Biobased Chemicals:
Today, Not Tomorrow

The valorization of functionalised chemicals from biomass resources compared to the conventional fossil production route by implementing a thermo-economic analysis.

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For quality of life

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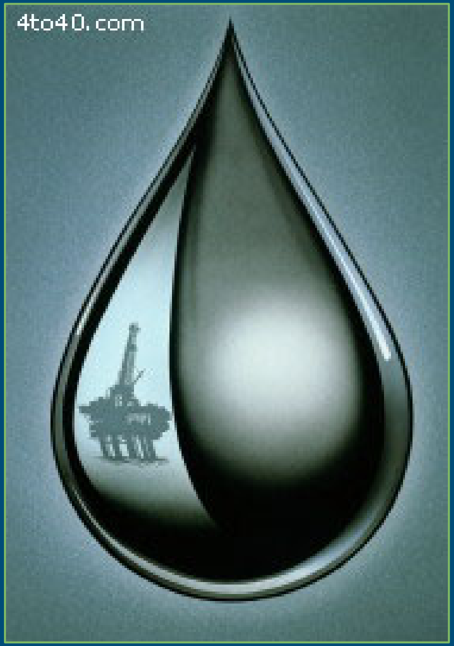
The Energy of Oil

- 1GJ of Oil ~ a full tank of petrol
- 1 barrel of Oil ~ 4GJ
- Oil has three main uses
  - Fuels (cheap transport)
    - Gasoline: 44.8GJ/ton
    - Diesel: 43.3GJ/ton
  - Energy (cheap electricity and heat)
    - Fuel Oil: 44.0GJ/ton
    - Electricity (45%): 19.8GJ/GJ or 71kW$_{el}$/ton
    - Heat (85%): 37.4GJ/GJ or 135kW$_{th}$/ton
  - Materials (cheap chemical building blocks)
    - Naphtha: 45.0GJ/ton
    - Chemical Energy: 15 – 100GJ/ton



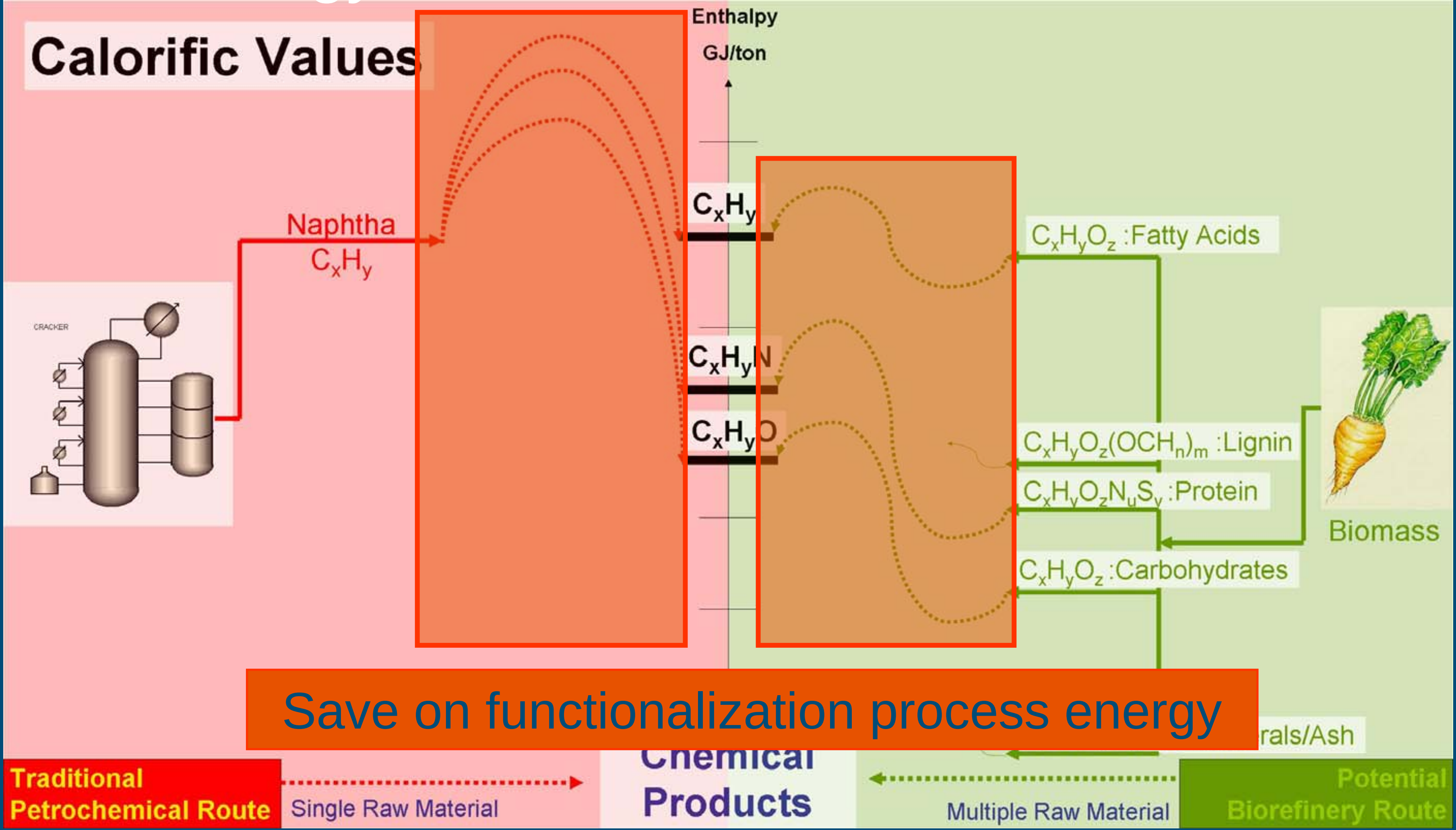
A lot of energy in just one drop

The Energy of Biomass

A lot less energy compared to oil

- 1GJ of biomass ~ a ¼ tank of petrol
- 1 barrel of biomass ~ 1GJ
- Biomass for the biobased economy also has three main uses
  - Fuels (transport)
    - Bioethanol: 27.5GJ/ton
    - Biodiesel: 39.2GJ/ton
  - Energy (electricity and heat)
    - Dry Biomass: 17.5GJ/ton
    - Electricity (33%): 5.8GJ/GJ or 5.8kW_{el}/ton
    - Heat (80%): 14.0GJ/GJ or 50.4kW_{th}/ton
  - Materials (cheap chemical building blocks)
    - Glucose: 13.1GJ/ton
    - Chemical Energy: 15 – 100GJ/ton

