TECHNO-ECONOMIC ANALYSIS OF E-METHANOL PRODUCTION UNDER FIXED OPERATING CONDITIONS IN GERMANY

Sustainable energy carrier for transportation and industry

14th European Congress of Chemical Engineering

CityCube Berlin, 18 September 2023

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German Aerospace Center (DLR), Institute of Engineering Thermodynamics

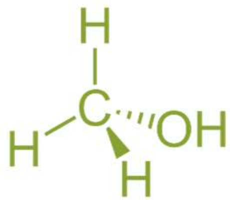
DLR

Outline

- Motivation
- Methodology
- e-MeOH plant for transportation sector
  - Process description, inputs, results
- Cleaner glass production using e-MeOH
  - Process description, inputs, results
- Conclusion and outlook

Motivation

- EU Climate Neutral Goal by 2050 (German already by 2045)[1][2]
- Potential to substitute fossil fuel



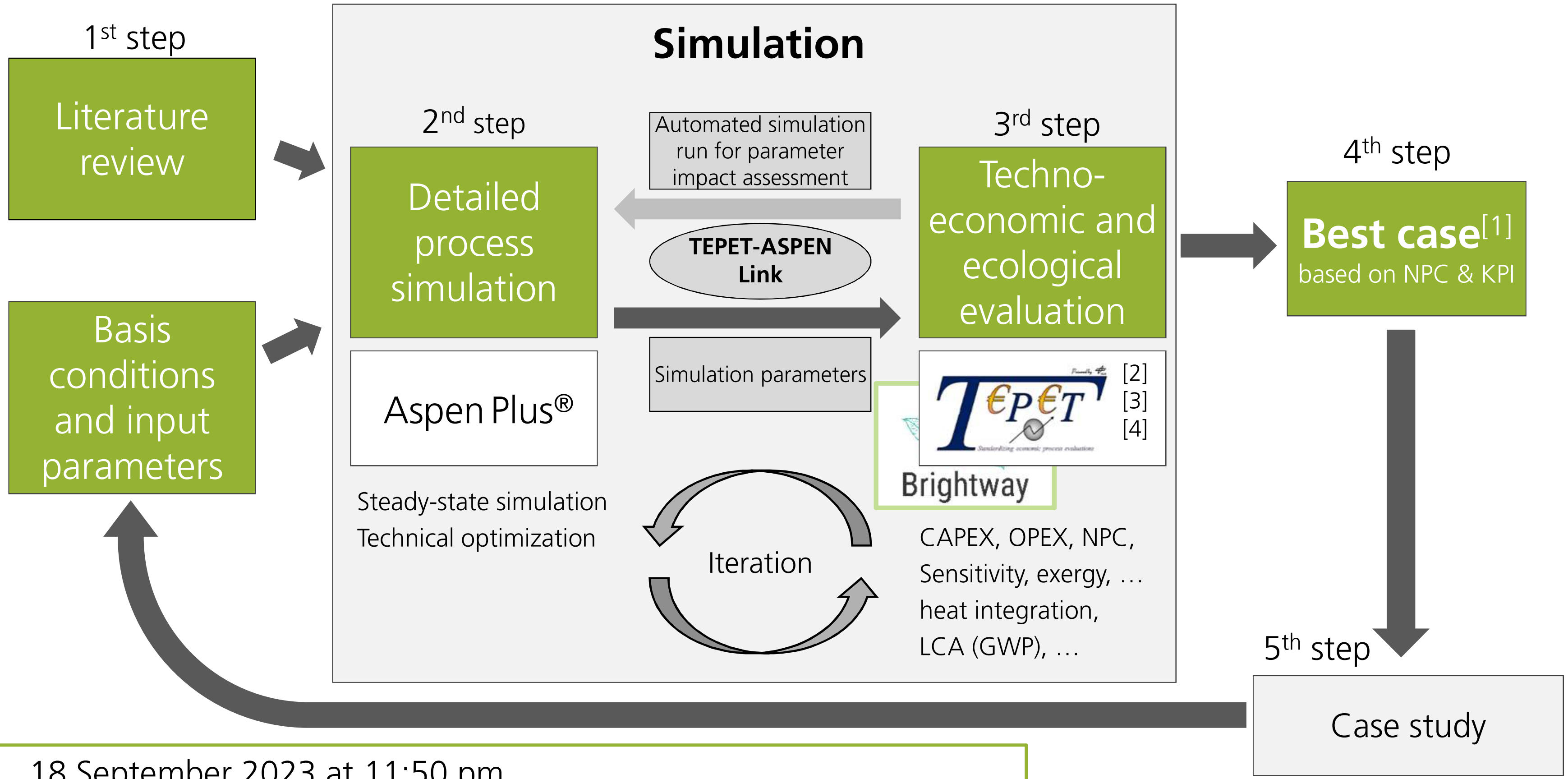
✔ Better vol. energy density than CH_4 or H_2[3]
✔ Suitable for land and maritime mobility[4]
→ M100 vehicles, incl. cars, vans, trucks & buses
→ MeOH-powered ferry, Stena Germanica
✔ Basic chemical
→ established infrastructure for distribution
✔ Raw material for MtK (SAF), DME, etc.
⚠ Cold start problem in ICE
⚠ Invisible flames
⚠ Water endangering

Goals:

- Techno-economic analysis of e-MeOH plant for transportation sector in Germany
- Techno-economic analysis of a cleaner glass production using e-MeOH

[1] European Climate Law (europa.eu)
[2] Jedamzik et al. (2020) Energiewende in Deutschland: Definition, Kosten & Ziele | co2online
[3] Bossel, Ulf (2003), The Physics of the Hydrogen Economy. European Fuel Cell News, Vol. 10, No. 2
[4] IRENA and Methanol Institute (2021) Innovation Outlook: Renewable Methanol, IRENA, Abu Dhabi.

Methodology[1]



Maier et al., 18 September 2023 at 11:50 pm
Room. A6 – Sustainability and circular (bio)economy – Process Systems Analysis I

Economic viability of e-MeOH

[1] Rahmat et al. (2023) Techno-economic and exergy analysis of e-MeOH production https://doi.org/10.1016/j.apenergy.2023.121738
[2] Albrecht et al. (2017). A Standardized Methodology for the Techno-Economic Evaluation of Alternative Fuels
[3] Maier et al. (2021) Techno-economically-driven identification of ideal plant configurations for a new biomass-to-liquid process
[4] Weyand et al. (2023) Process design analysis of a hybrid Power-and-Biomass-to-Liquid process

Methodology

Kinetic models & Key Performance Indicator (KPI)

Reactions[1]

$$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O \quad \Delta H_o = -49.8\,\frac{\text{kJ}}{\text{mol}} \quad (1)$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O$$

$$CO + 2H_2 \rightleftharpoons CH_3OH$$

3 moles H_2 converted into **1 mole MeOH**

Theoretical achievable η_{H_2tF} = **87.9 %**

KPI / efficiencies[3]

$$\eta_{PtF} = \frac{LHV_{\text{MeOH}} \cdot \dot{n}_{\text{MeOH}}}{\dot{P}_{\text{elec}}}$$

$$\eta_{H_2tF} = \frac{LHV_{\text{MeOH}} \cdot \dot{n}_{\text{MeOH}}}{LHV_{H_2} \cdot \dot{n}_{H_2}}$$

$$\eta_c = \frac{\dot{n}_{\text{MeOH}}}{\dot{n}_{CO_2}}$$

Vanden Bussche and Froment (VDB)[2]

