FAME/FAEE).
- These esters can be transformed to polymers.
- Glycerol is produced ~ 10% by weight in the process.
- Glycerol can be introduced to the propylene chain.

HYSYS Design of Transesterification Process

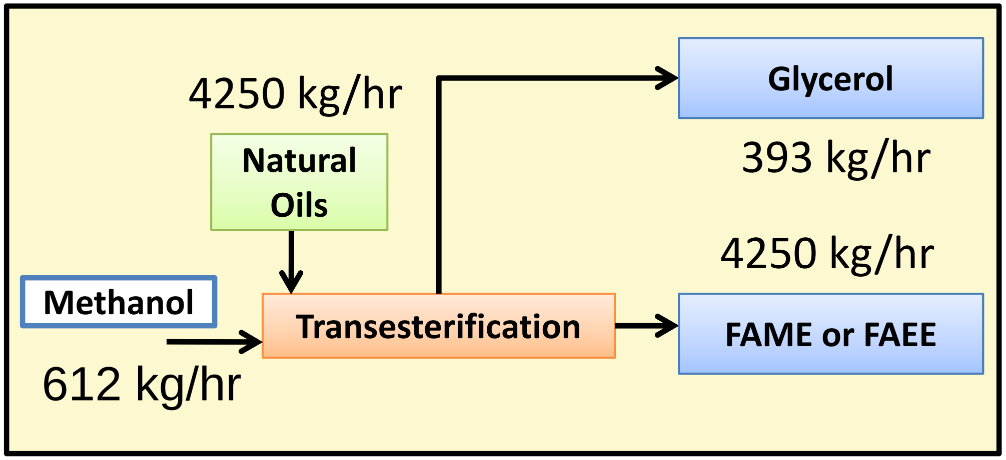


Transesterification Reaction

Methyl ester purification

Glycerol recovery and purification

Design Description of Transesterification



- The design is divided into three sections
    - Transesterification reaction
    - Methyl ester purification
    - Glycerol recovery and purification
- 10 million gallons per year [1] of Fatty Acid Methyl Ester (FAME) produced
- FAME is utilized in manufacture of polymers
- Glycerol is used in manufacture of propylene glycol
- This process can use Algae oil as feedstock
- The energy required for the process was comparable to the energy liberated

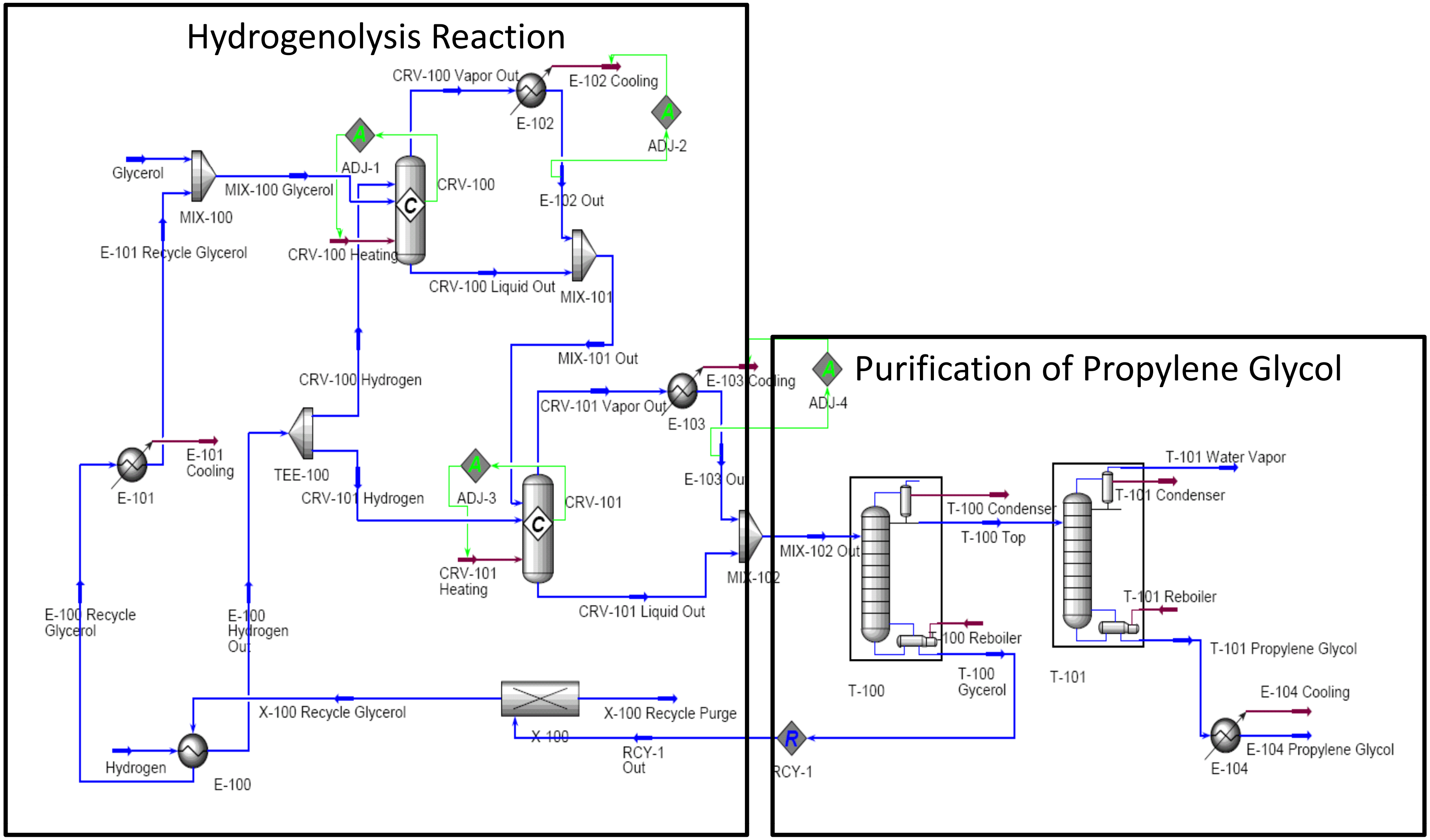
Transesterification	
Thermodynamic model	UNIQUAC
Reactants	Methanol Soybean Oil
Catalyst	1.78% (w/w) Sodium Methylate in methanol
Products	Methyl Ester Glycerol
Temperature	60°C
Methyl Ester Purification	
Wash agents	Water HCl
Glycerol Recovery and Purification	
Purification Agents	NaOH Water HCl

[1] *Design based on "A process model to estimate biodiesel production costs",M.J. Haas et al., Bioresource Technology 97 (2006) 671-678*

ICARUS Process Evaluator Economic Analysis of Transesterification

Economic Analysis		
Economic Life	10	years
Plant Capacity	10,300,000	gallons/year Methyl Ester
Total Project Capital Cost	6,930,000	USD
Total Operating Cost	22,600,000	USD/year
Total Raw Materials Cost	19,100,000	USD/year
Total Utilities Cost	139,000	USD/year
Total Product Sales	22,600,000	USD/year @2.18 USD/gallon of Methyl Ester

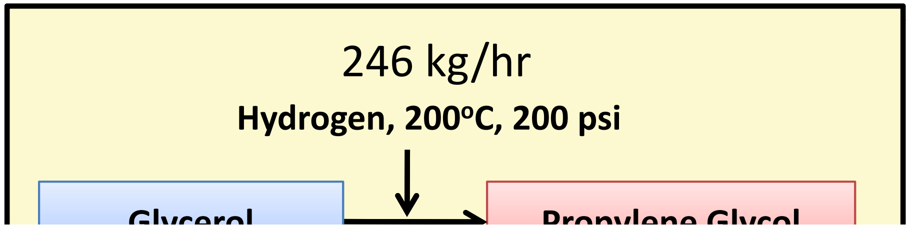
HYSYS Design of Glycerol to Propylene Glycol



Hydrogenolysis Reaction

Purification of Propylene Glycol

Design description of Propylene Glycol



246 kg/hr

Hydrogen, 200°C, 200 psi

Glycerol

Propylene Glycol

Hydrogenolysis	
Thermodynamic model	UNIQUAC
Reactants	Glycerol Hydrogen
Catalyst	Copper Chromite
Products	Propylene Glycol Water
Temperature	200°C
Pressure	200 psi

- The design is based on a low pressure (200 psi) and temperature (200°C) process for hydrogenation of glycerol to propylene glycol [1]
- ~65,000 metric ton of propylene glycol is produced per year[2]
- The energy required for the process was comparable to the energy liberated

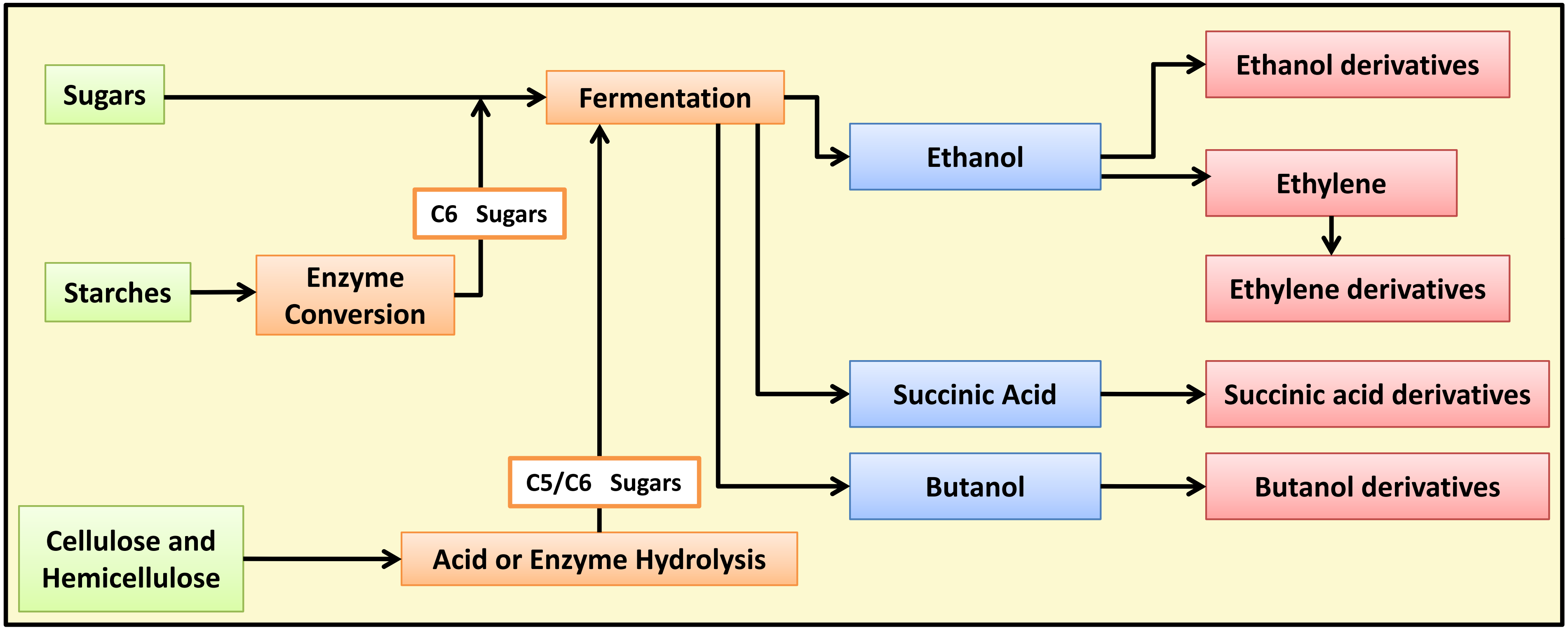
[1] *Design based on experimental results from* Dasari, M. A. et al. 2005, A*pplied Catalysis, A: General*, Vol. 281, p. 225-231.

[2] *Capacity based on Ashland/Cargill joint venture of process converting glycerol to propylene glycol*

