ADVANCES IN CATALYSIS FOR HYDROCARBONS

RESULTS FROM ZEOCAT-3D, C123 & BIZEOLCAT EU RESEARCH PROJECTS

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Conceptual process design, techno-economic and environmental assessment of C123 modular processes

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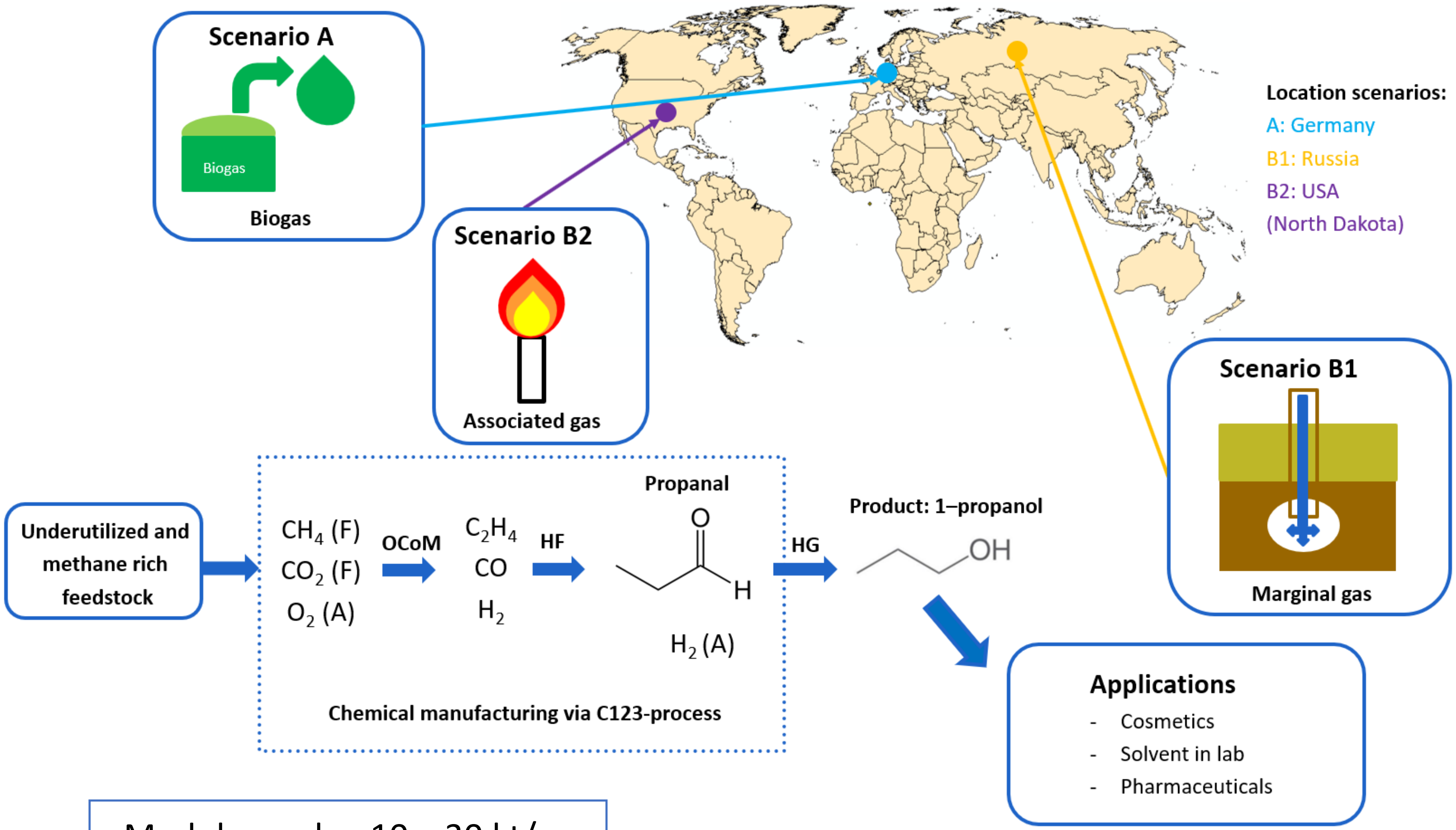
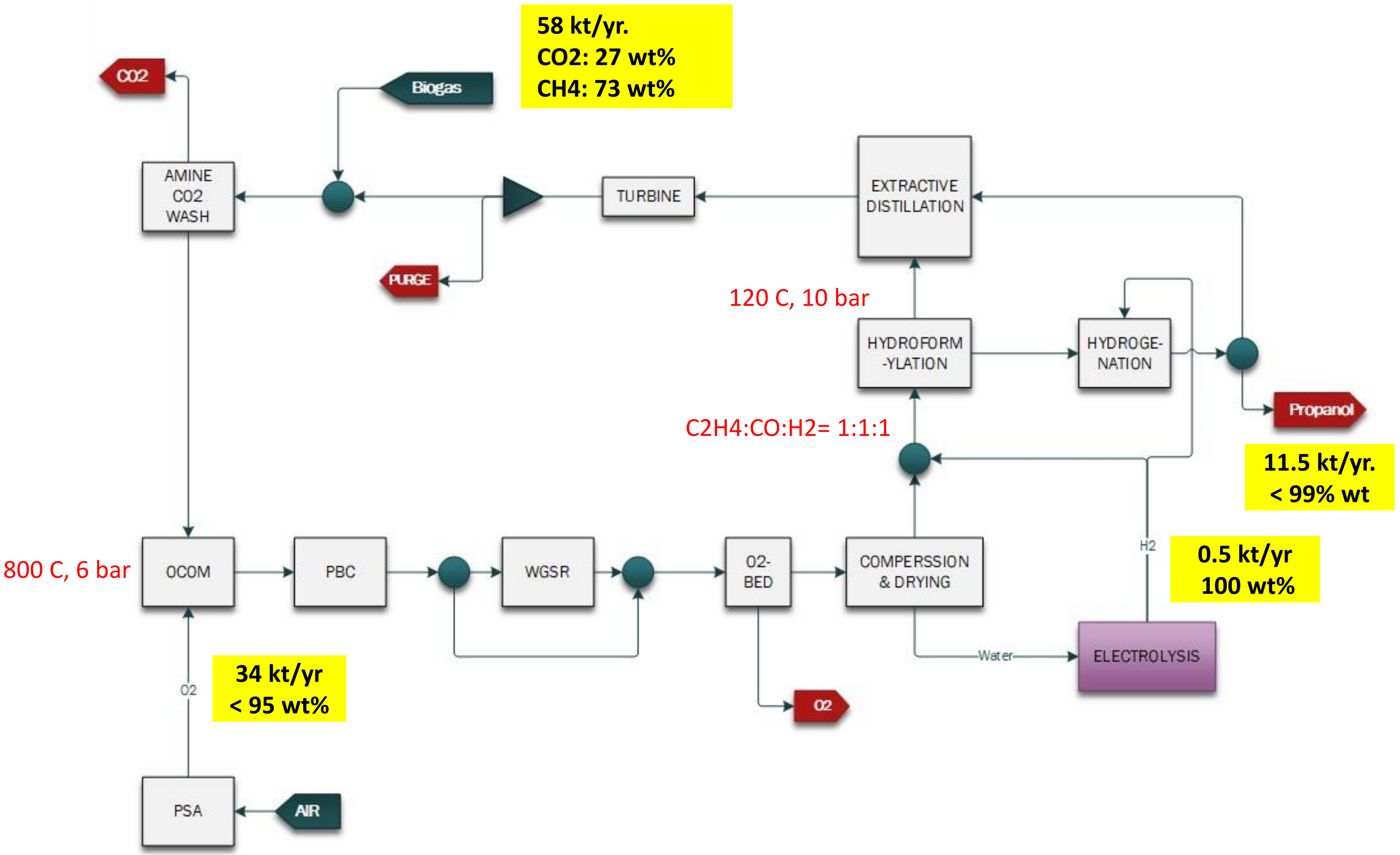
Introduction: C123-project