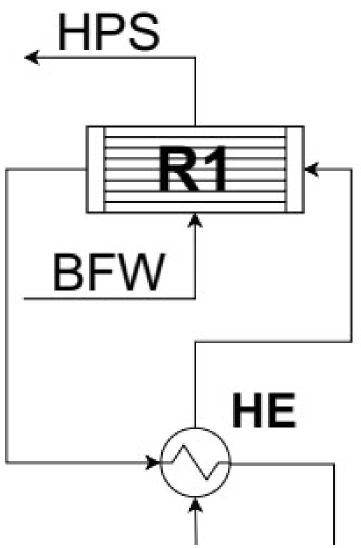
Only CO_2 hydrogenation & RWGS in the kinetic model

Reaction (3) is represented in reactions (1) and (2)

[1] Van-Dal and Bouallou (2013) Design and simulation of a methanol plant plant from CO_2 hydrogenation
[2] Vanden Bussche & Froment (1996) A steady-state kinetic model for methanol synthesis and the water gas shift reaction on a commercial Cu/ZnO/Al_2O_3 catalyst
[3] Rahmat et al. (2023) Techno-economic and exergy analysis of e-MeOH production https://doi.org/10.1016/j.apenergy.2023.121738

e-MeOH plant for transportation
Process description – reactor design and parameters[1]

AspenPlus® model: RPlug



Pressure drop[3]: Ergun's equation

$T_{in,R1}$ = 230 °C

p[1,2] = 80 bar

D_{shell}[6] = 120 in.

D_{tube}[4] = 2 in. OD

L_{tube}[5] = 5 m

N_{tube}[1,7] = 5154

GHSV[1] = 454 h^{-1}

Catalyst[3] $Cu/ZnO/Al_2O_3$

Bulk density[3] = 1065 kg m^{-3}

Particle diameter[3] = 5.5 mm

Lifespan[5] = 3 years

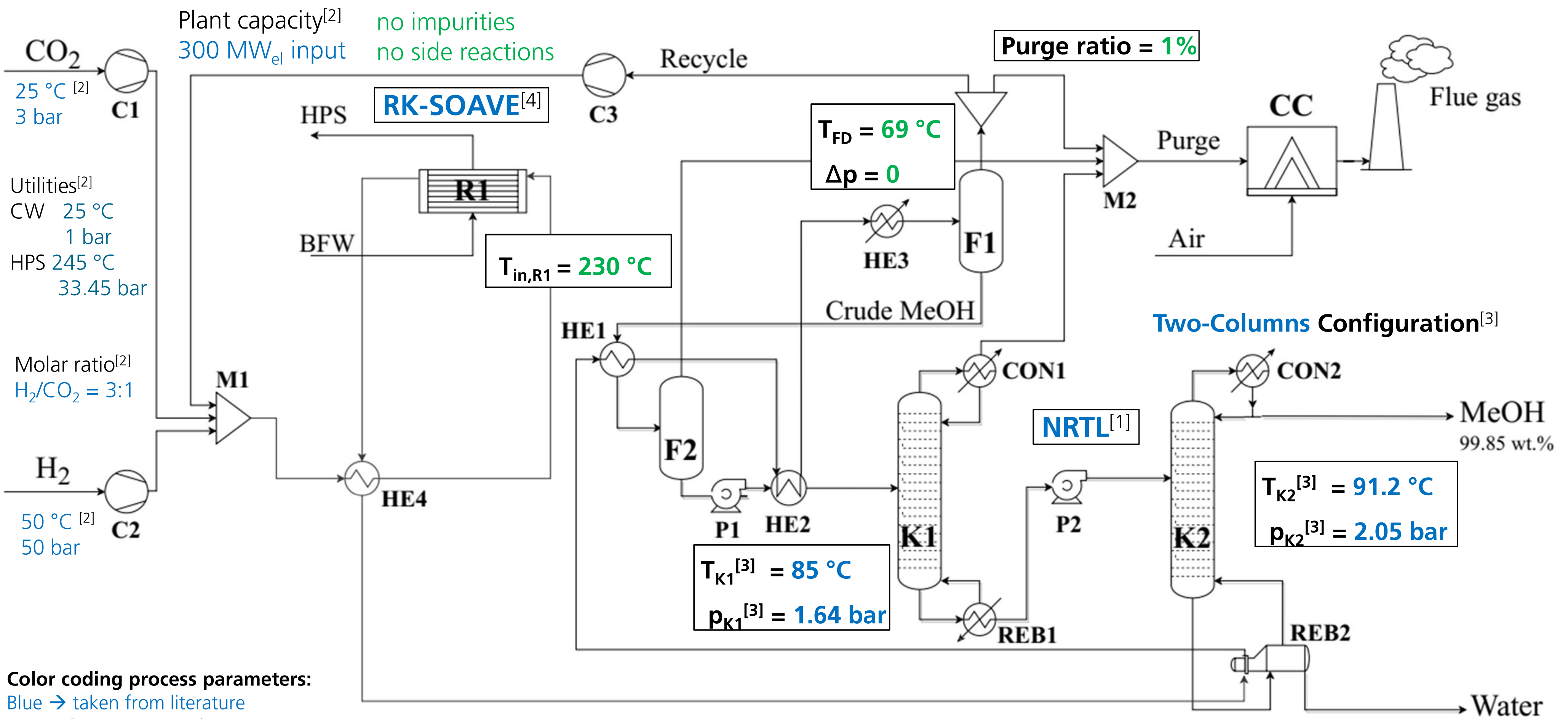
Dilution Factor[4] = 15 %

Color coding process parameters:
Blue → taken from literature
Green → own assumptions

✔ Better energy efficiency than quench/adiabatic
→ steam generated & feed pre-heated
⚠ More expensive CAPEX than quench/adiabatic

[1] Rahmat et al. (2023) Techno-economic and exergy analysis of e-MeOH production https://doi.org/10.1016/j.apenergy.2023.121738
[2] Metallgesellschaft AG (1996) – EP 0 790 226 B1
[3] Van-Dal and Bouallou (2013) Design and simulation of a methanol plant plant from CO_2 hydrogenation
[4] Doraiswamy and Sharma (1984) Heterogenous reactions: Analysis examples and reactor design
[5] Bartholomew and Farrauto (2006) Fundamentals of Industrial Catalytic Processes, 2. Ed.
[6] Serth and Lestina (2014) Process Heat Transfer: Principles, Applications and Rules of Thumb
[7] Rase (1990) Fixed-Bed Reactor Design and Diagnostics: Principles, Applications and Rules of Thumb

e-MeOH plant for transportation
Process description – flowsheet[1]