ICARUS Process Evaluator Economic Analysis of Propylene Glycol

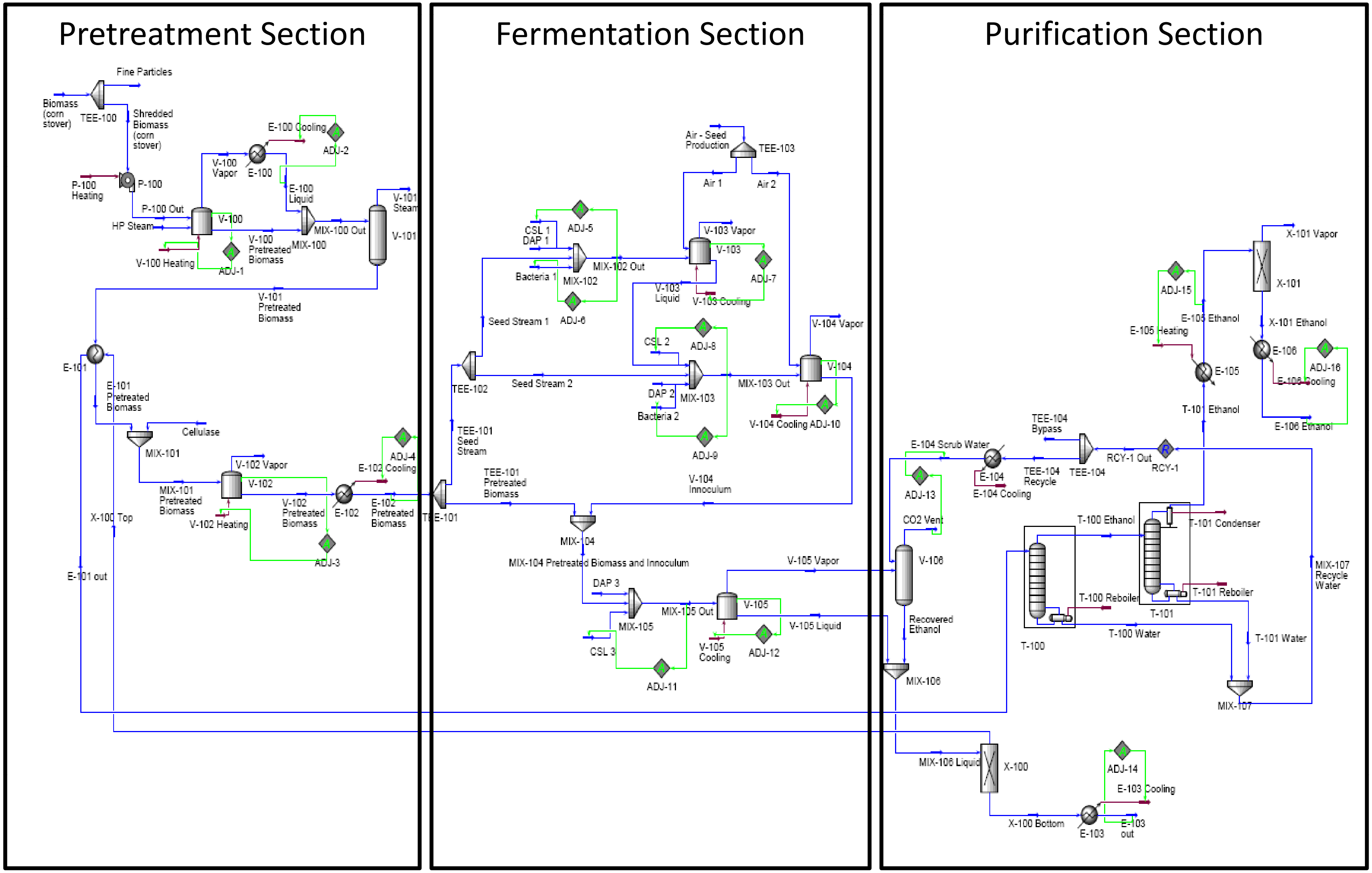
Economic Analysis		
Economic Life	10	Years
Plant Capacity	164,000,000	lb/Year propylene glycol
Total Project Capital Cost	6,580,000	USD
Total Operating Cost	83,400,000	USD/Year
Total Raw Materials Cost	73,300,000	USD/Year
Total Utilities Cost	2,410,000	USD/Year
Total Product Sales	133,000,000	USD/Year@ 0.82 USD/lb propylene glycol

Fermentation

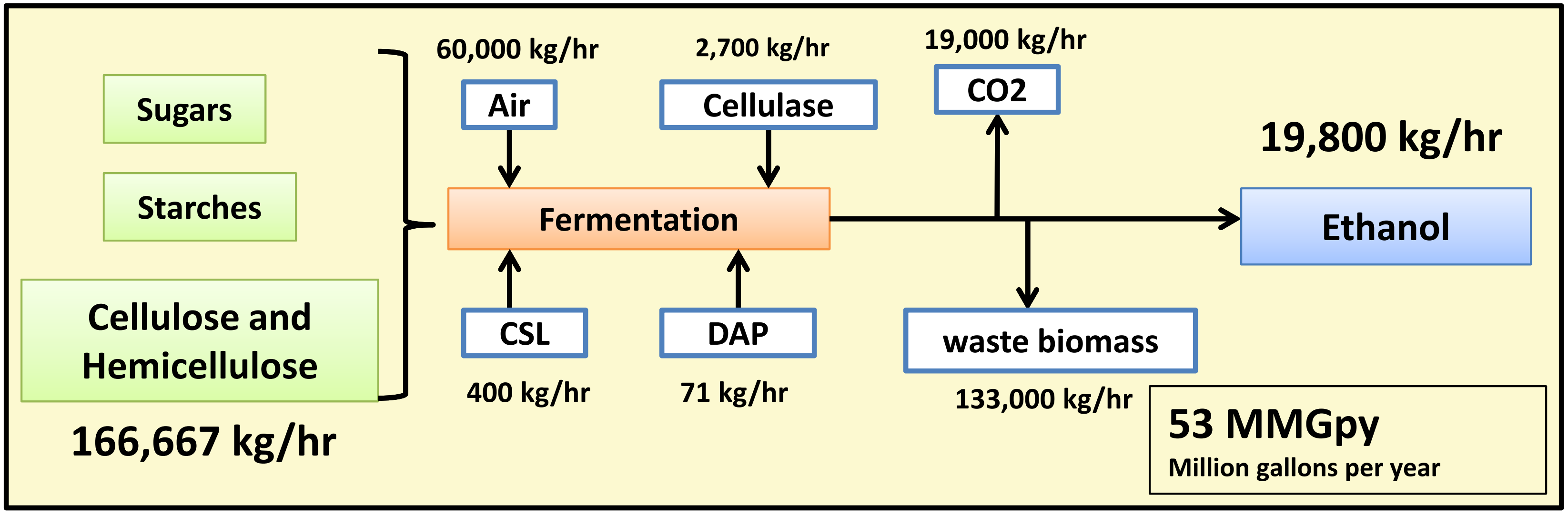


- Fermentation is the enzyme-catalyzed transformation of an organic compound.
- Fermentation enzymes react with hexose and pentose to form products.
- Enzyme selection determines product :-
  - *Saccharomyces Cervisiae* (C6), *Escherichia coli* (C5 & C6), *Zymomonas mobilis* (C6)– Ethanol
  - Engineered Eschericia coli, A. succiniciproducens – Succinic Acid
  - Engineeried microorganism - Butanol
  - Lactic Acid Producing Bacteria (LAB) – Lactic Acid

HYSYS Design of Fermentation



Design Description of Fermentation



- The design is based on NREL's[1] lignocellulosic biomass to ethanol process design which converts 2,000 metric tons/day of corn stover
- Waste treatment not considered
- Net energy was liberated from the system

Fermentation	
Thermodynamic Model	UNIQUAC
Reactants	Corn Stover
Enzyme (hydrolysis)	Cellulase (*Trichoderma reesei)*
Bacteria (fermentation)	*Z. mobilis*
Products	Ethanol, CO2, Waste
Nitrogen Sources	CSL, DAP

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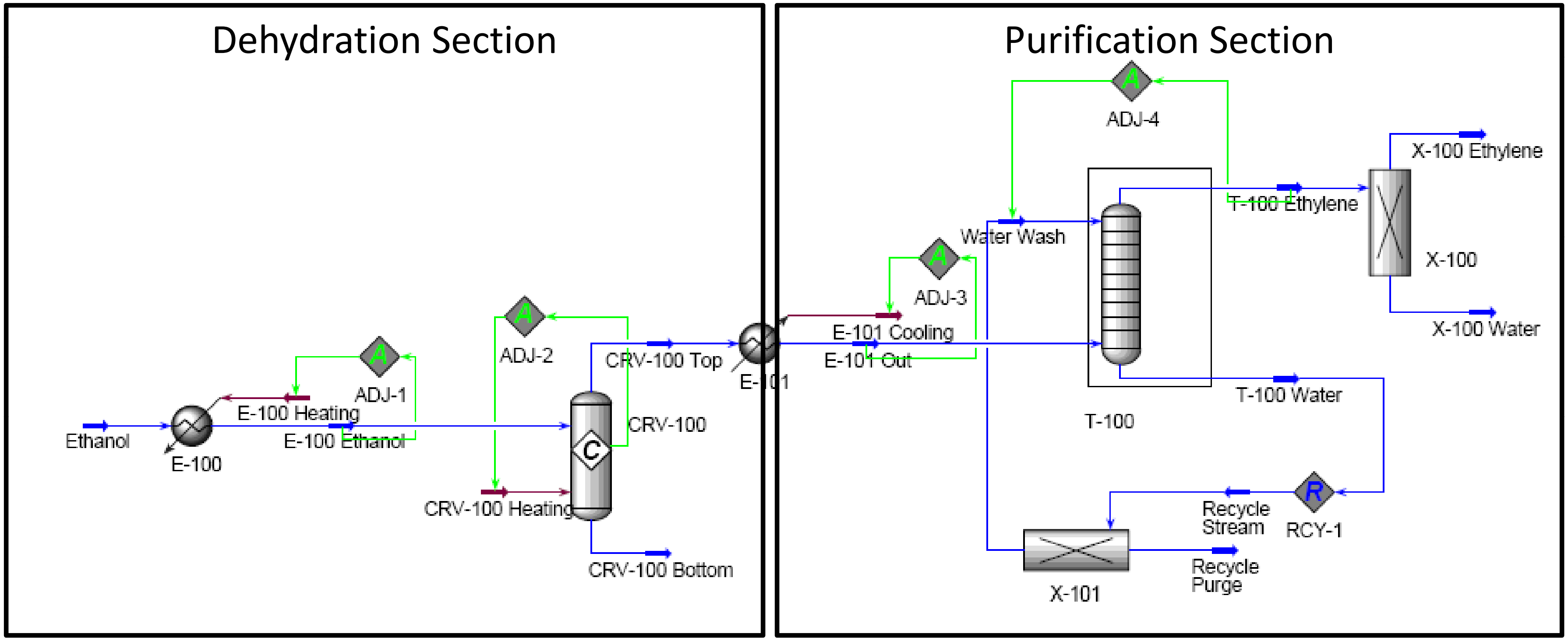
[1] *Design based on results from* Aden A. et al., NREL/TP-510-32438, National Renewable Energy Laboratory, Golden, CO, (June 2002)

ICARUS Process Evaluator Economic Analysis of Fermentation

Economic Analysis		
Economic Life	10	Years
Plant Capacity	53,000,000	gallons/Year ethanol
Total Project Capital Cost	20,000,000	USD
Total Operating Cost	81,000,000	USD/Year
Total Raw Materials Cost	54,000,000	USD/Year
Total Utilities Cost	17,000,000	USD/Year
Total Product Sales	106,000,000	USD/Year@ 1.50 USD/gallon ethanol

HYSYS Design of Ethanol to Ethylene



Description of Ethylene Process

300°C, Fluidized bed process, 99 % conversion

Ethanol → **Ethylene**

41,500 kg/hr → 25,000 kg/hr

- Design is based on dehydrogenation of ethanol to ethylene[1]
- The capacity of the plant is based on a 200,000 metric ton/year ethylene production facility proposed by Braskem in Brazil[2]
- Net energy was required by the system

Dehydrogenation	
Thermodynamic model	UNIQUAC
Reactants	Ethanol
Catalyst	Activated silica-alumina
Products	Ethylene Water
Temperature	300°C

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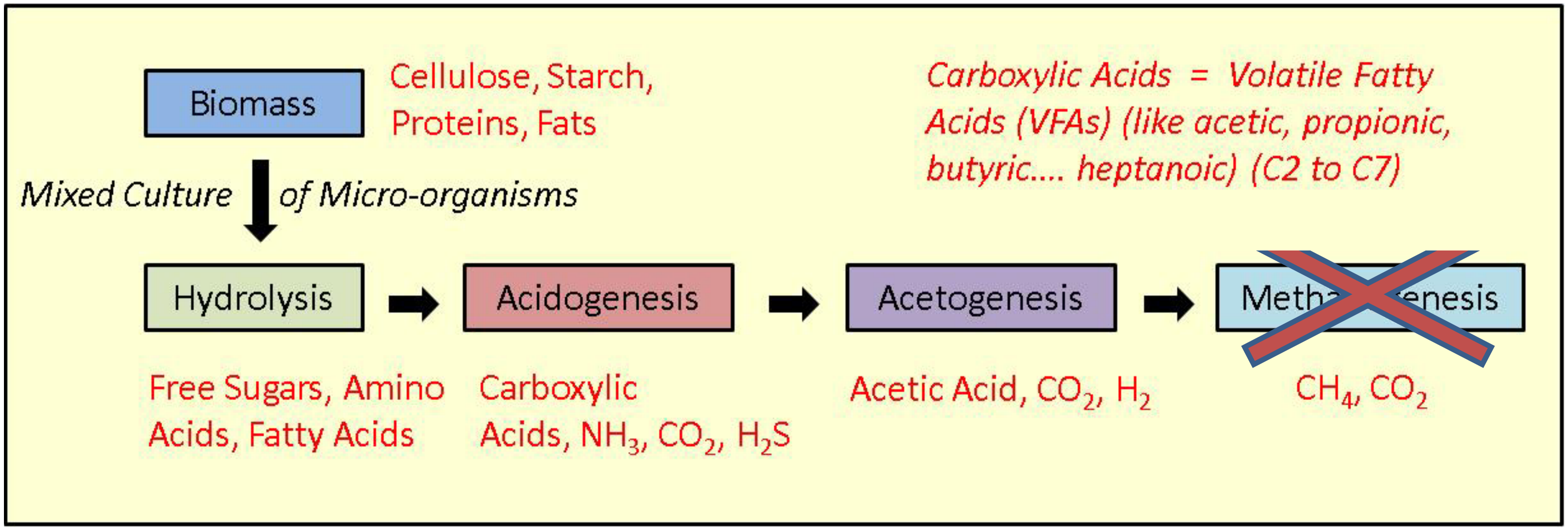
[1] *Design based on process described by* Wells, G. M., 1999, *Handbook of Petrochemicals and Processes*, Sec. Ed., Pg 207-208

[2] *Capacity based on Braskem proposed ethanol to ethylene plant in Brazil http://www.braskem.com.br/*

ICARUS Process Evaluator Economic Analysis of Ethylene

Economic Analysis		
Economic Life	10	Years
Plant Capacity	440,400,000	lb/Year ethylene
Total Project Capital Cost	3,000,000	USD
Total Operating Cost	186,000,000	USD/Year
Total Raw Materials Cost	169,000,000	USD/Year
Total Utilities Cost	3,000,000	USD/Year
Total Product Sales	186,000,000	USD/Year@ 0.42 USD/lb ethylene