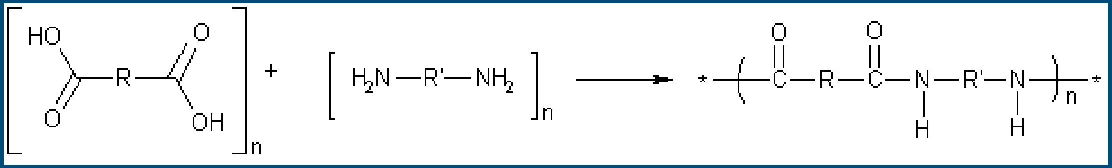
The Energy Reduction Potential of Biomass



Save on functionalization process energy

Chemical of a Functionalized Order

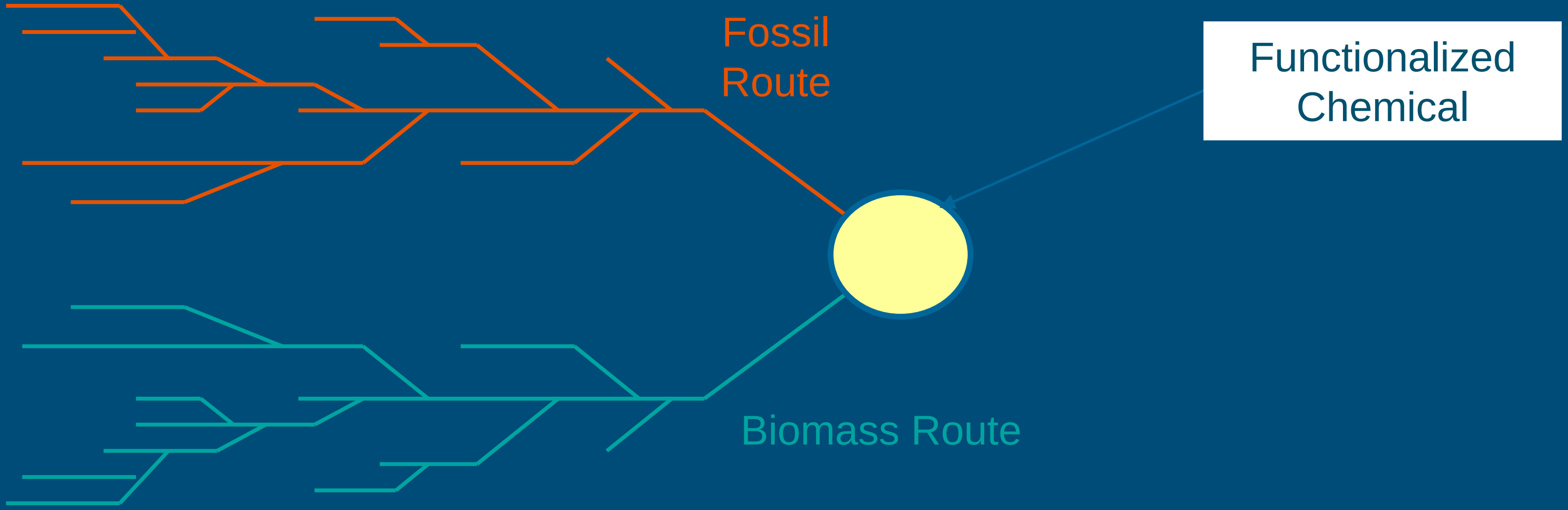
- Example: Nylon 6,6
- Cumulative Energy Demand (CED)
  - Feedstock cost and process energy cost
    - 154GJ/ton (Kindler)
    - 142GJ/ton (APME)
    - 143GJ/ton (BUWAL)
    - 163GJ/ton (Patel)



  - Biomass origin can use the existing functionalization of amino acids/proteins and alter under near atmospheric conditions
    - Expect between 5 – 30GJ/ton processing costs
    - **Huge energy saving potential!**

Method of Choice

- Comparative Exergetic Cradle-to-Factory Gate Analysis
  - Utilizes parts the ISO14040 series Life Cycle Assessment methodology – international norm
  - "*factory gate*" is the overlapping point on the horizontal chain
  - Compares the primary energy and material use for both routes
  - Incorporate thermodynamical energy efficiency (exergy)



Exergy

$$\boxed{Ex = Ex_{ph} + Ex_{chem} + Ex_{mix}}$$

$$\boxed{\sum Ex_{in} - \sum Ex_{out} = Loss(Anergy)}$$

- Thermodynamic Axiom
  - Based on the 2nd Law
  - Enthalpy (H) and Entropy (S) → Exergy
- Simple Terms
  - Useable energy
  - Quality of energy
- Simple Example
  - Waterfall
    - Top: high exergy
    - Bottom: low exergy

The Investigation

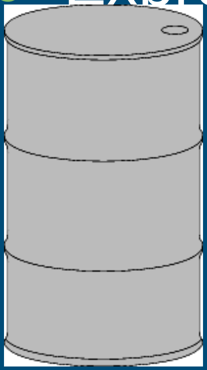
- 16 choice crops, common to the field of bioenergy and biomaterials, in most logical region

Crop	Continent	Country/Region
Common Name	Largest Producer	
Cassava	Africa	Nigeria
Grass	Europe	Holland
Lucerne	North America	South Dakota
Maize	North America	Iowa
Oil Palm	South Pacific	Malaysia
Potato	Europe	Holland
Rapeseed	Europe	Belgium
Sorghum	Africa	Kenya
Soya Beans	North America	Illinois
Sugar Beet	Europe	Germany
Sugar Cane	South America	Brazil
Sunflower	Europe	France
Switchgrass	North America	Iowa
Tobacco	South Pacific	Australia
Wheat	Europe	France
Willow Tree	Europe	Sweden

- Yields
  - Based on common practice in region Total biomass (except roots)
- Composition
  - Simple carbohydrates
  - Complex carbohydrates
  - Lignin
  - Protein
  - Fatty Acids
  - Ash (minerals)