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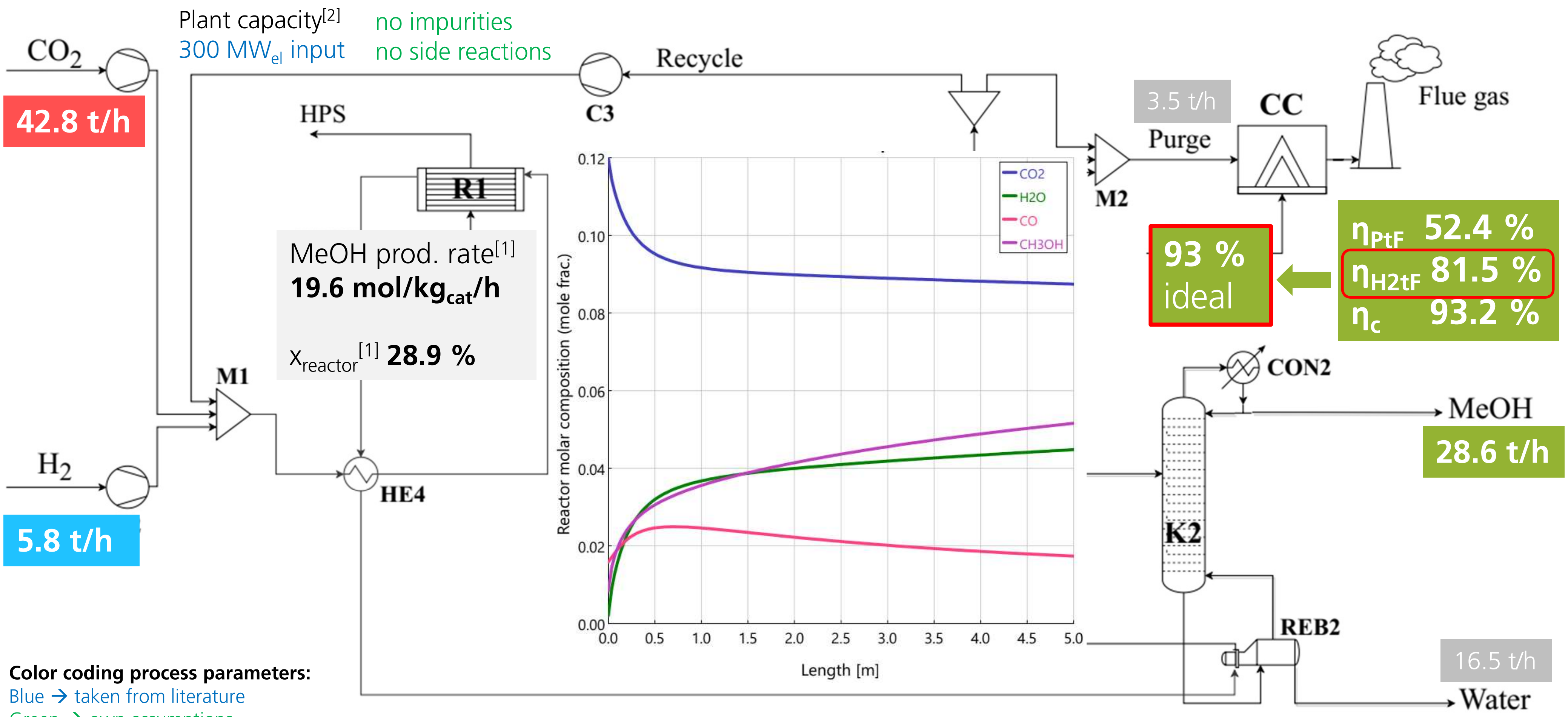
[2] Heimann et al. (2023) Contribution to the standardization of the economic and ecological analysis of PtX-process [in submission]
[3] Bertau et al. (2014) Methanol: The Basic Chemical and Energy Feedstock of the Future
[4] Graaf et al. (1986) Chemical equilibria in methanol synthesis

e-MeOH plant for transportation

Results[1] – KPI



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e-MeOH plant for transportation

Economic analysis – basis conditions, OPEX & NPC

Basis conditions	e-MeOH plant[1,2]
Plant location	Germany
Base year	2018
Basis currency	€
Full-load hours	8000 h/a
Plant lifetime (y)	20 a
Interest rate (IR)	5 %
Labor costs	41 €/h

BEniVer
Begleitforschung Energiewende im Verkehr

Raw materials	e-MeOH plant[1,2]
CO_2 [€/t]	68.95
H_2 [€/kg]	4.74
Electricity [€/MWh]	55.72
Utilities	taken from [2]

$$\sum OPEX_{dir}\left(\frac{€/\$}{a}\right) = \sum_{i=1}^{m} \dot{m}_{R\&B,\ i} \cdot c_{R\&B,\ i} + \sum_{j=1}^{n} E_{power_j} \cdot c_{power_j} + \sum_{k=1}^{p} W_{heat_k} \cdot c_{heat_k}$$

$$NPC\left(\frac{€/\$}{t}\right) = \frac{ACC + \sum OPEX_{dir} + \sum OPEX_{ind} + h_{labour} \cdot c_{labour}}{\dot{m}_{fuel}}$$ [2,3]

$$ACC = FCI * \left(\frac{IR * (1+IR)^y}{(1+IR)^y - 1} + \frac{IR * y}{(y-1)}\right)$$

See next slide!

$$FCI_i = EC_i \times \sum CAPEX\ cost\ factors$$ [3]

[1] Rahmat et al. (2023) Techno-economic and exergy analysis of e-MeOH production https://doi.org/10.1016/j.apenergy.2023.121738
[2] Heimann et al. (2023) Contribution to the standardization of the economic and ecological analysis of PtX-process [in submission]
[3] Peters et al. (2002) *Design and Economics for Chemical Engineers*. Europe: McGraw-Hill Education.

e-MeOH plant for transportation
Economic analysis – CAPEX

$$EC_i = EC_{ref} \times \left(\frac{sizing_i}{sizing_{ref}}\right)^n \times \left(\frac{CEPCI_i}{CEPCI_{ref}}\right) \times material\ factor \times pressure\ factor$$

$$EC_i = \left[e \cdot (sizing_i)^2 + f \cdot sizing_i + g \right] \times \left(\frac{CEPCI_i}{CEPCI_{ref}}\right) \times material\ factor \times pressure\ factor$$

Reference function	EC_{ref}	Currency	$sizing_{ref}$	Unit	n	$Year_{ref}$	Source
Compressor	3 035	$	1	kW	0.68	2002	[1]
Centrifugal pump	16 809	$	1	$m^3\ s^{-1}$	0.36	2002	[1]
Distillation column	286 343	$	100	size factor = $HxD^{1.5}$ [$m^{2.5}$]	0.53	2007	[2][3]
Combustion chamber	143 244	$	2	MW	0.87	2002	[1]
Polynomial function	**e**	**f**	**g**	**Sizing unit**	**Currency**	**$Year_{ref}$**	**Source**
Lurgi reactor, D_{tube} 2 in.*	0	156.03	11910	Number of tubes [-]	$	2002	[1]**
Shell & tube heat exchanger*	0	201.29	3853.3	Heat transfer area [m^2]	$	2002	[1]
Flash drum	-2.21	369.75	805.42	Length & diameter [m]	$	2002	[1]