Anaerobic Digestion



Biomass

Cellulose, Starch, Proteins, Fats

Mixed Culture of Micro-organisms

Hydrolysis → Acidogenesis → Acetogenesis → ~~Meth enesis~~

Free Sugars, Amino Acids, Fatty Acids

Carboxylic Acids, NH_3, CO_2, H_2S

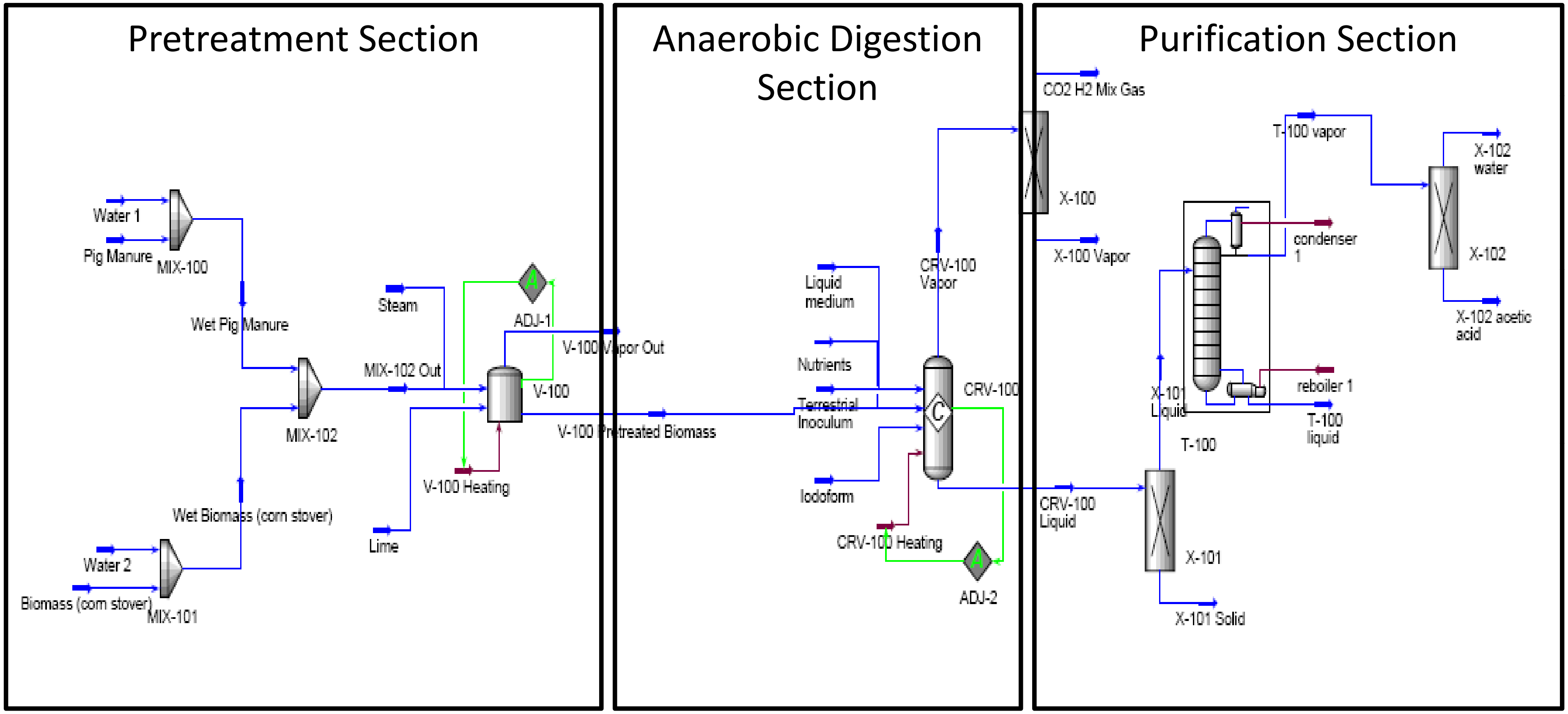
Acetic Acid, CO_2, H_2

CH_4, CO_2

Carboxylic Acids = Volatile Fatty Acids (VFAs) (like acetic, propionic, butyric.... heptanoic) (C2 to C7)

- Anaerobic digestion of biomass is the treatment of biomass with a mixed culture of bacteria in absence of oxygen to produce methane (biogas) and carbon dioxide.
- Four stages: hydrolysis, acidogenesis, acetogenesis and methanogenesis
- **MixAlco process** – Inhibits fourth stage of methane production using iodoform (CHI_3) or bromoform ($CHBr_3$). Reduces cost of process by using mixed culture of bacteria from cattle rumen. Produces mixed alcohols, carboxylic acids and ketones.

HYSYS Design of Anaerobic Digestion

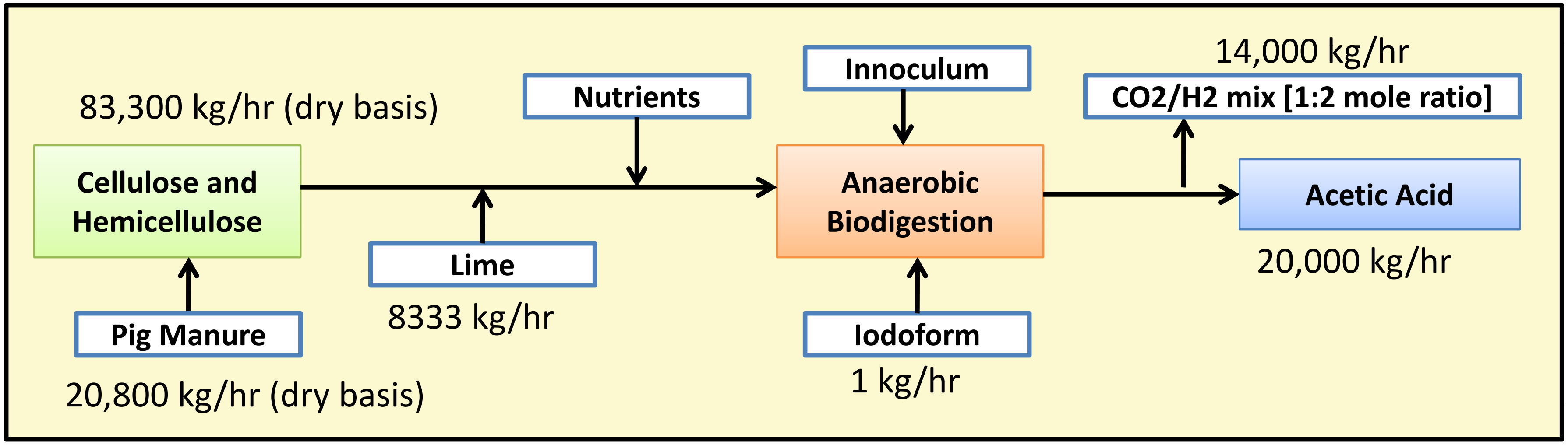


Pretreatment Section

Anaerobic Digestion Section

Purification Section

Design Description of Anaerobic Digestion



83,300 kg/hr (dry basis)

Cellulose and Hemicellulose

Pig Manure

20,800 kg/hr (dry basis)

Lime

8333 kg/hr

Nutrients

Innoculum

Anaerobic Biodigestion

Iodoform

1 kg/hr

14,000 kg/hr

CO2/H2 mix [1:2 mole ratio]

Acetic Acid

20,000 kg/hr

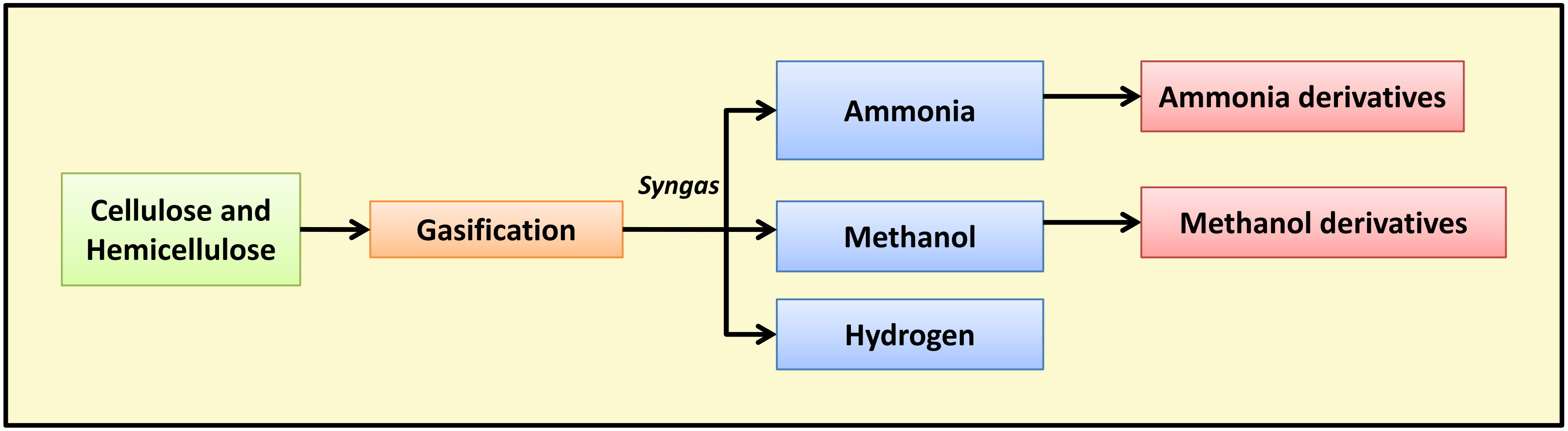
- Design is based on anaerobic digestion of corn stover to carboxylic acids [1]
- The capacity of the plant is based on a 2000 metric ton/day processing of biomass[2]
- Ketones can be produced by modifying process
- Energy recovered from the system

Anaerobic Digestion	
Thermodynamic model	UNIQUAC
Reactants	Corn Stover
Innoculum	Rumen Fluid
CH_4 Inhibitor	Iodoform
Products	Acetic Acid, CO_2,H_2

[1] *Design based on process described by* Thanakoses et al., "Fermentation of Corn Stover to Carboxylic Acids", Bio.Tech and Bio. Eng., Vol. 83, No. 2, 2003

[2] Aden A. et al., NREL/TP-510-32438, National Renewable Energy Laboratory, Golden, CO, (June 2002)

Gasification



Cellulose and Hemicellulose

Gasification

Syngas

Ammonia

Methanol

Hydrogen

Ammonia derivatives

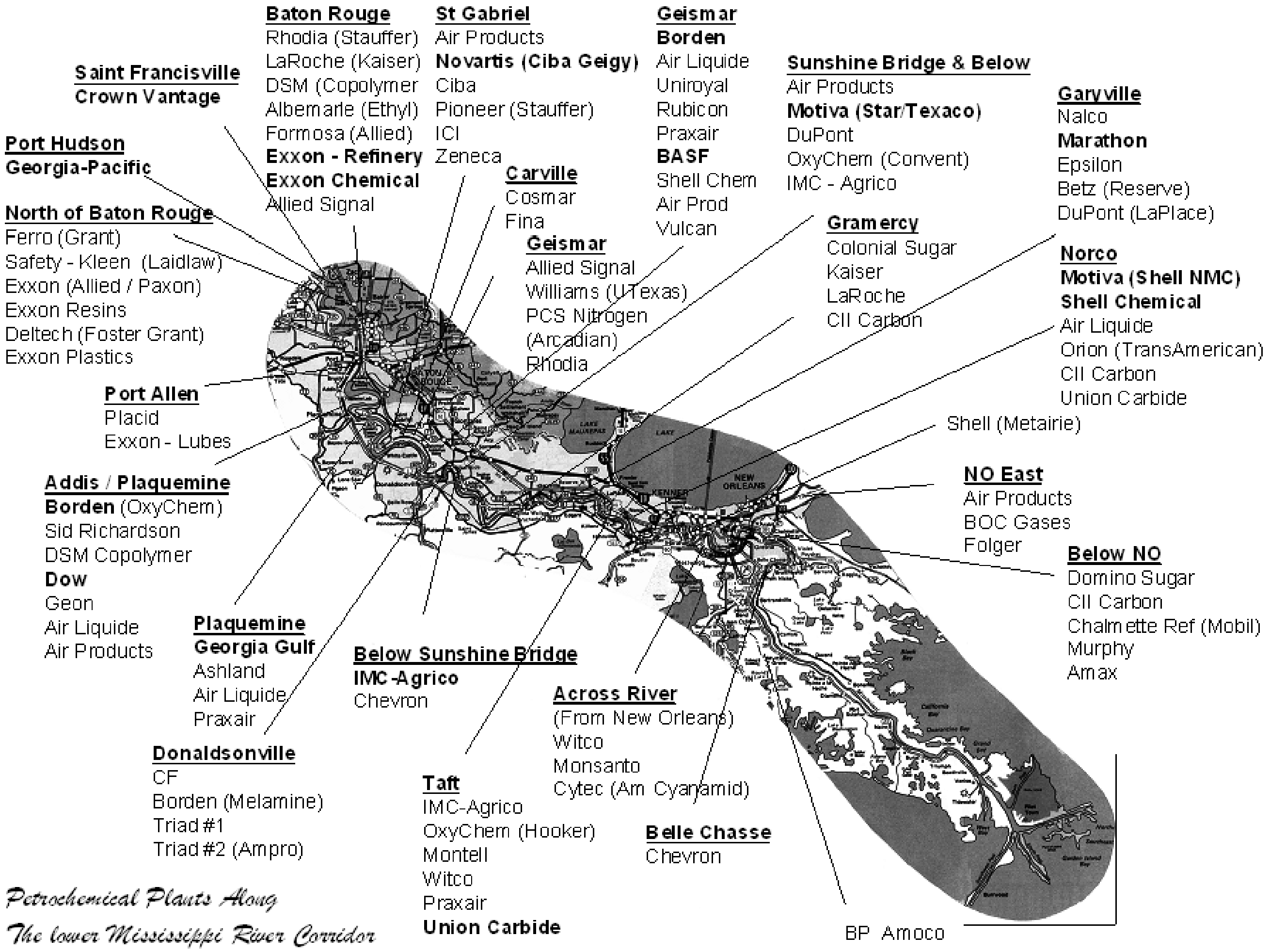
Methanol derivatives

- Biomass can be gasified to produce of syngas
- Syngas can be converted to chemicals like methanol, ammonia and hydrogen

