Making and Estimating Quantitative Comparisons

Fuel Options

Lots of money into alternative fuels

- Coal based liquid fuels
- Direct coal gasification
- Oil shale and other low-grade petroleum resources

In some ways these fuels illustrate the superior qualities of conventional fuels!

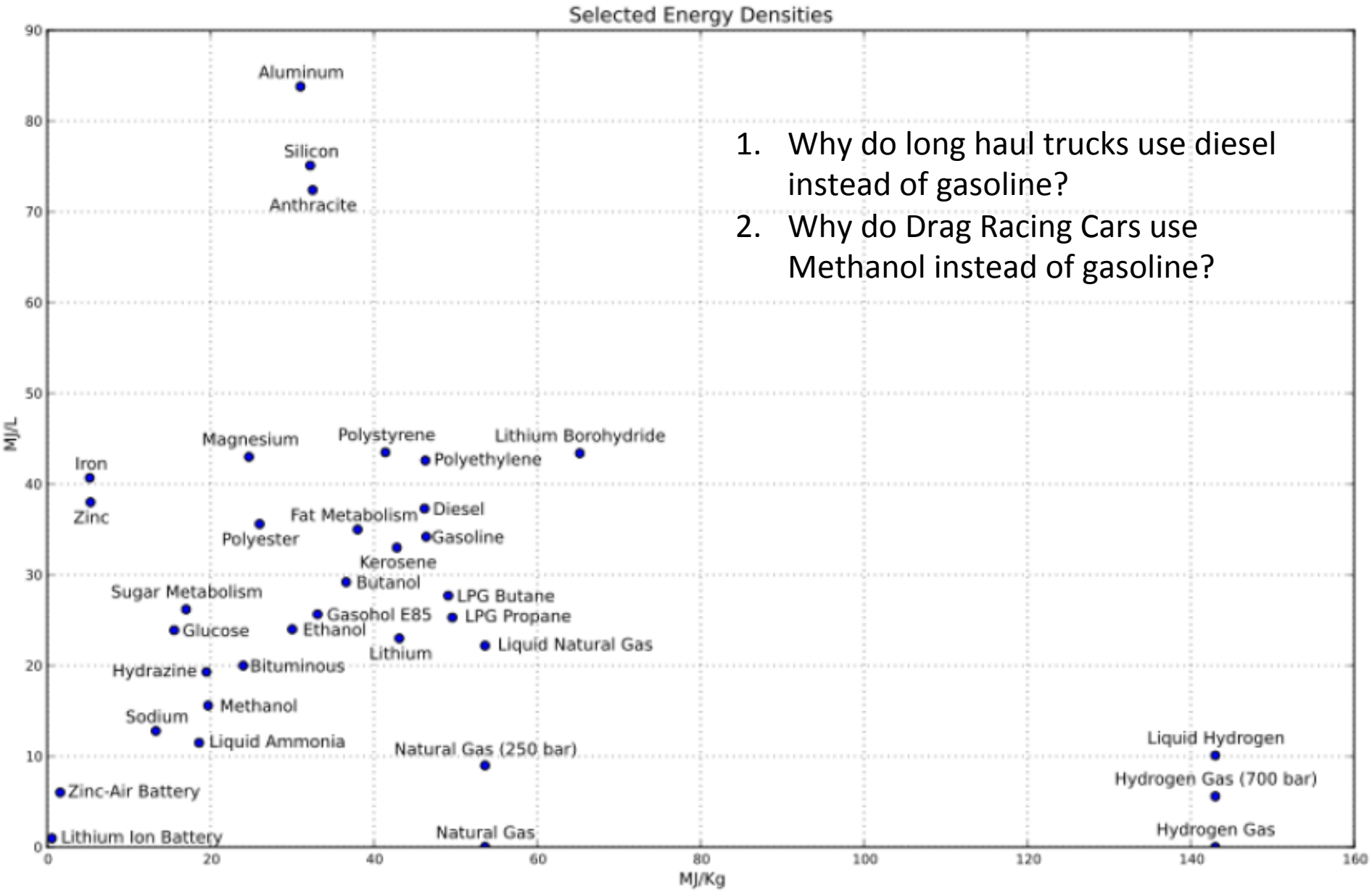
- Transport and movement by pump and tank
- Gas or fluid at ambient temperature and pressure
- High *energy density per-unit-mass* and *per-unit-volume*
- Comparing energy density per unit mass:
  - 110 lb Wood = **750** MJ
  - 110 lb Coal = **1465** MJ
  - 110 lb Oil = **2400** MJ
  - CH_4 = **37 – 40** MJ/m^3 ($2 – 5 mmBTU)

Energy Form	*Example Equivalent to 1,000 Joules*
Kinetic energy	A 150-lb person riding a bicycle at 12 miles per hour relative to a stationary object. Kinetic energy (KE) is a function of mass (m) and velocity (v), or $KE = \frac{1}{2}mv^2$.
Potential energy	The energy inherent in a 100 kilogram mass elevated 1 meter above the earth's surface due to the pull of gravity.
Chemical energy	The energy in 1/20 of a gram of sugar.
Light energy	The energy deposited by bright sunlight into your skin over a few seconds.
Sound energy	The energy emitted by powerful concert-style speakers at full blast in 15 minutes. (Notice that there is generally much less energy in everyday sound than in light.)
Nuclear energy	The energy that can be obtained from 1.2×10^{-8} grams of uranium.
Thermal energy	The energy required to make a teaspoon of hot tea.

Common energy units

http://www.onlineconversion.com/energy.htm

Energy conversion			
Unit	**Quantity**	**to**	**Note**
1 calorie =	4.1868000	Joule	
1 kiloWatt hour = kWh =	3600000	Joule	A power of 1 kW for a duration of 1 hour.
1 British Thermal Unit = btu	1055.06	Joule	It is a is a unit of energy used in North America.
1 ton oil equivalent = 1 toe	4.19E+010	Joule	It is the rounded-off amount of energy that would be produced by burning one metric ton of crude oil.
1 ton coal equivalent	2.93E+10	Joule	
1 ton oil equivalent = 1 toe	1 / 7.33	Barrel of oil	or 1 / 7.1 or 1 / 7.4 ...
1 cubic meter of natural gas	3.70E+07	Joule	or roughly 1000 btu/ft3
1000 Watts for one year	3.16E+010	Joule	for the 2000 Watt society
1000 Watts for one year	8.77E+006	kWh	for the 2000 Watt society
1 horsepower	7.46E+002	Watts	



1. Why do long haul trucks use diesel instead of gasoline?
2. Why do Drag Racing Cars use Methanol instead of gasoline?

Calculate Chemical Energy

Thermochemistry: Heat of Combustion (Ideal burning)

1. $\Delta H = H_{prod} - H_{react}$

Write a balanced reaction, find heats of formation, and calculate. (Note: This is assuming 25 ^{o}C, 1 atm and complete combustions)

For Methane:

	CH_4	+	$2\ O_2$	$\rightarrow$	CO_2	+	$2\ H_2O$
H_f (kJ/mol)	-75		0		-394		-242

$$\Delta H = -394 + 2(-242) - (-75) = -803 \text{ kJ/mol}$$

Or

Measure the Heat of Combustion using Calorimetry (It takes 4.18 J of energy to raise 1 g of water 1 ^{o}C.)

