Techno-economics of the synthesis route from CO_2 and clean H_2 to polycarbonate polyols

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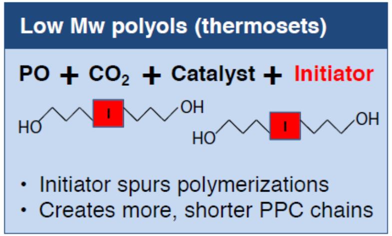
KEROGREEN Winter School
10.2.2022

Agenda

- Process route to polyols & background
- Results from preliminary TEA of BECCU-polyols
- Updated process simulation with Aspen Plus
- Suggested improvements & conclusions
- Discussion

Process route to polyols & background

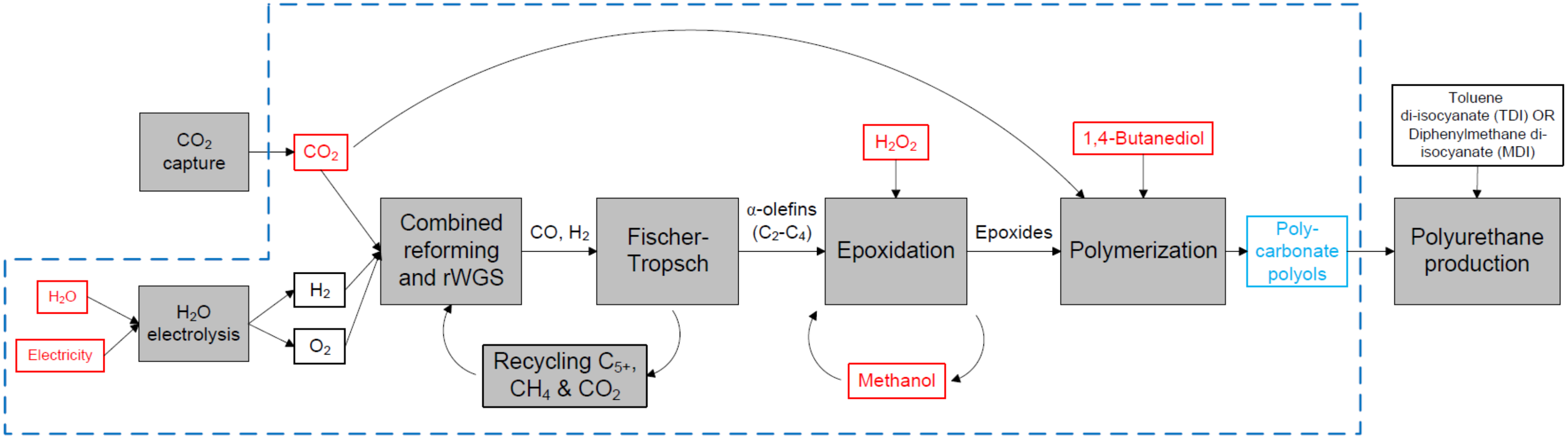
Polycarbonate polyols – high value chemicals and plastics

Term	Definition	Structural formula
Polycarbonate polyol	Low molecular weight polymer, linear aliphatic polycarbonate, derived from the copolymerization of carbon dioxide and an epoxide, containing two or more terminal hydroxyl groups (Qin & Wang, 2019)	 (Raschka et al., 2018)

- High value product, selling price can be even 6 000 €/tonne
- Applications: polyurethanes, coatings, adhesives, …

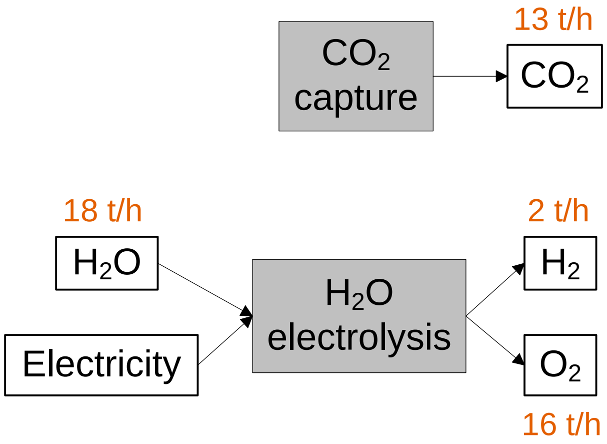
BECCU-polyols from biogenic CO_2 & green H_2

- The process is based on the **production of olefins** through reverse water-gas shift (rWGS) and Fischer-Tropsch (FT) reaction steps
- The olefins are further converted to epoxides through oxidation reactions by peroxides and epoxides are polymerized together with CO_2 to obtain polyols
- The yield of C_2-C_4 olefins is maximized to be used in polyol production



