STANDARDIZED TECHNO-ECONOMIC ANALYSIS OF PTX-FUELS

SNG- and HSNG-production in Germany

DECHEMA Jahrestreffen der Fachsektion Energie, Chemie und Klima
Frankfurt am Main, 12.03.2024

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Outline

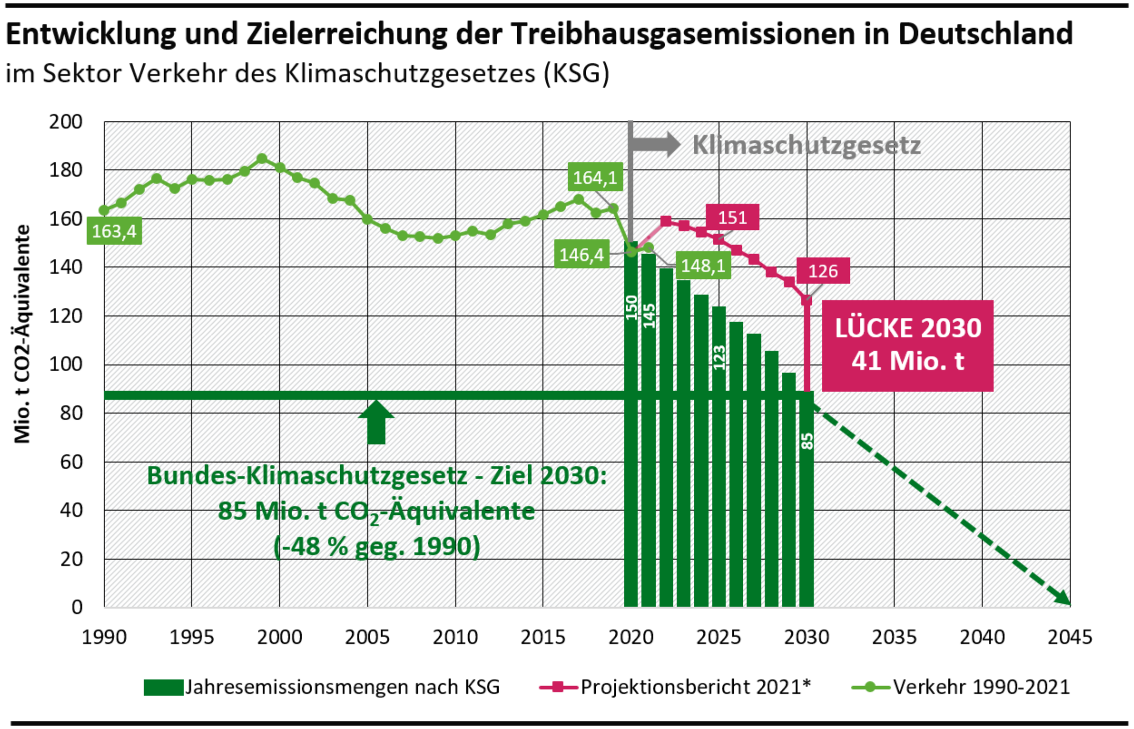
- Motivation
- Methodology
- SNG
- HSNG
- Comparison
- Conclusion and outlook

Rahmat et al., Sustainable glass production, DECHEMA, 12.03.2024

Motivation

- EU Climate Neutral Goal by 2050 (Germany already by 2045)[1][2]
- Renewable transport lacks behind
- Hart to abate: chemical energy carriers
    - But which?

Octanol
Butanol
Methane
FT-products
MeFo
OME
DME
DMC
Methanol
Hythane
Hydrogen
Ammonia
???


Entwicklung und Zielerreichung der Treibhausgasemissionen in Deutschland
im Sektor Verkehr des Klimaschutzgesetzes (KSG)

** Berechnete Werte des „Projektionsbericht 2021“(rote Linie, basierend auf Daten mit Stand August 2020) weichen für die Jahre 2020 und 2021 von den später veröffentlichten offiziellen IST-Werten (grüne Linie) ab.*

Quelle: UBA
22.03.2022

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[1] European Climate Law (europa.eu)
[2] Jedamzik et al. (2020) Energiewende in Deutschland: Definition, Kosten & Ziele | co2online

Motivation

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Energy transition in the transport sector (EiV) - BEniVer: Scientific supervision

BEniVer

Begleitforschung Energiewende im Verkehr

- EiV: funding 99 Mio. € | 16 projects | 100+ partner
- Renewable electricity based fuels

Cluster	Fuels in focus	Application
C3-Mobility	synth. Gasoline, DME, OME$_{3-5}$, Methanol, Butanol, Octanol	🚗 🚢
CombiFuel	Hythan (Hydrogen + Methane)	🚗
E2Fuels	Methanol, OME$_{3-5}$, Methan, Hythan	🚗 🚢 ⚡
FlexDME	Dimethylether (DME)	🚗
ISystem4EFuel	synth. Diesel, OME$_{3-5}$	🚢 ⚡
KEROSyN100	synth. Jet fuel	✈
LeanStoicH2	Hythan (Hydrogen+ Methane)	⚡
MEEMO	Methanol	🚗
MENA-Fuels	(Import strategies from MENA region)	
MethQuest	Methan, Methanol, Hydrogen	🚗 🚢 ⚡
NAMOSYN*	OME, Methylformiat (MeFo), Dimethylcarbonat (DMC)	🚗
PlasmaFuel	synth. Diesel	🚢
PowerFuel	synth. Jet fuel	✈
SHARC	(Smart energy management in harbors)	
SolareKraftstoffe	synth. Gasoline	🚗
SynLink	synth. Diesel, synth. Jet fuel, Methanol	🚗 ✈ 🚢

- Comparable assessment: BEniVer – Scientific supervision of „Energy transition in the transport sector (EiV)"