Fuel	HHV MJ/kg	HHV kJ/mol	LHV MJ/kg
Hydrogen	141.80	286	119.96
Methane	55.50	889	50.00
Methanol	22.7	726	
Ethanol	29.7	1,300	
Butane	49.5	2,877	45.75
Isobutanol	32.96	2,443	
Gasoline	47.3		44.4
Natural Gas	54.0		
Diesel	44.80		43.4
Carbon	32.8	393.5	
Coal (Anthracite)	32.50		
Coal (Lignite)	15.00		
Wood	21.7		
Peat (damp)	6.00		
Peat (dry)	15.00		

HHV (assumes water is a liquid)

LHV (assumes water stays in the gas phase)

Estimate how much energy will it take to dry 100 Kg of biomass that contains 20% water by weight, to 0.5% starting from room temperature.

Biomass source	Moisture Content (calculated on wet basis)
Wood chips	10-60 %
Straw	20-30 %
Cotton stalks	10-20 %
Switchgrass	30-70 %
Bagasse	40-60 %
Cow manure	88-94 %
Pig manure	90-97 %
Maize silage	65-75 %

http://www.biomassenergy.gr/en/articles/technology/biomass/251-significant-biomass-properties-part-1-moisture-content

Stoichiometry and CO_2 Imapacts

Source: *Life Magazine*, 1962

CO_2 Emmissions grams of CO_2 per KWHr electricity generation (World Ave. IEA)

Oil	796 g/KWHr
Coal	958 g/KWHr
Natural Gas	451 g/KWHr

http://www.iea.org/publications/freepublications/publication/name,4010,en.html

Using the data from combustion as well as balanced reactions compare the theoretical CO_2 emissions form: Methane (CH_4) and Ethanol (C_2H_6O), on a mass basis (Kg CO_2/Kg fuel) and then an energy basis (g CO_2/1000KJ).

Carbon	12.011 g/mol
Hydrogen	1.008 g/mol
Oxygen	15.999 g/mol

Air Pollutant Impacts

2 million people died in 2010 from disease related to high cholesterol.

3.2 million people died in 2012 form disease related to air pollution.

Blue Flame vs. Yellow and Red

What emissions come from each of these flames?

Gen. Gavin Power Plant – Original 1974 Schematic

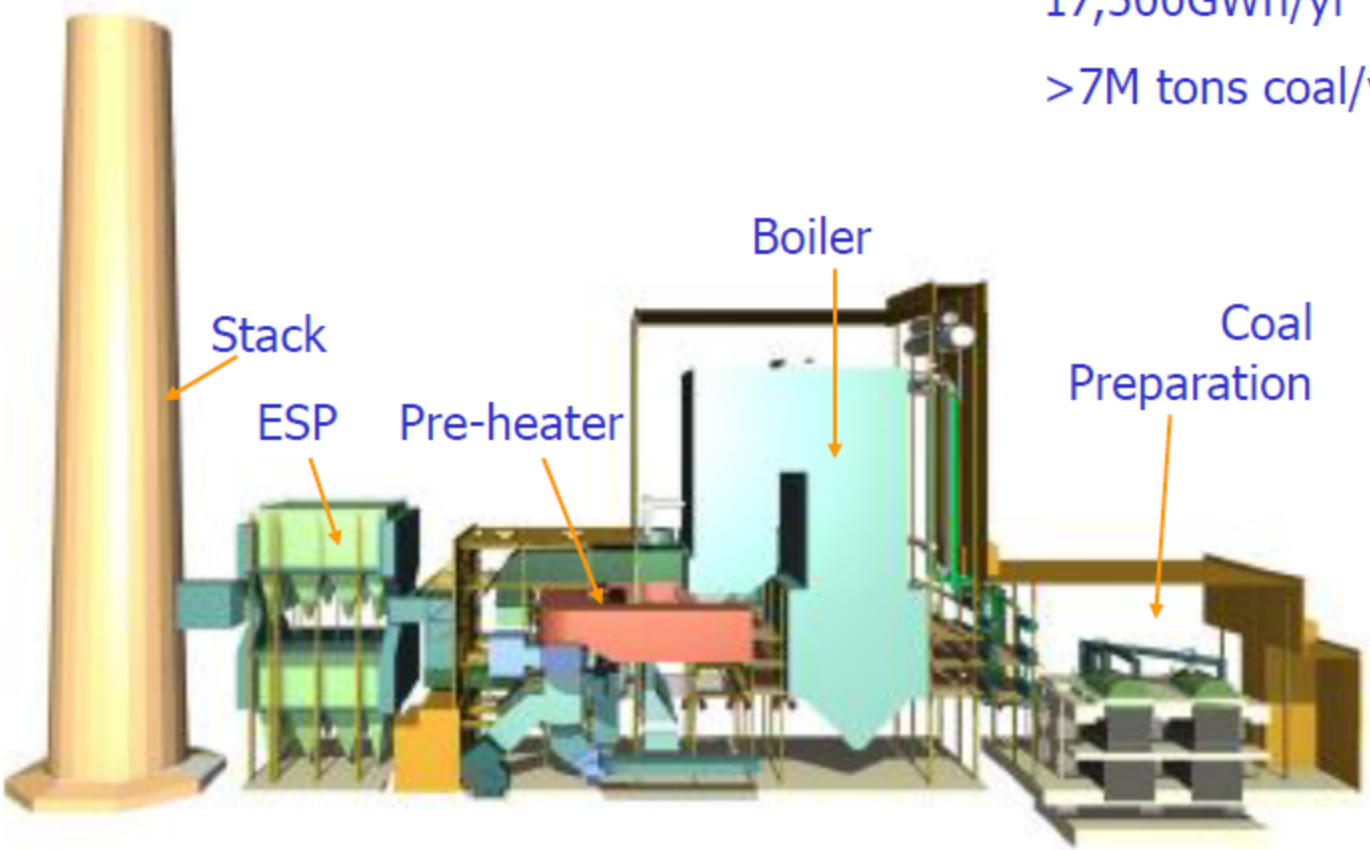
$1.7Billion (1999$)