Industries in Louisiana

- Petrochemical complex in the lower Mississippi River Corridor
  - Dow
  - DuPont
  - BASF
    Shell
  - Exxon
  - Monsanto
  - Mosaic
  - Union Carbide

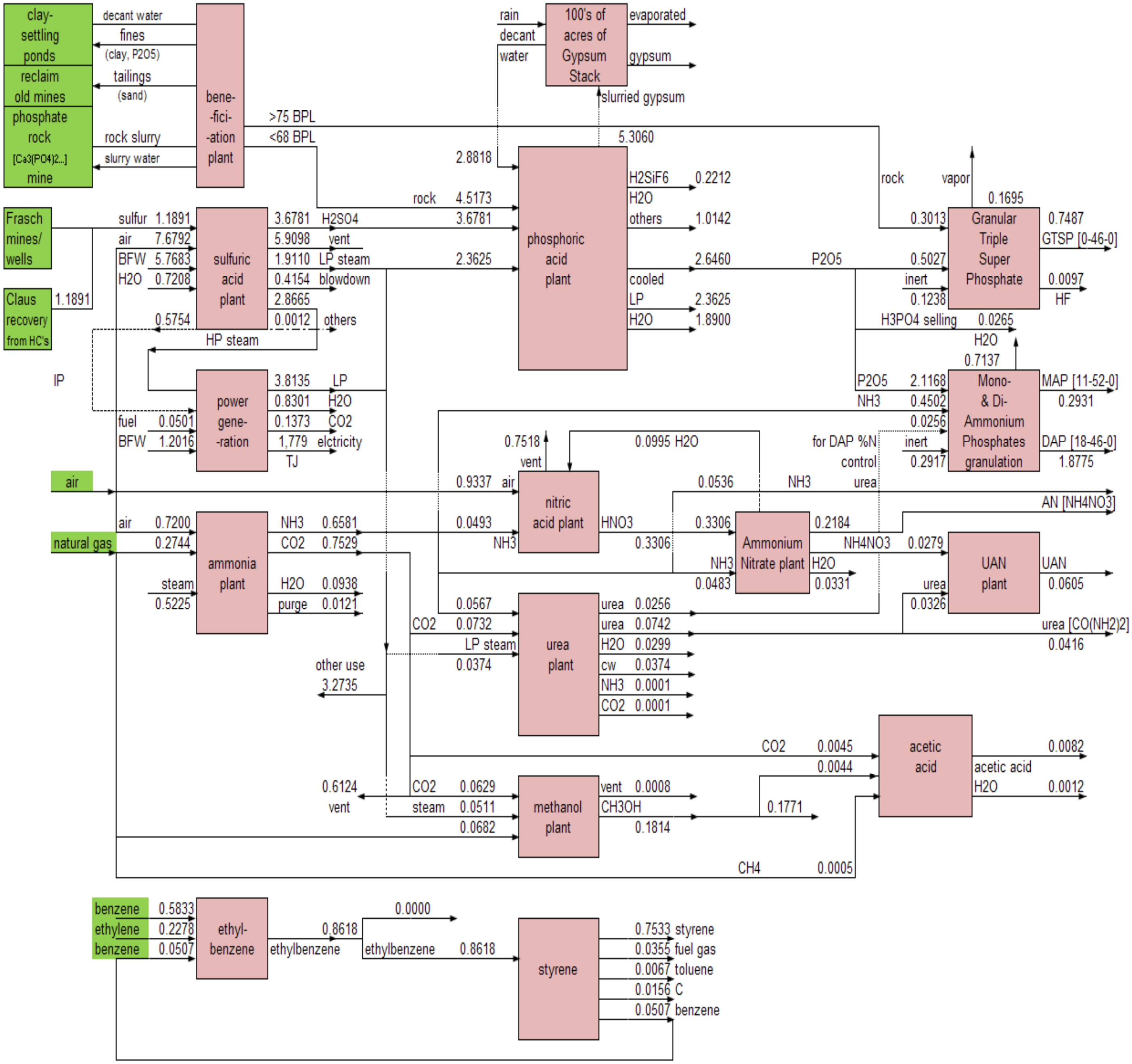
  …. and others



Petrochemical Plants Along The lower Mississippi River Corridor

Photo: Peterson, 2000

Base Case of Plants in the Lower Mississippi River Corridor



clay-settling ponds

reclaim old mines

phosphate rock [Ca3(PO4)2..] mine

decant water

fines (clay, P2O5)

tailings (sand)

rock slurry

slurry water

bene-fici-ation plant

>75 BPL

<68 BPL

rain

decant water

100's of acres of Gypsum Stack

evaporated

gypsum

slurried gypsum

5.3060

2.8818

rock 4.5173

3.6781

2.3625

phosphoric acid plant

H2SiF6 0.2212

H2O

others 1.0142

2.6460

cooled

LP 2.3625

H2O 1.8900

Frasch mines/ wells

Claus recovery from HC's

1.1891

sulfur 1.1891

air 7.6792

BFW 5.7683

H2O 0.7208

0.5754

sulfuric acid plant

3.6781 H2SO4

5.9098 vent

1.9110 LP steam

0.4154 blowdown

2.8665

0.0012 others

HP steam

IP

power gene-ration

fuel 0.0501

BFW 1.2016

3.8135 LP

0.8301 H2O

0.1373 CO2

1,779 elctricity TJ

air

air 0.7200

natural gas 0.2744

steam 0.5225

ammonia plant

NH3 0.6581

CO2 0.7529

H2O 0.0938

purge 0.0121

other use 3.2735

0.7518 vent

0.9337 air

0.0493 NH3

nitric acid plant

HNO3 0.3306

0.0995 H2O

0.0536

NH3

0.3306

Ammonium Nitrate plant

NH3 0.0483

0.2184

NH4NO3 0.0279

H2O 0.0331

AN [NH4NO3]

UAN plant

urea 0.0326

UAN 0.0605

CO2 0.0567

0.0732

LP steam 0.0374

urea plant

urea 0.0256

urea 0.0742

H2O 0.0299

cw 0.0374

NH3 0.0001

CO2 0.0001

urea [CO(NH2)2] 0.0416

rock

vapor

0.1695

0.3013

0.5027

inert 0.1238

Granular Triple Super Phosphate

0.7487 GTSP [0-46-0]

0.0097 HF

P2O5

H3PO4 selling 0.0265

H2O 0.7137

P2O5 2.1168

NH3 0.4502

0.0256

inert 0.2917

for DAP %N control

urea

Mono- & Di- Ammonium Phosphates granulation

MAP [11-52-0] 0.2931

DAP [18-46-0] 1.8775

CO2 0.0045

0.0044

acetic acid

acetic acid 0.0082

H2O 0.0012

0.6124 vent

CO2 0.0629

steam 0.0511

0.0682

methanol plant

vent 0.0008

CH3OH 0.1814

0.1771

CH4 0.0005

benzene 0.5833

ethylene 0.2278

benzene 0.0507

ethyl-benzene

ethylbenzene 0.8618

0.0000

ethylbenzene 0.8618

styrene

0.7533 styrene

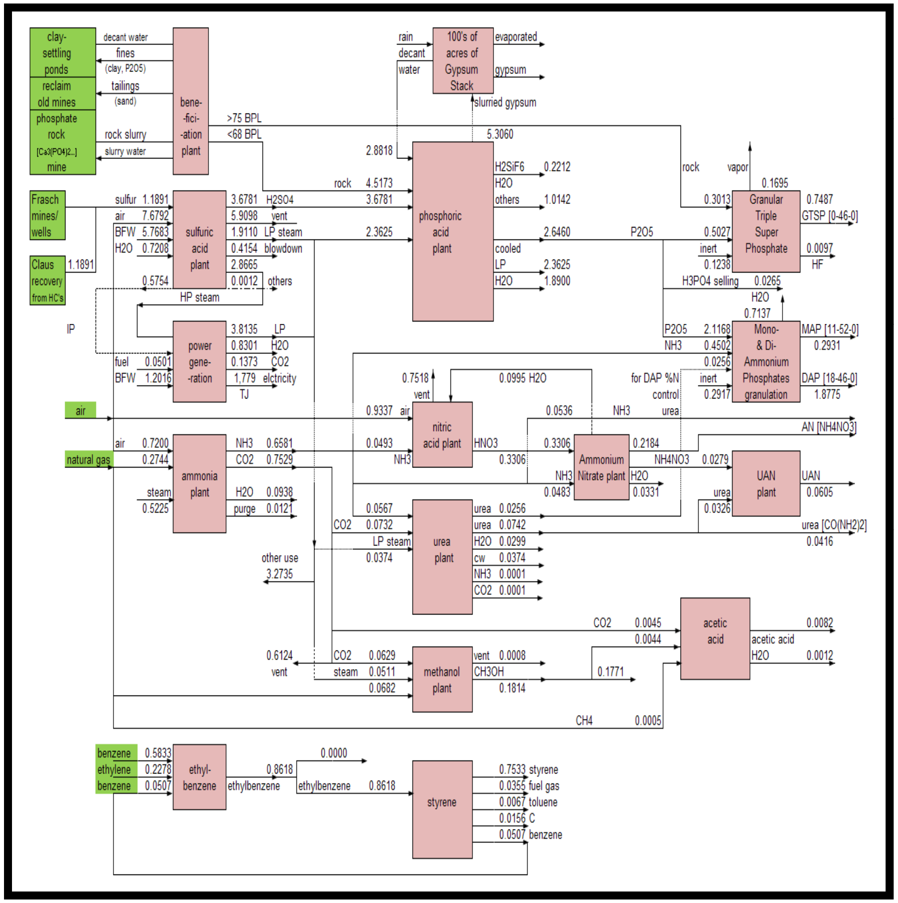
0.0355 fuel gas

0.0067 toluene

0.0156 C

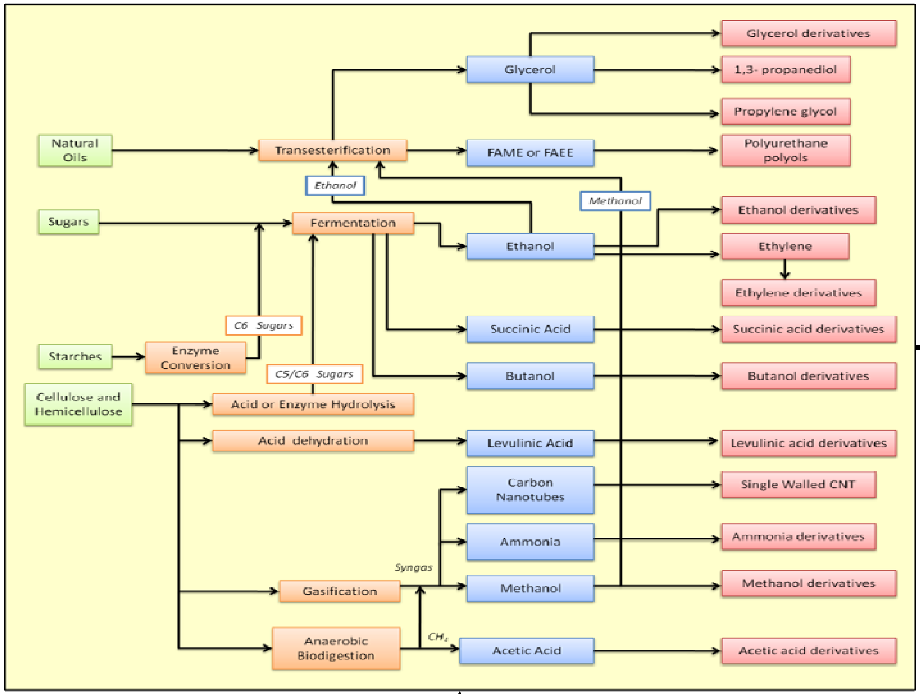
0.0507 benzene

Plants in the Base Case



- Ammonia
- Nitric acid
- Ammonium nitrate
- Urea
- UAN
- Methanol
- Granular triple super phosphate
- MAP & DAP
- Contact process for Sulfuric acid
- Wet process for Phosphoric acid
- Acetic acid
- Ethylbenzene
- Styrene