DLR

izes gGmbH
Institut für ZukunftsEnergie- und Stoffstromsysteme

FfE

HELMHOLTZ
ZENTRUM FÜR UMWELTFORSCHUNG
UFZ

DBFZ

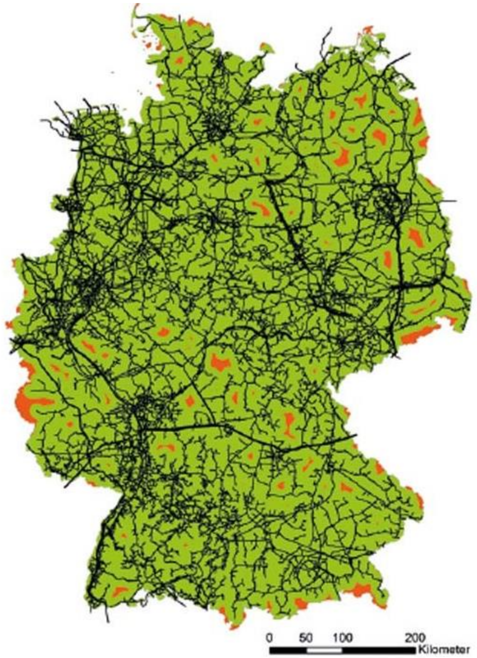
GWS
SPECIALISTS IN EMPIRICAL ECONOMIC RESEARCH

DECHEMA

DGMK

Motivation: SNG

- Potential of SNG and HSNG:
  - Application proven
  - Little CO_2 needed per molecule
  - Existing infrastructure



Gas-grid >4 bar
Image: DVGW

Image: Volvo Trucks

Source: Wolfgang Jargstorff / Fotolia.com

Image: Avenir LNG

Image: Daimler

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[1] European Climate Law (europa.eu)
[2] Jedamzik et al. (2020) Energiewende in Deutschland: Definition, Kosten & Ziele | co2online

Motivation: HSNG

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Combifuel project of Graforce GmbH, Berlin

- Addition of H_2 to SNG → less CO_2 needed
- Up to 30 % H_2 tested


[1]


[1]

[1] Schlussbericht CombiFuel, FKZ 03EIV091A, Graforce GmbH, Synreform GmbH, 2022

Motivation: HSNG

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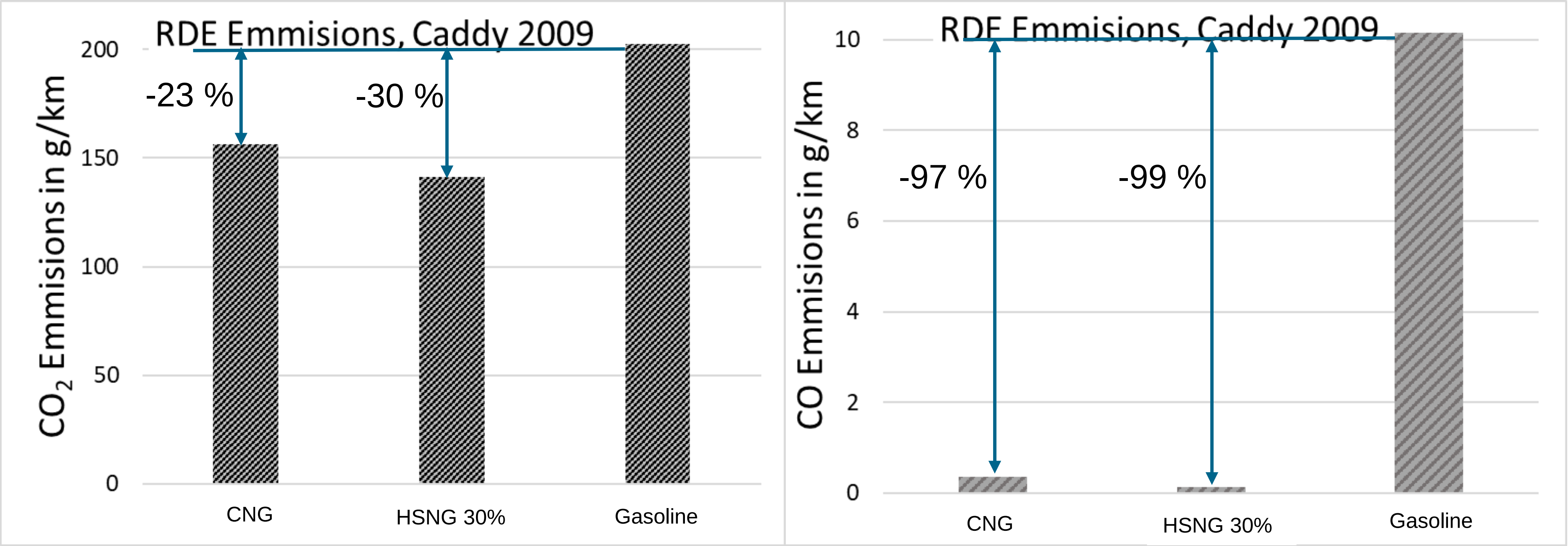
Begleitforschung Energiewende im Verkehr