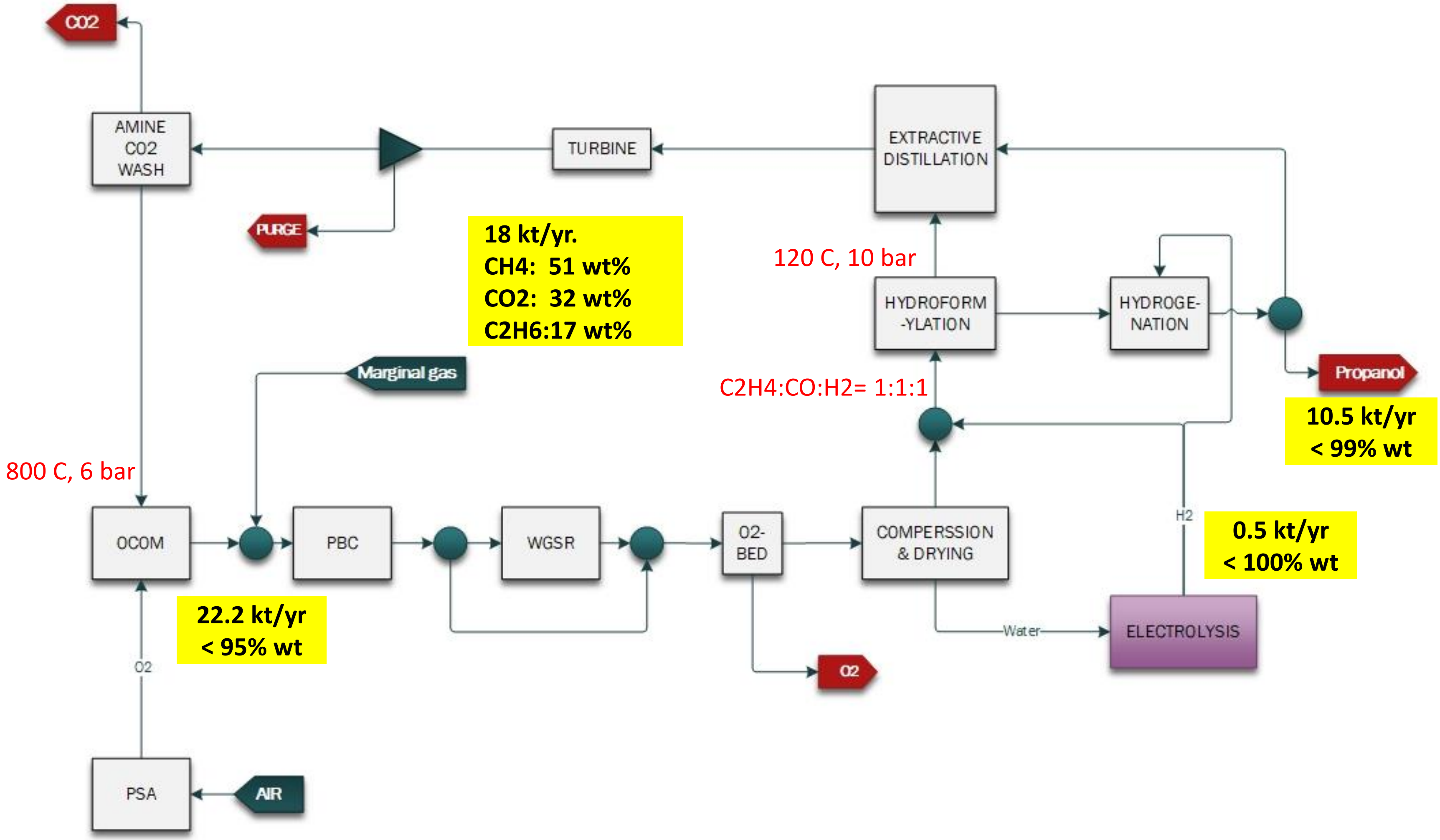
Modular scale : 10 – 30 kt/yr.