Carbon dioxide & hydrogen as starting materials

- CO_2 from biogenic sources with MEA
  - 50 €/tonne capture & processing cost assumed
- H_2 from alkaline electrolysis (AEC)
  - 100 MW electrolyser (η=67%)
  - 60 M€ electrolyser & costs of water and electricity



Results from preliminary TEA of BECCU-polyols

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Assumptions & results

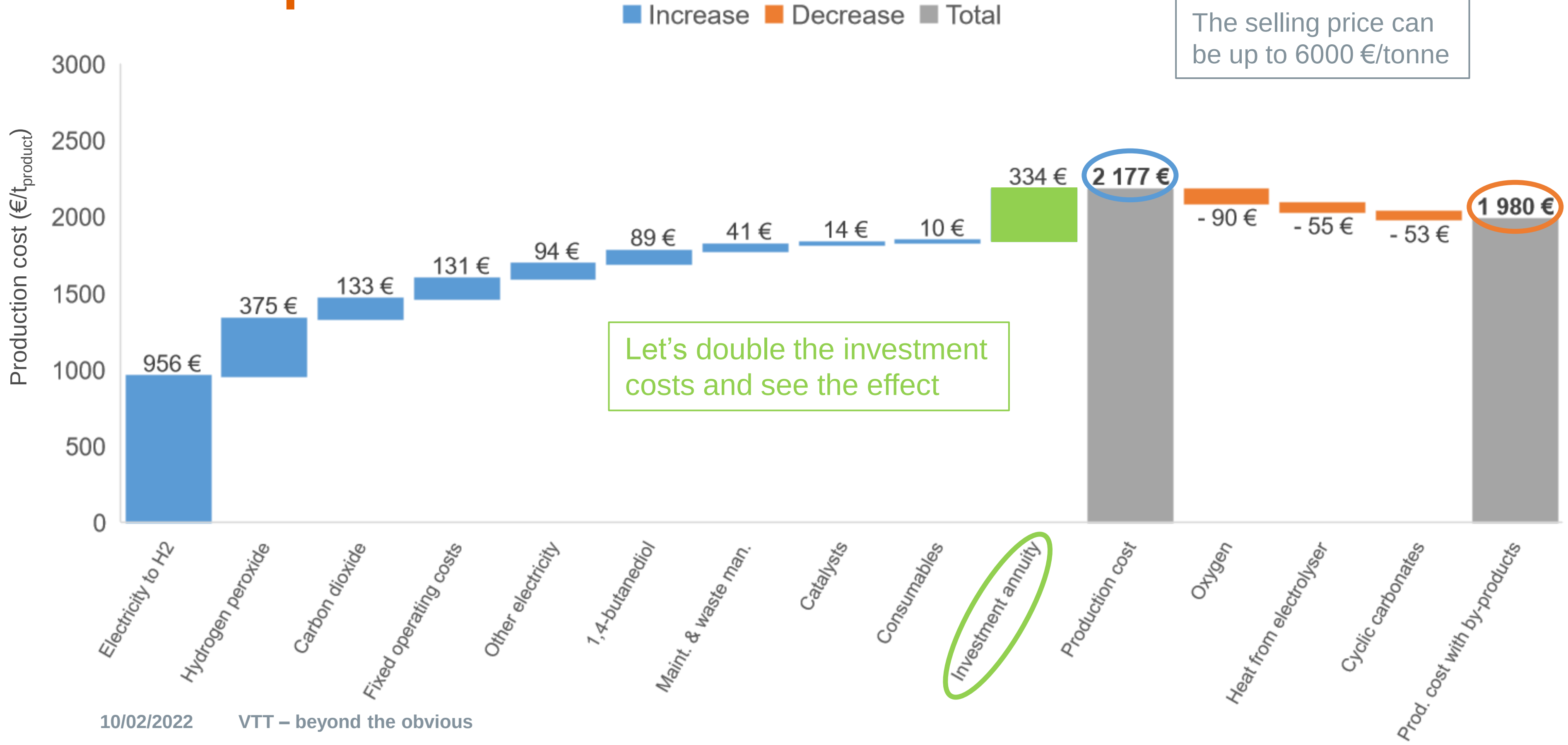
Inputs	Price	Outputs	Price
Electricity (total)	45 €/MWh	Cyclic carbonates	900 €/t
Hydrogen peroxide	550 €/t	By-product heat	20 €/MWh
CO_2 supply	50 €/t	By-product oxygen	40 €/t