Met NSR requirements

2x 1300 MW units

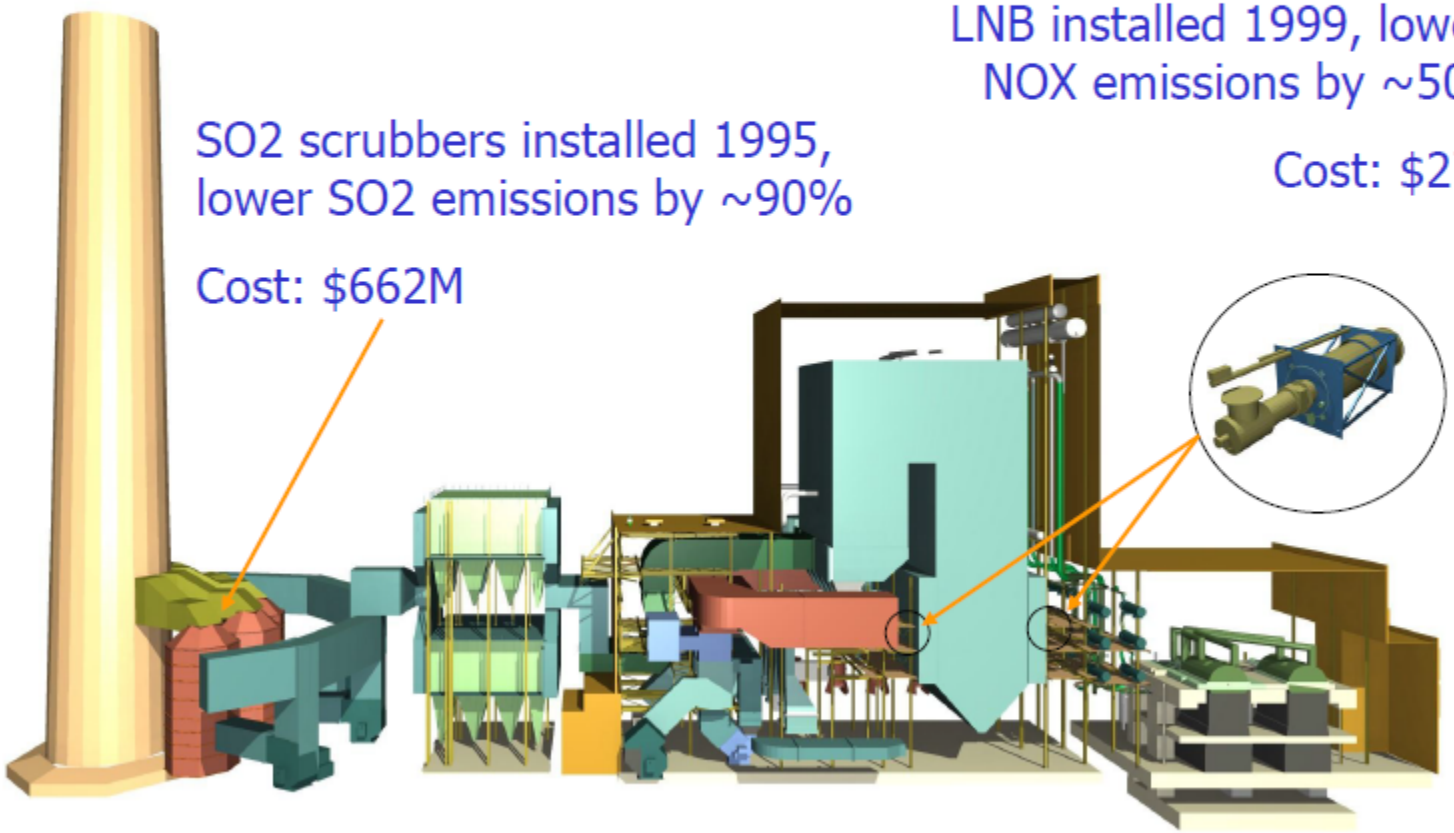
17,500GWh/yr

>7M tons coal/yr.



What additional emissions come from this power plant?

