Economic and environmental assessment of biological conversions of Agile BioFoundry (ABF) bio-derived chemicals

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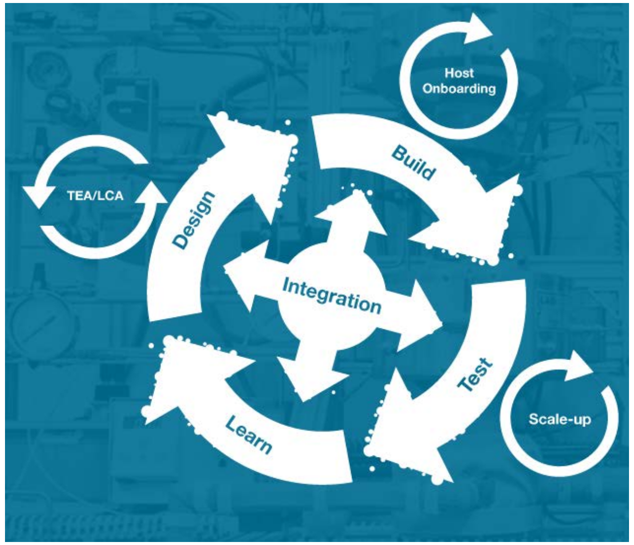
Introduction

The **Agile BioFoundry (ABF)** consortium goal: enable biorefineries to achieve **50% reductions** in time to **bioprocess scale-up** as compared to the current average of around 10 years by establishing a distributed Agile BioFoundry to productionize synthetic biology. https://agilebiofoundry.org/

Integrated Analysis team goal

- Help to quantify the ultimate **economic and environmental** sustainability potential for a given beachhead molecule/ product pathway of interest,
- Compare different products or synthesis routes to understand relative merits or drawbacks,
- Highlight key TEA/LCA drivers for prioritizing R&D focus areas

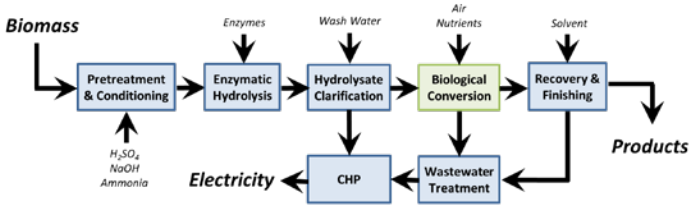


Goal of this presentation

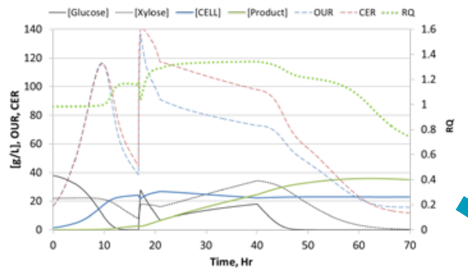
- Present a methodology to select a single exemplar product molecule to represent each beachhead pathway based on similarities
- Present techno-economic analysis (TEA) and life-cycle analysis (LCA) for two selected ABF technology pathways to bio-derived chemicals:
  - ✓ **adipic acid** production via muconic acid fermentation from mixed sugars with *Pseudomonas putida*
  - ✓ **cineole** via geranyl diphosphate with *Rhodosporidium toruloides*

TEA/LCA approach

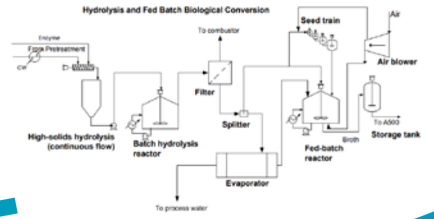
1) Conceptual process is **formulated or refined based on current research** and expected chemical transformations. Process flow diagram is synthesized.



2) Individual unit operations are **designed and modeled using experimental data**. Process model outputs are used to size and cost equipment.



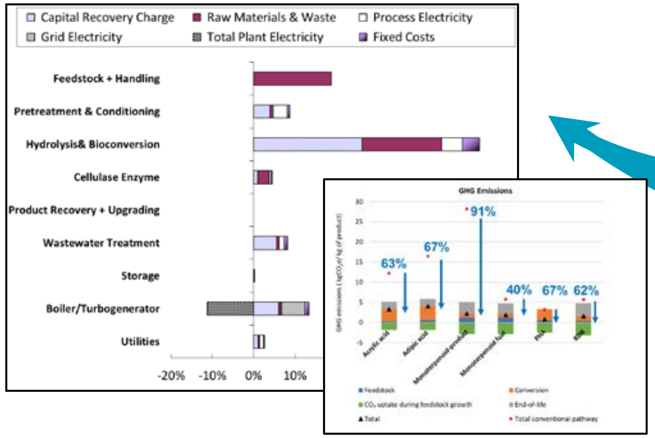
3a) Capital and operating costs are input into an economic model to **identify the major cost drivers**.



GREET
LIFE-CYCLE MODEL

3b) Material and Energy flows are input into a life cycle model to **identify the major sustainability drivers**.

4) Results and **new understanding is fed back** into step 1) and the process iterates.