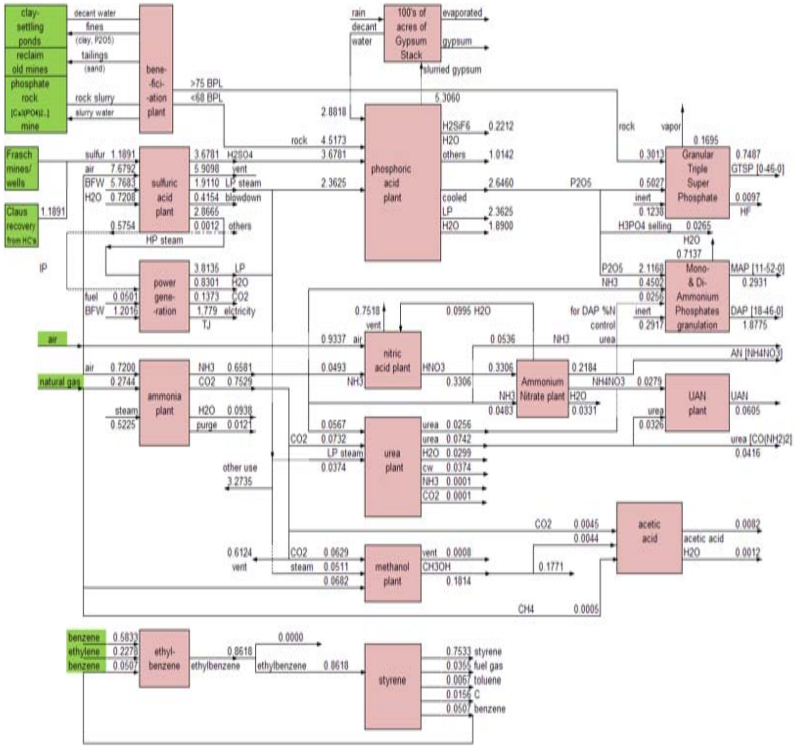
Integrated Chemical Production Complex



Biomass Complex

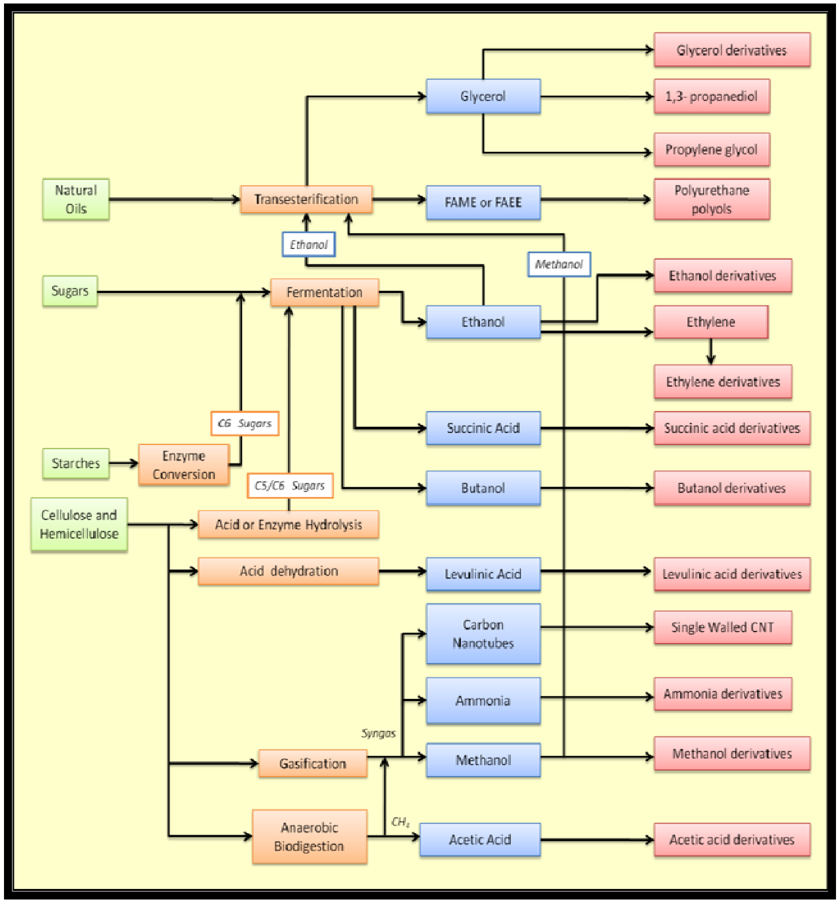
Utilities, CO_2

Methanol, DAP, Acids

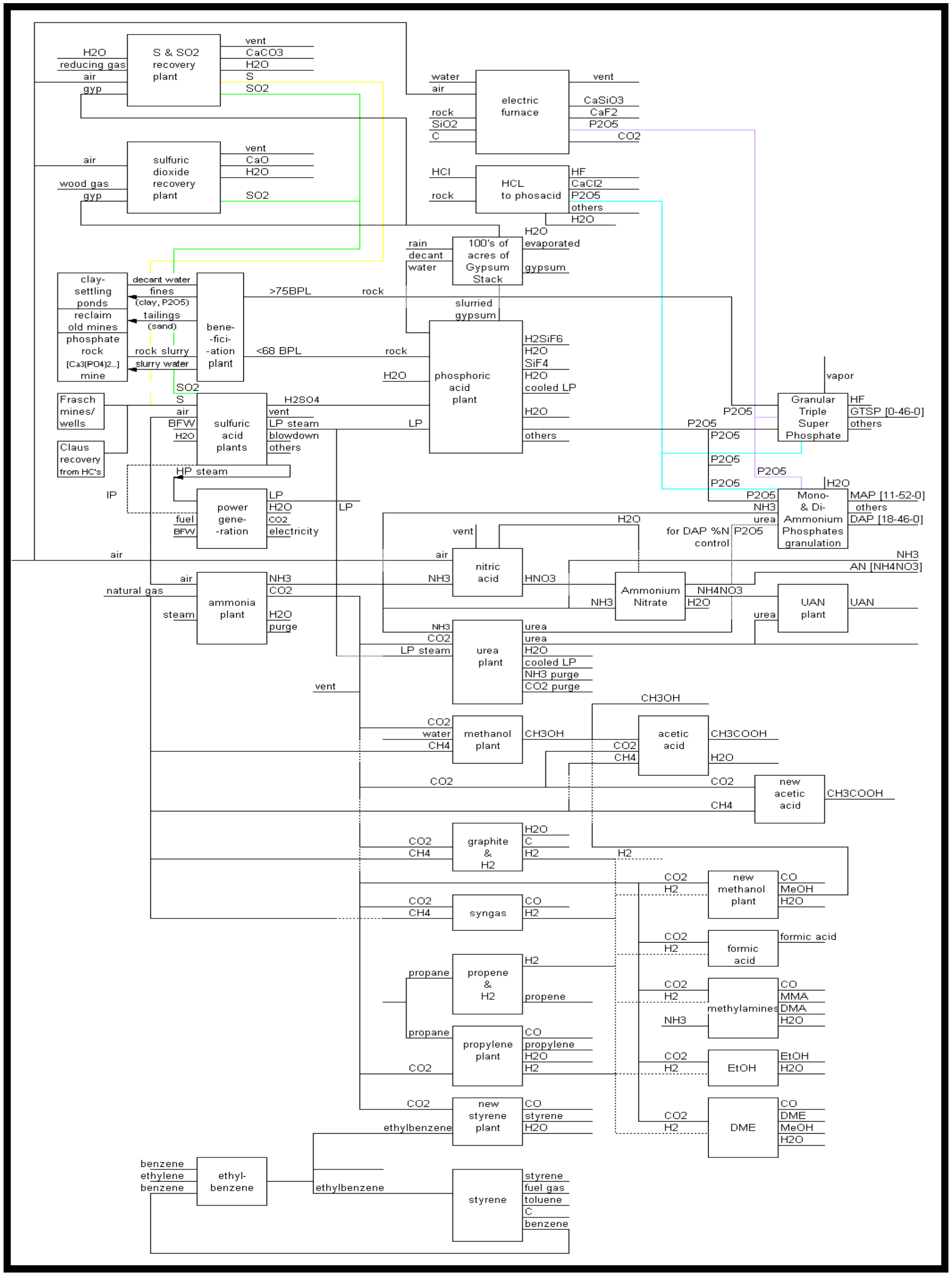


Base Case Complex

New Processes Utilizing Biomass Feedstock



- Fermentation to Ethanol,CO_2
- Ethanol to Ethylene process
- Transesterification to FAME, Glycerol
- Glycerol to Propylene Glycol process
- Anaerobic Digestion to Acetic Acid, H_2, CO_2
- Gasification to Syngas



Superstructure with New Processes Utilizing CO2 Integrated into Base Case

- Electric furnace process for phosphoric acid
- HCl process for phosphoric acid
- SO_2 recovery from gypsum
- S & SO_2 recovery from gypsum
- Acetic acid from CO_2 & CH_4
- Graphite & H_2
- Syngas from CO_2 & CH_4
- Propane dehydrogenation
- Propylene from propane & CO_2
- Styrene from ethylbenzene & CO_2
- Methanol from CO_2 & H_2
- Formic acid
- Methylamines
- Ethanol
- Dimethylether

Past work done by our group where CO2 is utilized to make chemicals and integrated into base case

Processes in the Optimal Structure

Plants in the Base Case

- Ammonia
- Nitric acid
- Ammonium nitrate
- Urea
- UAN
- Methanol
- Granular triple super phosphate
- MAP & DAP
- Contact process for Sulfuric acid
- Wet process for phosphoric acid
- Ethylbenzene
- Styrene

Not in the Base Case

- Acetic acid

New Plants in the Optimal Structure

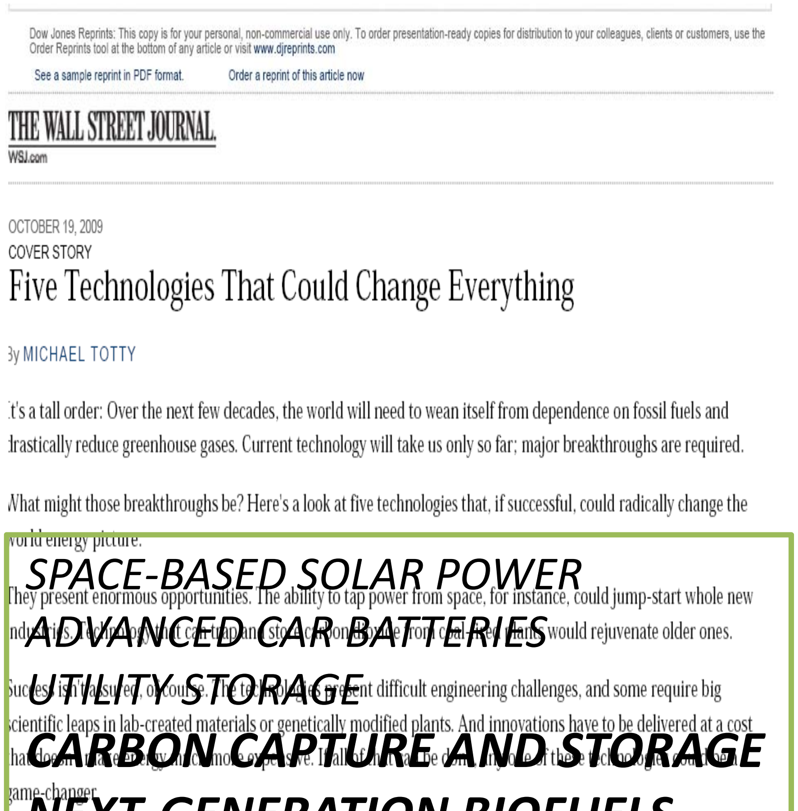
- Acetic acid from CO_2 & CH_4
- Graphite & H_2
- Syngas from CO_2 & CH_4
- Formic acid
- Methylamines

Plants Not in the Optimal Structure

- Electric furnace process for phosphoric acid
- HCl process for phosphoric acid
- SO_2 recovery from gypsum
- S & SO_2 recovery from gypsum
- Propane dehydrogenation
- Propylene from propane & CO_2
- Styrene from ethylbenzene & CO_2
- Methanol from CO_2 & H_2
- Ethanol
- Dimethylether

Algae - New Feedstock Option that use CO2

- Algae
  - Consumes CO_2 in a continuous process using exhaust from power plant (40% CO_2 and 86 % NO)
  - Can be separated into oil and carbohydrates
  - Upto 5,000 gallons/acre of yield of alcohol produced compared to 350 gallons/acre corn based ethanol[1]
  - Upto 15,000 gallons/acre of algae oil produced compared to 60 gallons/acre for soybean oil[2]
  - Water used can be recycled and waste water can be used as compared to oilseed crops' high water demand
  - High growth rates, can be harvested daily



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OCTOBER 19, 2009
COVER STORY

Five Technologies That Could Change Everything

By MICHAEL TOTTY

t's a tall order: Over the next few decades, the world will need to wean itself from dependence on fossil fuels and rastically reduce greenhouse gases. Current technology will take us only so far; major breakthroughs are required.

Vhat might those breakthroughs be? Here's a look at five technologies that, if successful, could radically change the vorld energy picture.

They present enormous opportunities. The ability to tap power from space, for instance, could jump-start whole new ndustries. Technology that can trap and store carbon dioxide from coal-fired plants would rejuvenate older ones.

uccess isn't assured, of course. The technologies present difficult engineering challenges, and some require big cientific leaps in lab-created materials or genetically modified plants. And innovations have to be delivered at a cost hat doesn't make energy much more expensive. If all of that can be done, any one of these technologies could be a ame-changer.