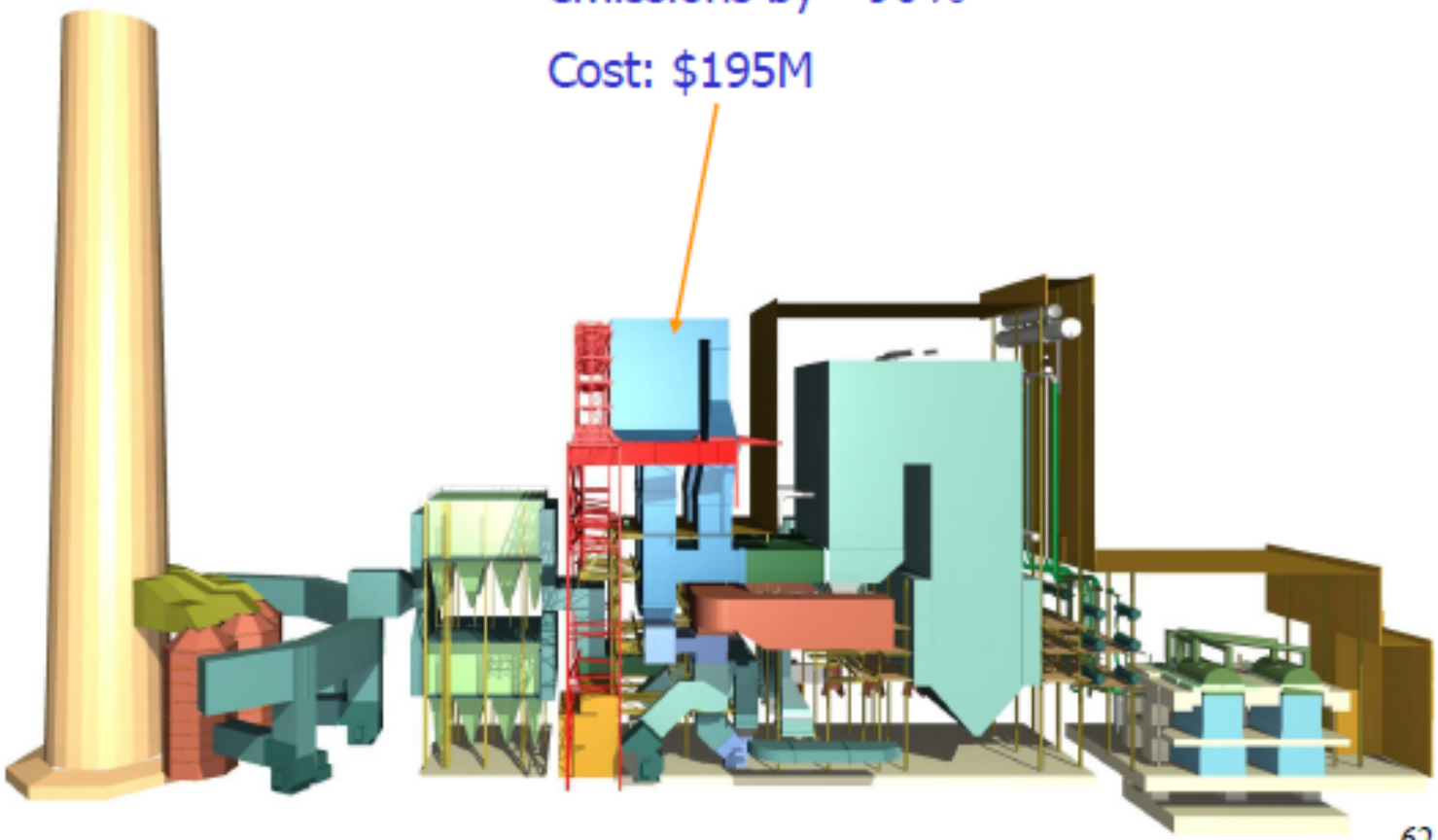
Gavin – 1990 Clean Air Act



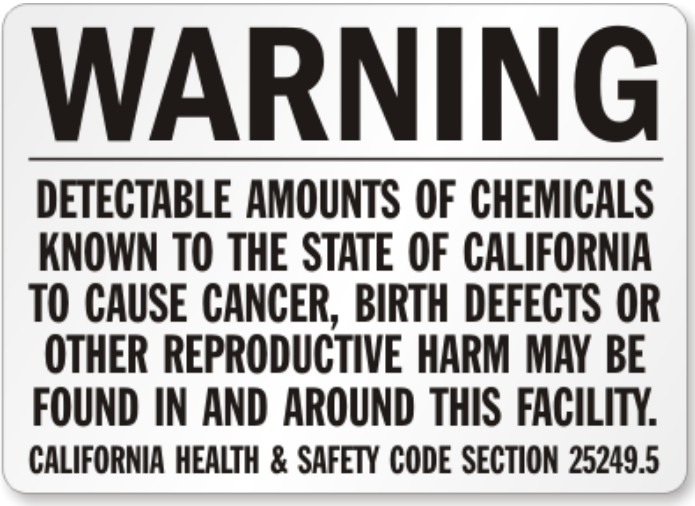
Gavin – NO_X SIP Call

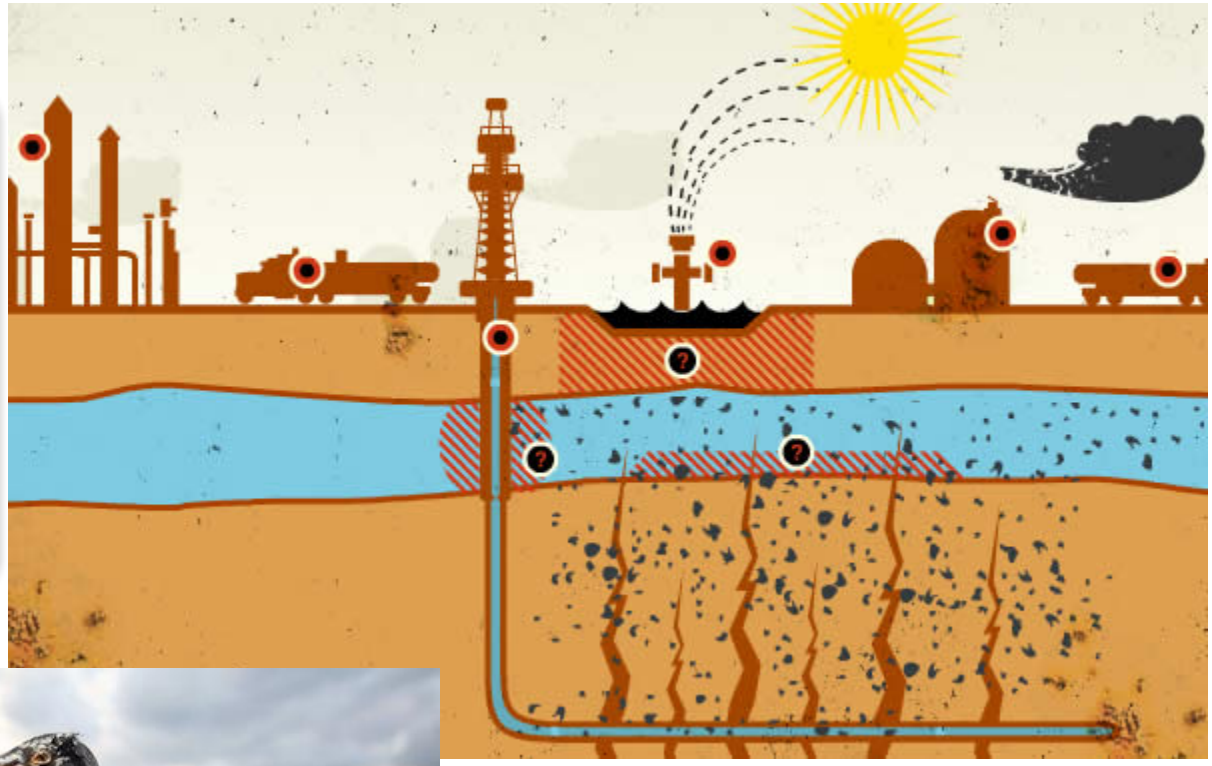
SCR installed 2001, lower SO2 emissions by ~90%

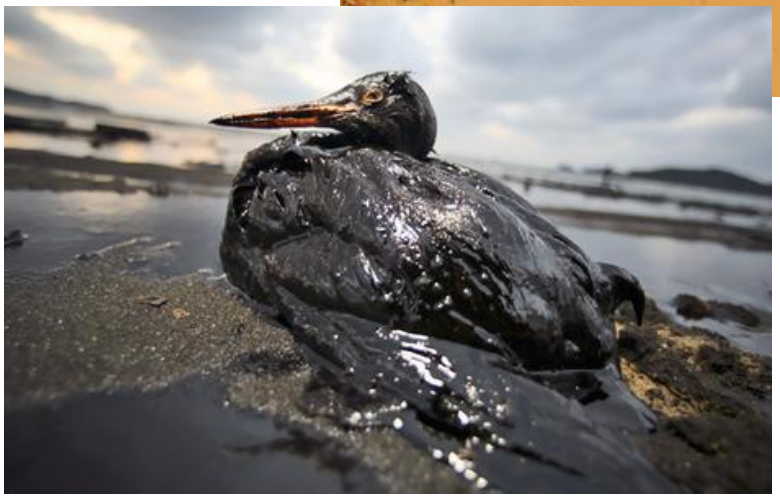
Cost: $195M



Greening Other Parts of the Life Cycle: Oil has non-combustion related risks.