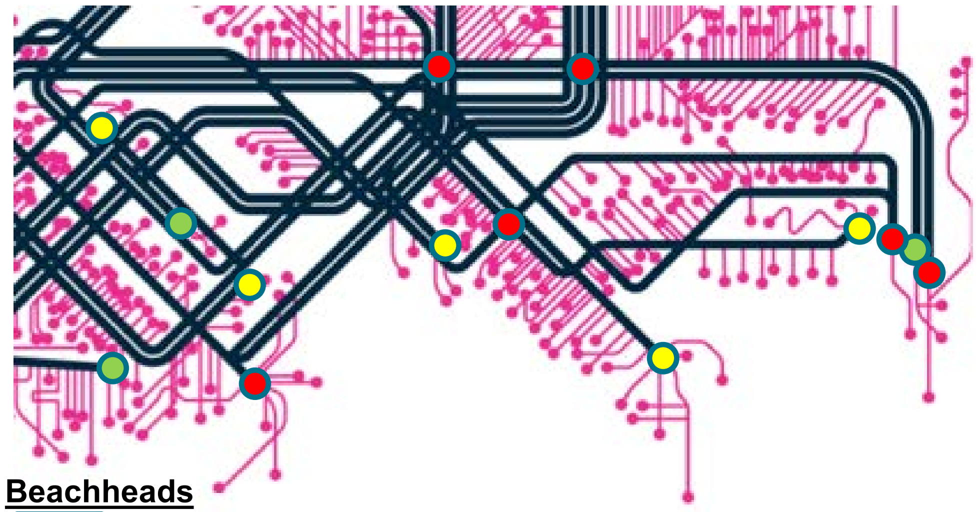


TEA
Minimum selling price
$/kg

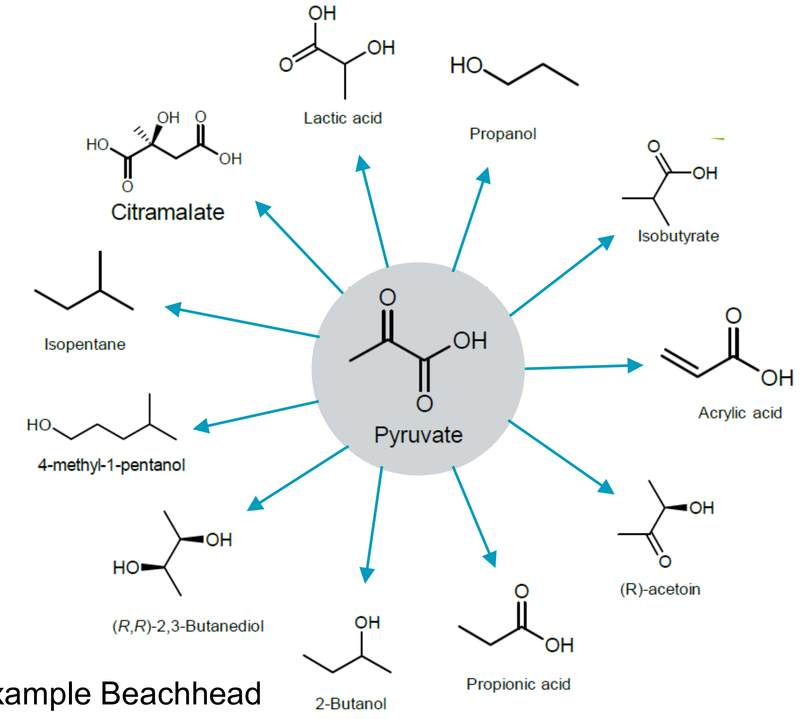
LCA
GHG emissions
kg CO_2e/kg

Beachhead Molecules

- Beachheads are metabolites that can be converted into many different bioproducts
- ABF will develop >15 beachhead strains to enable rapid development of a wide range of downstream bioproducts



Beachheads
- Developed (7)
- Mid Goal (3 additional FY20Q2)
- FY22 Goal (15+ total)



Example Beachhead

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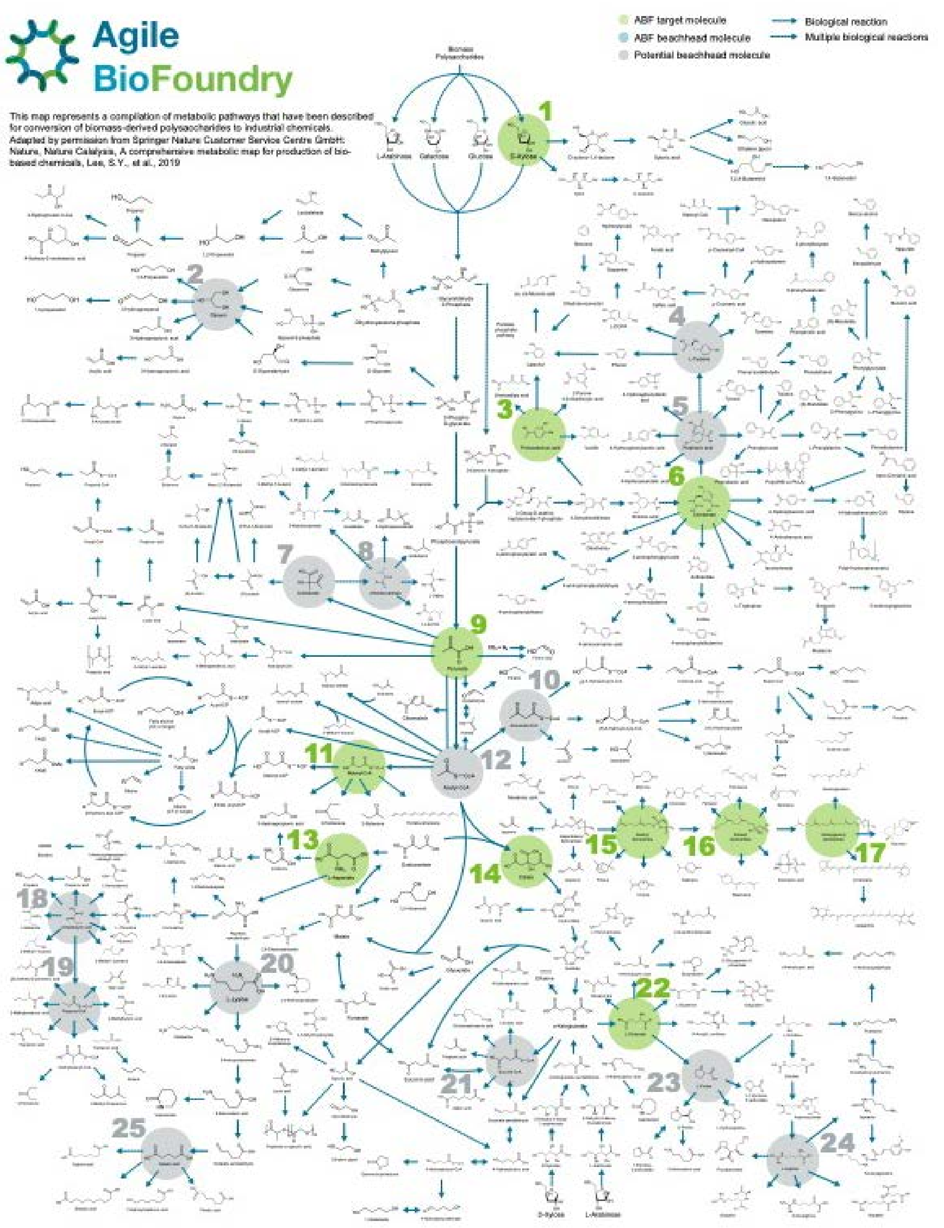
Beachhead map