SPACE-BASED SOLAR POWER
ADVANCED CAR BATTERIES
UTILITY STORAGE
CARBON CAPTURE AND STORAGE
NEXT-GENERATION BIOFUELS

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1 Wall Street Journal Oct 19, 2009
2 National Geographic, October 2007

Algae Feedstock

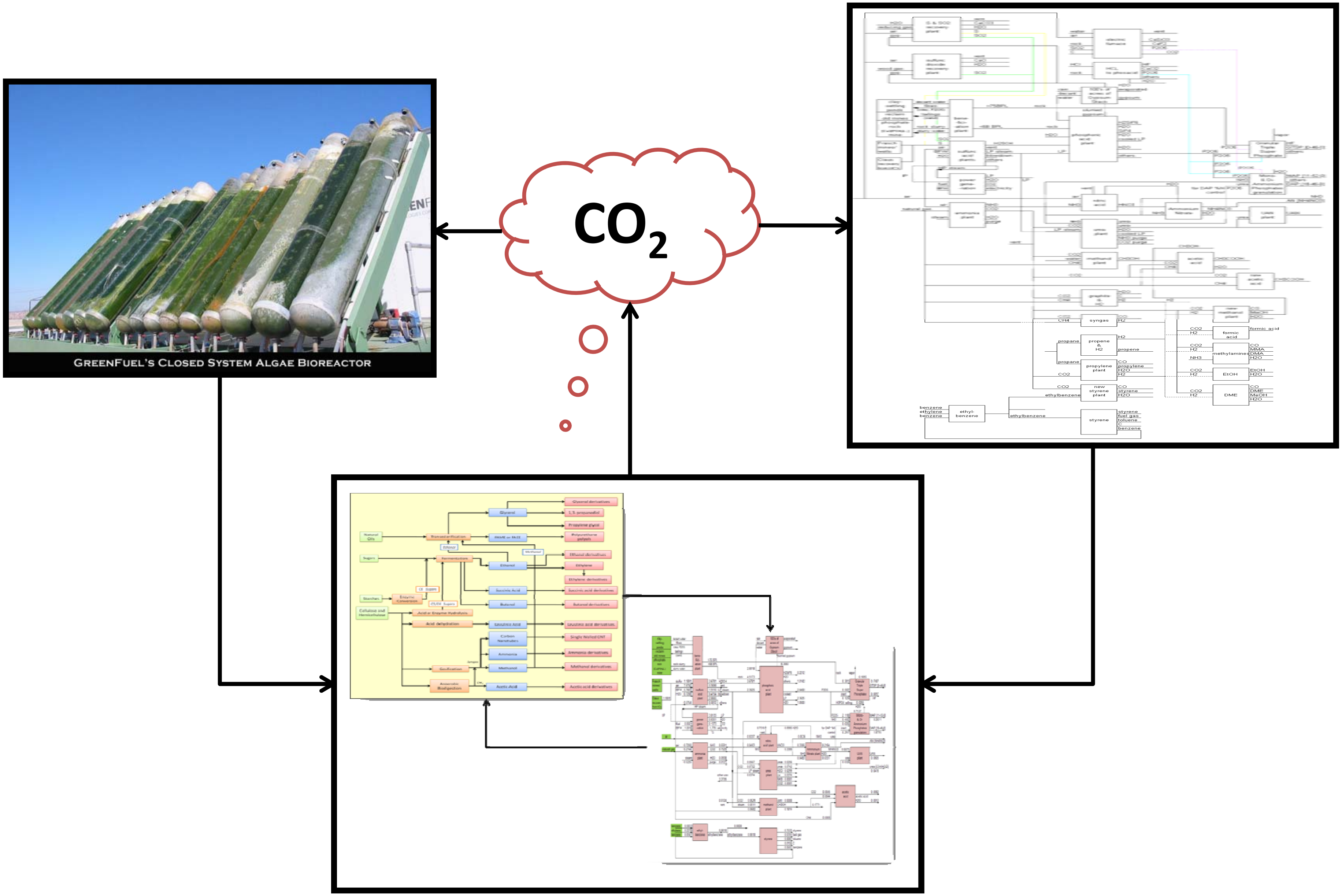
— **ExxonMobil Announcement** - it will invest more than $600 million in algae-based biofuels in association with Synthetic Genomics Inc. [1]

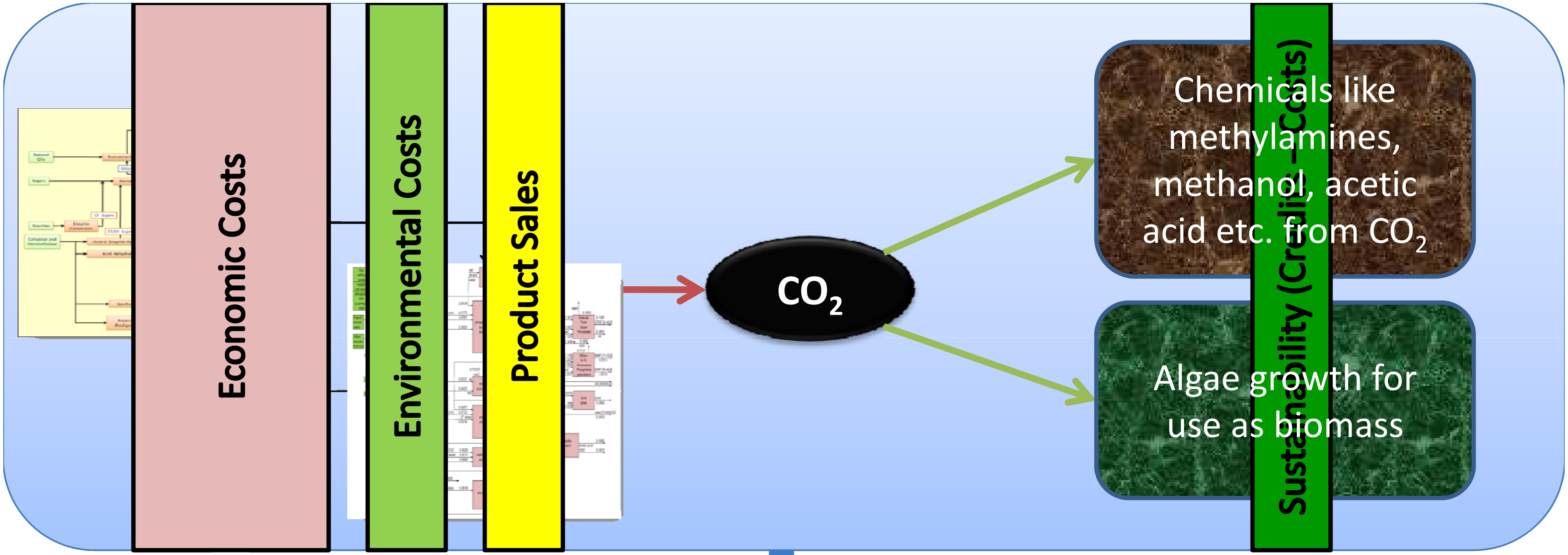
— **Dow Announcement –** Algenol and Dow Chemical Company announced a pilot scale Algae-based process to convert CO_2 to ethanol[2]

Algenol Biofuels Inc. algae to ethanol test facility in Florida

1 Biodiesel Magazine, July 2009
2 and Photo: Ethanol Producer Magazine September 2009

Integrated Chemical Production Complex





Economic Costs

Environmental Costs

Product Sales

CO_2

Chemicals like methylamines, methanol, acetic acid etc. from CO_2

Algae growth for use as biomass

Sustainability (Credits – Costs)

Multicriteria Optimization Problem

Maximize: $\mathbf{w_1P+w_2S}$

$$\mathbf{P = \Sigma\ \text{Product Sales} - \Sigma\ \text{Economic Costs} - \Sigma\ \text{Environmental Costs}}$$

$$\mathbf{S = \Sigma\ \text{Sustainability (Credits – Costs)}}$$

$$\mathbf{w_1 + w_2 = 1}$$

Subject to:

Multiplant material and energy balance
Product demand
Raw material availability
Plant capacities

Costs in the Triple Bottom line

- **Economic Costs**
  - Icarus Process Evaluator results for capital costs
  - Icarus Process Evaluator results for operating costs, including raw material costs and utilities
- **Environmental costs**
  - AIChE/TCA report [1] lists environmental costs as approximately 20% of total manufacturing cost and raw material as 30% of manufacturing costs (data provided by Amoco, DuPont and Novartis).
  - Environmental cost estimated as 67% of raw material cost.
- **Sustainable costs**
  - Sustainable costs were estimated from results given for power generation in AIChE/TCA report [1].
  - Alternate methods to estimate sustainable costs are being evaluated.

Component	**Sustainable Cost ($/m.t.)**
Carbon Dioxide	3.25
NO_x	1,030
SO_x	192

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[1] *Constable, D. et al., "Total Cost Assessment Methodology; Internal Managerial Decision Making Tool", AIChE, ISBN 0-8169-0807-9, July ,1999.*

Raw Material and Product Prices (Base Case)

Raw Materials Cost ($/mt)
Natural Gas 172
Phosphate Rock
wet process
24
HCl process
27
GTSP process 30
electrofurnace
HCl
25
Sulfur
Frasch 42
Claus
C electrofurnace 760
Ethylene 446
38
Benzene 257
Propane 163
50

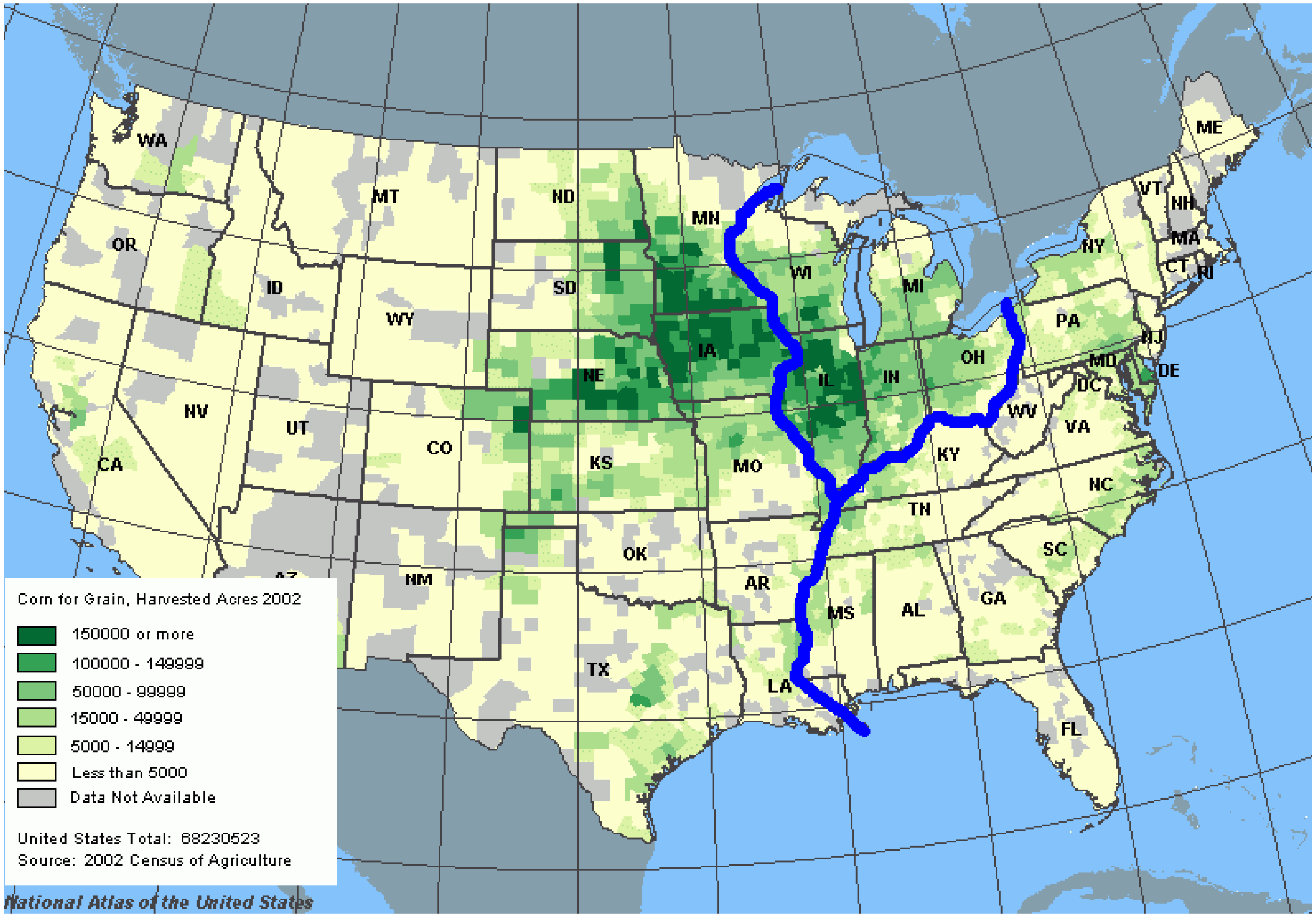
Raw Materials Cost ($/mt)
Market cost for short term purchase
Reducing gas
Wood gas
Sustainable Costs and Credits
1394
Credit for CO_2 6.50
Consumption
Debit for CO_2
Production
634
Methanol
Credit for HP Steam 10
3.25
Credit for IP Steam 6.4
Credit for gypsum 5
Consumption
Debit for gypsum 2.5
NH
Debit for NO_x 1025
Production
Debit for SO_2 150
Propene
Styrene

Products Price ($/mt)
Ammonia 150
300
Acetic Acid 1034
GTSP 142
MAP 180
DAP 165
$_4NO_3$ 153
UAN 112
Urea 154
H_3PO_4
Ethanol 670
Ethylbenzene 551
320
240
CO 31
Graphite 882
H_2 796
705
Toluene 238
Fuel Gas 596
Formic Acid 690
1606
1606
DME 946