Scenario A : Biogas _ Modular scale



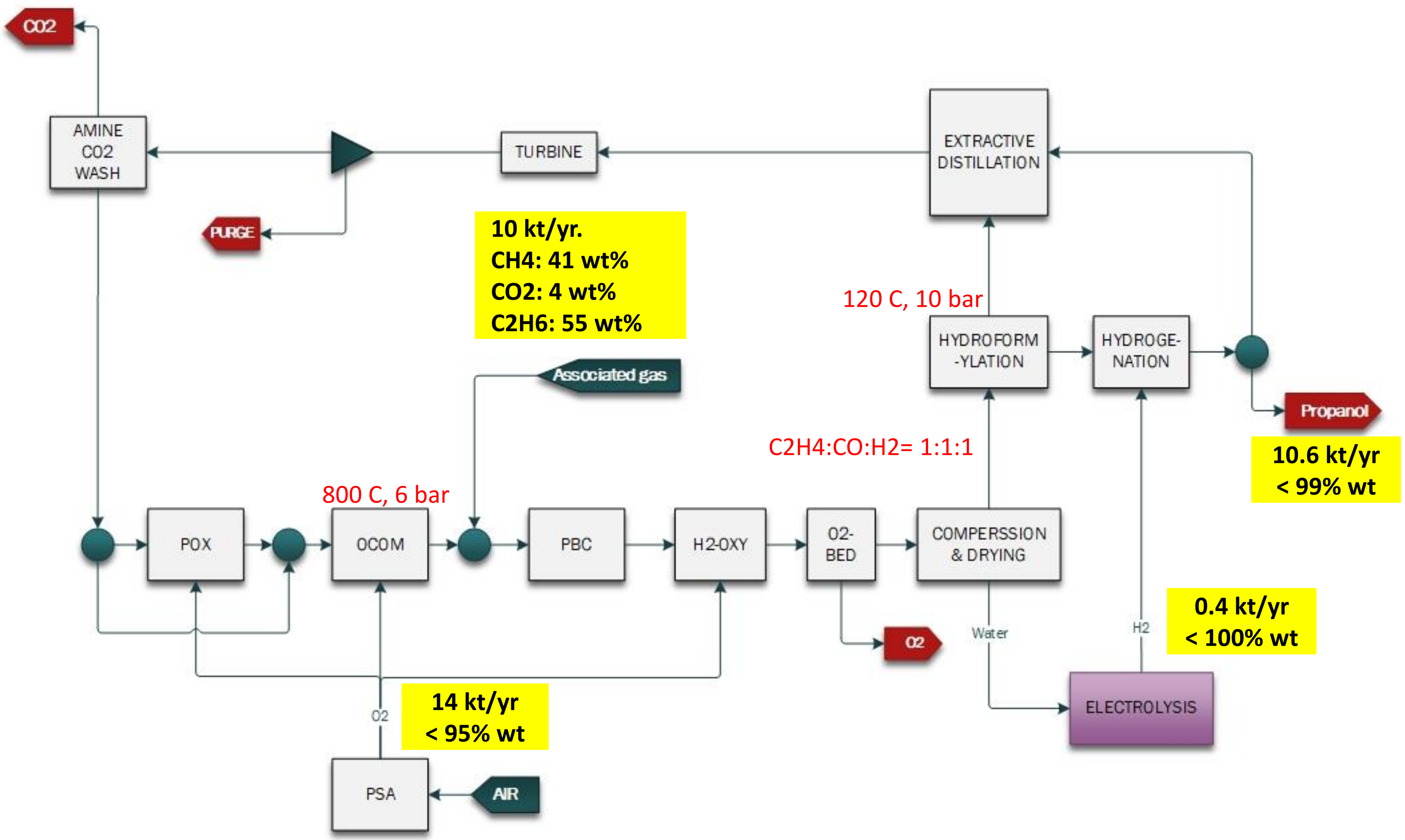
- Large quantities of CO_2 present in the fresh Feed.
- 99 % of CO_2 is captured
- X-CH_4 : 35% per pass
- PBC is used to a convert ethane to H_2 and ethylene
- Water gas shift reactor adjust the C_2H_4:CO to 1:1
- Process water removed is sufficient to supply water demand for electrolysis.

Scenario B1: Marginal gas _ Modular scale



- Considerable quantities of **Ethane** is present in the feed.
- Marginal gas is fed directly to PBC ➔ ethane cracking
- The OCOM reactor feed is the recycle stream leaving the CO2 wash unit
- X-CH4 : 35% per pass
- PBC is used to a convert ethane to H2 and ethylene
- Water gas shift reactor adjust the C2H4:CO to 1:1
- Process water removed is sufficient to supply water demand for electrolysis.

Scenario B2: Associated gas _ Modular scale



- Large quantities of **Ethane** is present in the feed.
- Marginal gas is fed directly to PBC ➔ ethane cracking
- Excess H2 is selectively oxidized.
- Partial oxidation of C1 & C2+ is used to adjust the ratio of C2H4:CO: H2 to 1:1:1
- The OCOM reactor feed is the recycle stream leaving the partial oxidation reactor.
- X-CH4 : 35% per pass
- PBC is used to a convert ethane to H2 and ethylene
- Process water removed is sufficient to supply water demand for electrolysis.
- No additional H2 is needed for Hydroformylation.

EU-project Horizon 2020 GA No. 814557 C123 Methane oxidative conversion and hydroformylation to propylene

Modular Scale Plant

- What is Modular plant?
  - Smaller, standardized, and pre-fabricated modules that can be easily assembled, transported, and interconnected at the site of installation.

- Why Modular scale Plant?
  - Efficient use of resources ➔ Utilizing smaller feedstocks.
  - Difficulty to build onsite ➔ very remote locations such as scenarios B1 & B2
  - Economy of scale is a challenge ➔ resolved by implementing number-up approach.
  - Flexibility ➔ Easier to modify and expand the plant as needed.
  - Reduced construction time and cost ➔ pre-fabrication off-site reduce construction time and plant site is significantly reduced, leading cost savings.
  - Safety ➔ minimizes on-site work, reducing the potential for accidents and injuries.
  - Transport ➔ Pre-fabricated modules are containerized which makes it easier transport.
  - Easier maintenance and repair ➔ exchange of damaged equipment with new ones

https://www.prweb.com/releases/2013/5/prweb10705036.htm

Modular scale plant : Design considerations

- Production scale 10 -30 kt/yr.
- Modules should fit in container ➔limited to the following maximum dimensions:
  - Length: 12.2 m
  - Height: 2.39 m
  - Width: 2.35
  - Maximum gross weight : 30.5 tonne
- Maximize the selectivity and conversions of the reactors
- Minimize the intermediate separation steps.

- Cost-effectiveness ➔ optimizing the process design for maximum efficiency and productivity.
- Portability ➔ designed to be easily transported and installed on site.
- Integration ➔ designed to be integrated with other process equipment and systems to ensure smooth operation and efficient production