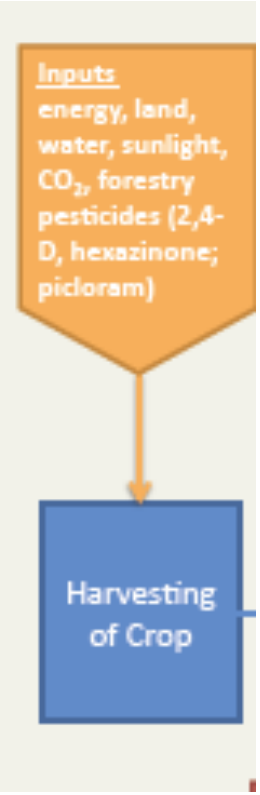




Identifying the indirect chemical inputs/ impacts by process.

- Does this step differentiate us from other fuels?
- What are the competing technologies for any given step
  - Which are most relevant?
- What are all of the chemical characteristics that we can identify?
  - Water content
  - Carbon Content
  - Impurities (metal, biological, chemical)
- If there are classes of chemicals identified (ie. alcohols, or pesticides)
  - Which 3-5 chemical species are most relevant?
    - Ethanol, Methanol, or Attrizine, 2,4 D..

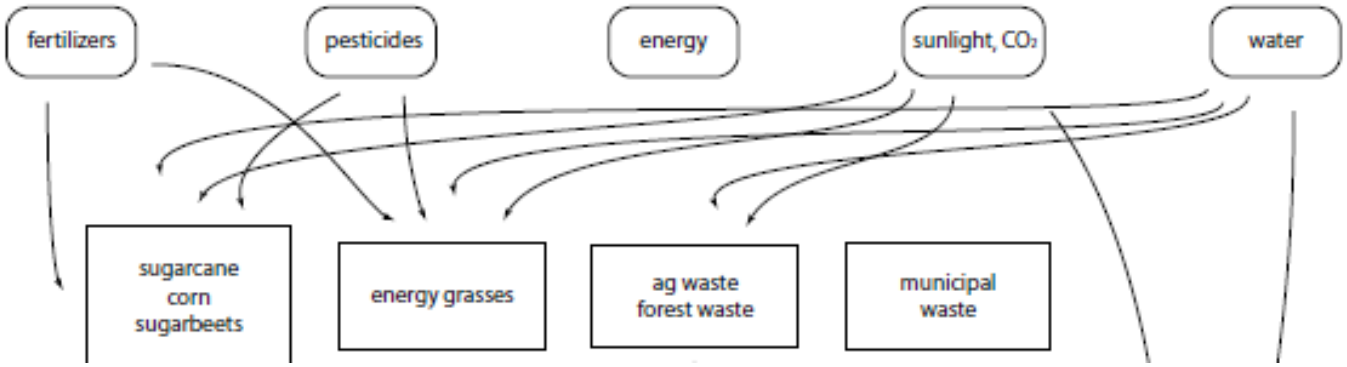
Source Material for each group

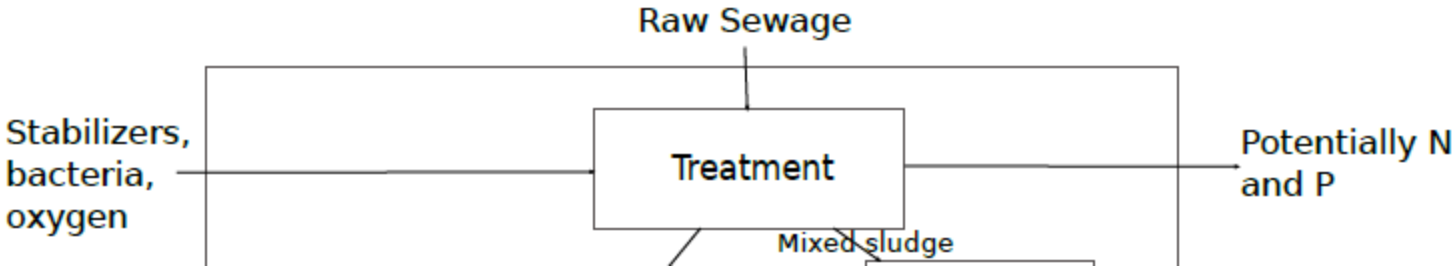


Feedstock

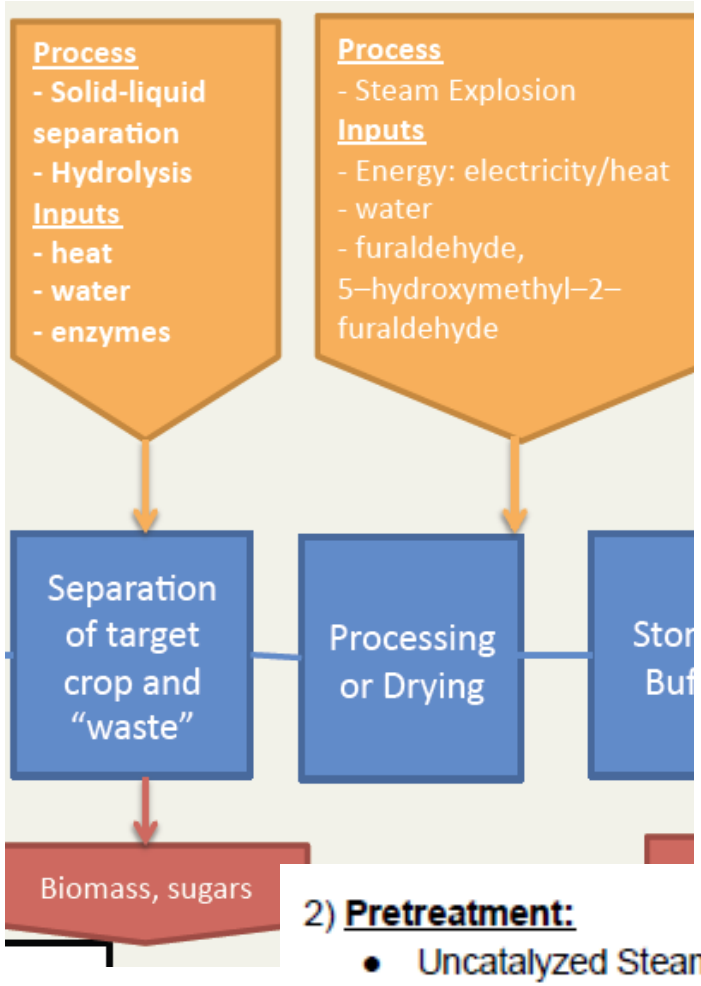
- **Input**: Municipal solid waste (plant-based, pre-treated)
- **Output**: Carbohydrates, cellulose, fats, proteins