Other parameters	
Electrolyser electricity input	100 MW_e
Annual plant operation time	8 000 h
Total investment cost estimate *(20 years and 8% WACC for annuity)*	124 M€

IN	
CO_2 need	100 kt/a
H_2 need	16 kt/a

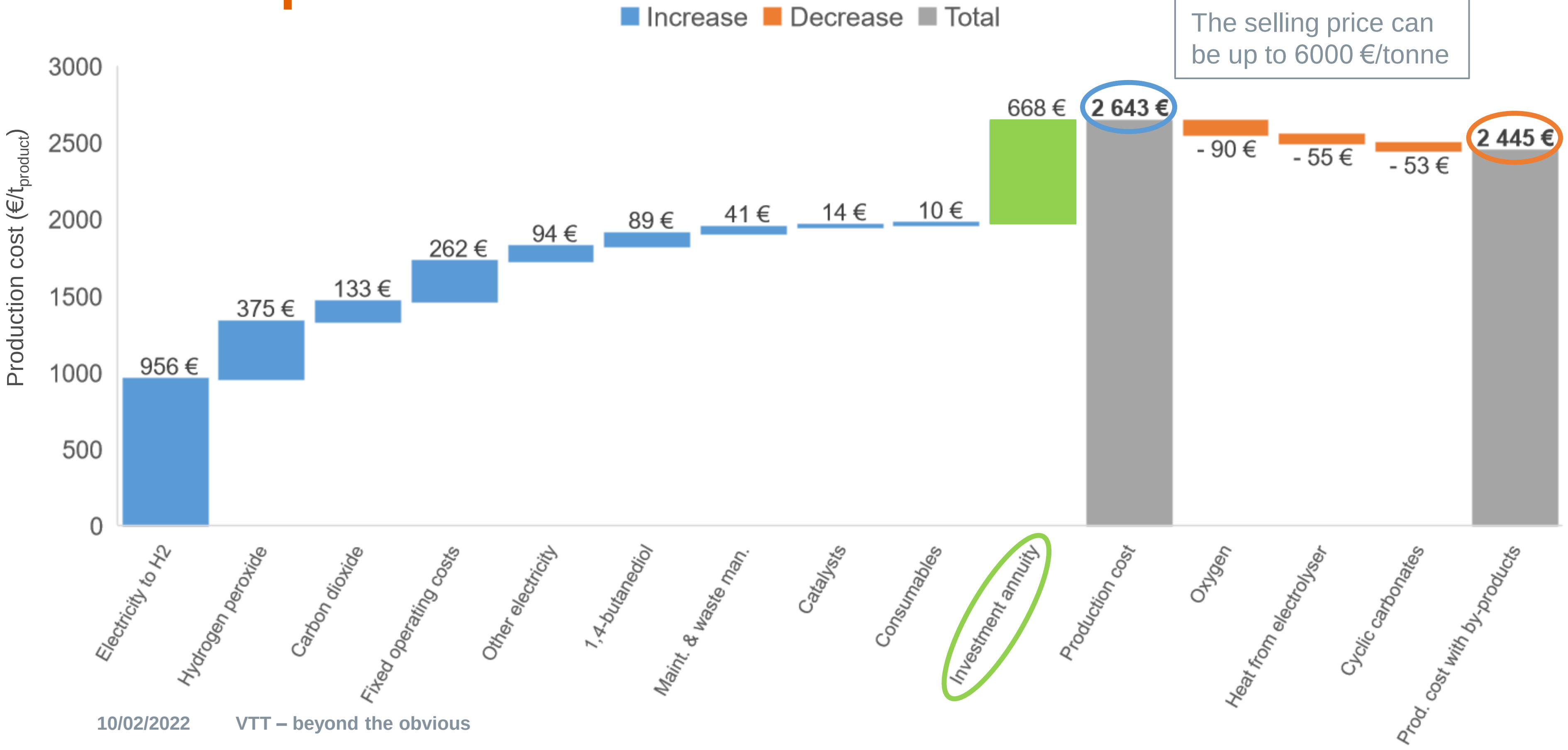
OUT	
Polycarbonate polyols	38 kt/a
Cyclic carbonates	2 kt/a
Excess oxygen	84 kt/a