Production

Productio

Transportation to Gulf Coast

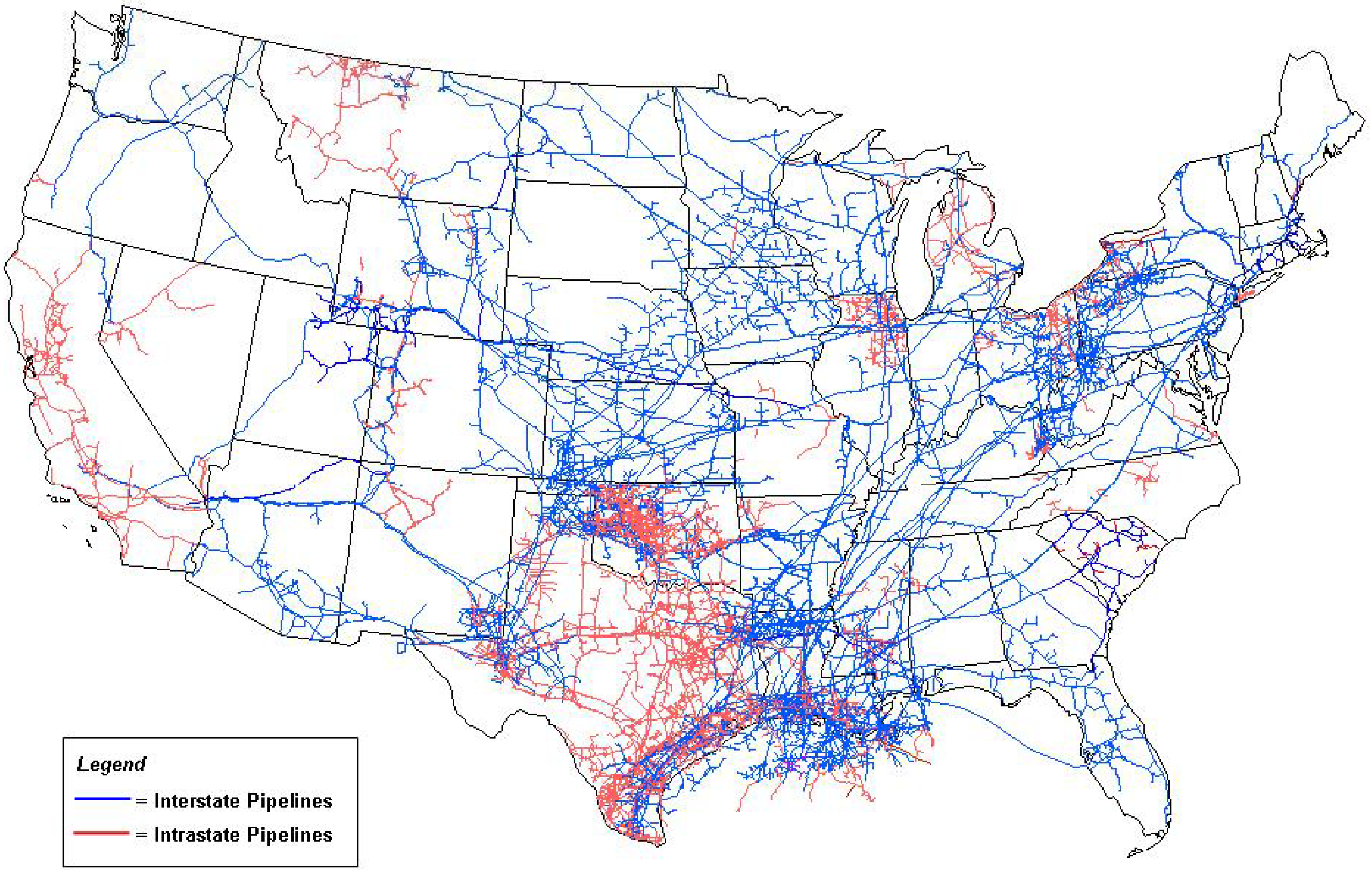


Waterways from the midwestern states can provide excellent transport for biomass feedstock to the Gulf Coast.

Industries in the Lower Mississippi River Corridor can receive the feedstock and convert to chemicals.

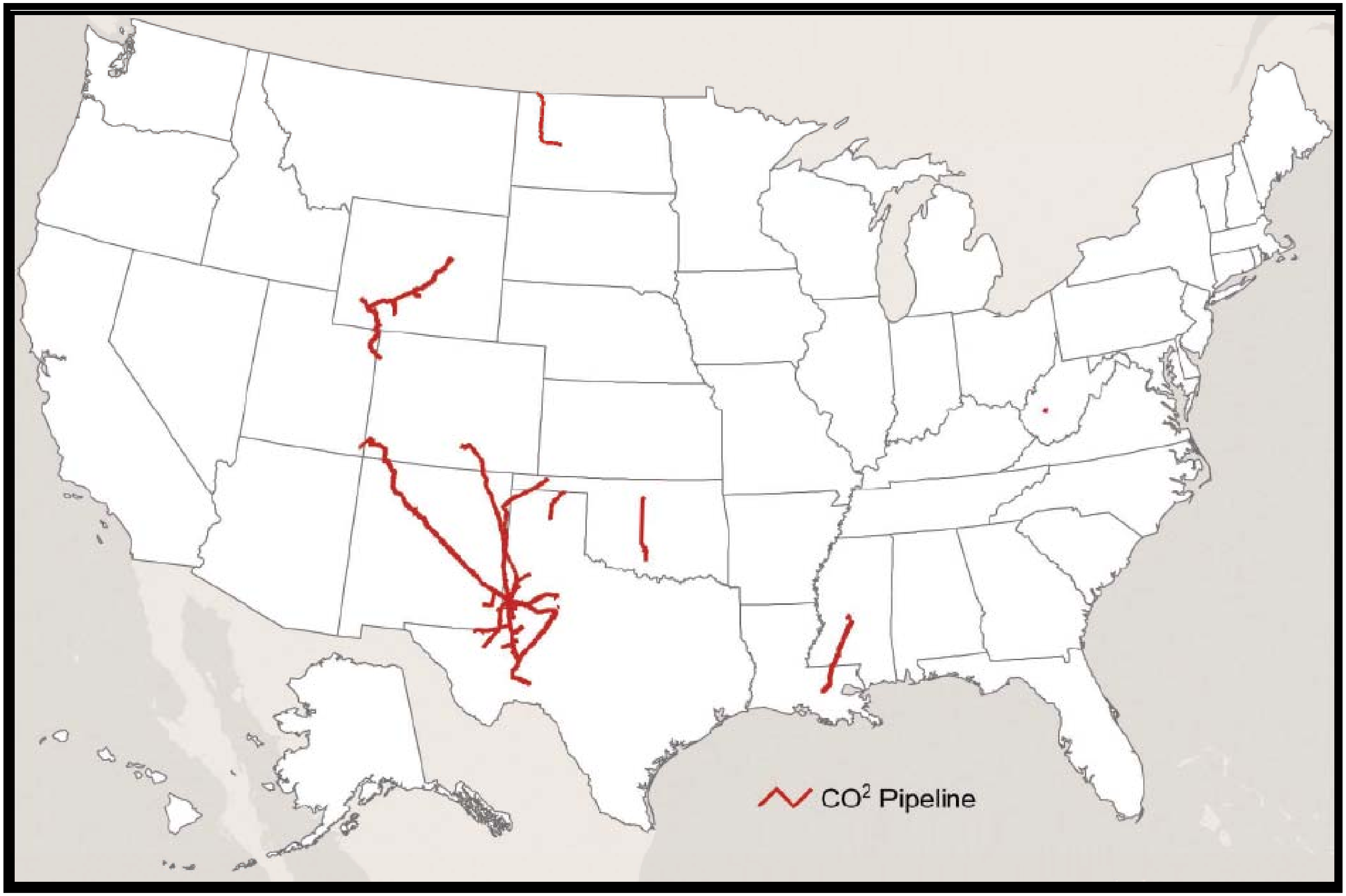
Map created from http://nationalatlas.gov/

Natural Gas Pipelines in the United States



Source: Energy Information Administration, Office of Oil & Gas, Natural Gas Division, Gas Transportation Information System

Major CO2 Pipelines in the United States



Source: http://ncseonline.org/nle/crsreports/07may/rl33971.pdf

Summary

Extend the Chemical Production Complex in the Lower Mississippi River Corridor to include:

- Biomass based chemical production complex
- CO_2 utilization from the complex

Obtained the relations for the above chemical plants:

- Availability of raw materials
- Demand for product
- Plant capacities
- Material and energy balance equations

Assigned Triple Bottomline costs:

- Economic costs
- Environmental costs
- Sustainable credits and costs

Summary

- Solve Multicriteria Optimization Problem with constraints
- Use Mixed Integer Non Linear Programming Global Optimization Solvers to obtain Pareto optimal solutions of the problem below.

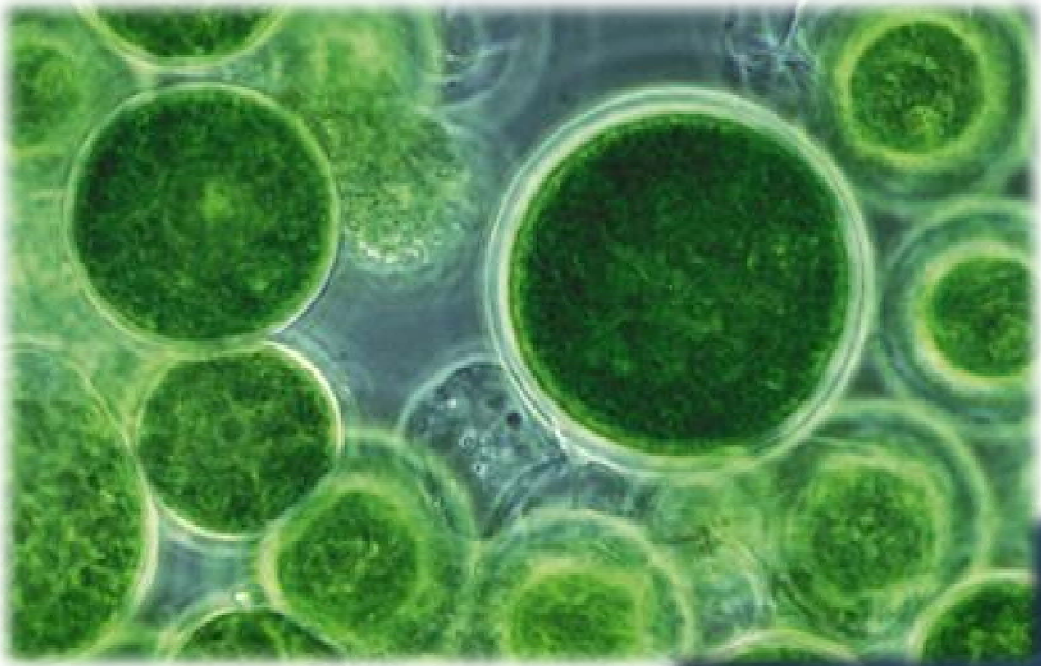
Optimise: w_1P+w_2S

$P = \Sigma$Product Sales – ΣEconomic Costs – ΣEnvironmental Costs

$S = \Sigma$Sustainability (Credits – Costs)

$w_1 + w_2 = 1$

- Use Monte Carlo Analysis to determine sensitivity of the optimal solution.
- Follow the procedure to include plants in the Gulf Coast Region (Texas, Louisiana, Mississippi, Alabama)
- Methodology can be applied to other chemical complexes of the world.



Questions

Comments

Research White Paper and Presentation available at www.mpri.lsu.edu

TCA Cost Explanations

Cost Type	Description	Examples
I. Direct costs	Manufacturing site costs	Capital investment, operating, labor, materials, and waste disposal costs
II. Indirect costs	Corporate and manufacturing overhead	Reporting costs, regulatory costs, and monitoring costs
III. Future and contingent liability costs	Potential fines, penalties and future liabilities	Clean-up, personal injury, and property damage lawsuits; industrial accident costs.
IV. Intangible internal costs (Company-paid)	Difficult-to-measure but real costs borne by the company	Cost to maintain customer loyalty, worker morale, union relations, and community relations.
V. External costs (Not currently paid by the company)	Costs borne by society	Effect of operations on housing costs, degradation of habitat, effect of pollution on human health