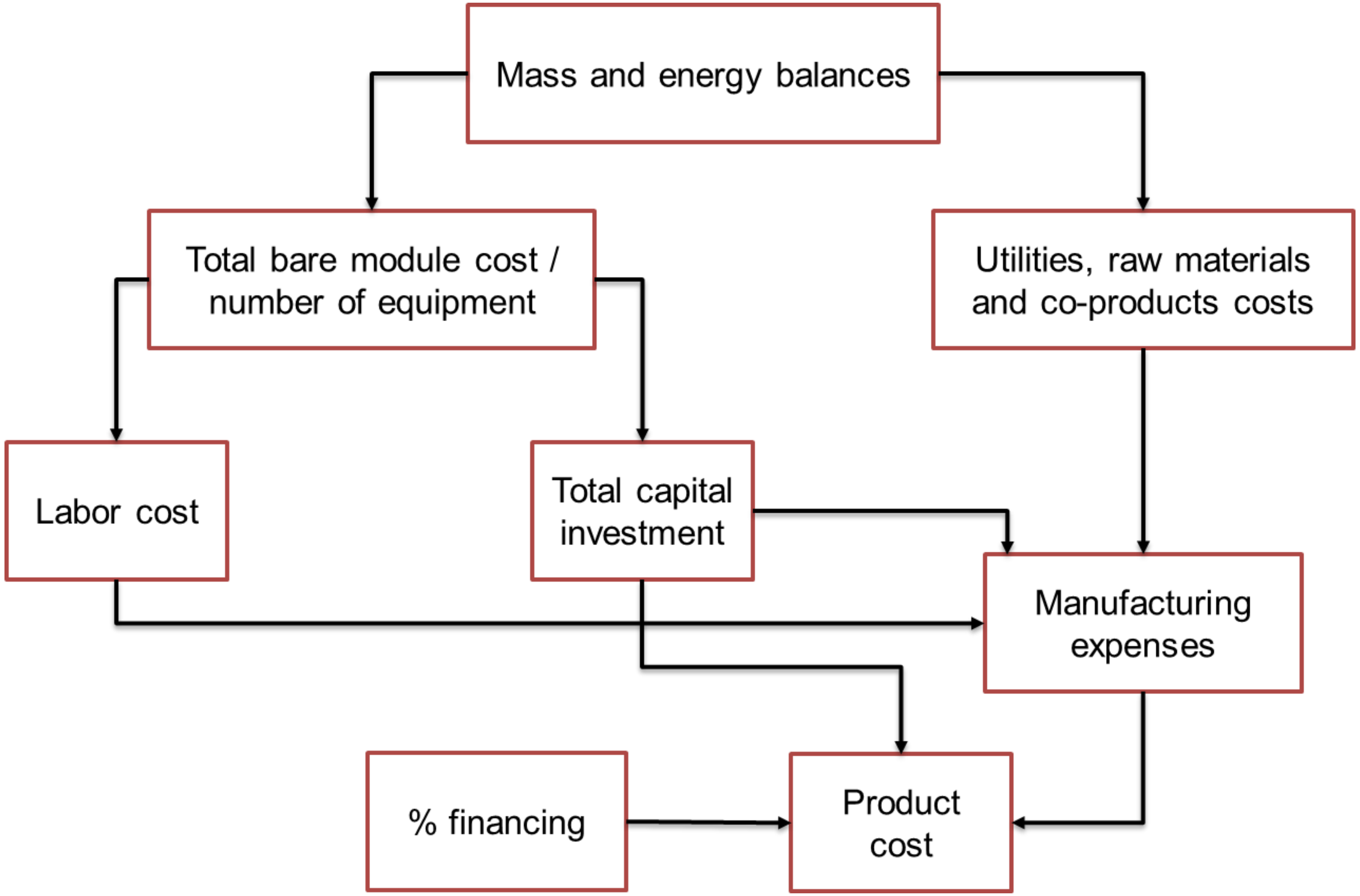
Preliminary Techno-Economic Assessment

- Costing tool : PROSYN® costing
- Basic data
  - Cost date — September 2021
  - Currency — US Dollar
  - Location details

    Scenario A : Germany — Location factor : 0.81 (vs. USGC)
    Scenario B : US Midwest — Location factor : 1.02 (vs. USGC)
- General
  - Utilities ISBL
    - Natural gas
  - Utilities OSBL
    - Cooling water
    - MP steam (and LPS return)
    - Power generation
    - Electrolysis + PSA
    - Waste water treatment
    - Hydrogen Production

- Assumptions and considerations
  - Space velocities / residence times from literature were used to size OCoM section reactors, Hydroformylation reactor and propanal hydrogenation reactor.
  - Catalysts and catalysts regenerations were not considered in this study.