*stainless steel as the material construction
**with own reformulation

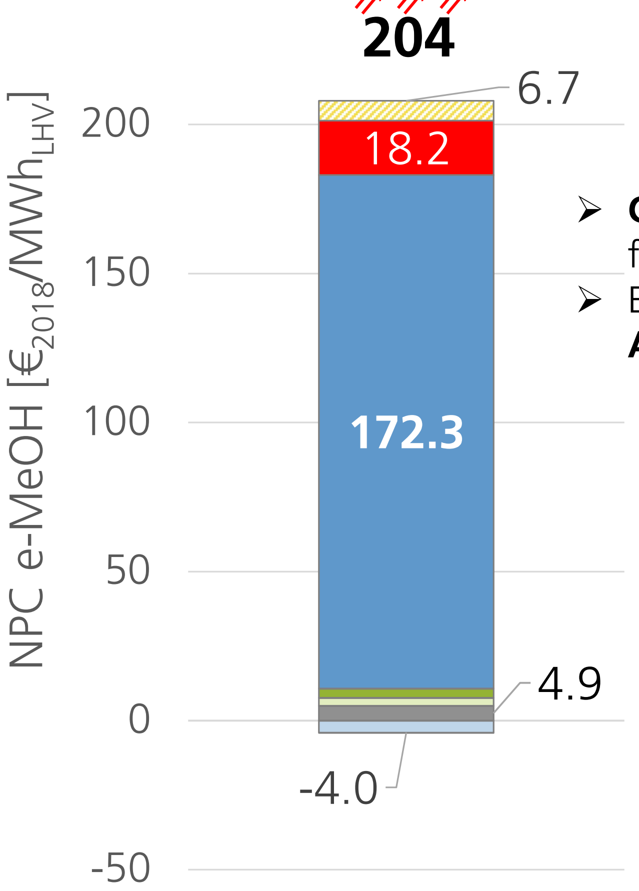
[1] Peters et al. (2002) *Design and Economics for Chemical Engineers*. Europe: McGraw-Hill Education.
[2] Woods (2007) Rules of Thumb in Engineering Practices
[3] Towler (2008) Chemical Engineering Design

e-MeOH plant for transportation

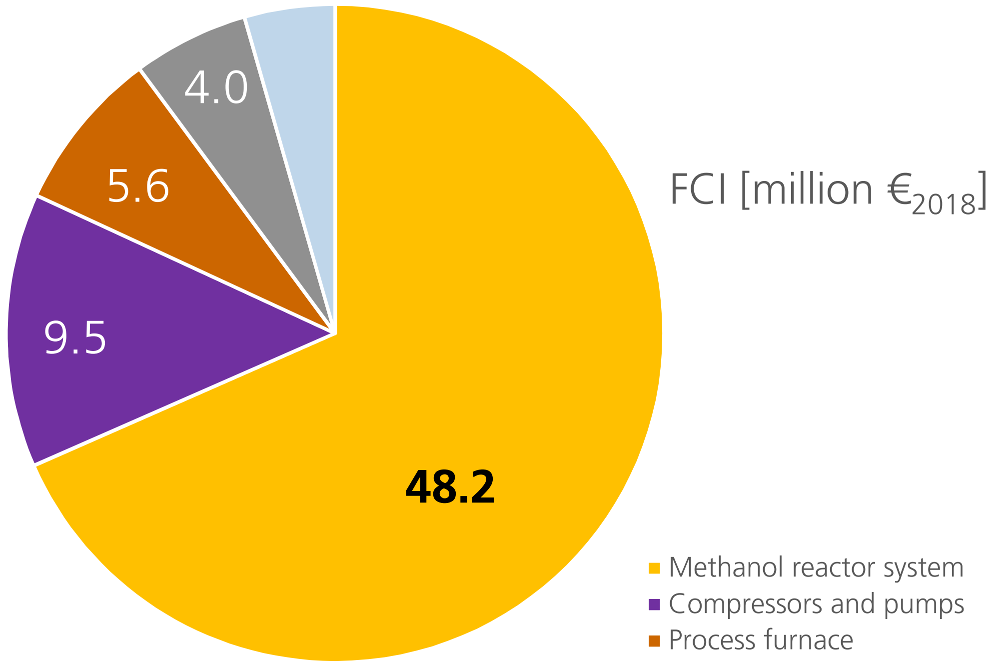
Results[1] – NPC & FCI

2-3x more expensive

European market price[2]
400 – 600 $€_{2018}$/t
73 – 109 $€_{2018}/MWh_{LHV}$



- **Cost driver is H_2**
  f(electricity costs)
- Electrolyzers[3] for H_2
  AEL, PEM, SOEC



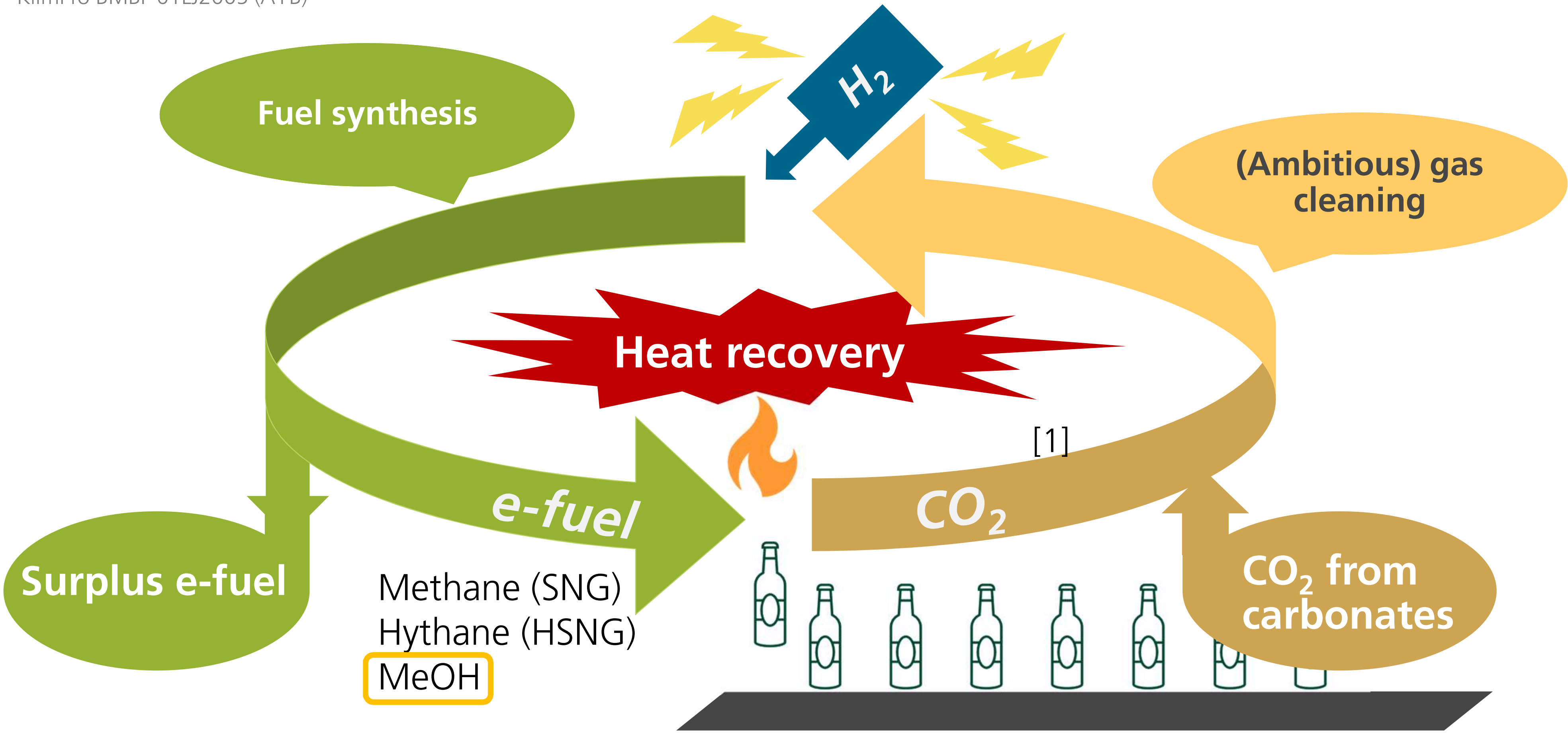
70.5 million $€_{2018}$

[1] Rahmat et al. (2023) Techno-economic and exergy analysis of e-MeOH production https://doi.org/10.1016/j.apenergy.2023.121738
[2] Methanol Price|Methanol Institute|www.methanol.org
[3] Heimann et al. (2023) Contribution to the standardization of the economic and ecological analysis of PtX-process [in submission]