01 Xylose
02 Glycerol
03 Protocatechuic acid
04 L-Tyrosine
05 Prephenic acid
06 Chorismate
07 Acetolactate
08 2-Ketoisovalerate
09 Pyruvate
10 Acetoacetyl-CoA
11 Malonyl-CoA
12 Acetyl-CoA
13 L-Aspartate
14 Citrate
15 Geranyl diphosphate
16 Farnesyl diphosphate
17 Geranylgeranyl diphosphate
18 2-ketobutyric acid
19 Propionyl-CoA
20 L-Lysine
21 Succinyl-CoA
22 L-Glutamate
23 L-Proline
24 L-Arginine
25 Glutaric acid

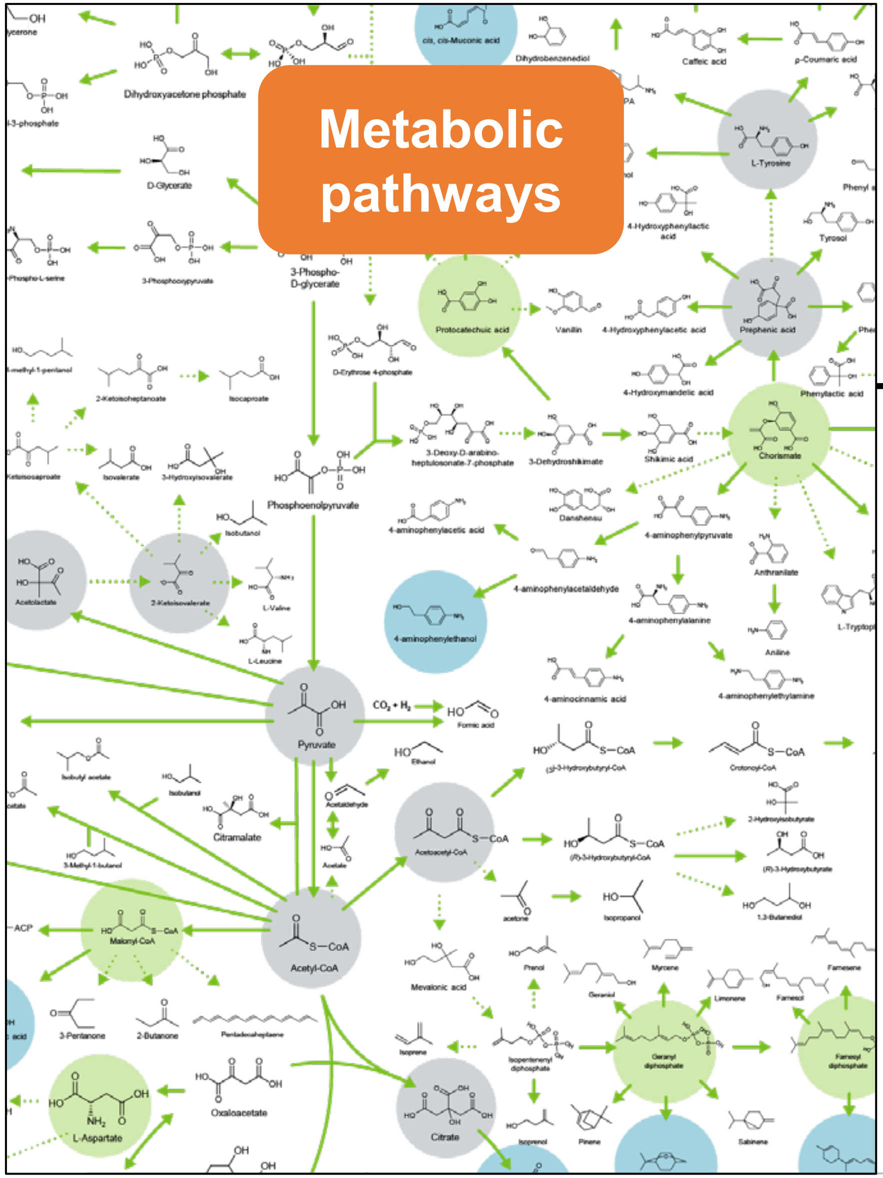
ABF Metabolic Coverage Map

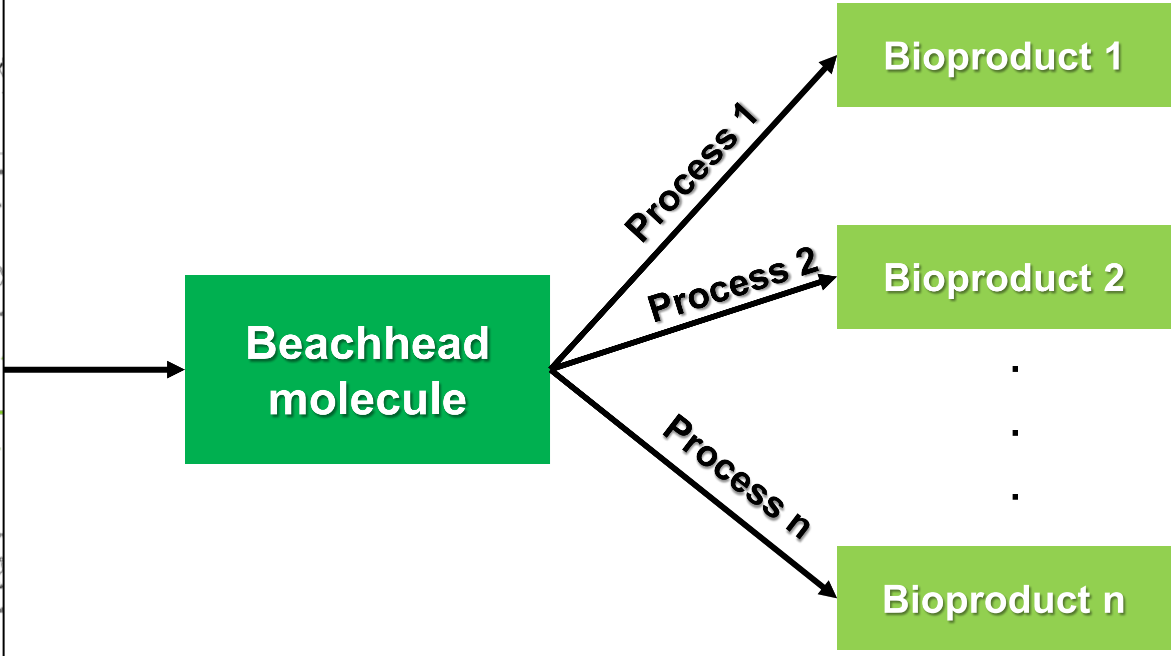
- ABF beachhead molecules
- Potential beachhead molecules