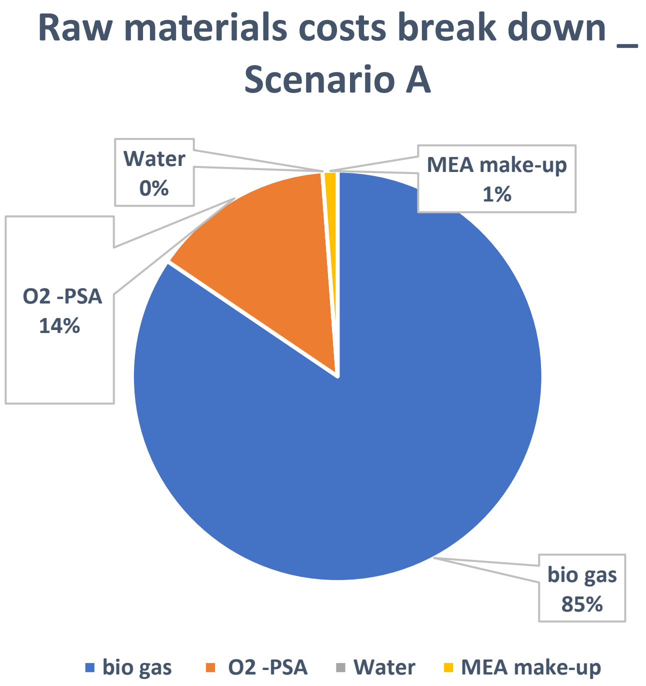
Process economics estimation approach

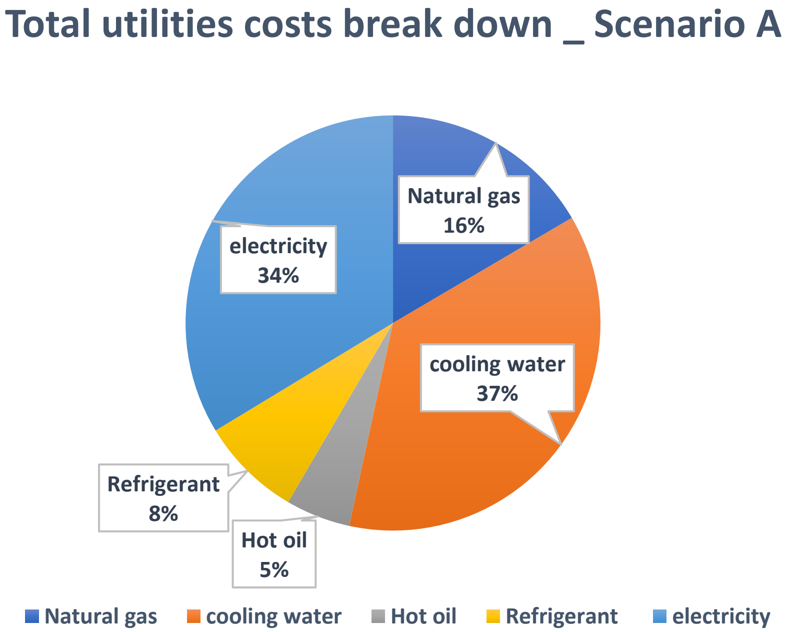


Capital cost

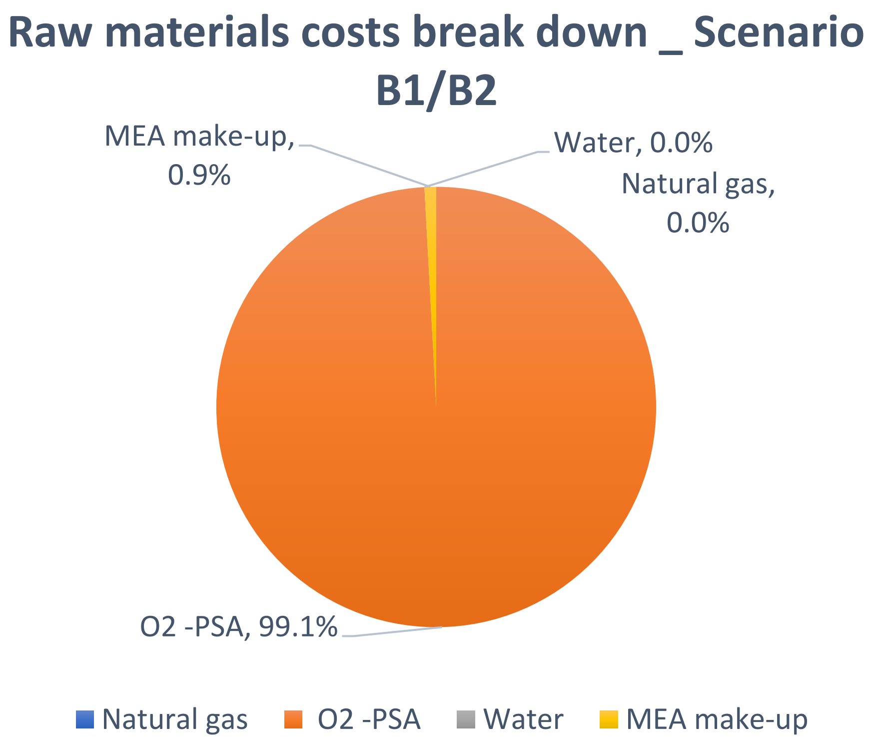
		Scenario A	Scenario B1/B2
Capital cost calculation		x 1000 $	
Heat exchangers		$ 653	$ 619
Process vessels		$ 3,156	$ 4,976
Pumps and compersso rs		$ 3,155	$ 3,222
Drives		$ 244	$ 261
Furnaces		$ 582	$ 679
Quoted equipment		$ 12	$ 14
Unlisted equipment	15%	$ 1,170	$ 1,466
Total bare module cost		**$ 8,972**	**$ 11,238**
Contingency	15%	$ 1,346	$ 1,686
Fee	3%	$ 269	$ 337
Total module capital cost		**$10,588**	**$ 13,261**
Land cost	3%	$ 262	$ 296
site development	5%	$ 437	$ 493
auxilary buildings	4%	$ 350	$ 395
off-site facilities	25%	$ 2,185	$ 4,935
total grass roots capital		**$13,821**	**$ 19,380**
startup expenses	2%	$ 276	$ 388
working capital	15%	$ 2,073	$ 2,907
total capital investment		**$16,171**	**$ 22,675**

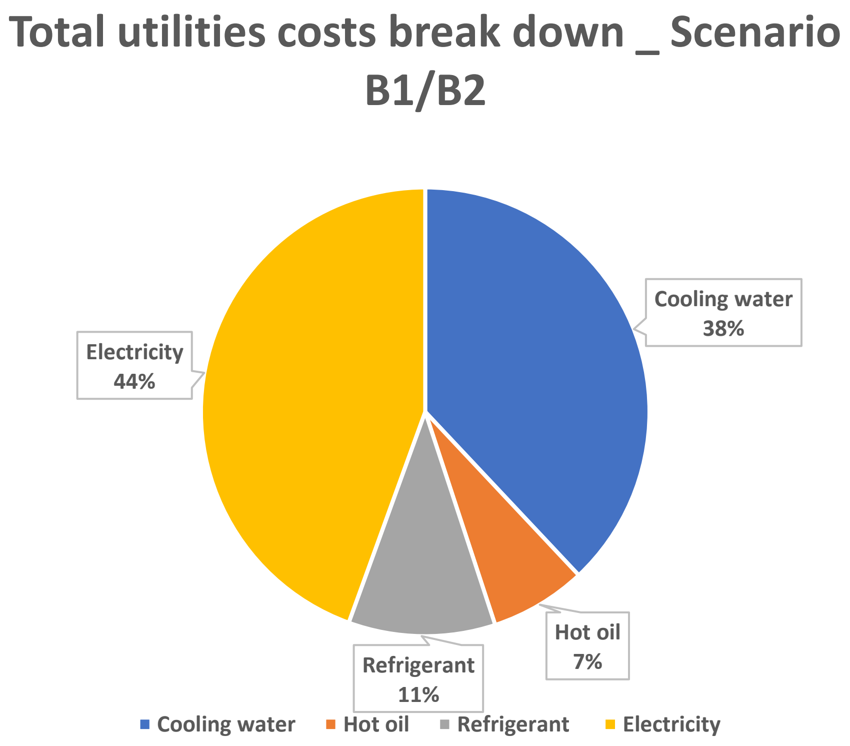
Scenario A: Utilities, raw materials, co-products and wastes





Scenario B1/B2: Utilities, raw materials, co-products and wastes





Manufacturing expenses

Manufacturing expenses (annual)			Scenario A $/yr	Scenario B1/B2 $/yr
Direct				
Raw materials			$ 9,825,628	$ 1,278,431
operating labour			$ 1,394,640	$ 1,394,640
supervisory and clerical labour	15%	of operating labour	$ 209,196	$ 209,196
utilities			$ 2,050,613	$ 1,418,643
maintenance and repairs	6%	of grass roots capital	$ 829,288	$ 1,162,803
operating supplies	10%	of maintenance	$ 82,929	$ 232,561
laboratory charges	15%	of operating labour	$ 209,196	$ 209,196
patents and royalties	3%	of manufacturing expenses excl. financing	$ 650,516	$ 377,051
SUM				
Indirect				
Overhead, packaging, and storage	50%	of labour, supervision, maintenance	$ 1,216,562	$ 1,659,983
local taxes	1%	of grass roots capital	$ 138,215	$ 193,800
insurance	1%	of grass roots capital	$ 138,215	$ 193,800
SUM				
General expenses				
Administrative costs	25%	of overhead	$ 304,141	$ 414,996
distributing and selling	10%	of manufacturing expenses excl. financing	$ 2,168,386	$ 1,256,836
Research and development	5%	of manufacturing expenses excl. financing	$ 1,084,193	$ 628,418
SUM				
Depreciation				
Depreciation	10%	of grass roots capital	$ 1,382,147	$ 1,938,005
SUM				
Total			**$ 21,683,864**	**$ 12,568,358**
Plant capacity (N-propanol produced)		kton/year	13	11
Manufacturing product cost price		**$/ton**	**$ 1,613**	**$ 1,096**

Summary of results

	Case 1a	Case 2a	Case 1b	Case 2b
	Scenario A : 10bar + PSA	*Scenario A: 10bar + PSA*	*Scenario B1/B2 : 10bar + PSA*	*Scenario B1/B2 : 10bar + PSA*
Production capacity (kt/yr)	**13**	**30**	**12**	**30**
Total capital investment (M$)	**16.2**	**28.3**	**22.7**	**39.6**
Manufacturing expenses (M$)	**21.7**	**44.1**	**12.1**	**21.9**
Product cost (k$/tonne)	**1.61**	**1.47**	**1.00**	**0.73**
Market price (k$/tonne)		**1.68**		

Notes
- Case 2a has the lowest manufacturing product cost prices due to the effect of economy of scale.
- Heat integration is not fully considered.
- Economy of scale is very prominent.
- Catalyst and catalyst regeneration costs were not considered.