Cleaner glass production using e-MeOH

Project Glas-CO2[1]

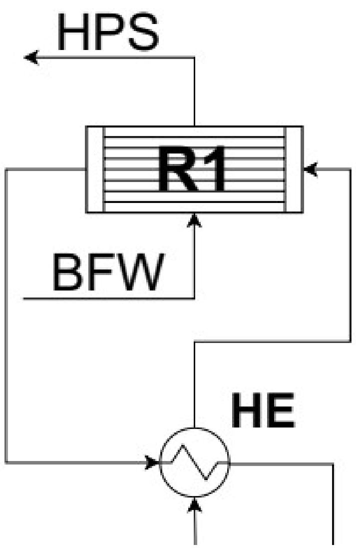
Carbon Capture and Utilization Cycles for a CO_2 Neutral Glass Production
KlimPro BMBF 01LJ2005 (A+B)



[1] Drünert et al. (2023) Techno-economic assessment of carbon capture and utilization concepts for a CO2 emission-free glass production.

Cleaner glass production using e-MeOH
Process description – reactor design and parameters

AspenPlus® model: RPlug



Pressure drop[3]: Ergun's equation

$T_{in,R1}$ = 230 °C

p[1,2] = 80 bar

D_{shell}[6] = 120 in.

D_{tube}[4] = 2 in. OD

L_{tube}[5] = 5 m

N_{tube}[7] = 1088

Catalyst[3] $Cu/ZnO/Al_2O_3$

Bulk density[3] = 1065 kg m^{-3}

Particle diameter[3] = 5.5 mm

Lifespan[5] = 3 years

Dilution Factor[4] = 15 %

Color coding process parameters:
Blue → taken from literature
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⇉ fewer N_{tube} due to smaller e-MeOH production capacity

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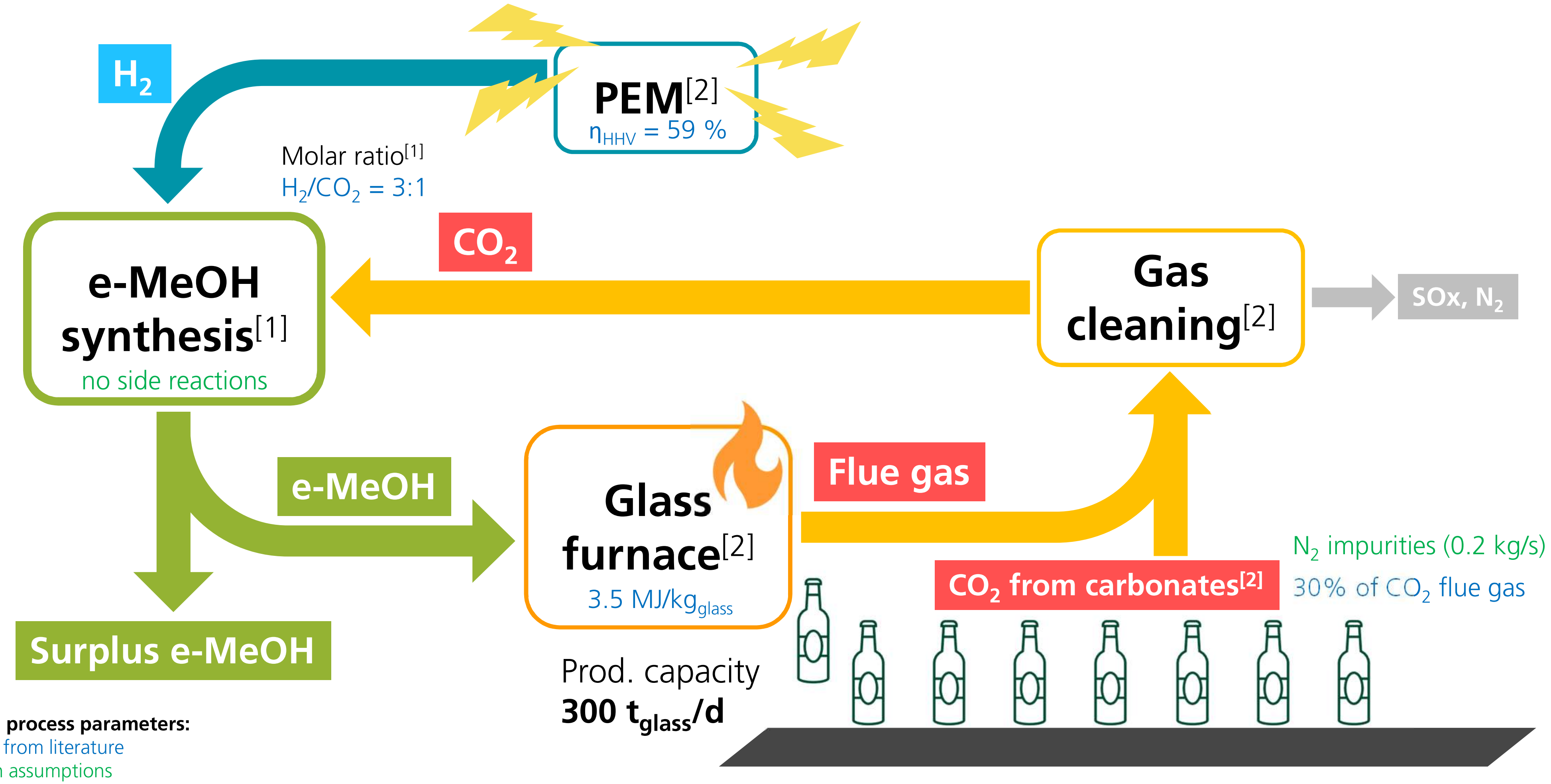
[7] Rase (1990) Fixed-Bed Reactor Design and Diagnostics: Principles, Applications and Rules of Thumb