POC: Christopher Johnson, christopher.johnson@nrel.gov

Future directions: beachhead intermediates

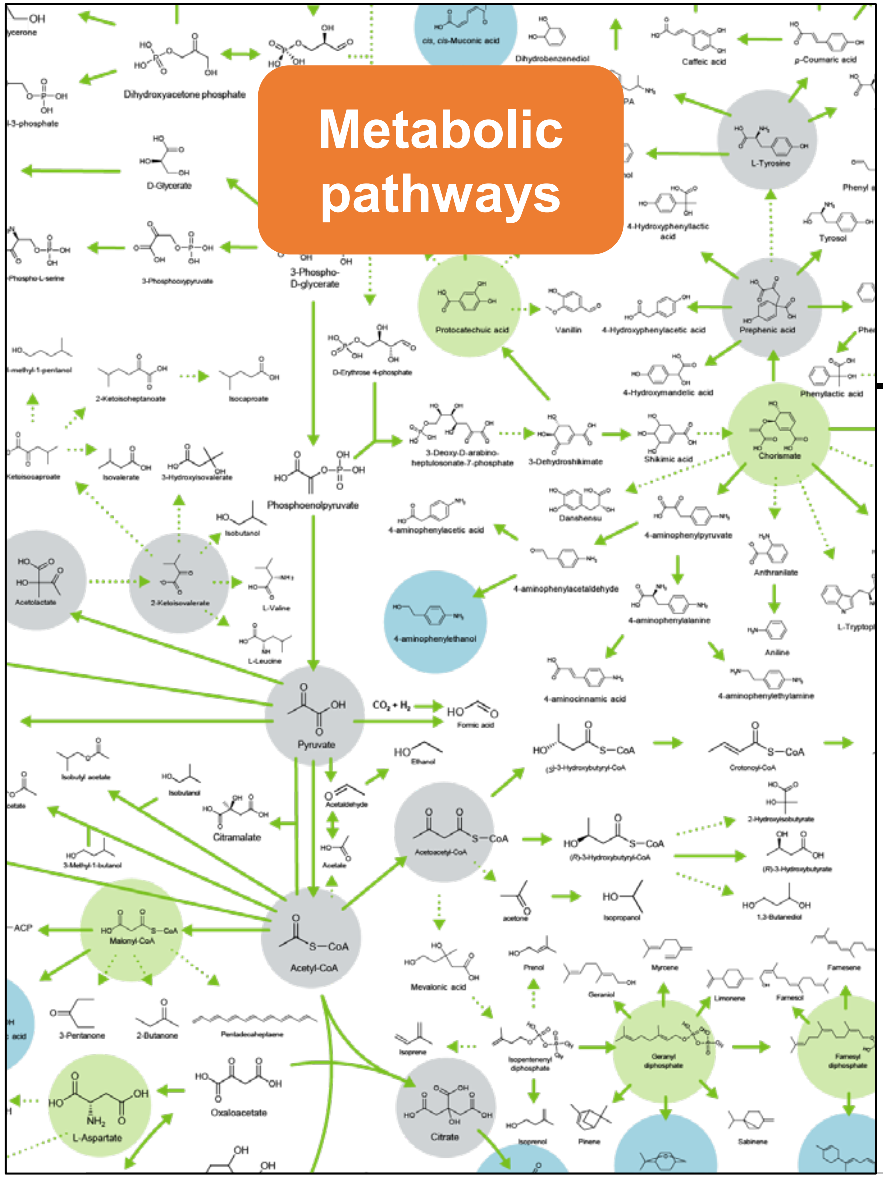




TEA/LCA for all possible bioproducts is not feasible

Instead: select a single exemplar molecule to represent each pathway

Future directions: beachhead intermediates



Beachhead molecule → **Exemplar molecule**

Similar processing parameters

- T/R/Y
- Downstream
- Aeration
- …

Fatty acids Isoprenoids Organic acids
Shikimate-derived compounds PHAs
Polyketides Flavonoids others