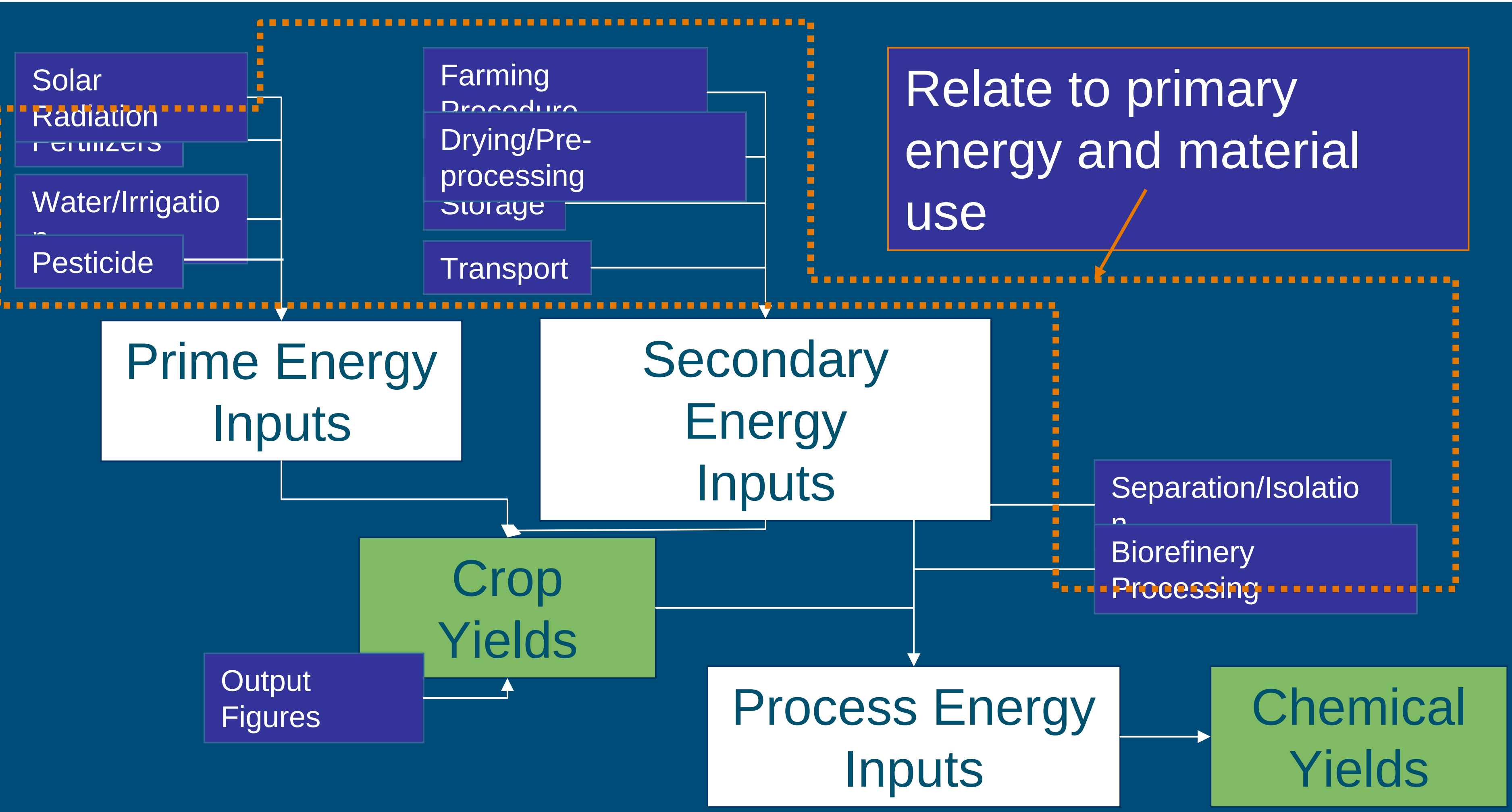
Purpose of Study

- To create a matrix calculation model linking the different regions, crops and biorefinery concepts together using exergy
- Determine the best combination supplying the chemical industry with an alternative feedstock
- Strive for maximum fossil fuel energy savings
  - Expression Terms:



    - Net Energy (Exergy) Value: NEV or NExV
    - Breeding Factor
    - GJ/ton chemicals produced
    - GJ/ton biomass cultivated
    - GJ/ha