Cleaner glass production using e-MeOH

Process description – block flow diagram



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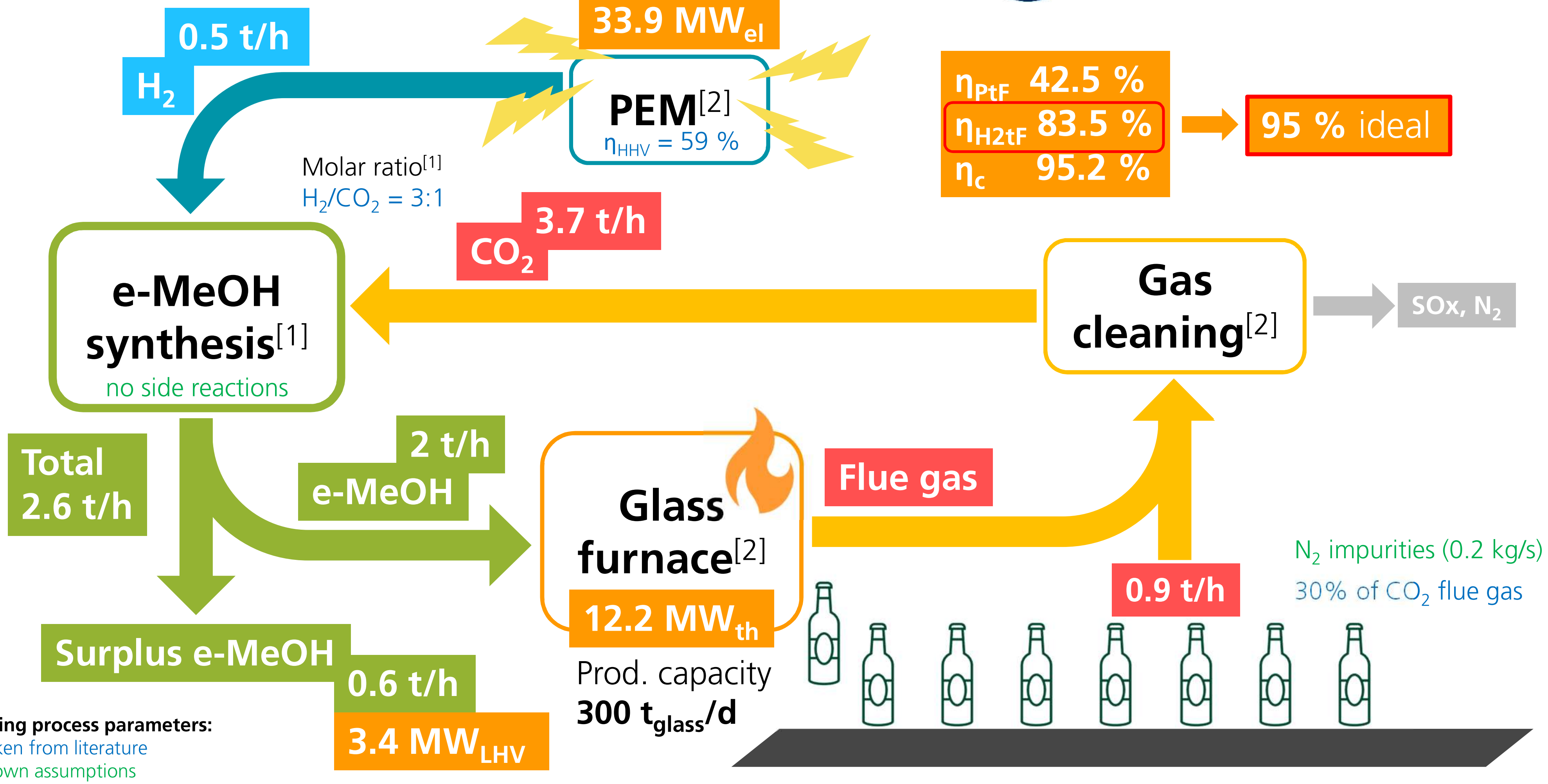
[2] Drünert et al. (2023) Techno-economic assessment of carbon capture and utilization concepts for a CO2 emission-free glass production.

Cleaner glass production using e-MeOH
Results – KPI



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Cleaner glass production using e-MeOH
Economic analysis – basis conditions & OPEX

Basis conditions	e-MeOH plant[1,2]
Plant location	Germany
Base year	2018
Basis currency	€
Full-load hours	8000 h/a
Plant lifetime (y)	20 a
Interest rate (IR)	5 %
Labor costs	41 €/h

Raw materials	e-MeOH plant[1,2]
CO_2 [€/t]	68.95
H_2 [€/kg]	4.74
Electricity [€/MWh]	55.72
Utilities	taken from [2]

- Different basis conditions
- Raw materials costs depend on the process
  - **CO_2** from **flue gas** and **carbonates**
  - **H_2** from **electricity**

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[3] Drünert et al. (2023) Techno-economic assessment of carbon capture and utilization concepts for a CO2 emission-free glass production.

Cleaner glass production using e-MeOH
Economic analysis – CAPEX

$$EC_i = EC_{ref} \times \left(\frac{sizing_i}{sizing_{ref}}\right)^n \times \left(\frac{CEPCI_i}{CEPCI_{ref}}\right) \times material\ factor\ \times pressure\ factor$$

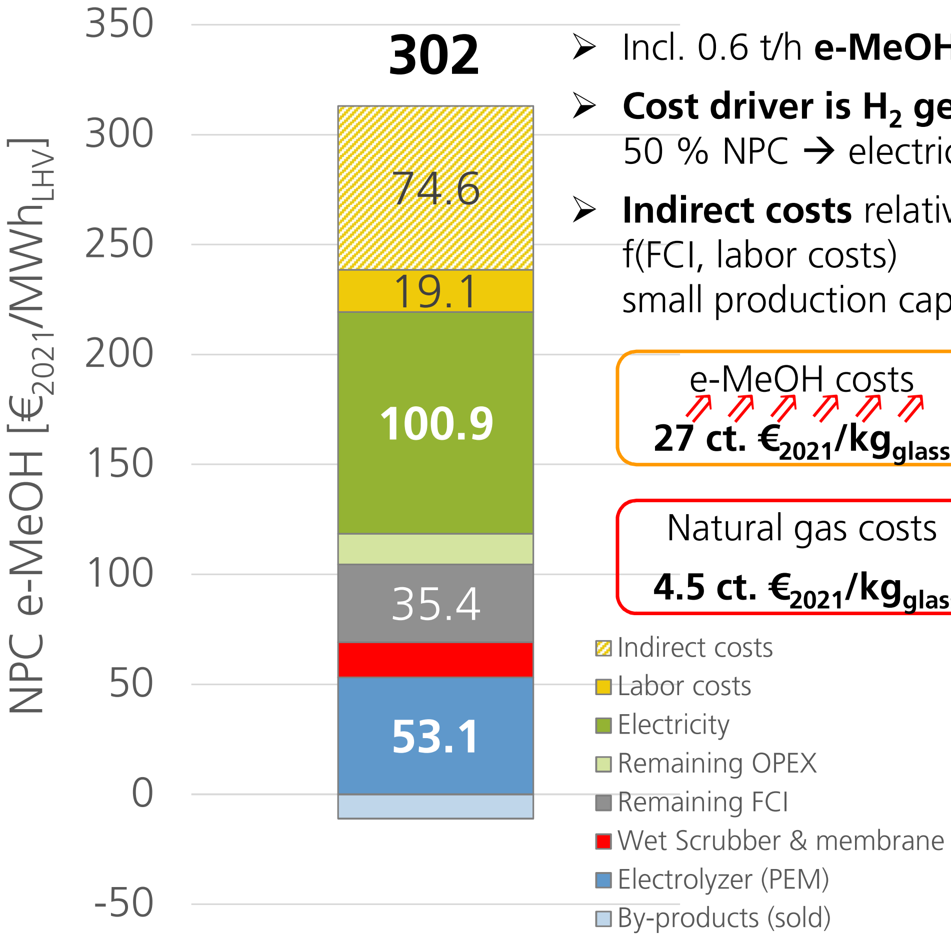
Reference function	EC_{ref}	Currency	$sizing_{ref}$	Unit	n	$Year_{ref}$	Source
PEM electrolysis	957	€	1	kW	1	2016	[1]
Wet scrubber (limestone)	13 061	k$	14	MW	0.72	2012	[2]
Membrane PMP	9.76	m$	525.6	kmol/h	0.6	2020	[3]*

*with own reformulation

- Same equipment cost functions as for e-MeOH plant
- Additional equipment
  - PEM electrolysis for **H_2 production**
  - Wet scrubber & membrane for **gas cleaning**