Production cost estimation with preliminary assumptions



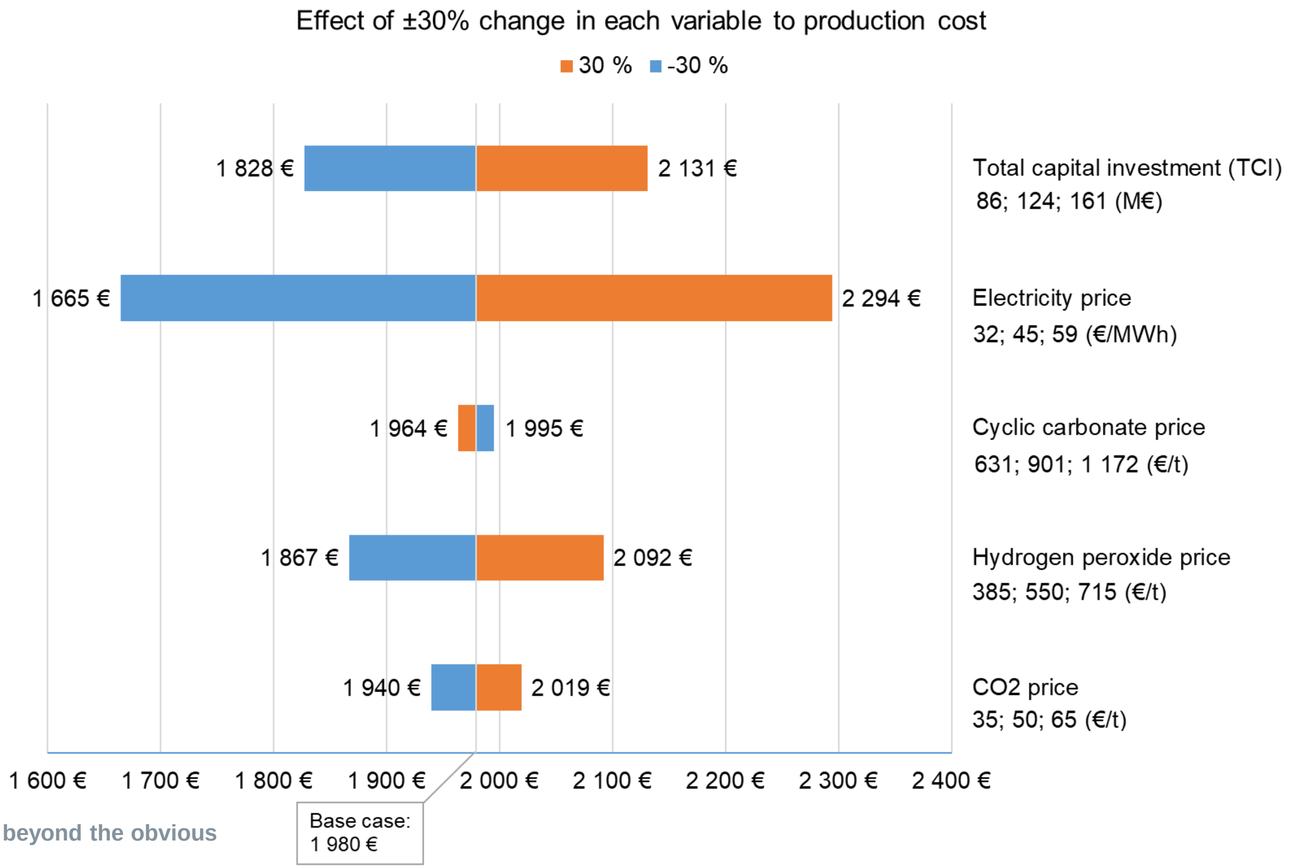
The selling price can be up to 6000 €/tonne