DLR

Combifuel project of Graforce GmbH, Berlin

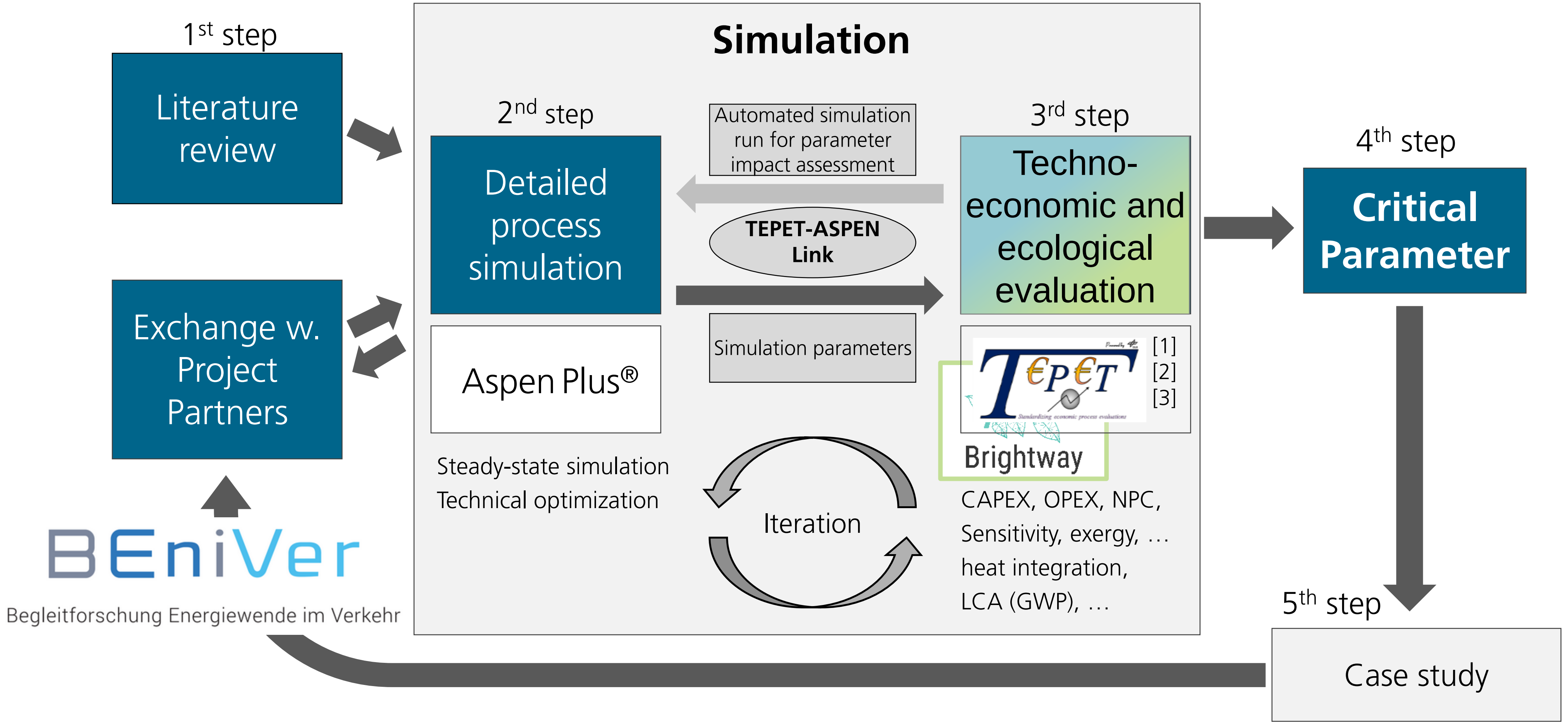
- Addition of H_2 to SNG → less CO_2 needed
- Up to 30 % H_2 tested
- Emission reduction: CO_2, CO, HC, increase: NO_x



[1] Schlussbericht CombiFuel, FKZ 03EIV091A, Graforce GmbH, Synreform GmbH, 2022

METHODOLOGY

Assessment Workflow



1st step

Literature review

Exchange w. Project Partners

BEniVer

Begleitforschung Energiewende im Verkehr

Simulation

2nd step

Detailed process simulation

Aspen Plus®

Steady-state simulation

Technical optimization

Automated simulation run for parameter impact assessment

TEPET-ASPEN Link

Simulation parameters

Iteration

3rd step

Techno-economic and ecological evaluation

TEPET [1] [2] [3]

Brightway

CAPEX, OPEX, NPC,

Sensitivity, exergy, …

heat integration,

LCA (GWP), …

4th step

Critical Parameter

5th step

Case study

Economic / ecological viability of e-fuels production

[1] Albrecht et al. (2017). A Standardized Methodology for the Techno-Economic Evaluation of Alternative Fuels

[2] Maier et al. (2021) Techno-economically-driven identification of ideal plant configurations for a new biomass-to-liquid process

[3] Weyand et al. (2023) Process design analysis of a hybrid Power-and-Biomass-to-Liquid process

Methodology: technical analysis

Key performance indicator (KPI)

KPI / efficiencies[1]

$$\eta_{PtF} = \frac{LHV_{Fuel} \cdot \dot{n}_{Fuel}}{\dot{P}_{el}}$$

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

4 moles H_2 converted into 1 mole Methane

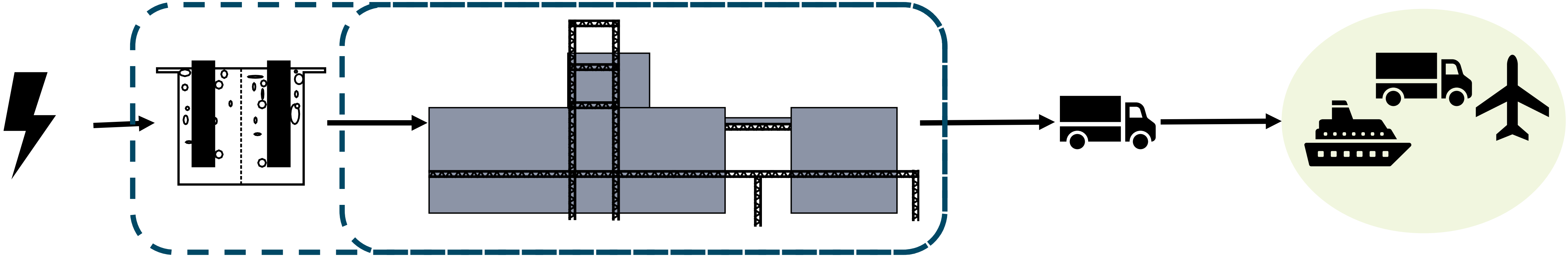
$\eta_{H_2tF,\,ideal}$ = 83.3 %

Methane synthesis reactions[2]

$$CO + 3H_2 \rightleftharpoons CH_4 + H_2O \qquad \Delta H_o = -164\,\frac{kJ}{mol} \quad (1)$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \qquad \Delta H_o = +41.2\,\frac{kJ}{mol} \quad (2)$$

$$CO_2 + 4H_2 \rightleftharpoons CH_4 + 2H_2O \qquad \Delta H_o = -206\,\frac{kJ}{mol} \quad (3)$$



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

[2] Rönsch, S., et al., Review on methanation – From fundamentals to current projects. Fuel, 2015. 166: p. 276-296.