[1] DLR, Ludwig Bölkow Systemtechnik, Fhg ISE, KBB (2014) Abschlussbericht der Studie Plan-DelyKad, Stuttgart.
[2] Sorrels (2021) Chapter 1 – Wet and Dry Scrubbers for Acid Gas Control. www.epa.gov
[3] Samei and Raisi (2022) Separation of nitrogen from methane by multi-stage membrane. https://doi.org/10.1016/j.jngse.2021.104380

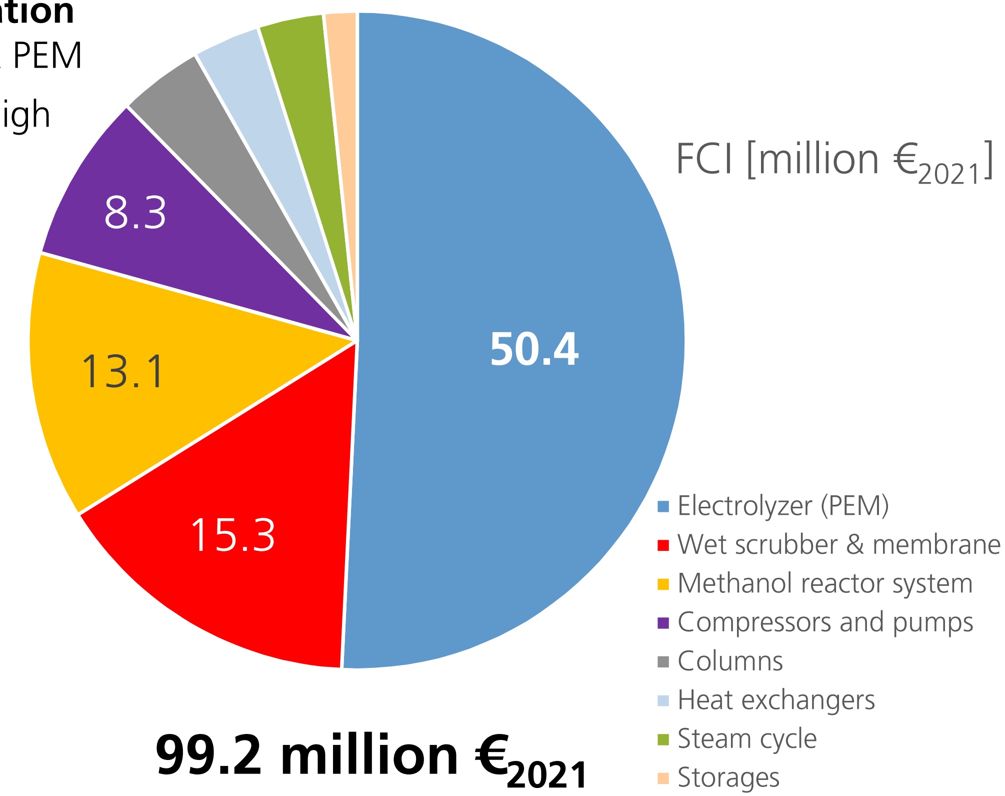
Cleaner glass production using e-MeOH
Results – NPC & FCI



- Incl. 0.6 t/h **e-MeOH surplus**
- **Cost driver is H_2 generation**
  50 % NPC → electricity & PEM
- **Indirect costs** relatively high
  f(FCI, labor costs)
  small production capacity

e-MeOH costs
27 ct. $€_{2021}/kg_{glass}$

Natural gas costs
4.5 ct. $€_{2021}/kg_{glass}$



99.2 million $€_{2021}$

Conclusion

- e-MeOH plant for transportation sector in Germany
- Implementation in industrial sector for a cleaner glass production (Glas-CO2)
- KPI η_{PtF} 52.4 %, η_{H2tF} 81.5 % and η_c 93.2 % can be achieved by e-MeOH plant[1]
  - With AEL + PEM + SOEC, exothermic process, equilibrium-limited reactions, CO-based syngas is preferred, purge stream
- KPI η_{PtF} ⇘ 42.5 %, η_{H2tF} ⇗ 83.5 % and η_c ⇗ 95.2 % can be achieved in Glas-CO2
  - Only with PEM (flexible operation), no purge, reactor size 21 % with 11 % prod. capacity
- NPC e-MeOH
  - ⇗⇗⇗ 204 $€_{2018}/MWh_{LHV}$ in e-MeOH plant[1]
    → **2-3 times more expensive** than market price
  - 302 $€_{2021}/MWh_{LHV}$ in Glas-CO2
    → fuel costs **27 ct. $€_{2021}/kg_{glass}$** ⇗⇗⇗⇗⇗⇗
    → **6 times more expensive** than with natural gas

Realization = f(**user-acceptance**)
Transportation? Industry?

[1] Rahmat et al. (2023) Techno-economic and exergy analysis of e-MeOH production https://doi.org/10.1016/j.apenergy.2023.121738