Cradle-to-Factory Gate Overview



Solar Radiation

Fertilizers

Water/Irrigation

Pesticide

Farming Procedure

Drying/Pre-processing

Storage

Transport

Relate to primary energy and material use

Prime Energy Inputs

Secondary Energy Inputs

Separation/Isolation

Biorefinery Processing

Crop Yields

Output Figures

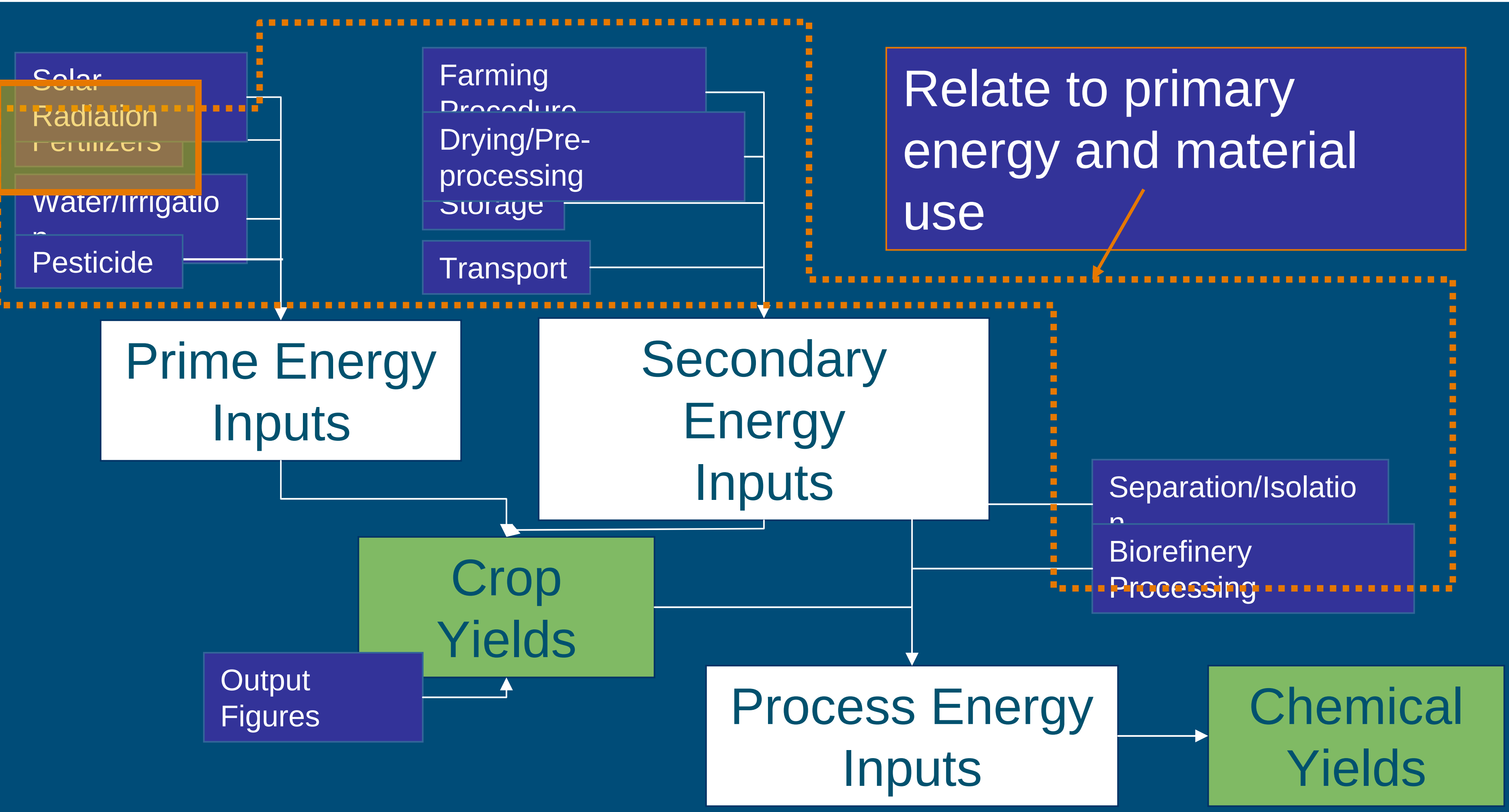
Process Energy Inputs

Chemical Yields

Scope of the Cradle

- All inputs related to initial fossil fuel input
  - Processed oil, diesel, gasoline, etc.
  - Based on amount and calorific values/exergy
  - Example: Steam calculated to initial fossil fuel input (heating oil)
    - 1ton at 8bar = 3.5GJ energy and 0.78GJ exergy
    - In a typical boiler the steam generation (taking into account co-generation) the efficiency is 85% for energy and 50% for exergy
    - **→ 1ton, 8bar steam = 4.1GJ energy and 1.6GJ exergy**
- *"Cradle"* has been set at the horizontal process chain including extraction of material and minerals
  - Mining, related to extraction energy plus material exergy
  - Not included is manufacturing of equipment, facilities, etc. Only process costs, assumed similar on both sides of the comparison.
- Exergy adds the extra dimension for non-renewable materials

Example: Fertilizer Chain



Relate to primary energy and material use

Solar Radiation

Fertilizers

Water/Irrigation

Pesticide

Farming Procedure

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Prime Energy Inputs

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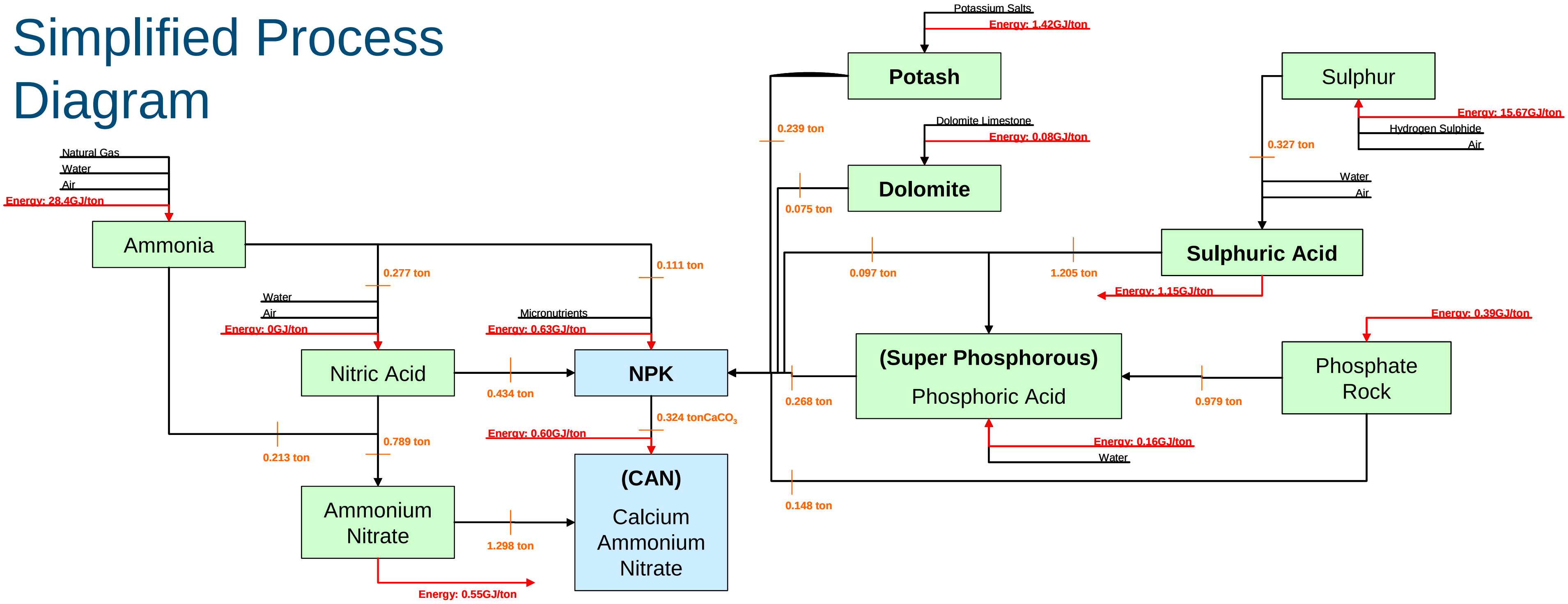
Example: Fertilizer Production Route