About adipic acid & cineole

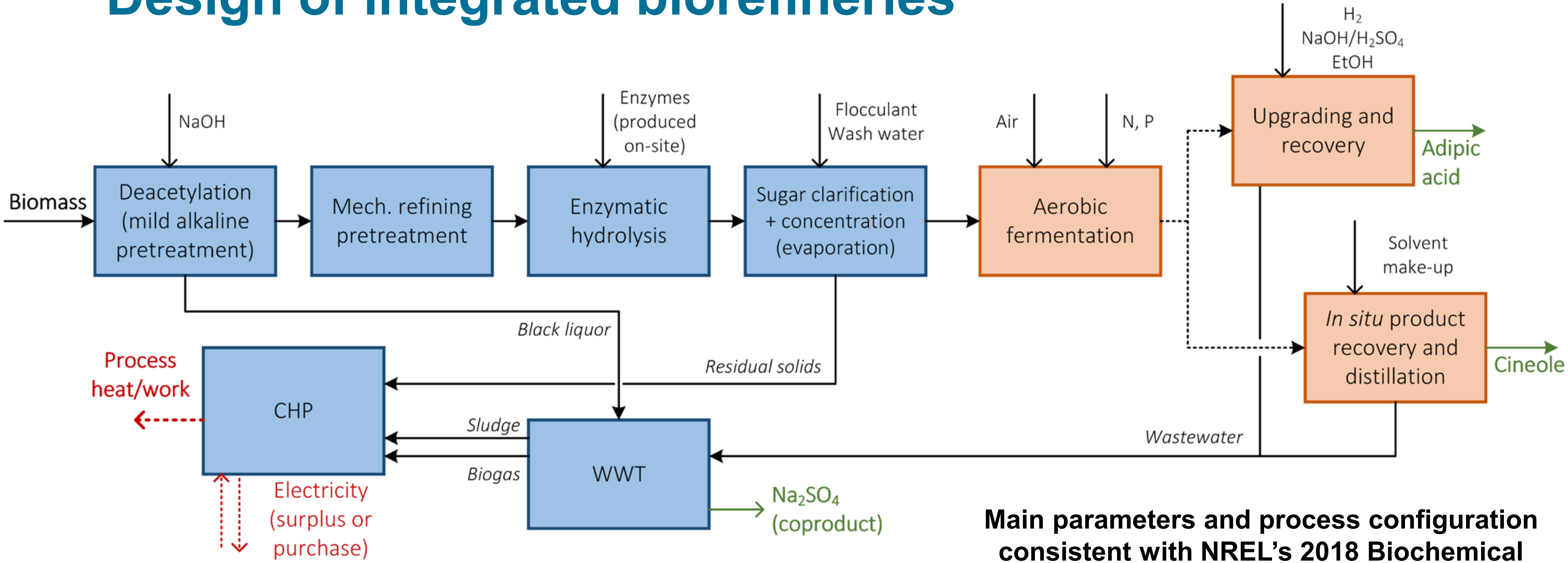
Adipic acid

- Widely used dicarboxylic acid
- High-value chemical with a market volume of ~2.6 million tons per year
- Demand expected to growth 3-5% globally
- Industrial applications include production of Nylon 66, polyurethanes, plasticizers, and food additives
- US is the leading producer (net exporter) and consumer of the compound

Cineole

- Natural organic compound, used as a fragrance (known as eucalyptol in lower purities)
- Mainly obtained through extraction from eucalyptus leaves
- Market likely restricted to hundreds of tons per year; high price
- New applications such as a natural insecticide, an industrial solvent, a backbone for organic synthesis, or a high-octane number gasoline blendstock

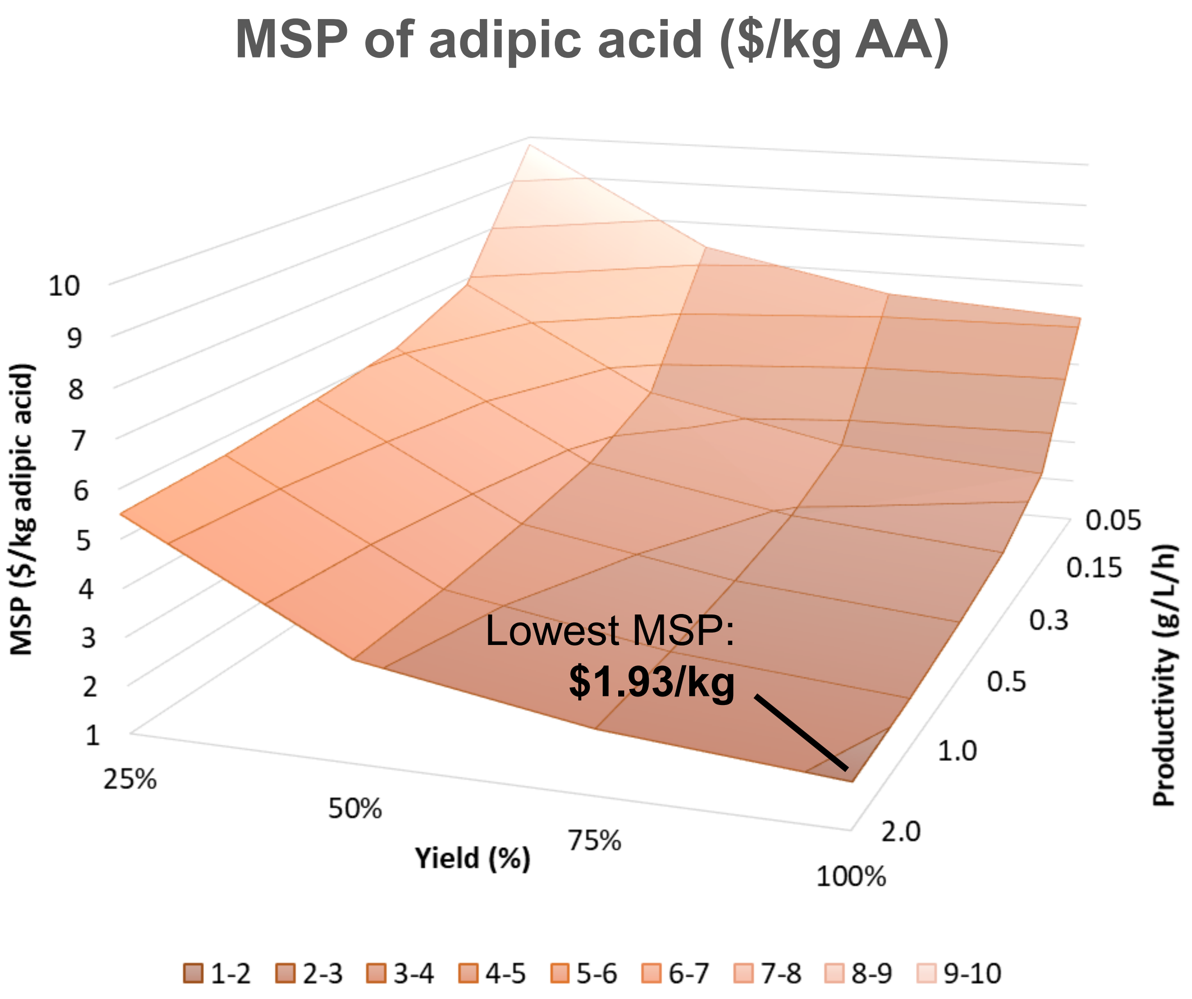
Design of integrated biorefineries



Main parameters and process configuration consistent with NREL's 2018 Biochemical Design Report
https://www.nrel.gov/docs/fy19osti/71949.pdf