Methodology: Economical Analysis

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Peters et.al. [1]

$$\boldsymbol{NPC}\left[\frac{€}{L}\right] = \frac{\boldsymbol{ACC} + \sum OPEX_{ind} + \sum OPEX_{dir} + t_{labor}c_{labor}}{\frac{\dot{m}_{fuel}}{\rho_{fuel}} \cdot \frac{\omega_{fuel}}{\omega_{reference}}}$$

$$\boldsymbol{ACC}\left[\frac{€}{a}\right] = \boldsymbol{FCI} \cdot \left(\frac{IR\cdot(1+IR)^{y}}{(1+IR)^{y}-1} + \frac{IR\cdot y}{9}\right)$$

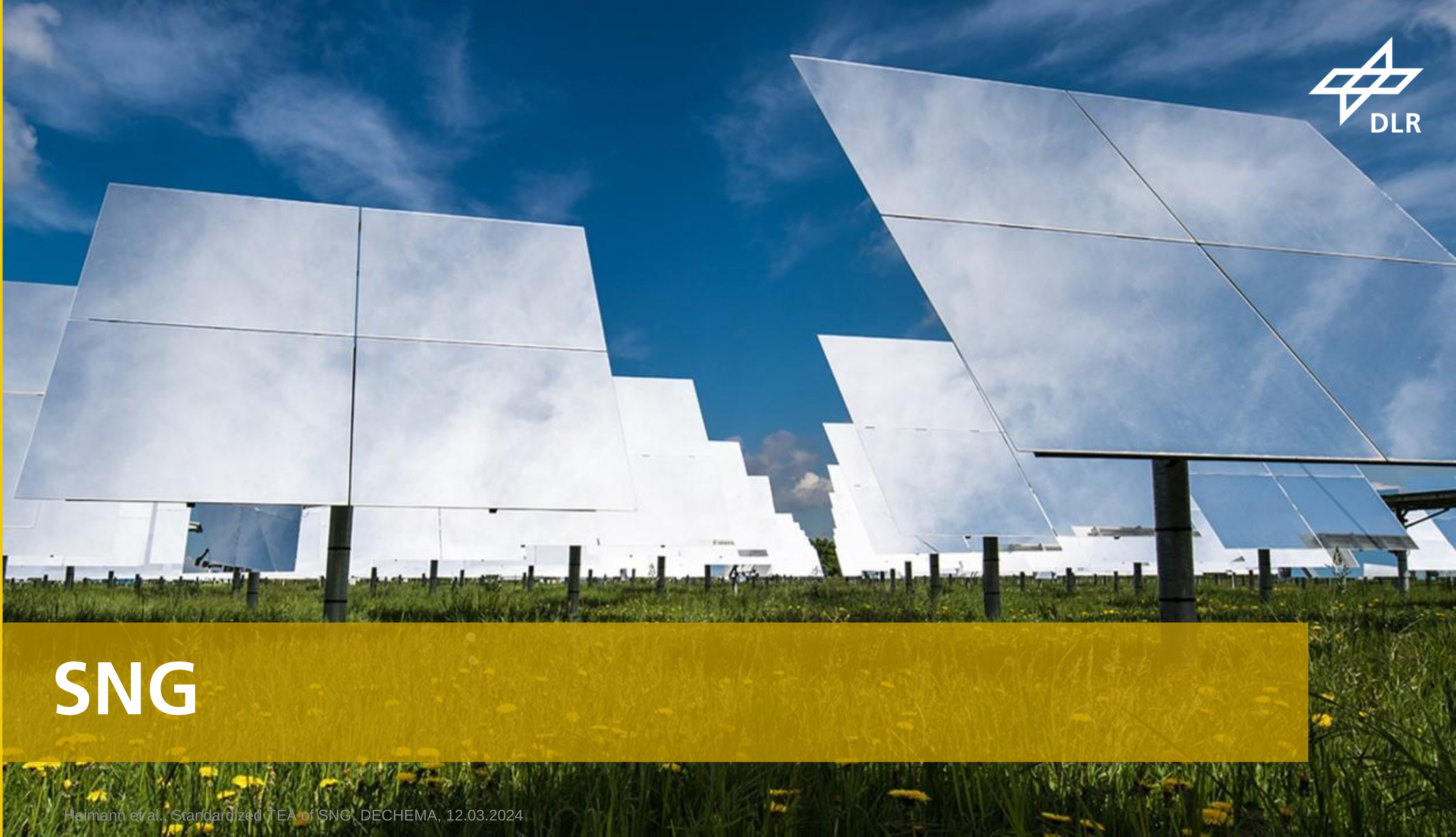
$$\boldsymbol{FCI} = \sum_{i=1}^{m} \boldsymbol{EC_i} \cdot \left(1 + \sum_{j=1}^{10} F_{ind,i,j}\right) \cdot \left(1 + \sum_{j=11}^{12} F_{ind,i,j}\right) \quad i,j \in \mathbb{N}$$

$$\boldsymbol{EC_i} = \boldsymbol{f_i}(\boldsymbol{S_{i,1}};\ \boldsymbol{S_{i,2}};\ \ldots\ \boldsymbol{S_{i,k}}) \cdot \left(\frac{CEPCI}{CEPCI_{ref}}\right) \cdot F_{pre,i} \cdot F_{mat,i} \cdot \left(1 - L_i^{\log_2(n)}\right), \qquad n,i,k \in \mathbb{N}$$

$$\boldsymbol{f_i}(\boldsymbol{S_{i,1}};\ \boldsymbol{S_{i,2}};\ \ldots\ \boldsymbol{S_{i,k}}) = f_i(S_i) = EC_{ref,i} \cdot \left(\frac{S_i}{S_{ref,i}}\right)^{d_i}$$