Simplified Process Diagram



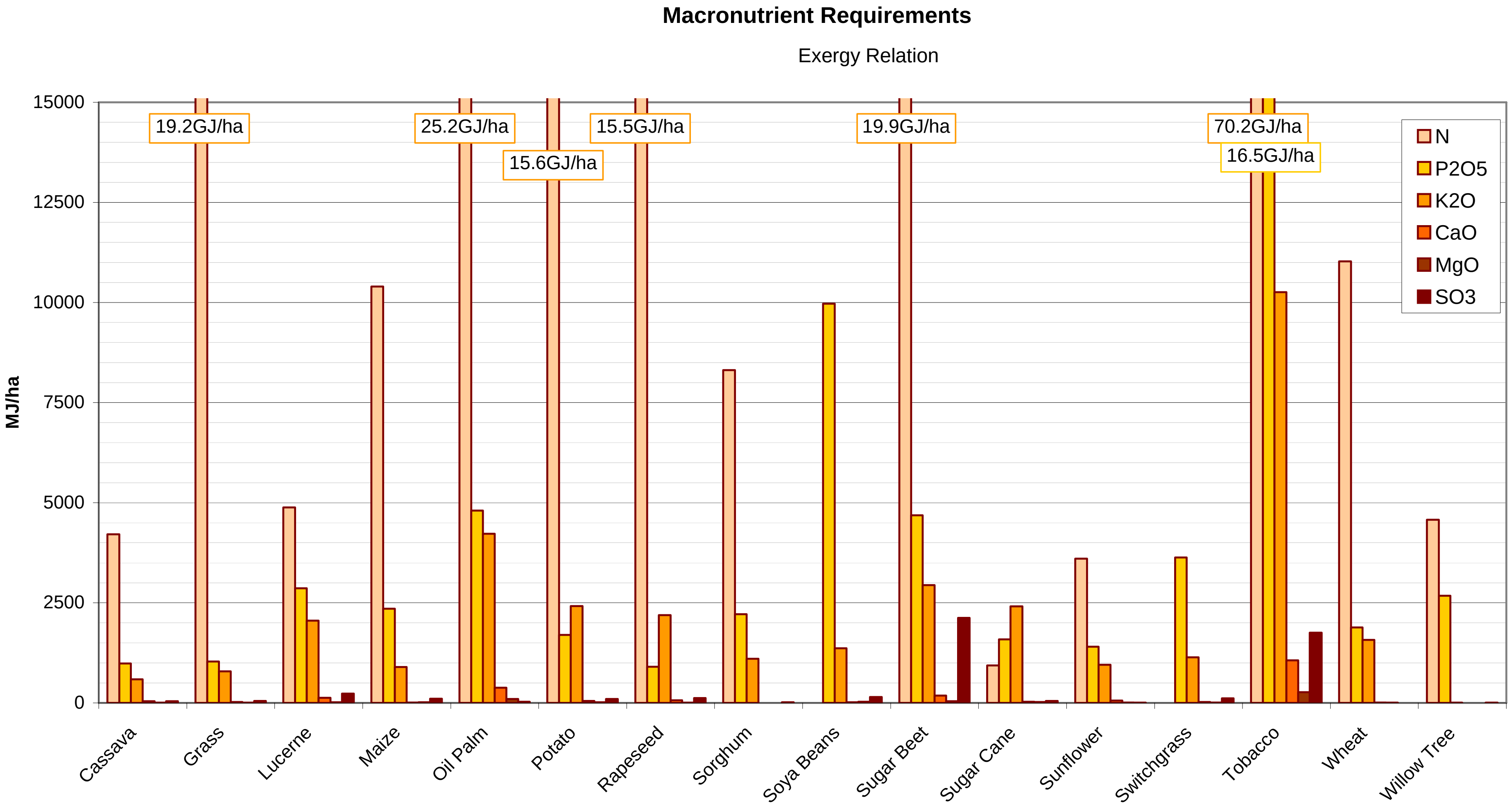
- Best Available Technology (as of 2002)
- Most common and advanced fertilizer in Europe (EFMA, IFA)
- Covers both complex and straight routes
- Related to nutrient content as expressed in the industry

Example: Fertilizer Energy/Exergy Cost

- Cumulative energy requirements for main macronutrients per unit (MJ/kg)
  - Listed as: N, P, K, Ca, Mg, S
  - Expressed as: N, P_2O_5, K_2O, CaO, MgO, SO_3
- In “crop output” determined nutrient uptake figures based on chemical composition analysis
  - Source IFA
- Link to total nutrient uptake levels of the crops
  - ton/ton → kg/ha → MJ/ha
- Assumptions
  - When any of the macronutrients is larger than 25% of N level, the non-NPK route will be used for the dividend
  - UAN will be used when N is more than PK combined for the dividend

Overview			
Macronutrients			
Nutrient	Route	Energy	Exergy
		MJ/kg	
(N) Nitrogen	NPK+CAN	50.90	53.99
(N) Nitrogen	UAN	49.02	50.22
(P) Phosphorous	NPK+CAN	25.06	31.63
(P) Phosphorous	SuperP	7.28	17.48
(K) Potassium	NPK+CAN	5.10	6.31
(K) Potassium	Potash	3.22	4.11
(S) Sulphur	NPK+CAN	1.94	5.16
(S) Sulphur	H_3SO_4	1.94	5.16
(Ca) Calcium	NPK+CAN	0.94	0.74
(Ca) Calcium	Dolomite	0.16	0.34
(Mg) Magnesium	NPK+CAN	0.19	0.40
(Mg) Magnesium	Dolomite	0.19	0.40
Micronutrients			
Nutrient	Route	Energy	Exergy
		MJ/kg	
Various	Ore	20.0	25.0