Evaluate sensitivity drivers to key fermentation parameters (rate, yield) over a range of achievable values towards impacts on MSP and GHG emissions

TEA: adipic acid

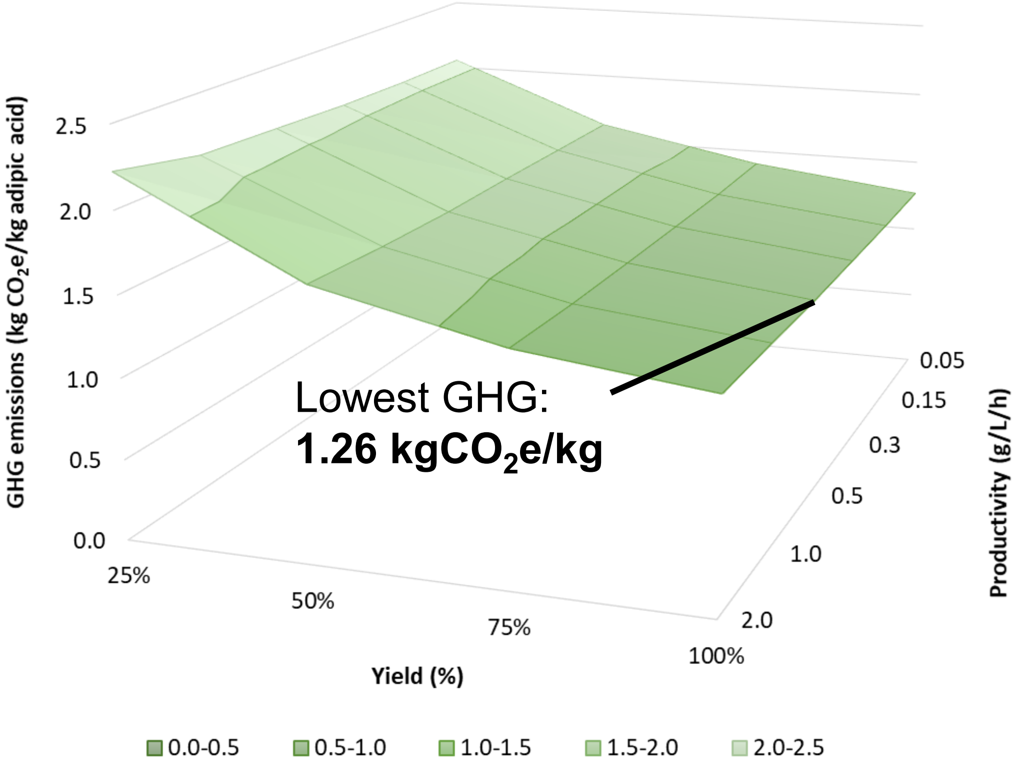


Reference market price: $1.89/kg AA

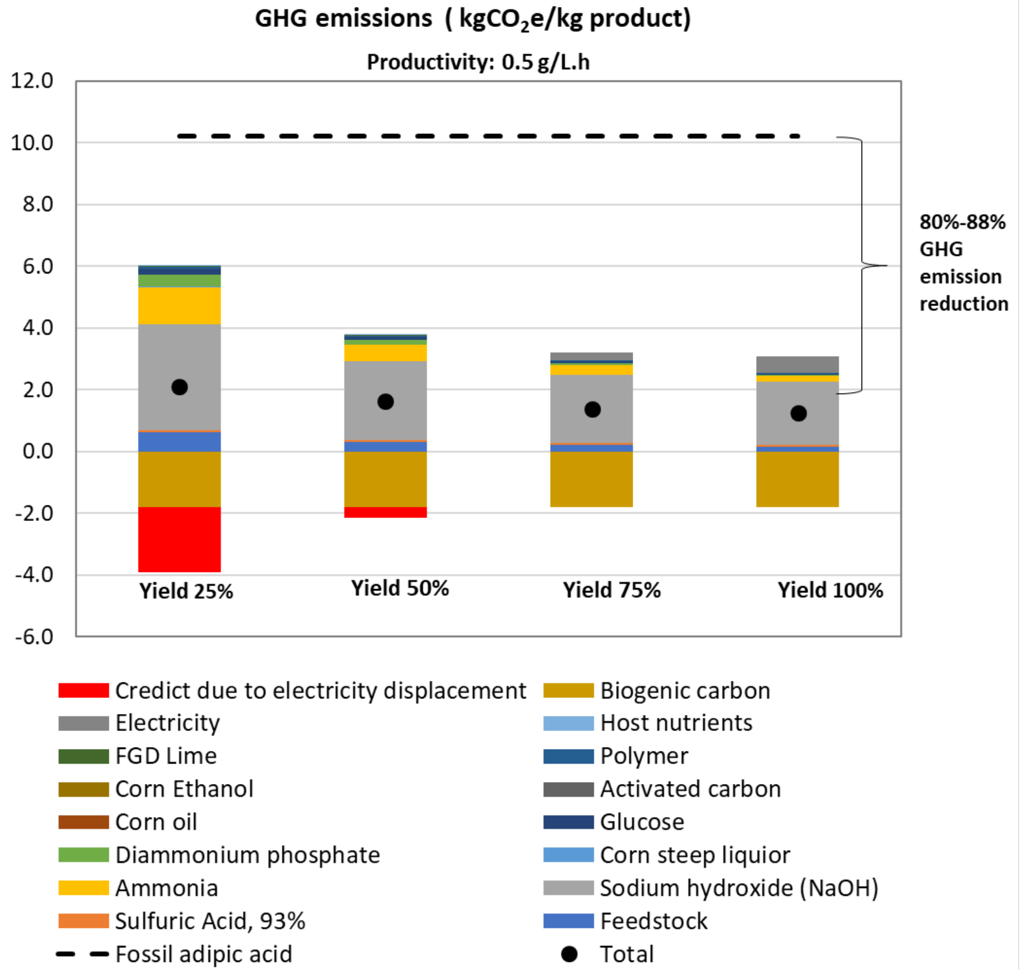
- MSP driven strongly by productivity below 0.3 g/L.h, starts to plateau at productivities higher than 0.3 – 0.5 g/L.h
- Considerable influence of MA yield when passing from 25% to 50% of theoretical yield
- Strategies to further reduce MSP:
  - Lowering feedstock costs
  - Increasing biorefinery scale
  - Using lower-cost separation strategy
  - Adding value to lignin