Basic conditions	[3]
Base Year	2018
Location	Germany
Currency	$€_{2018}$
Electricity input (plant + electrolysis)	300 MW_{el}
Full-load Hours	8,000 h/a
Electricity	56 $€_{2018}$/MWh
H_2 cost	4,742 $€_{2018}$/t
H_2 feed conditions	50 bar; 50 °C
CO_2 cost	69 $€_{2018}$/t
CO_2 feed conditions	3 bar; 25 °C
Interest Rate	5 %
Labor cost	41 $€_{2018}$
Plant lifetime	20 a

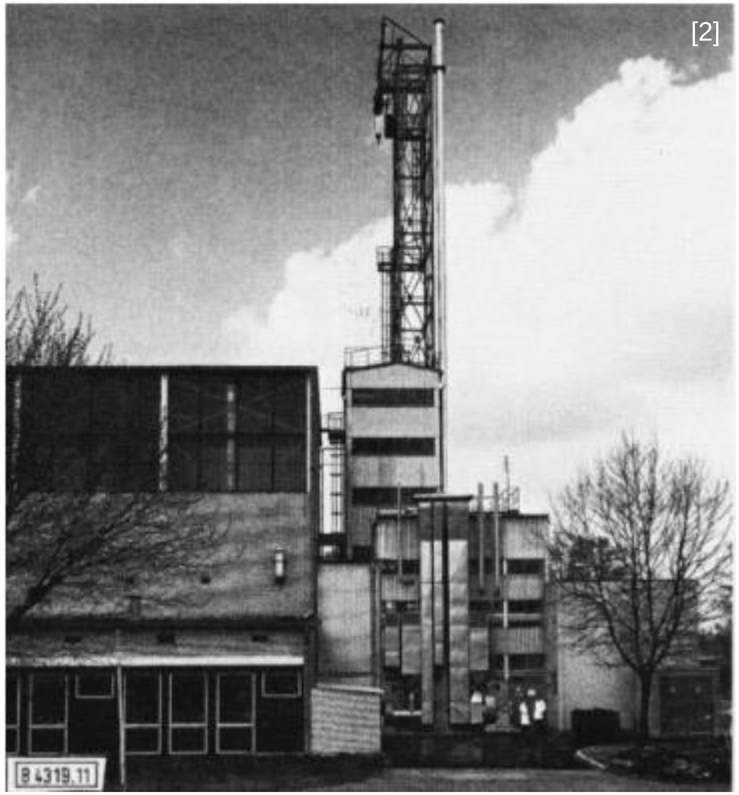
[1] M. Peters, K. Timmerhaus, R. West, 2004.
[2] F. G. Albrecht, D. H. König, N. Baucks, R.-U. Dietrich, 2017
[3] Heimann, N. et al (2023), submitted.



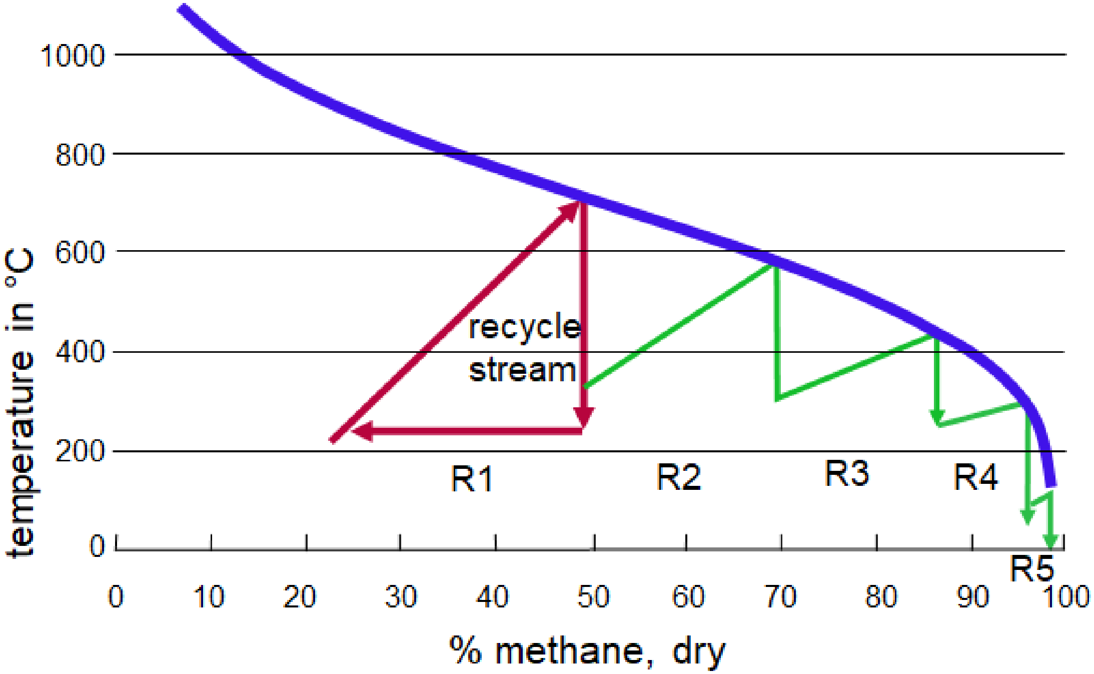
SNG

Large scale e-Methane production (SNG w. 98 vol.% CH_4)

Advanced TREMP™-process [1]


[2]

- Composition adjustment
  Transport: DIN EN 16723-2:2017-10
  Gas grid: DVGW G260
  - Polishing reactor & water removal



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[1] Topsøe, H., From coal to clean energy. 2011
[2] Harms, H., B. Höhlein, and A. Skov, 1980, Methanisierung kohlenmonoxidreicher Gase beim Energie-Transport. Heimann,
[3] N. et al., 2023, Standardized TEA of sCNG and HCNG, to be submitted