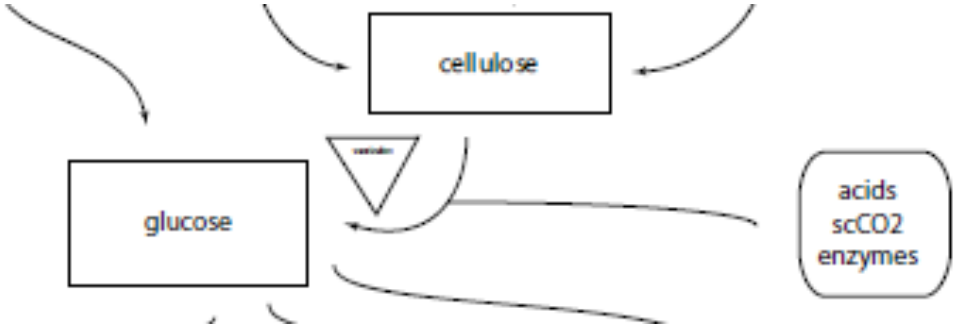
1) **Cellulosic Biomass:** Pesticides: Metam-Sodium, Pandimethalin (Source: http://pesticideinfo.org/airpic/ap_step3.jsp)





Pretreatment for Cellulosic





Hydrolysis

- **Input**: Carbohydrates, cellulose, fats, proteins, hydrolytic bacteria (such as Thermoanaerobacter Brockii), hydrolase
- **Output**: Monomers/simple sugars, fatty acids, aminoacids

2) **Pretreatment:**

- Uncatalyzed Steam Explosion: Steam(water)
- Catalyzed Steam Explosion: Water, SO2 or H2SO4, gypsum, xylose
- Ammonia Fiber Expansion: Ammonia
- Dilute Acid Hydrolysis:H2SO4, aliphatic acids, furan derivatives and phenolic compounds
- *All pretreatment steps produce oligosaccharides(C5 and C6) and lignin

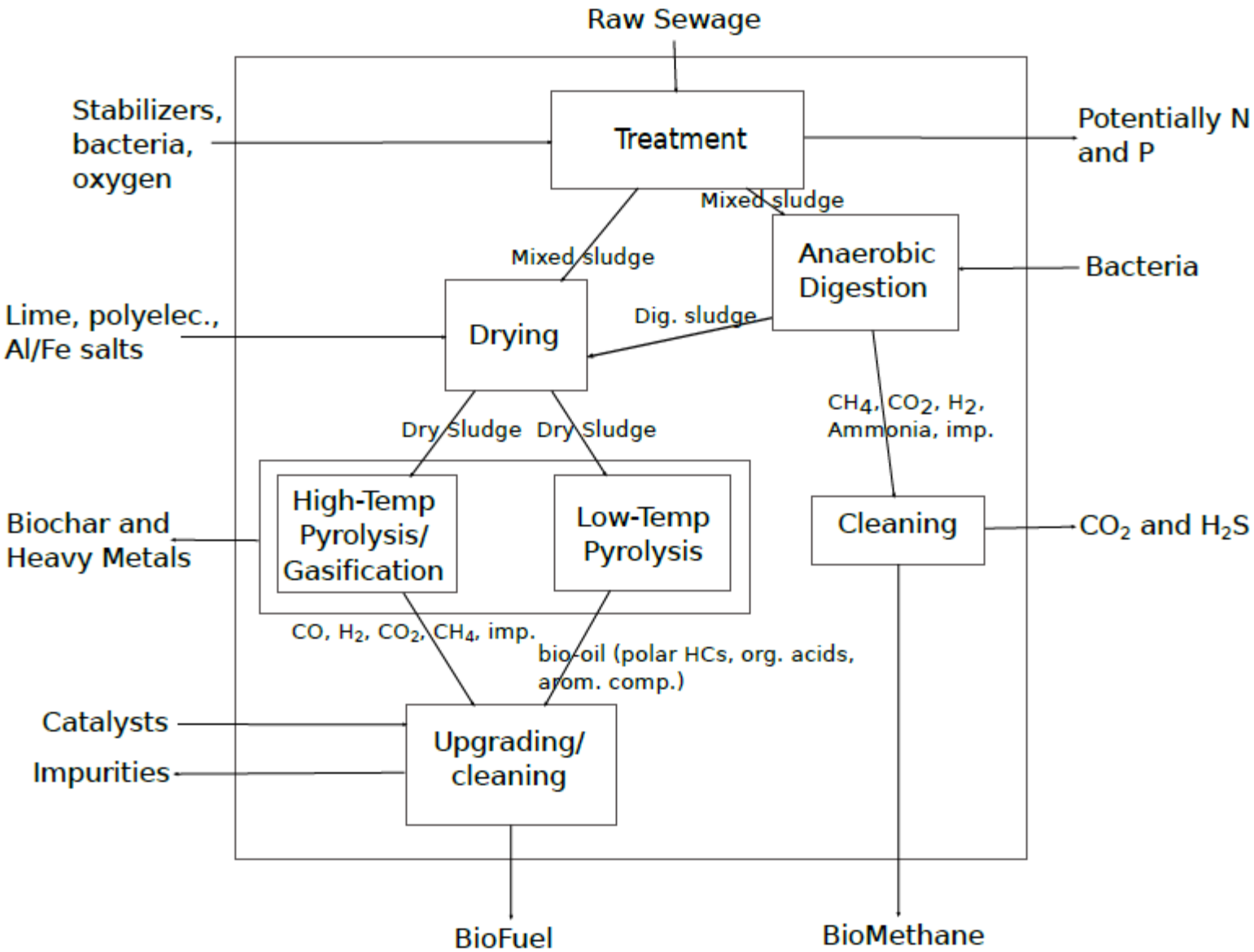
Advanced Biofuels Pretreatment technologies

Brainstorm pretreatment strategies.