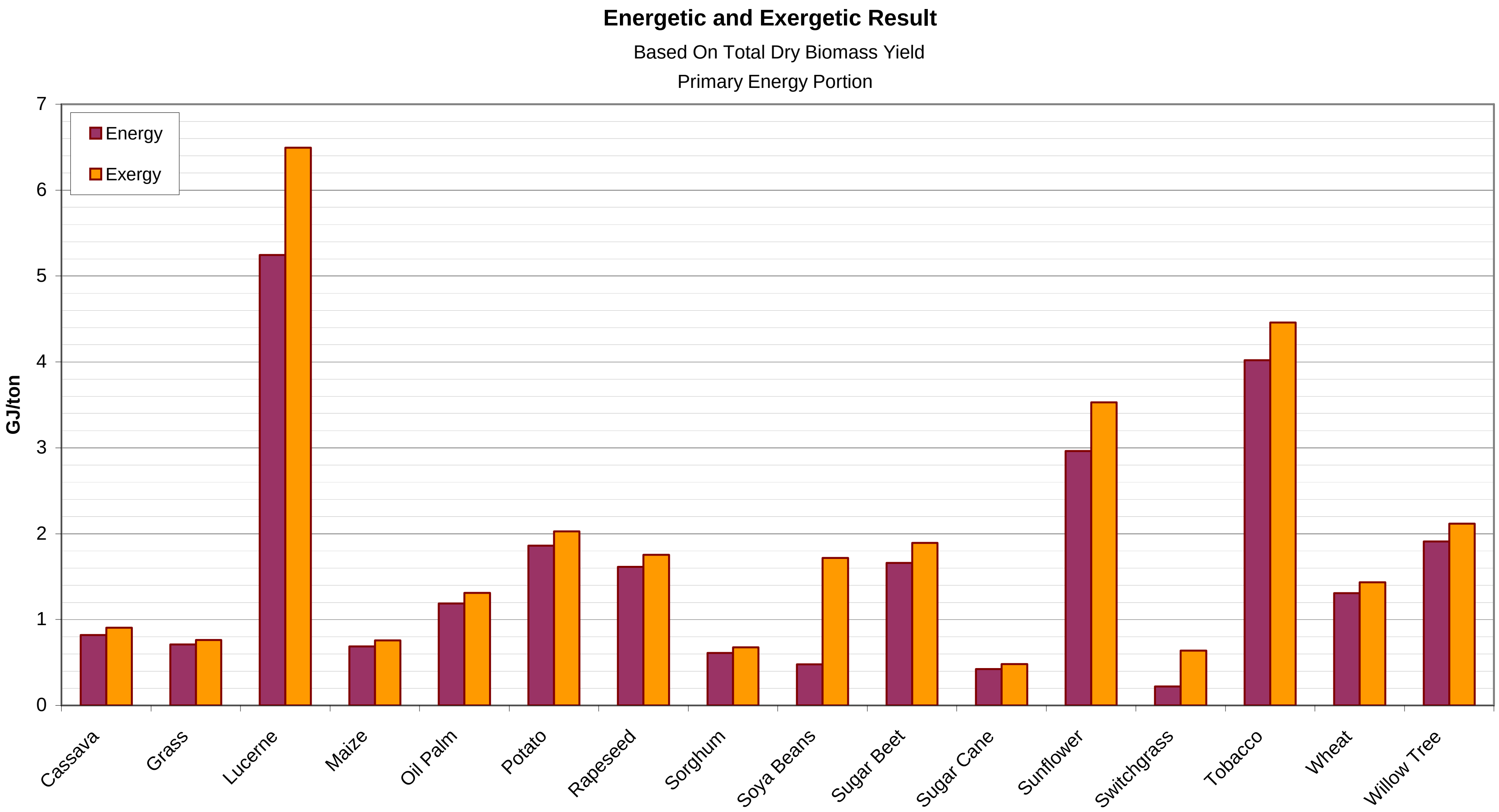
Example: Fertilizer Exergy Cost



Data Input

- All other input follow same procedure as with the fertilizer section
  - Best available technology, crop dependent, regionally dependent, all related to MJ/ha and MJ/ton biomass
- Primary Energy Input: Completed
  - Water
    - Irrigation/drainage, monthly crop water demands, regional monthly effective rainfall, typical regional systems and source of water, etc.
  - Pesticides
    - BAT for 40 typical pesticides, crop protection demands, regionally application practices, etc.
- Secondary and Process Energy Input: Pending
  - Preliminary and other source data used for model creation

Resulting Biomass Cumulative Process



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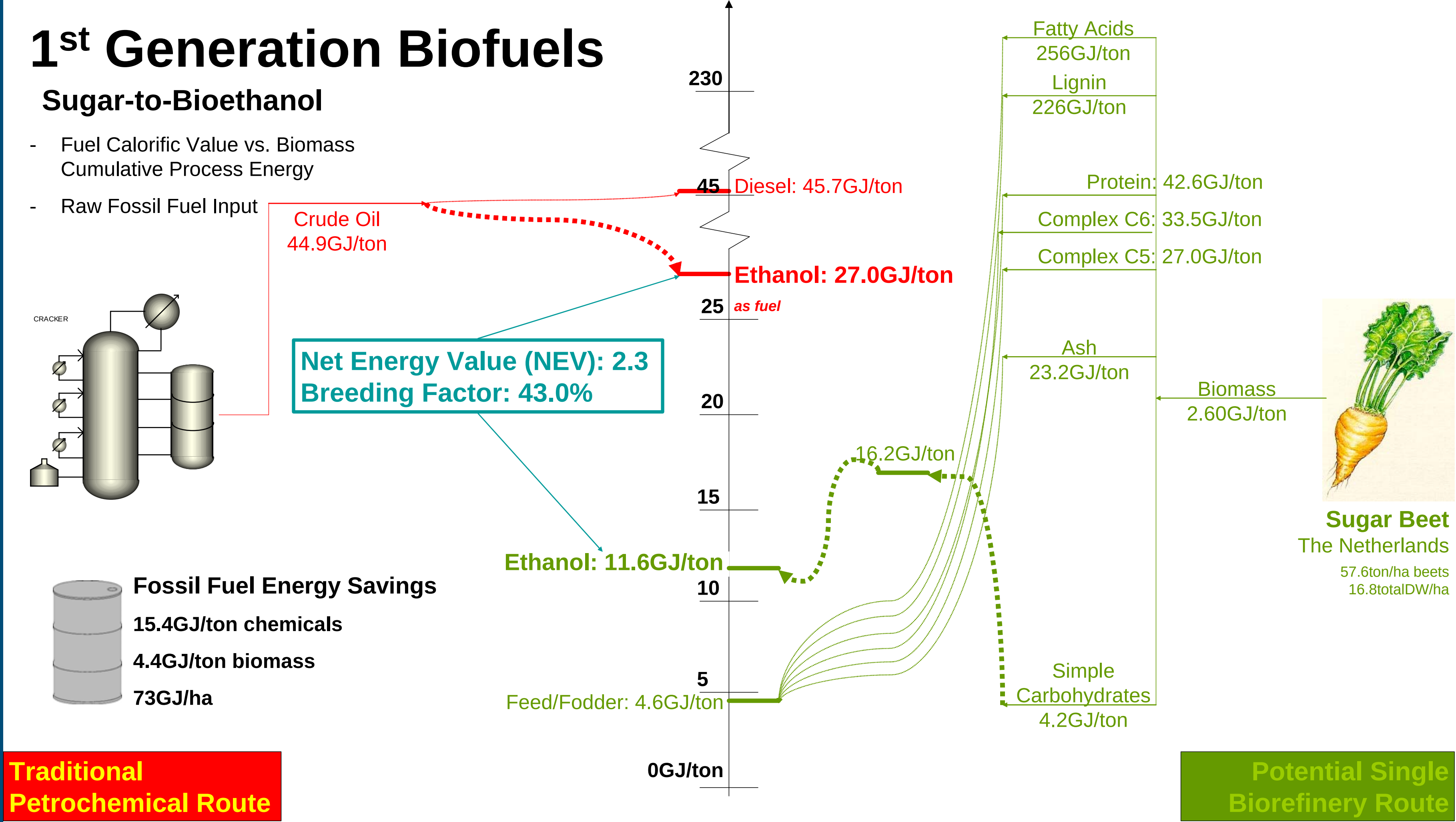