Large scale e-Methane production (SNG w. 98 vol.% CH_4)

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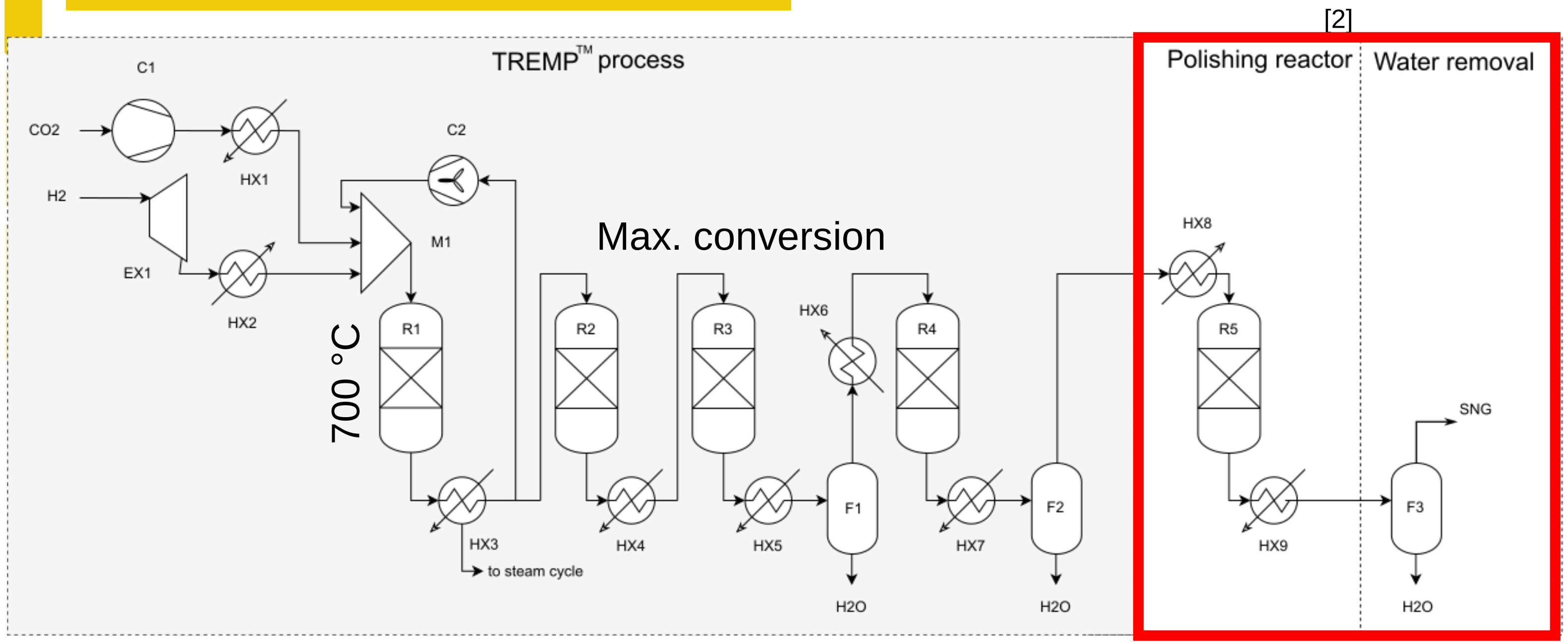

- Composition adjustment
  Transport: DIN EN 16723-2:2017-10
  Gas grid: DVGW G260
  - Polishing reactor & water removal

	R1	R2	R3	R4	R5
t [°C]	700	545	400	428	427
GHSV	8900	8800	4200[2]	4200[2]	4200[2]

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[1] Topsøe, H., From coal to clean energy. 2011
[2] Harms, H., B. Höhlein, and A. Skov, 1980, Methanisierung kohlenmonoxidreicher Gase beim Energie-Transport. Heimann,
[3] N. et al., 2023, Standardized TEA of sCNG and HCNG, to be submitted

Process description (SNG w. 98 vol.% CH_4)

Catalysis

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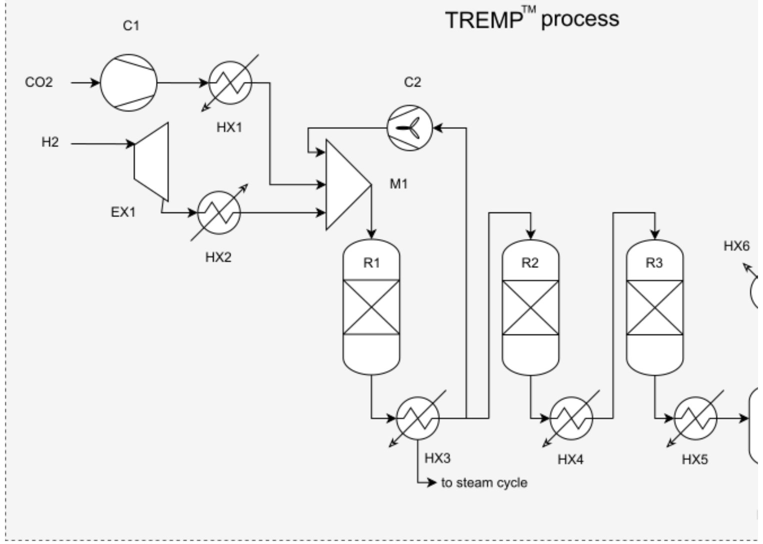
Advanced TREMP™-process [1]



Reaction kinetic: Rönsch et.al. [3-5]
Combination of WGS and CO-Mathanation

AspenPlus® model: RPlug

$T_{max,R1}$[3] = 700 °C

$T_{in,R1}$ = 250 °C

p[2] = 20-30 bar

$L_{reactor}$ = 2 m

$D_{reactor}$ = f(GHSV)

GHSV[2] = 4200-8900

Pressure drop: Ergun's equation

Catalyst[2] MCR-2X (22 % Ni)