LCA: adipic acid

GHG emissions of adipic acid ($kg\ CO_2e/kg\ AA$)

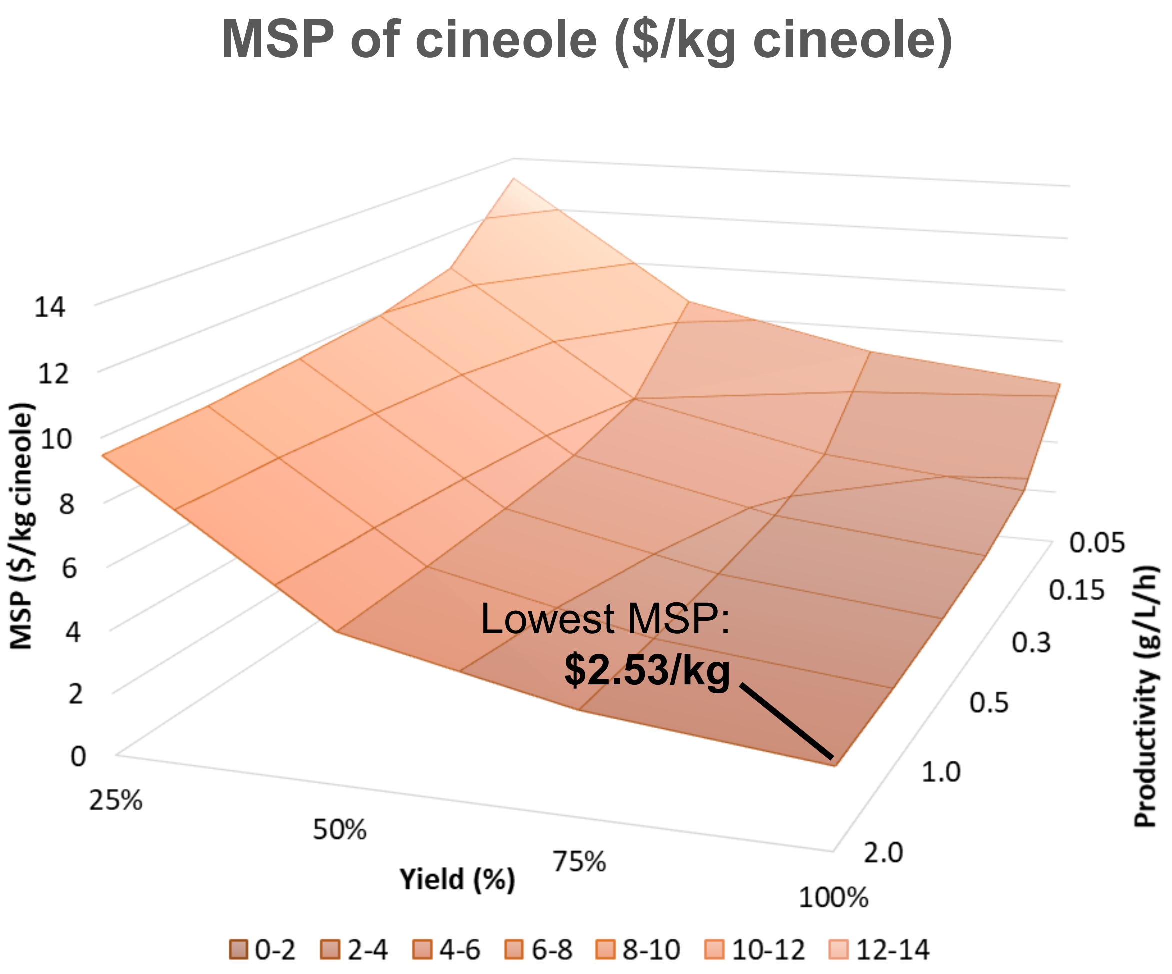


Productivity plays a considerably smaller role on LCA than it does on TEA



The lowest GHG emission value is obtained with the highest yield at different productivities (0.5; 0.3;0.15)

TEA: cineole



Reference market price: $30/kg cineole

- Biorefinery able to deliver cineole at MSP lower than $5/kg with productivities above 0.5 g/L.h and product yield of 50%
- Low market volume likely limits deployment of multiple full scale biorefineries
  - Development of new applications such as an industrial solvent, insecticide/repellant, or backbone for organic synthesis could enable reaching larger markets