Life Cycle analysis

Jordy Motte

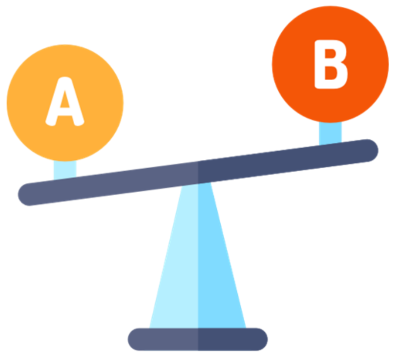
Methodology

Environmental performance assessment

Resource efficiency analysis

Methodology: Environmental performance assessment

Goal



Comparison
C123 scenarios

Scope

Cradle-to-gate

Functional unit

1 kg propanol

(With purity of
99.5 weight%)

Selected KPIs

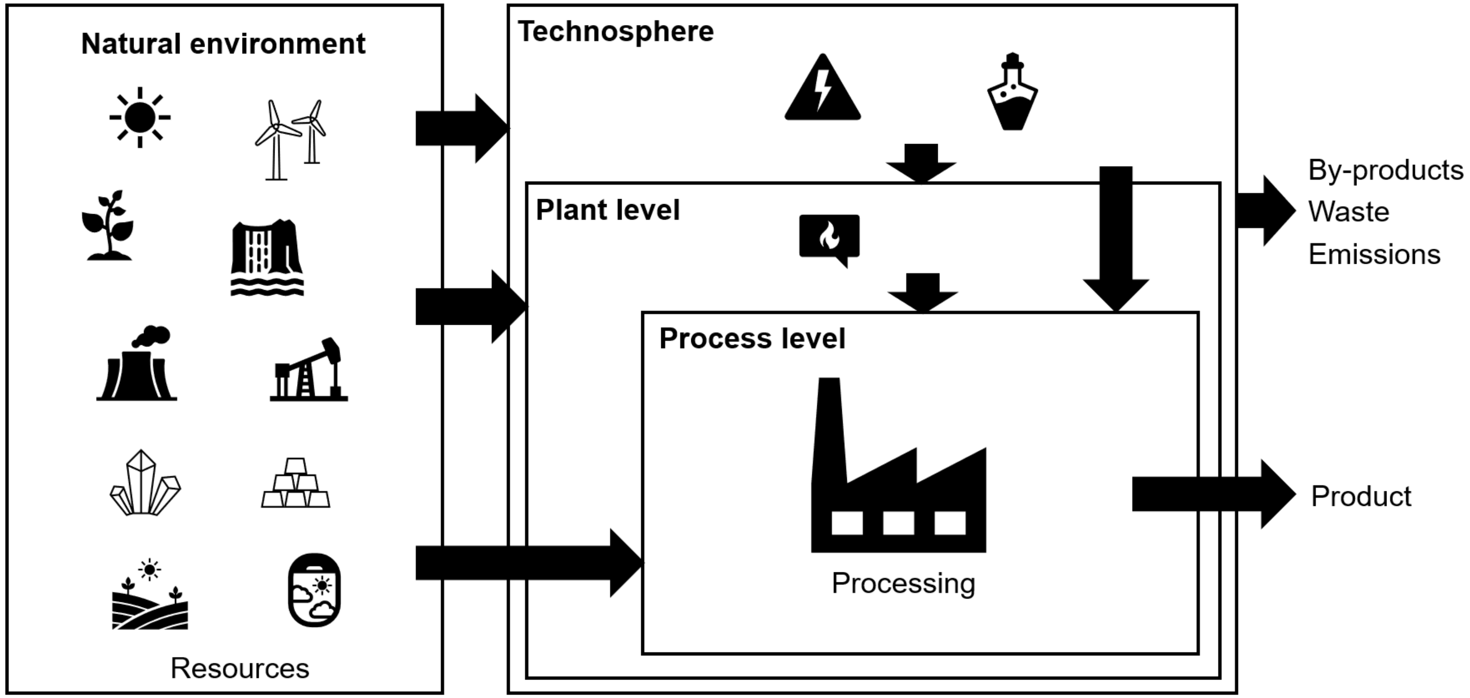
- Global warming burden
- Energy input + % from fossil resources
- Water consumption
- Human health damage

Retrieved from sustainability metrics of IChemE

Data collection: - Aspen simulations for C123 process
- Literature and Ecoinvent database for supporting processes (e.g., oxygen production, electricity production)

For more details: https://doi.org/10.1021/acs.iecr.2c00808

Methodology: Resource efficiency analysis



At life cycle level:

CEENE method (Dewulf et al., 2007)

$$CDP = \frac{Ex_{product} + Ex_{by-products}}{CEENE}$$

CDP = cumulative degree of perfection
CEENE = cumulative exergy extraction from the natural environment

At process and plant level:

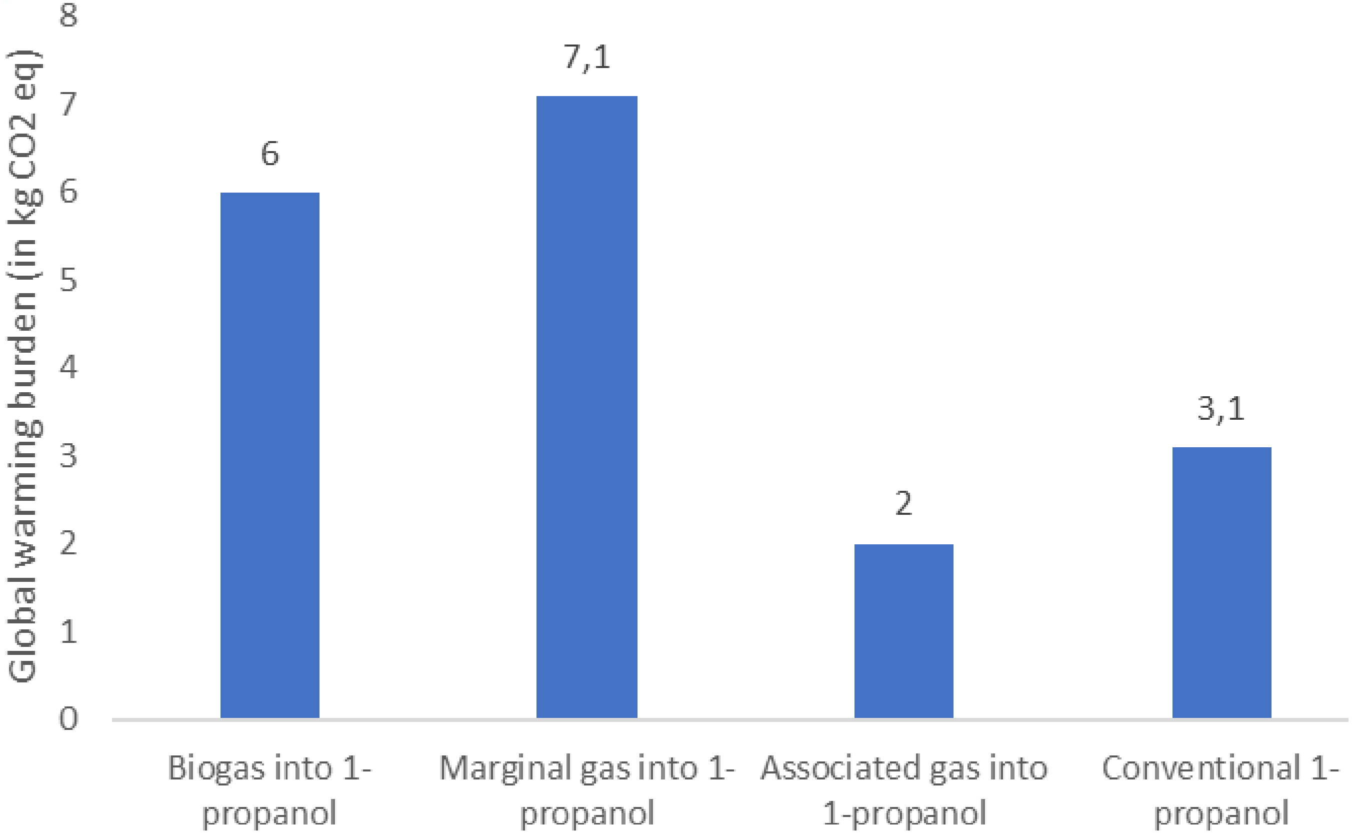
Exergy calculations, Exergy = useful part of energy

$$\eta_r = \frac{\sum Ex_{useful\ outputs}}{\sum Ex_{inputs}}$$

For more details: https://doi.org/10.1016/j.jclepro.2022.134843

EU-project Horizon 2020 GA No. 814557 C123 Methane oxidative conversion and hydroformylation to propylene

Preliminary results environmental performance assessment



(Scenario A) (Scenario B1) (Scenario B2)

Including avoided flaring

Main contributors:

Only for scenario A:

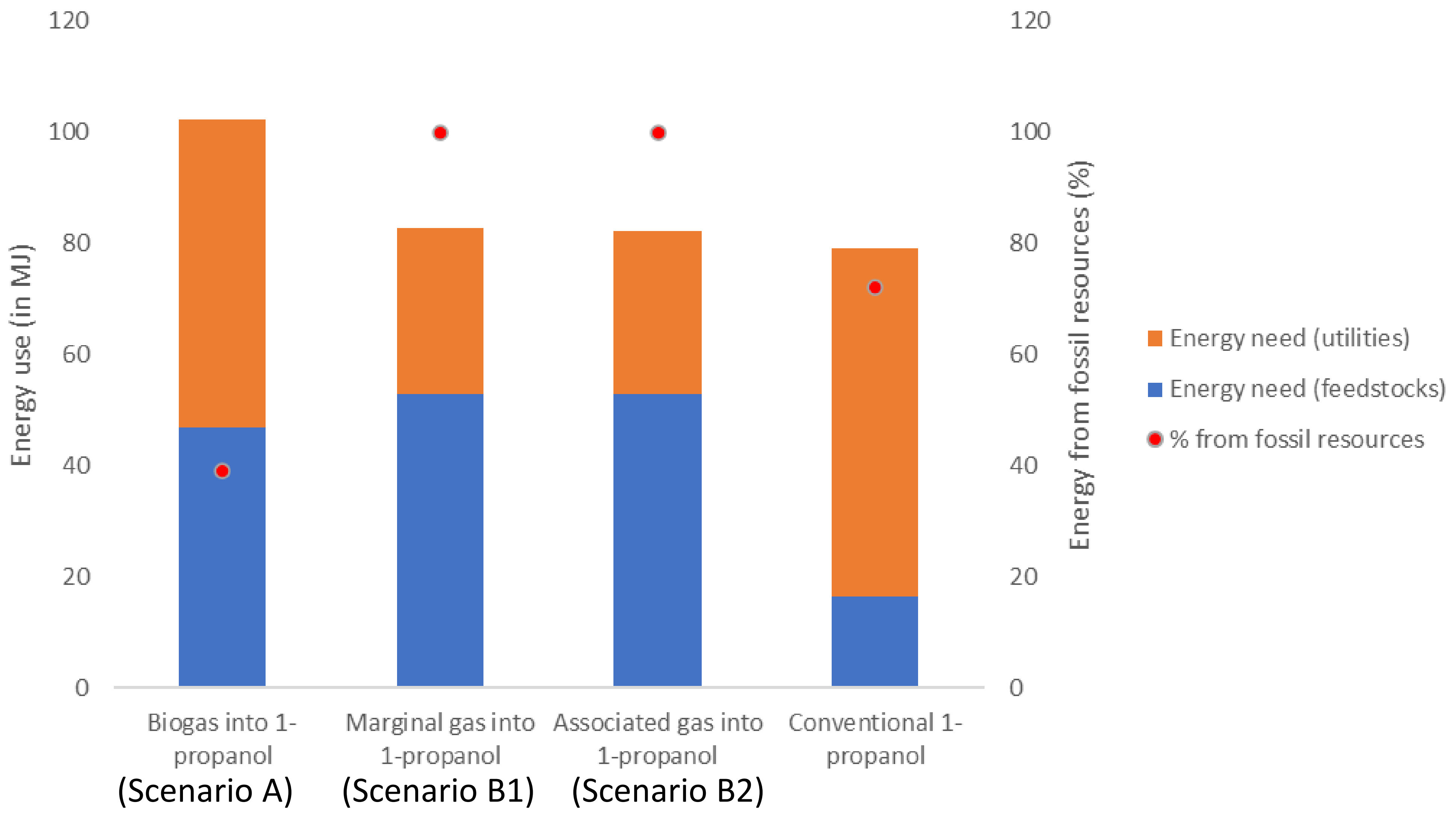
- Biogas production & upgrading

For all scenarios:

- Oxygen production for oxidative conversion of methane (OCoM)
- Electricity production (for compression, hydrogen production)
- Direct CO_2 emission in CO_2 reduction stage (except scenario BG)
- Heat production for preheating (e.g., OCoM)

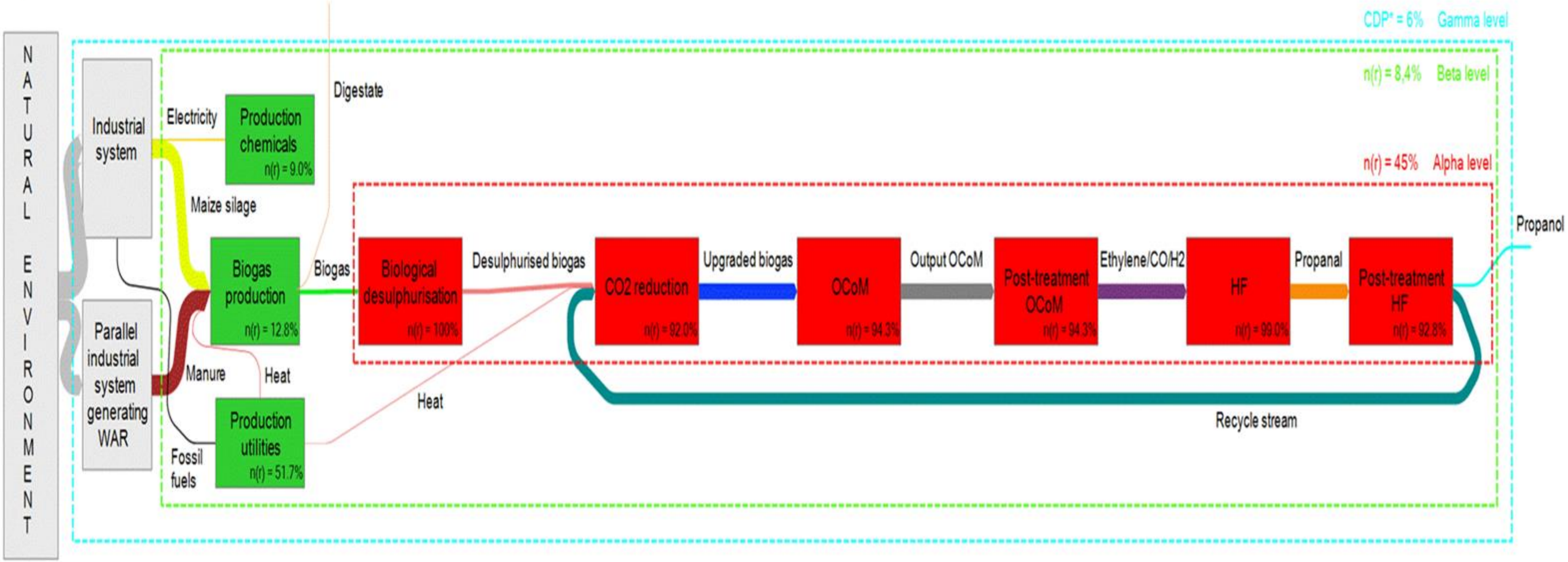
Comparsion with 1-propanol not fair at this moment due to different technology readiness level!

Preliminary results environmental performance assessment



Preliminary results resource efficiency analysis

Scenario A:



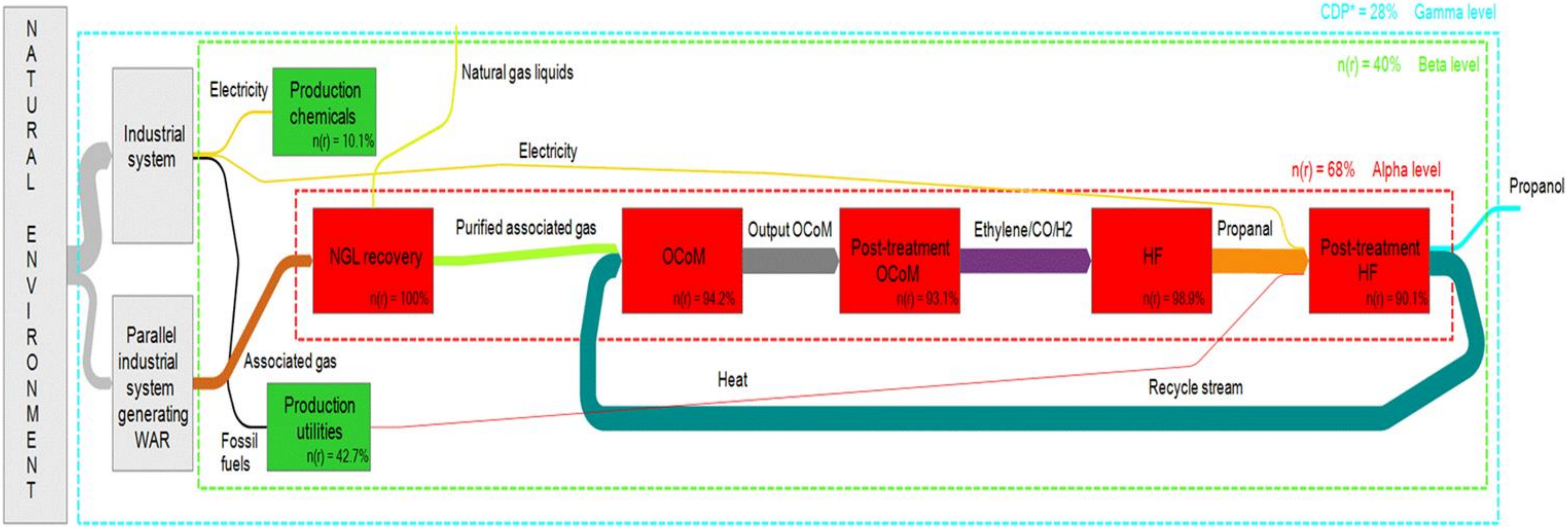
All C123 production steps have a high exergetic efficiency

Low exergetic efficiency for biogas production

Low methane conversion into propanol per pass due to high exergy content of recycling stream

Preliminary results resource efficiency analysis

Scenario B2:



Higher CDP than scenario A

However, scenario A uses more renewable resources and can be part of a circular economy (open loop)

Preliminary conclusions

- Environmental assessment:
  - The lowest impact on climate change ➔ Scenario B2
  - The highest exergetic efficiency on life cycle level ➔ Scenario B2

- Modular scale plants can utilize widely available and wasted resources
  - Easier to design and build ➔ Cost reductions and easier to modify and transport
  - Economy of scale is the main challenge ➔ resolved by number-up approach

THANK YOU

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