Bulk density[2] = 1000 kg m^{-3}

Bed voidage[2] = 0.3

Lifespan[5] = 1 year

Color coding process parameters:
Blue → taken from literature
Green → own assumption/calculation

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[1] Topsøe, H., From coal to clean energy. 2011
[2] in range of: Harms, H., B. Höhlein, and A. Skov, 1980, Methanisierung kohlenmonoxidreicher Gase beim Energie-Transport.
[3] Rönsch et al., 2016, Review on methanation – From fundamentals to current projects.
[4] Klose, J., 1984, Kinetics of the methanation of carbon monoxide on an alumina-supported nickel catalyst. Journal of Catalysis
[5] Zhang, J., et al., 2013, Kinetic investigation of carbon monoxide hydrogenation under realistic conditions of methanation of biomass derived syngas
[6] Meylan et al., 2016, Material constraints related to storage of future European renewable electricity surpluses with CO2 methanation

Results KPI

SNG w. 98 vol.% CH_4

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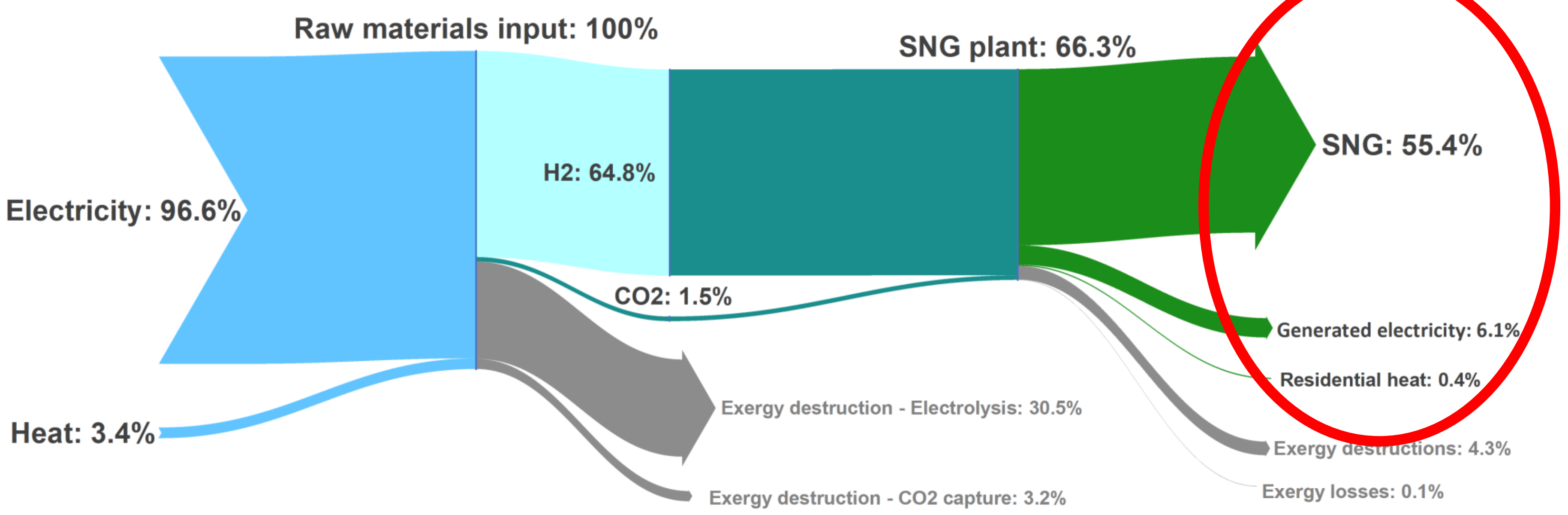
KPI / efficiencies