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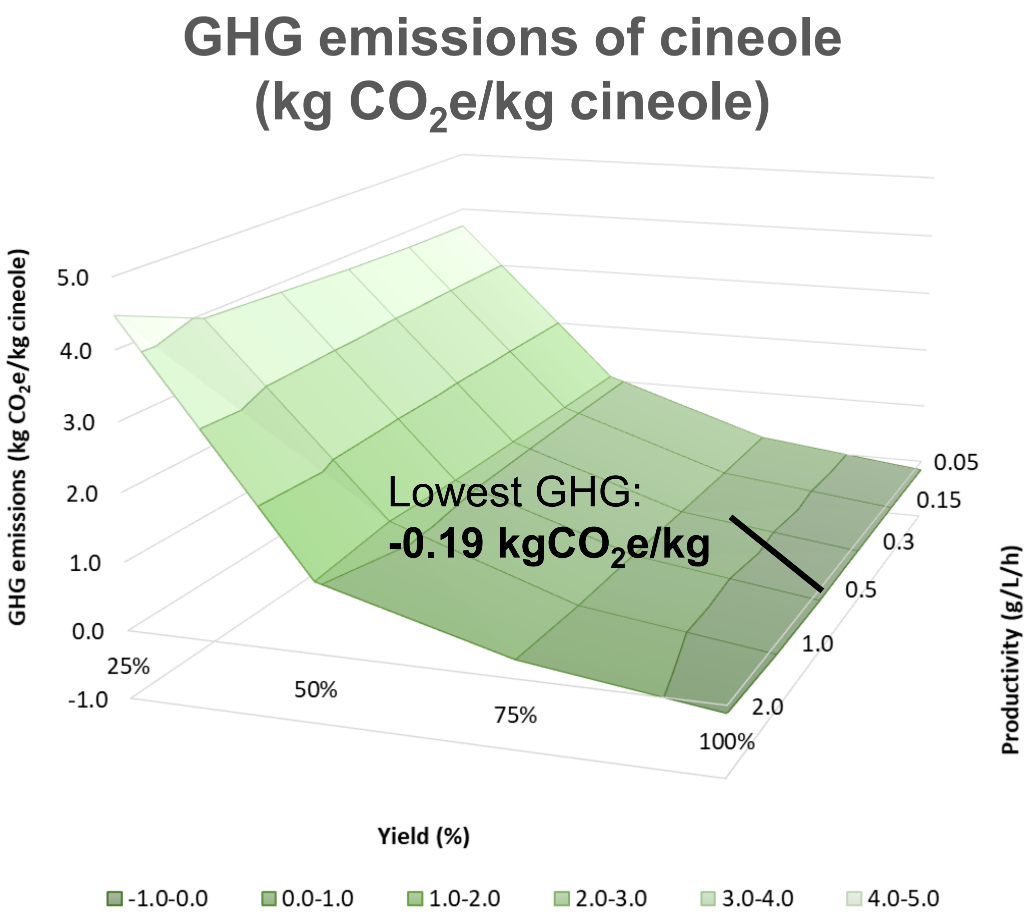
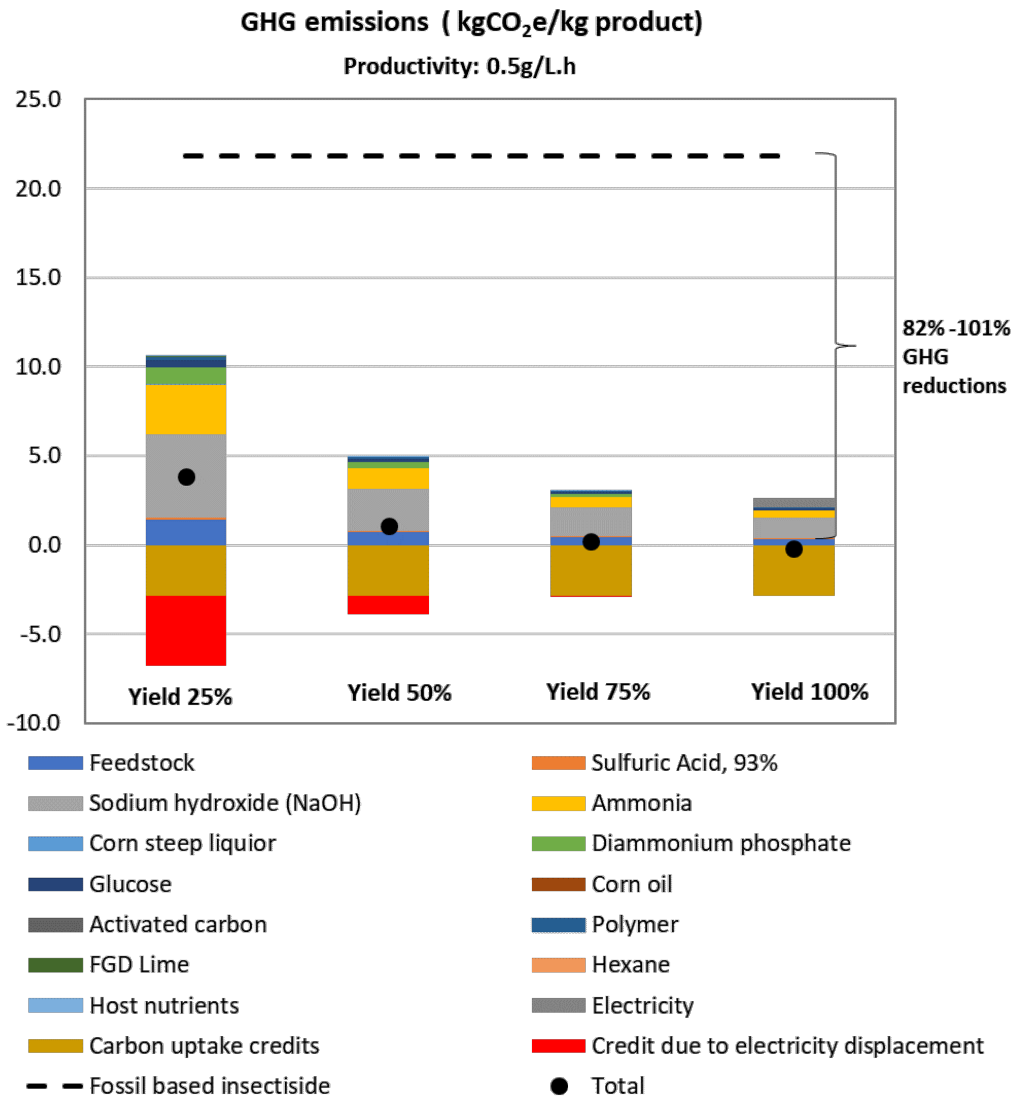
LCA: cineole





GHG emissions varied greatly at lower yields

GHG emissions decrease as the yield improves

Conclusions

- Two selected BH/EX pairs were assessed in this work:
  - Protocatechuate to muconic acid/adipic acid
  - Geranyl diphosphate to cineole

- The proposed agile TEA/LCA approach to scan metabolic pathways was able to provide insights into the main barriers for development of bioproducts
  - **TEA**: minimum production conditions for economical production of adipic acid and cineole were determined
  - **LCA**: improvement in terms of GHG emissions in comparison to fossil-based counterparts was seen under any fermentation conditions

- Future developments will expand this type of analysis to other BH/EX pairs
  - Covering the full metabolic space of interest to ABF and the industry
  - Informing ABF R&D priorities

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Thank you!

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Questions?