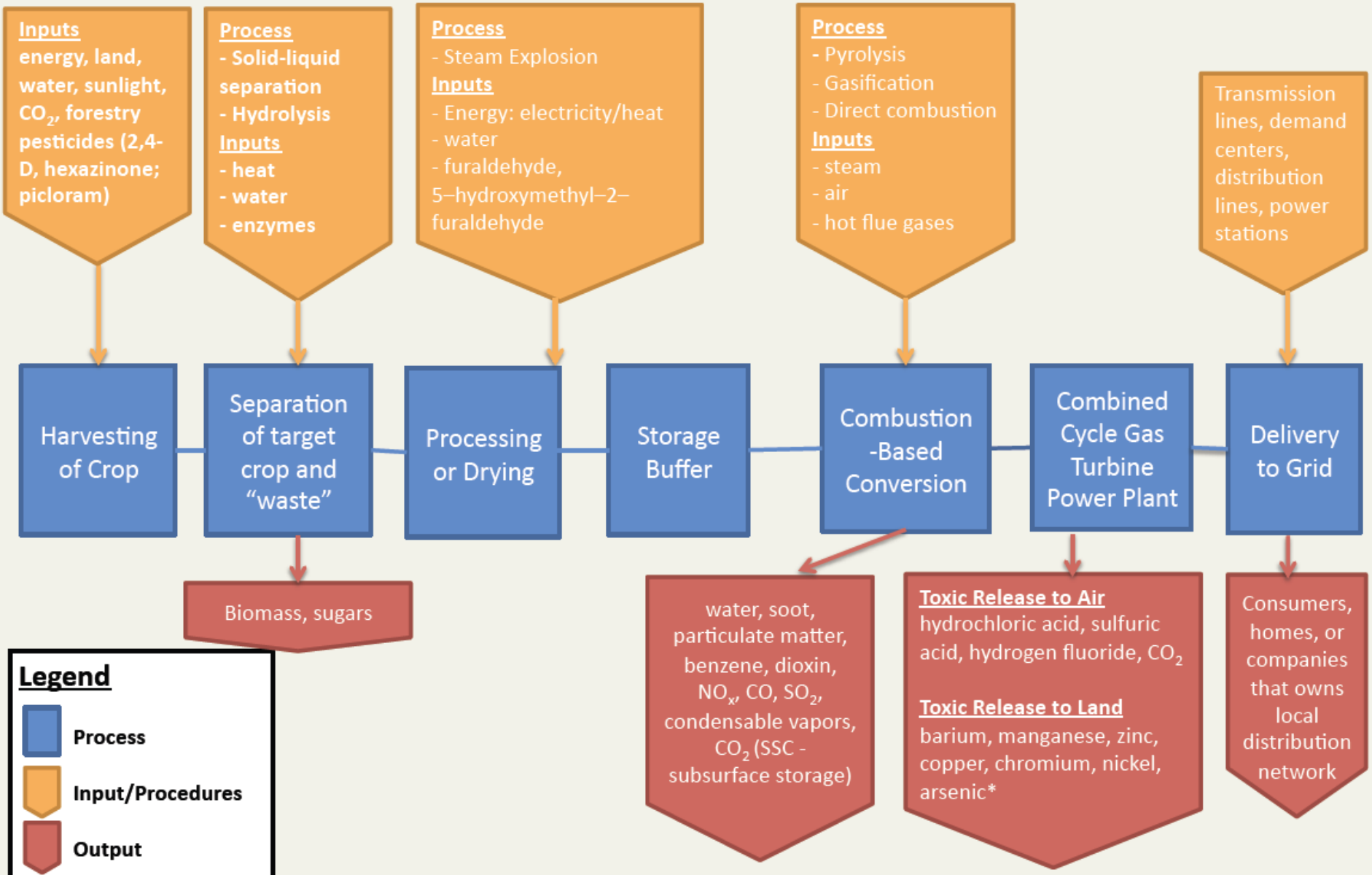
Pick one of the strategies to fill in around the room

For each strategies identify:

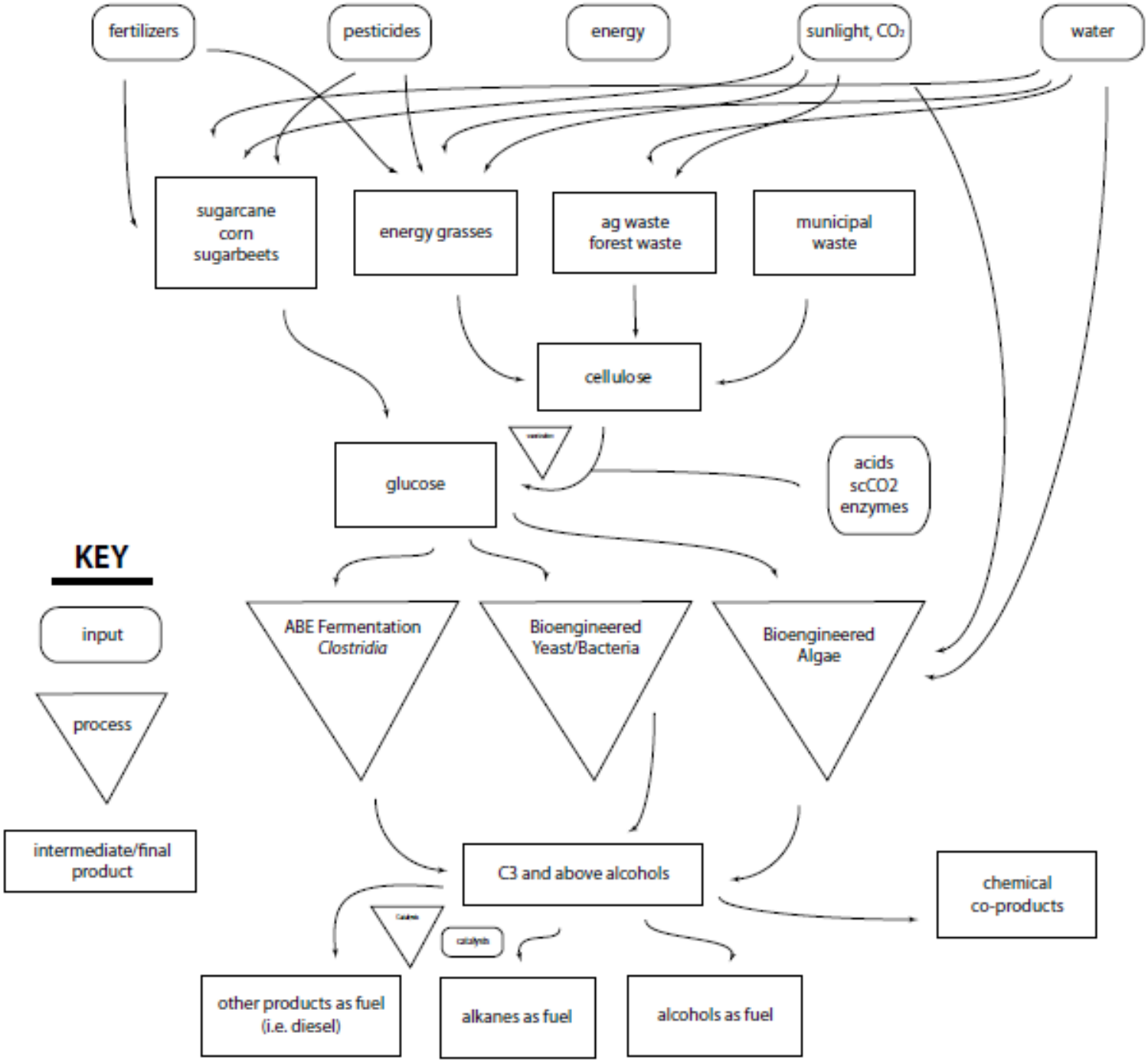
1) Which starting materials are relevant?
2) What type of products are made?
3) The relevant chemicals used.