Biomass Components

Biomass

Starch

Cellulose

Hemicellulose

Lignin

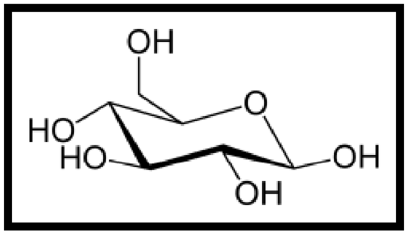
Oils

α links

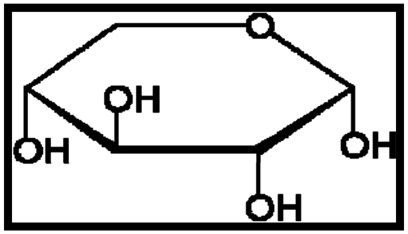
β links

C6 polysaccharides

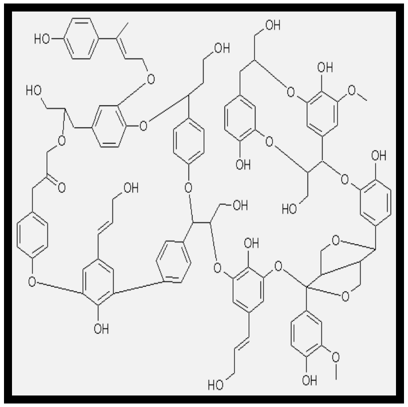
C5 polysaccharides



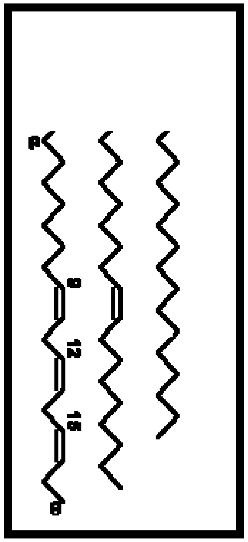
Hexose



Pentose



Complex polymer containing phenolic compounds

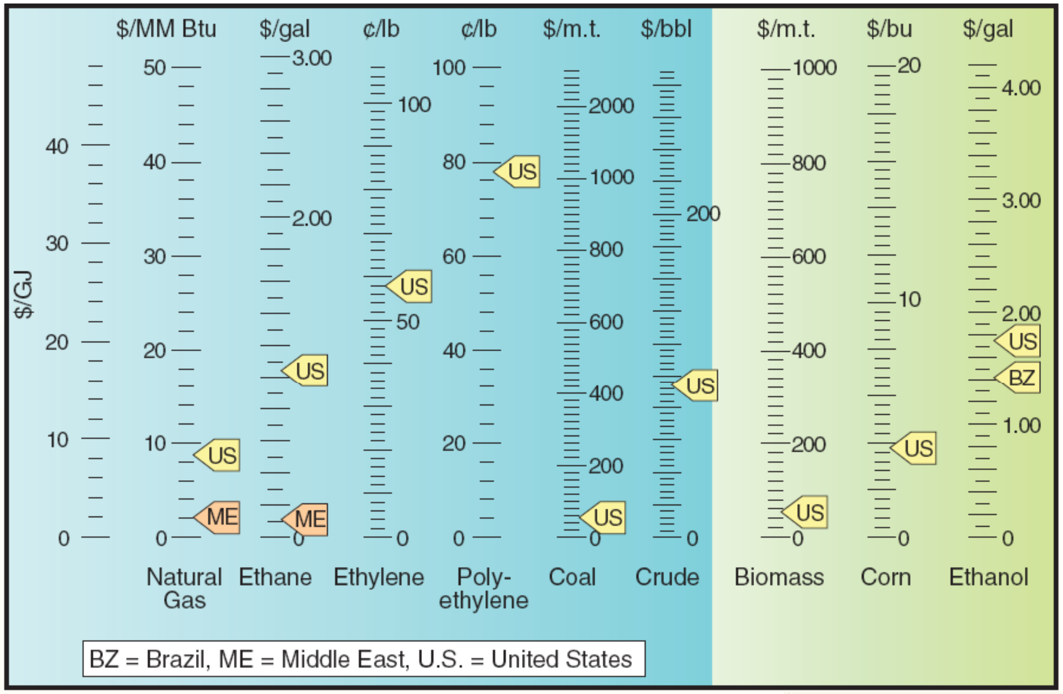


Triglycerides

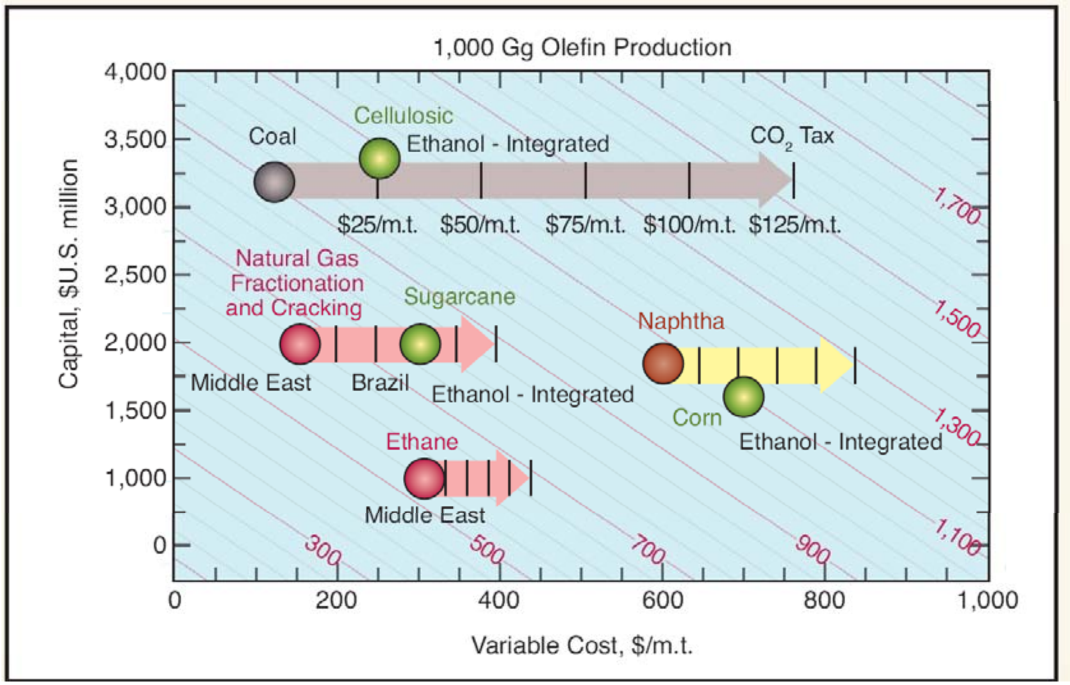
Algae Species

- The following species listed are currently being studied for their suitability as a mass-oil producing crop, across various locations worldwide
- *Botryococcus braunii*
- *Chlorella*
- *Dunaliella tertiolecta*
- *Gracilaria*
- *Pleurochrysis carterae* (also called CCMP647)[39] .
- *Sargassum*, with 10 times the output volume of *Gracilaria*.[40]

Costs in the Triple Bottom line



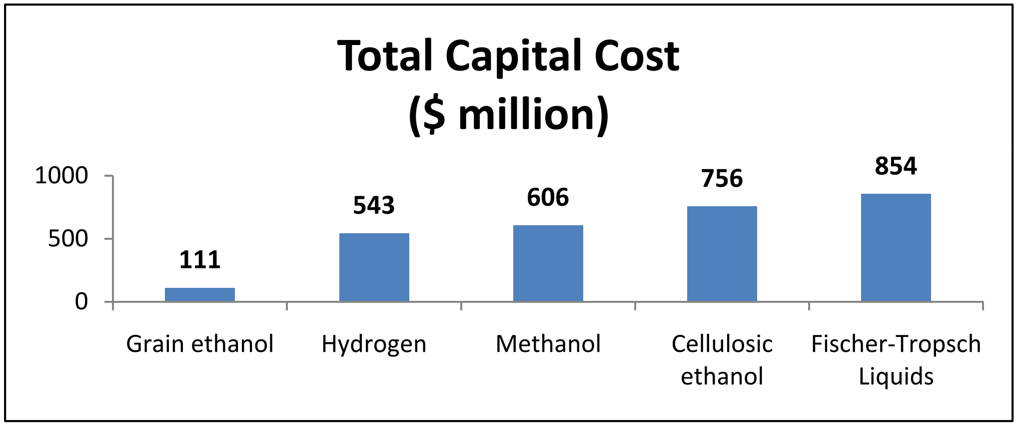
Relative Price per unit energy of various feedstocks and products, quoted in their traditional units and calibrated to $/GJ

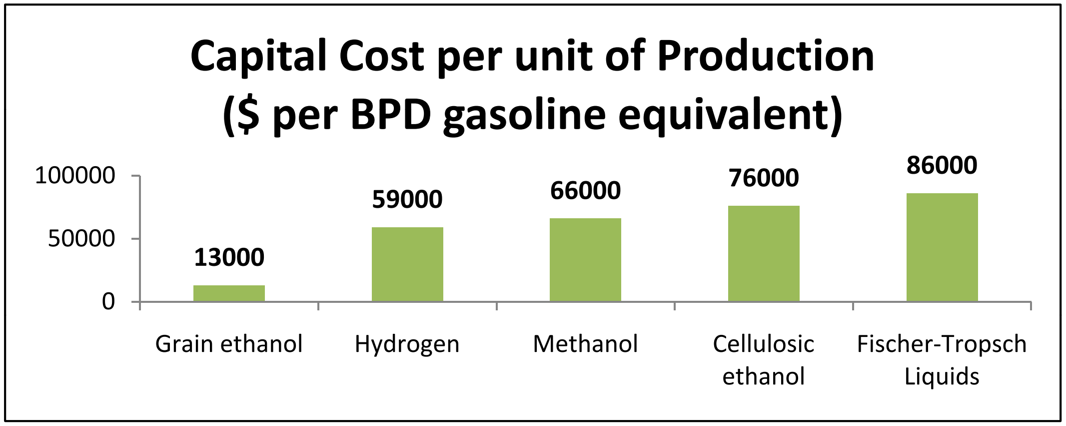


Contour plot of production cost plus return on investment as a function of capital and variable costs (based on 1000Gg/year of olefin production)

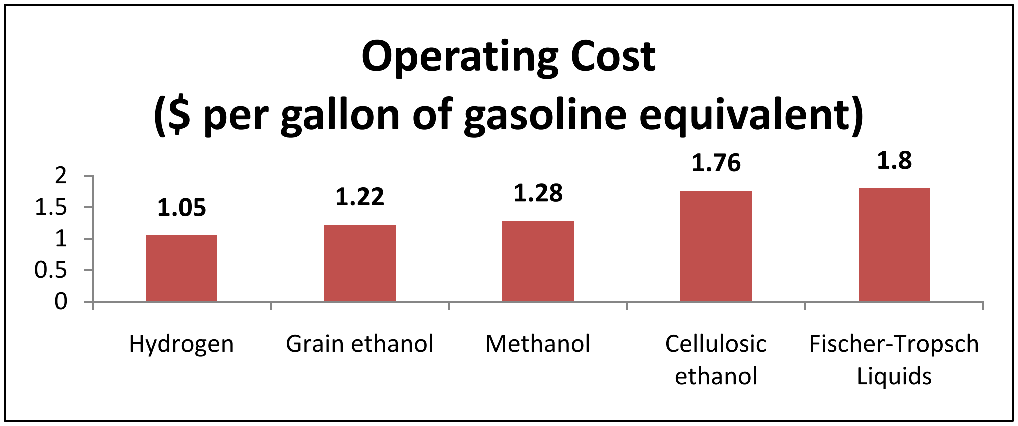
CEP, March 2008, Pg S7-S14

Costs in the Triple Bottom line





Capital and operating costs for 150 million gallons per year (MMGPY) of gasoline equivalent plants, 2005 dollars



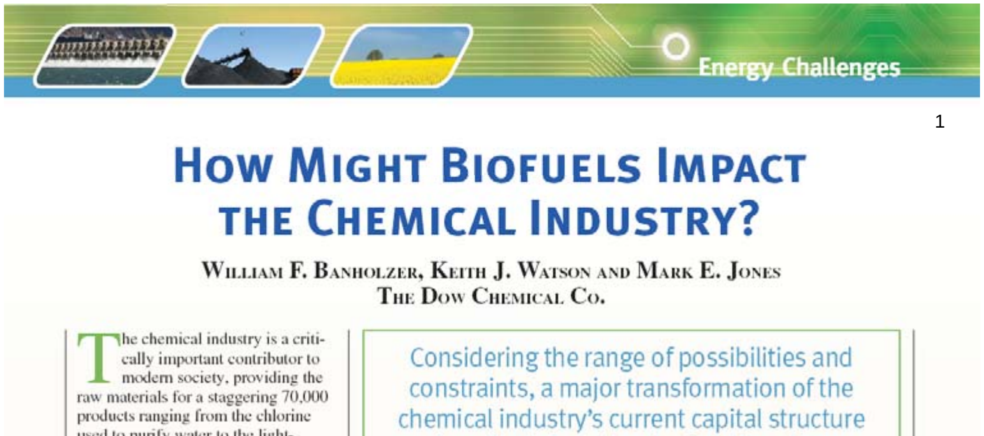
Biofpr, 1:49-56 (2007)

Industry Perspective

Ethylene and Propylene are basic building blocks for polymers and chemical intermediates

Approximately 1% of global energy market and 3% of global oil and gas market is used as chemical feedstock

½ of the energy and ¾ mass of the chemical feedstock is retained in the end product



1

How Might Biofuels Impact the Chemical Industry?

William F. Banholzer, Keith J. Watson and Mark E. Jones
The Dow Chemical Co.

The chemical industry is a critically important contributor to modern society, providing the raw materials for a staggering 70,000 products ranging from the chlorine

Considering the range of possibilities and constraints, a major transformation of the chemical industry's current capital structure
cades.

aints — a dramatic
he chemical industry
tional feedstocks to-
highly unlikely to be
next few decades.

fuels
propylene serve as
g blocks from which
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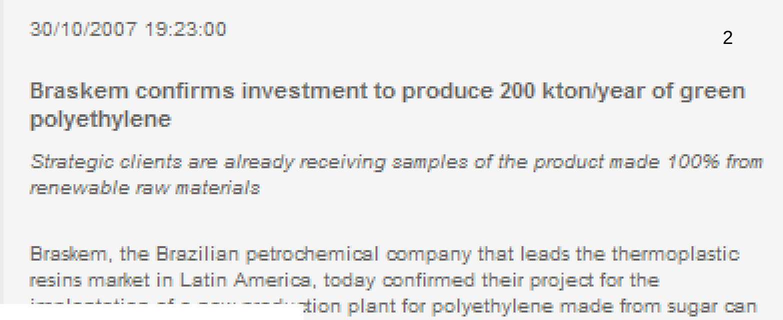

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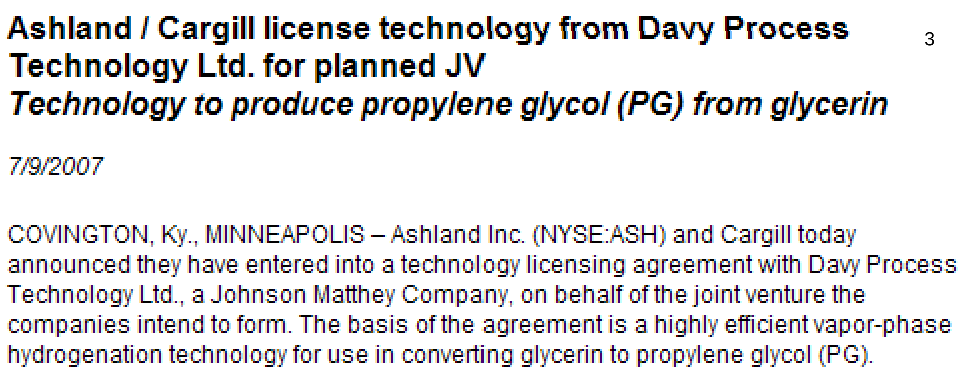
2

Braskem confirms investment to produce 200 kton/year of green polyethylene

Strategic clients are already receiving samples of the product made 100% from renewable raw materials

Braskem, the Brazilian petrochemical company that leads the thermoplastic resins market in Latin America, today confirmed their project for the
tion plant for polyethylene made from sugar can
ons at the end of 2009 and with a capacity of 200
e news was officially relayed by José Carlos
who is in Germany to take part in the K 2007
largest international event for the petrochemical



Ashland / Cargill license technology from Davy Process Technology Ltd. for planned JV
Technology to produce propylene glycol (PG) from glycerin

3

7/9/2007

COVINGTON, Ky., MINNEAPOLIS – Ashland Inc. (NYSE:ASH) and Cargill today announced they have entered into a technology licensing agreement with Davy Process Technology Ltd., a Johnson Matthey Company, on behalf of the joint venture the companies intend to form. The basis of the agreement is a highly efficient vapor-phase hydrogenation technology for use in converting glycerin to propylene glycol (PG).

1 CEP, March 2008, Pg S7-S14
2 http://www.braskem.com.br/site/portal_braskem/en/sala_de_imprensa/sala_de_imprensa_detalhes_6970.aspx
3 http://www.ashland.com/press_room/news_detail.asp?s=1543