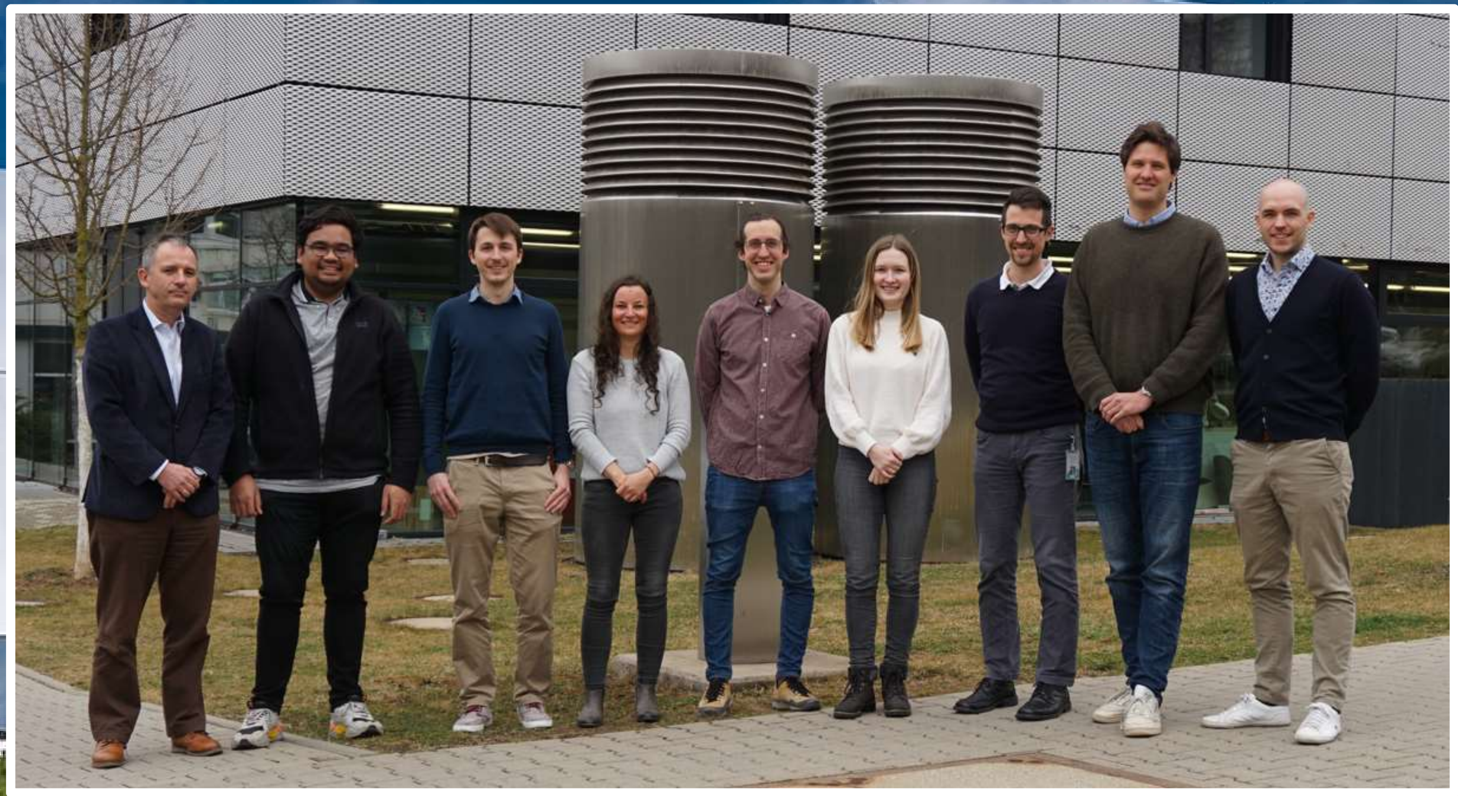
Outlook

- Using our methodology for other possible e-fuels syntheses
  e.g. **synthetic methane (SNG)** and **hythane-30 (HSNG)** in Glas-CO2

  → Dietrich et al., 19 September 2023 at 12:50 pm
  Room. A1 - Climate and energy - Hydrogen and fuels

- Implementation of the concept for other carbon intensive industries
  e.g. **cement, steel, petrochemicals, etc.**

We are looking forward to a cooperation in any project idea to make our **world better**!



THANK YOU FOR YOUR ATTENTION!

Yoga.Rahmat@dlr.de

Impressum

Thema: **Techno-economic analysis of e-methanol production under fixed operating conditions in Germany**
A case study – Cleaner glass production using e-MeOH
14th European Congress of Chemical Engineering, CityCube Berlin

Datum: 18.09.2023

Autor: Yoga Rahmat (Yoga.Rahmat@dlr.de)

Institut: Technische Thermodynamik

Cleaner glass production using e-MeOH

Results – Fuel costs with e-MeOH and natural gas

- NPC e-MeOH **302 €$_{2021}$/MWh$_{LHV}$**
- European **market price**[1] up to **100 €$_{2021}$/MWh$_{LHV}$**
- 0.6 t/h (3.4 MW$_{LHV}$) **e-MeOH surplus sold** with market price
- Production capacity 300 t$_{glass}$/d → **12.5 t$_{glass}$/h**
- Furnace heat demand **12.2 MW$_{th}$** ⇒
- **Glass production plant** is assumed **fully depreciated**

Natural gas

Avg. market price[2] 46.33 €$_{2021}$/MWh$_{LHV}$

Fuel costs **5 ct. €$_{2021}$/kg$_{glass}$**

For 12.5 t$_{glass}$ hourly production

e-MeOH fuel → 12.2 MWh$_{LHV}$ * 302 €$_{2021}$/MWh$_{LHV}$ = 3684 €$_{2021}$

e-MeOH sale → 3.4 MWh$_{LHV}$ * 100 €$_{2021}$/MWh$_{LHV}$ = 340 €$_{2021}$ –

Glass hourly total production costs = 3344 €$_{2021}$

Fuel costs → 3344 €$_{2021}$ / 12.5 t$_{glass}$ = **27 ct. €$_{2021}$/kg$_{glass}$**

[1] Methanol Price|Methanol Institute|www.methanol.org
[2] EU Natural Gas - 2023 Data - 2010-2022 Historical - 2024 Forecast - Price - Quote (tradingeconomics.com)

Cleaner glass production using e-MeOH

Results – KPI

Plant capacity
300 t_{glass}/d

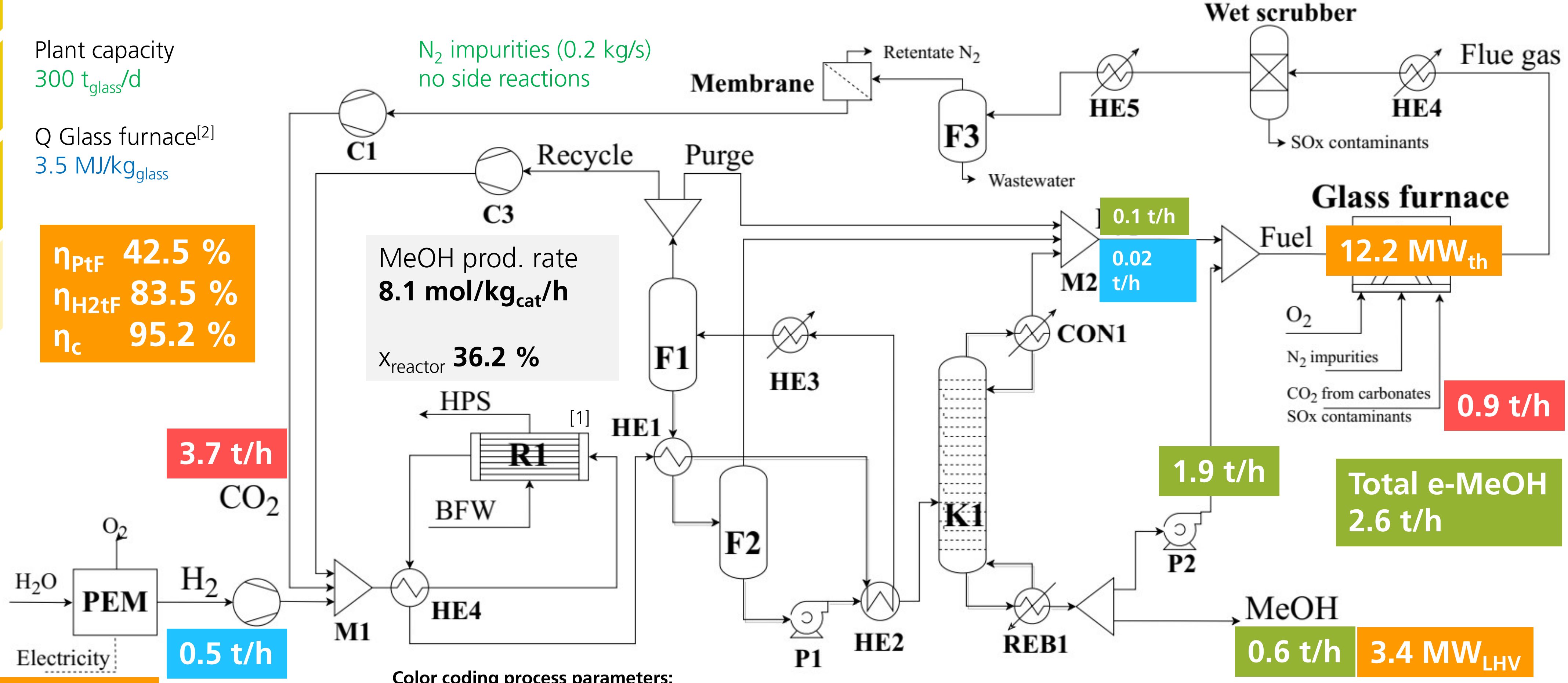
Q Glass furnace[2]
3.5 MJ/kg_{glass}

η_{PtF} 42.5 %
η_{H2tF} 83.5 %
η_{c} 95.2 %

N_2 impurities (0.2 kg/s)
no side reactions

MeOH prod. rate
8.1 $mol/kg_{cat}/h$

$x_{reactor}$ **36.2 %**



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