1^{st} Generation Biofuels

Sugar-to-Bioethanol

- Fuel Calorific Value vs. Biomass Cumulative Process Energy
- Raw Fossil Fuel Input

Net Energy Value (NEV): 2.3
Breeding Factor: 43.0%

Fossil Fuel Energy Savings

15.4GJ/ton chemicals

4.4GJ/ton biomass

73GJ/ha

Traditional Petrochemical Route

Potential Single Biorefinery Route

Introduction | Goal and Scope | Inventory | Data | **Interpretation**

- Secondary Input: from other sources, so not validated
- Bio-processing Input: rough estimates, so not validated

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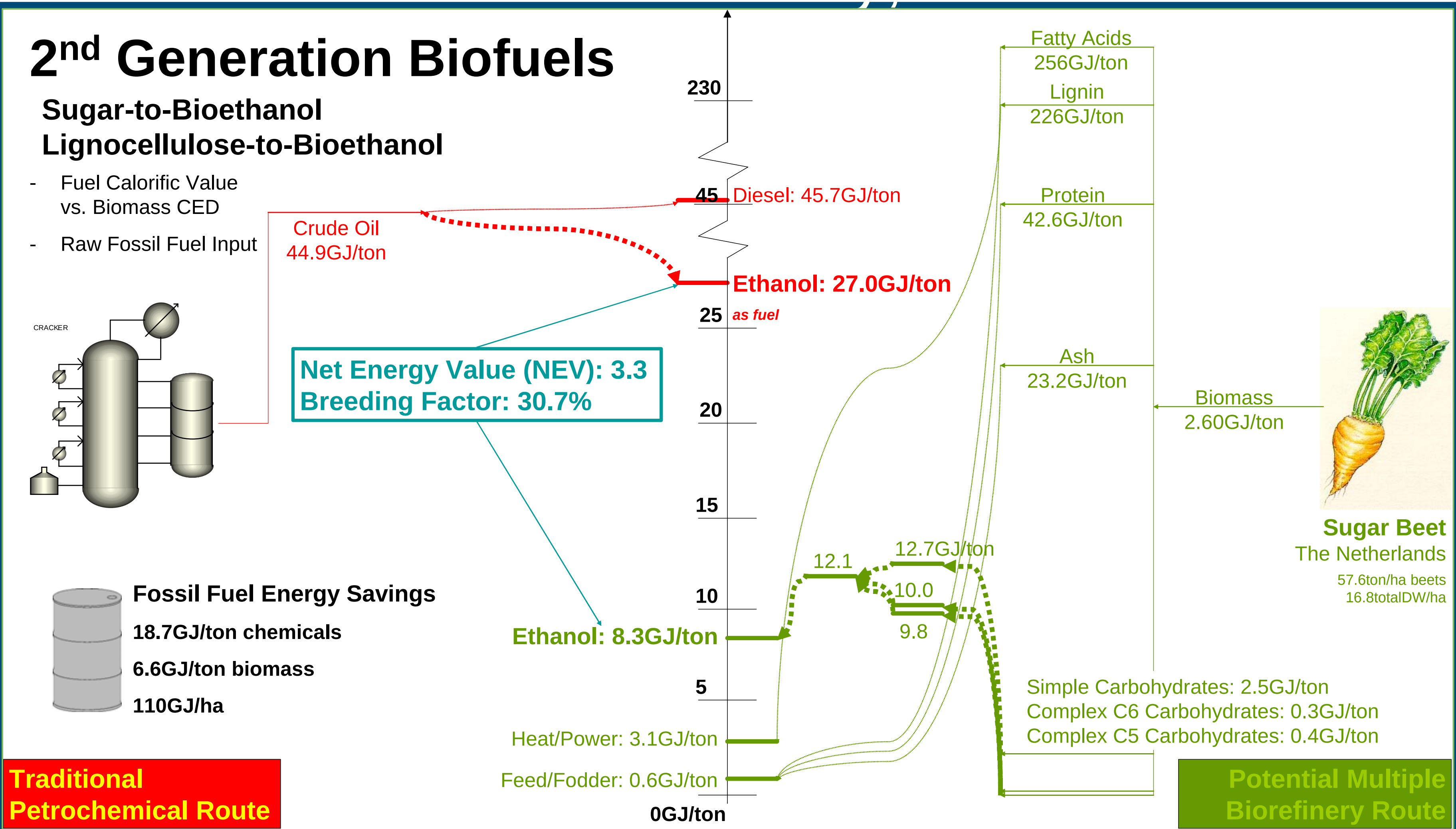