Production cost estimation with preliminary assumptions



The selling price can be up to 6000 €/tonne

The production costs are heavily dependent on the price of electricity



Updated process simulation with Aspen Plus

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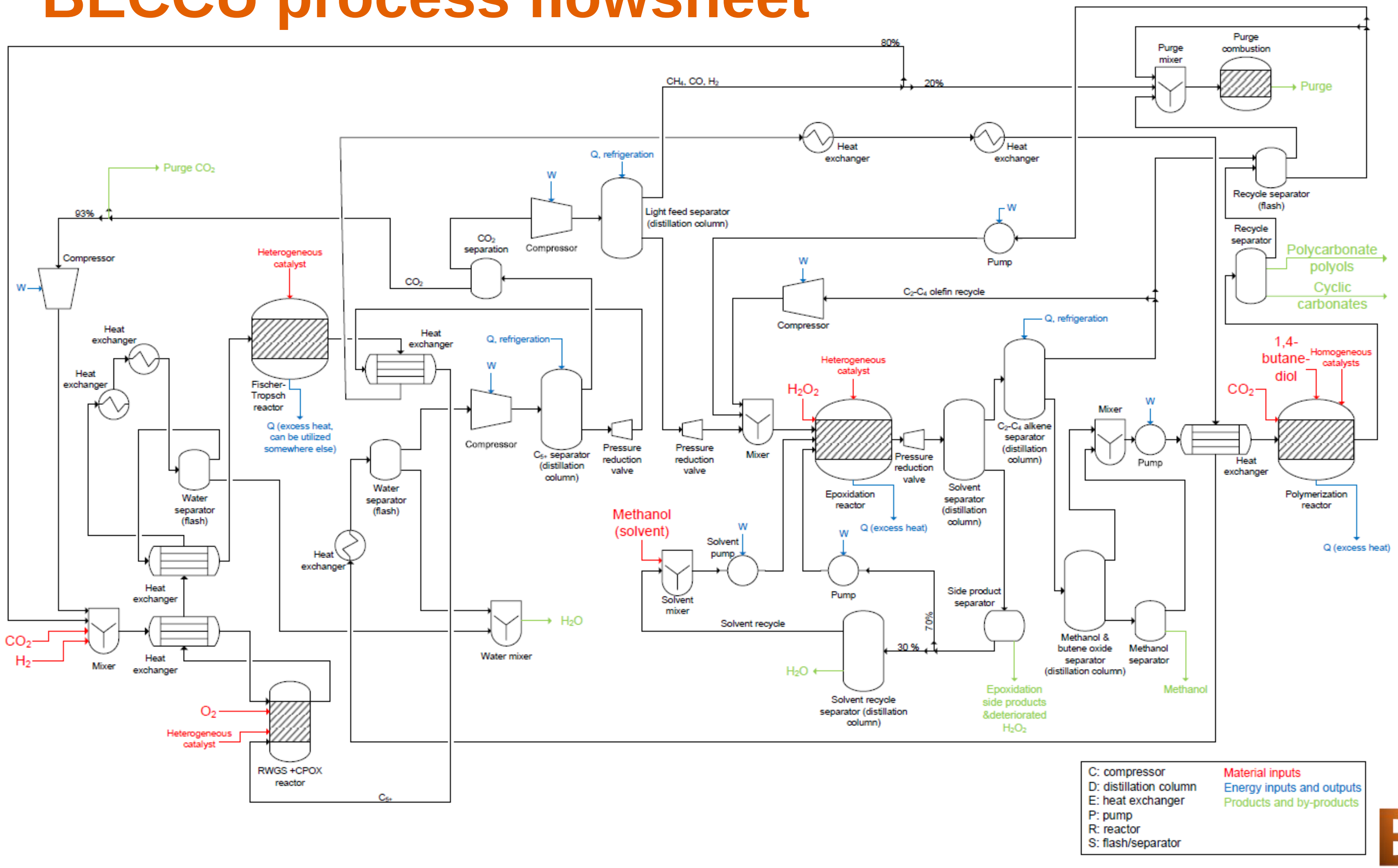
Simulation model improved since the preliminary TEA results

- Raw material in epoxidation, ethene, is difficult to separate from other light substances when there is CO_2 in the feed
  - CO_2 freezes in temperatures needed for cryogenic separation
  - ➢ We assume a separation method for CO_2 and are able to retrieve ethene to epoxidation
- Recycle loop added for epoxidation solvent (methanol)
  - Energy consumption of separations optimized
- Experimentally discovered side products have been added to the model
- Reactor performances have been revised and updated

BECCU process flowsheet



Suggested improvements & conclusions

Room for improvements after BECCU project

Separation of CO_2 after Fischer-Tropsch (FT)

- FT catalyst is both rWGS and WGS active, so there should be some CO_2 in the feed to FT
- Further investigation needed to find the most suitable separation method

Separation of side products of epoxidation

- Side products form azeotropes with methanol, water and other components, so the separation seems challenging

Epoxidation solvent (methanol) and product (1-butene oxide) have boiling points very close to each other, and they form azeotropes

- Difficult to separate
- Liquid-liquid extraction process should be further investigated

The modelling of polycarbonate polyols

- Polymer modelling requires thermodynamic data
- The products are not added to Aspen model

Conclusions

- BECCU production route seems competitive & profitable
  - Production cost was found lower than the expected selling price
- Sensitivity analysis showed that the process is most sensitive to changes in electricity price
  - TCI and H_2O_2 price have the second and third greatest effect

➢ An improved TEA is in the making, with the updated process model and experimental findings

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10/02/2022

Questions & Discussion