Raw Sewage
Stabilizers, bacteria, oxygen
Treatment
Potentially N and P
Mixed sludge
Mixed sludge
Anaerobic Digestion
Bacteria
Lime, polyelec., Al/Fe salts
Drying
Dig. sludge
CH4, CO2, H2, Ammonia, imp.
Dry Sludge
Dry Sludge
High-Temp Pyrolysis/ Gasification
Low-Temp Pyrolysis
Cleaning
Biochar and Heavy Metals
CO2 and H2S
CO, H2, CO2, CH4, imp.
bio-oil (polar HCs, org. acids, arom. comp.)
Catalysts
Impurities
Upgrading/ cleaning
BioFuel
BioMethane

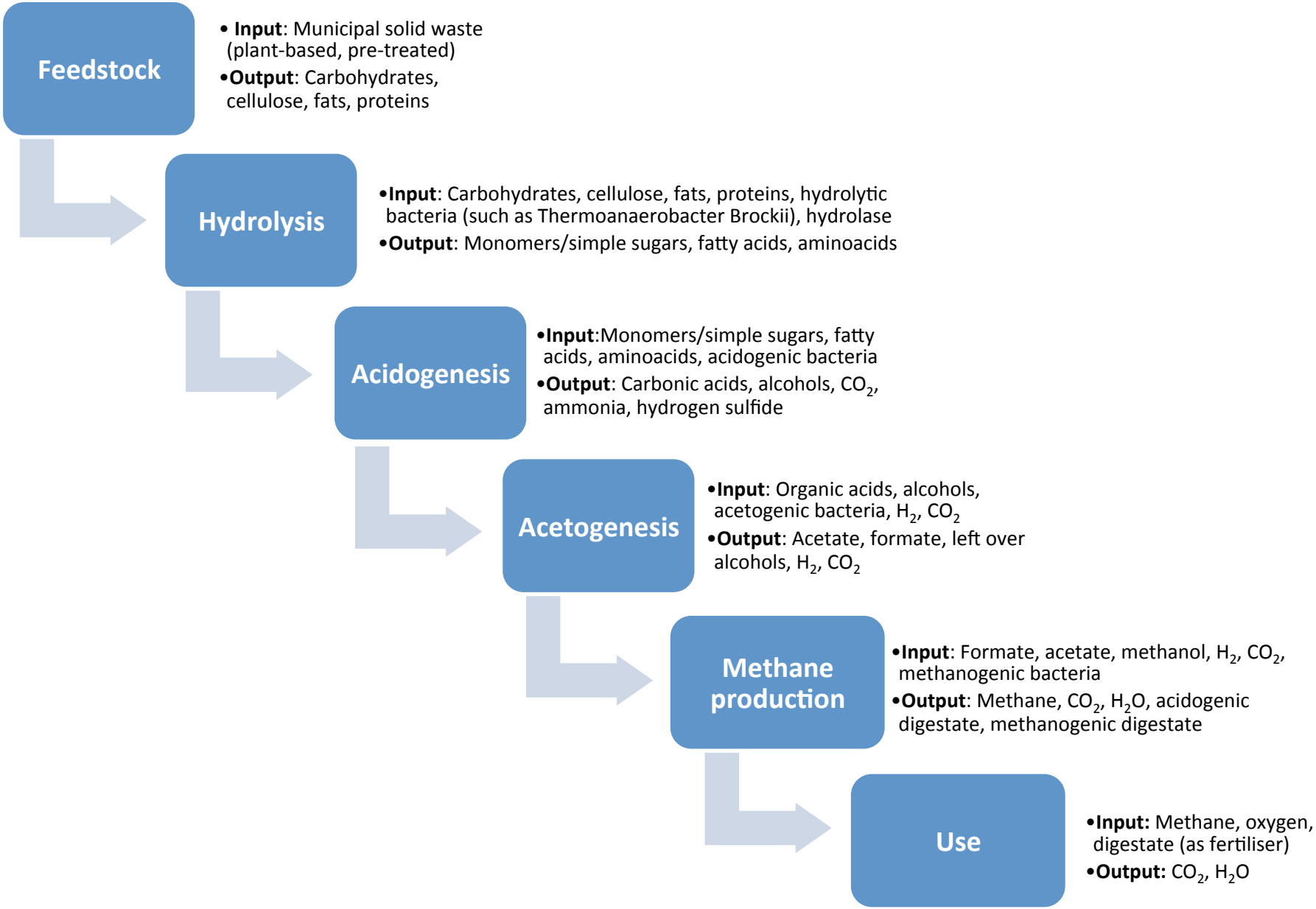
Biomass to Electricity Process Flow Diagram



*Rubin, E., "Toxic Releases from Power Plants." *Env.Sci.Techn.*, 33(18), 1999


fertilizers
pesticides
energy
sunlight, CO_2
water
sugarcane
corn
sugarbeets
energy grasses
ag waste
forest waste
municipal
waste
cellulose
glucose
acids
scCO2
enzymes
KEY
input
process
intermediate/final
product
ABE Fermentation
Clostridia
Bioengineered
Yeast/Bacteria
Bioengineered
Algae
C3 and above alcohols
chemical
co-products
catalysts
other products as fuel
(i.e. diesel)
alkanes as fuel
alcohols as fuel

Anaerobic Digestion Process



Major Processes - Cellulosic Biofuels

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3) **Hydrolysis:**
- Accellerase 1000
- Multifect Xylanase
- Multifect Pectinase

4) **Fermentation:**
- Ethanol major
- Minor Methanol
- Acetone, butyl alcohol, etc.

5) **Distillation/Blending:**
- Distillation, Molecular Sieves and Desiccants (Uses: Cornmeal, Straw, or Synthetic Zeolite)
- Membranes and Reverse Osmosis
- Usually gets blended with gasoline or exclusively with water for certain vehicles.

6) **Uses:**
- As a fuel, it's burning results in atmospheric particulates, NOx, SOx, and Ozone

Final activity/Next step for your diagrams

- Now with your group do the same thing for at least two of your process steps where you are able to choose from multiple technology platforms.

- Come up with a list of chemicals that are individually identifiable.