2nd Generation Biofuels

Sugar-to-Bioethanol
Lignocellulose-to-Bioethanol

- Fuel Calorific Value vs. Biomass CED
- Raw Fossil Fuel Input

Crude Oil 44.9GJ/ton

Diesel: 45.7GJ/ton

Ethanol: 27.0GJ/ton

as fuel

Net Energy Value (NEV): 3.3
Breeding Factor: 30.7%

Fossil Fuel Energy Savings

18.7GJ/ton chemicals

6.6GJ/ton biomass

110GJ/ha

Ethanol: 8.3GJ/ton

Heat/Power: 3.1GJ/ton

Feed/Fodder: 0.6GJ/ton

0GJ/ton

Fatty Acids 256GJ/ton

Lignin 226GJ/ton

Protein 42.6GJ/ton

Ash 23.2GJ/ton

Biomass 2.60GJ/ton

Sugar Beet
The Netherlands
57.6ton/ha beets
16.8totalDW/ha

Simple Carbohydrates: 2.5GJ/ton
Complex C6 Carbohydrates: 0.3GJ/ton
Complex C5 Carbohydrates: 0.4GJ/ton

Traditional Petrochemical Route

Potential Multiple Biorefinery Route

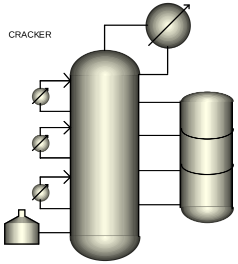
- Secondary Input: from other sources, so not validated
- Bio-processing Input: rough estimates, so not validated

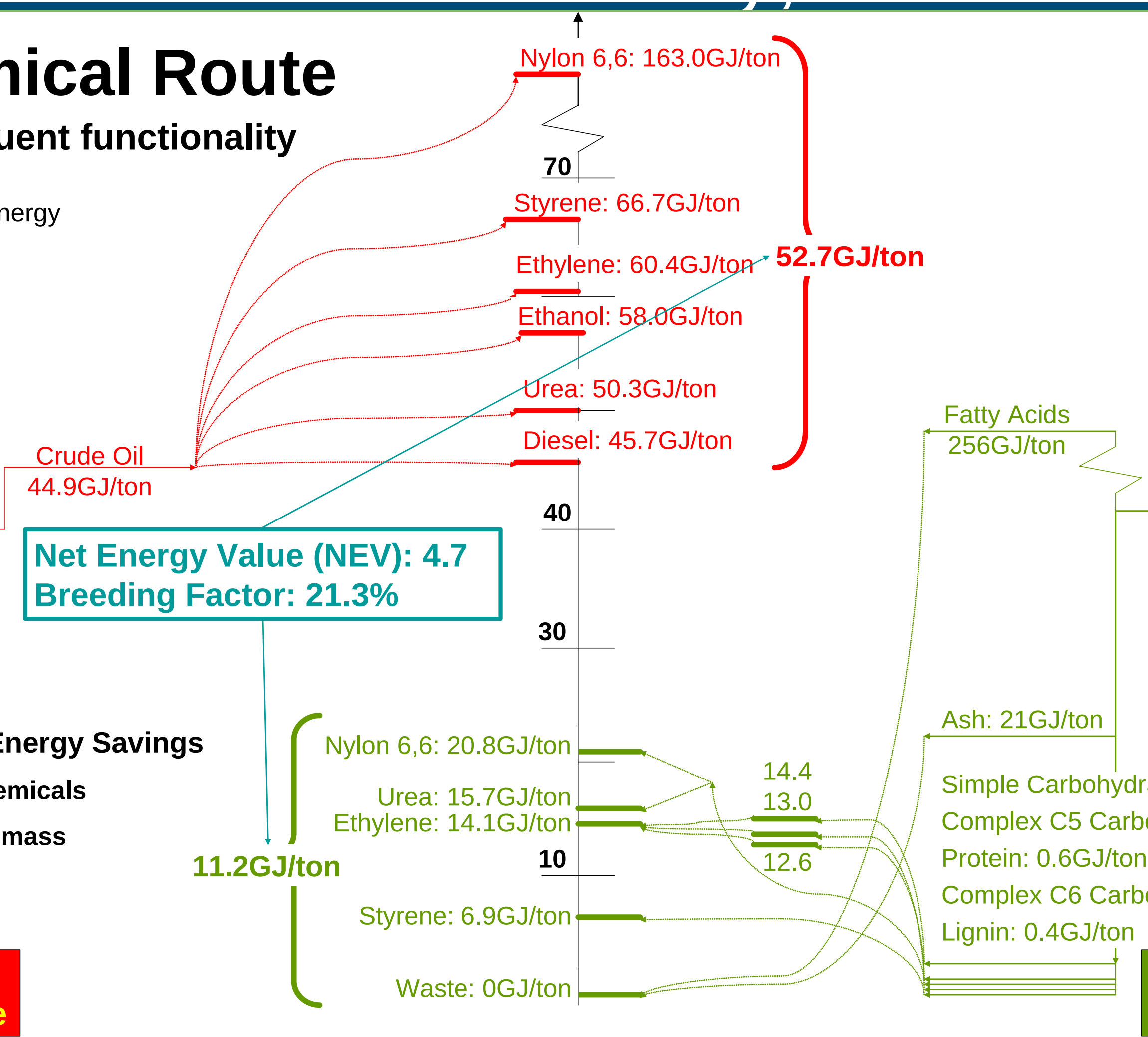
Biobased Chemicals: Today, Not Tomorrow

Full Chemical Route

Utilizing constituent functionality

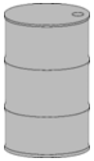
- Chemical vs. Biomass Cumulative Process Energy
- Raw Fossil Fuel Input





Net Energy Value (NEV): 4.7
Breeding Factor: 21.3%

Sugar Beet
The Netherlands
57.6ton/ha beets
16.8totalDW/ha



Fossil Fuel Energy Savings
41.5GJ/ton chemicals
15.4GJ/ton biomass
259GJ/ha

Traditional Petrochemical Route

Potential Chemical Biorefinery Route

- Secondary Input: from other sources, so not validated
- Bio-processing Input: rough estimates, so not validated

Biobased Chemicals

- **Biomass Best as Feedstock for Chemical Industry!**
- Compared to other utilization options, using current state-of-the-art techniques, a potential biorefinery for chemical feedstock will mitigate the most fossil energy, reduce the most CO2, maximize sustainability and place the least burden on land availability.

Fossil Fuel Savings	1st Generation	2nd Generation	Biorefinery
GJ/ton Chemicals	15.4	18.7	41.5
GJ/ton Biomass	4.4	6.6	15.4
GJ/ha	73	110	259

- Preliminary results using the sugar beet under Dutch conditions

Conclusion

- Questions?
- Suggestions?