η_{H_2tF} = 82 %

η_{PtF} = 57 %*

SNG production exergy flow

61,9 % of exergy used

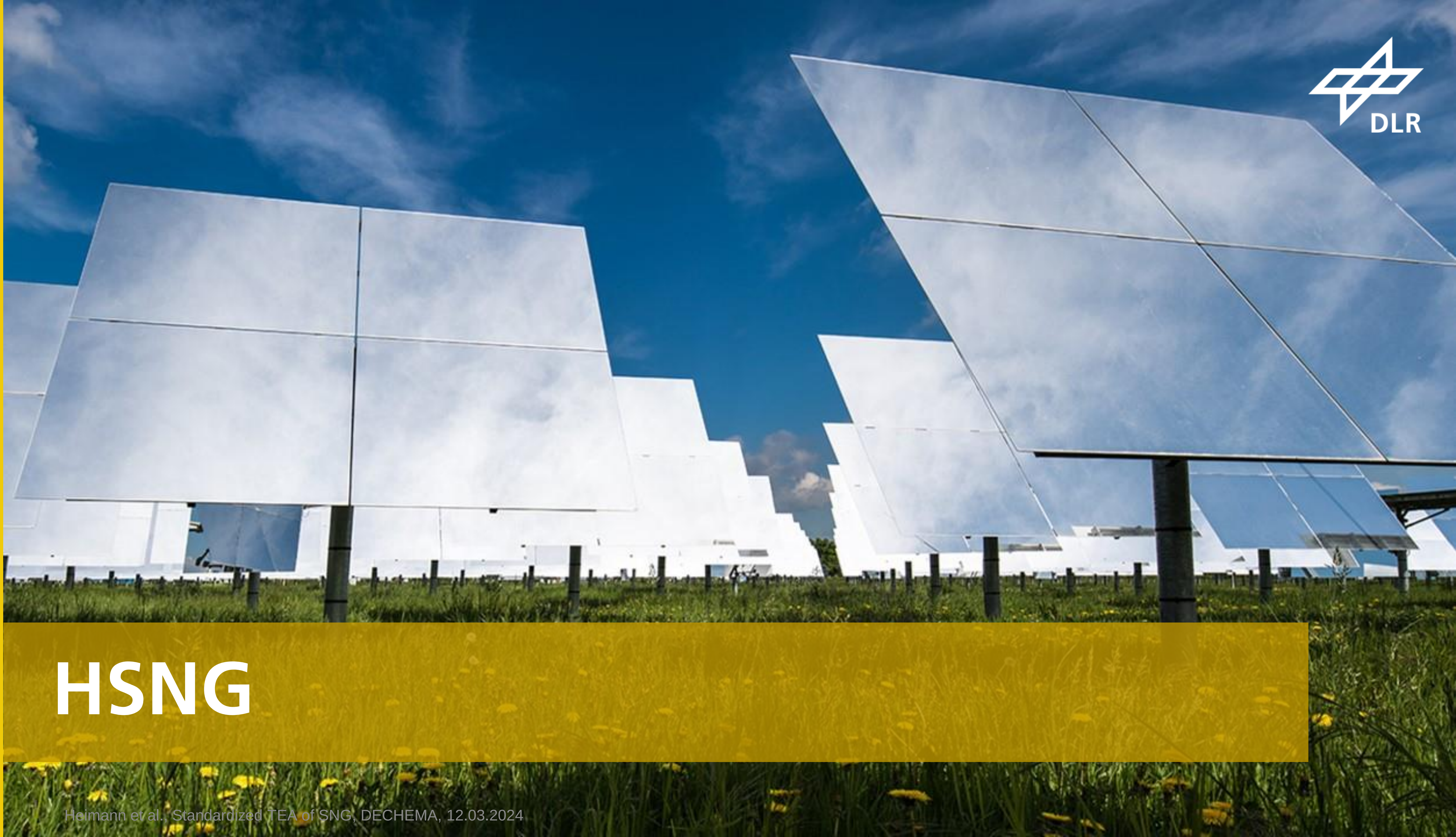


*Electrolysis combined efficiency 69.2 % P_{el}/LHV: assumed: 1/3 PEM, AEL, SOEC each[1-3]

- Exergy reuse: steam-cycle and residential heat
- Highly exergy efficiency optimized

[1] Noack et al., 2015
[2] Jansen et al., 2018, p. 36
[3] BEniVer assumptions

Heimann et al., Standardized TEA of SN



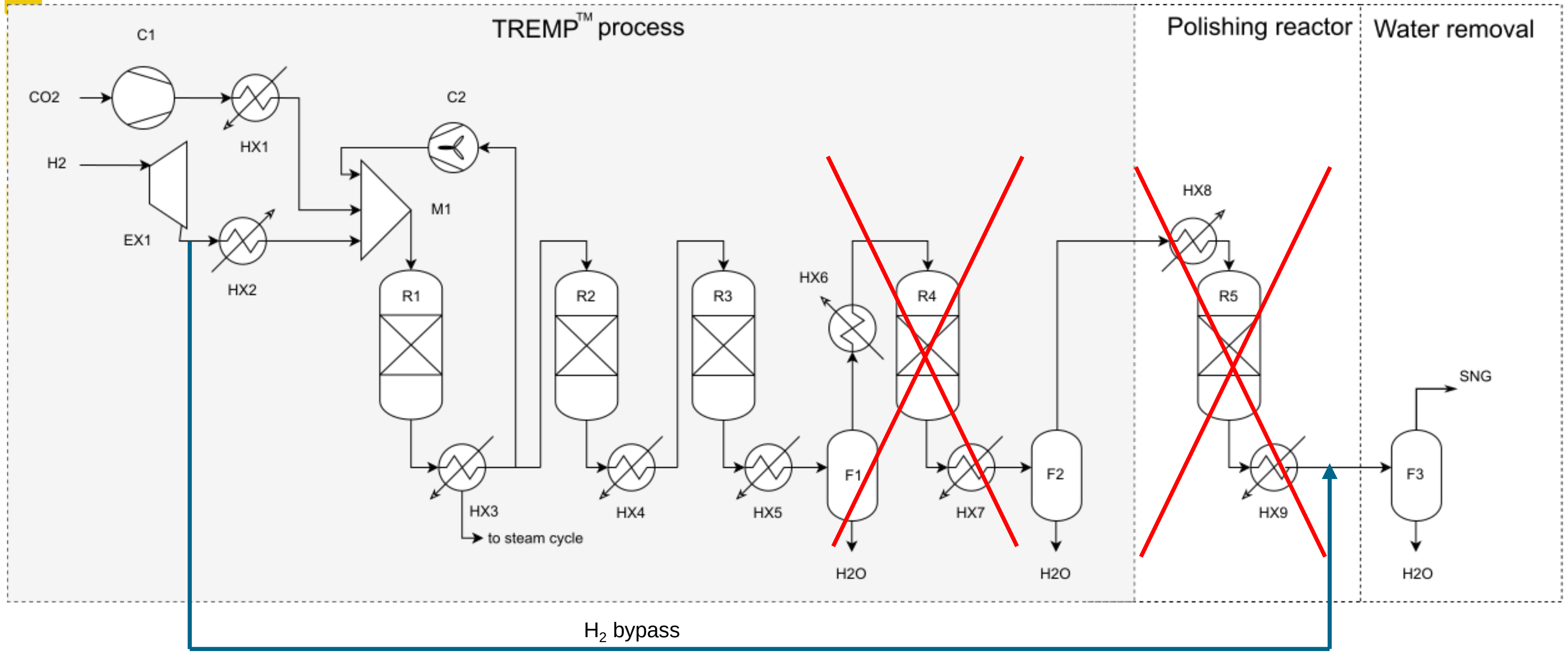
HSNG

Large scale HSNG production

HSNG w. 30 vol.% H_2

Adapted TREMP™ process [2]

[1]



- High temperature in R1
  - Steam cycle
- Composition adjustment
  30 vol.% H_2 content → HSNG-30
  - Number of reactors reduced
  - Partial H_2 bypass
  - Smaller reactors for same output
  - less H_2O production

Assumptions in the simulation:

- No impurities
- No side reactions

[1] Rönsch, S., et al., 2016
[2] Heimann, et al 2023, to be submitted

Large scale e-Hythane production (HSNG-30)

KPI / efficiencies

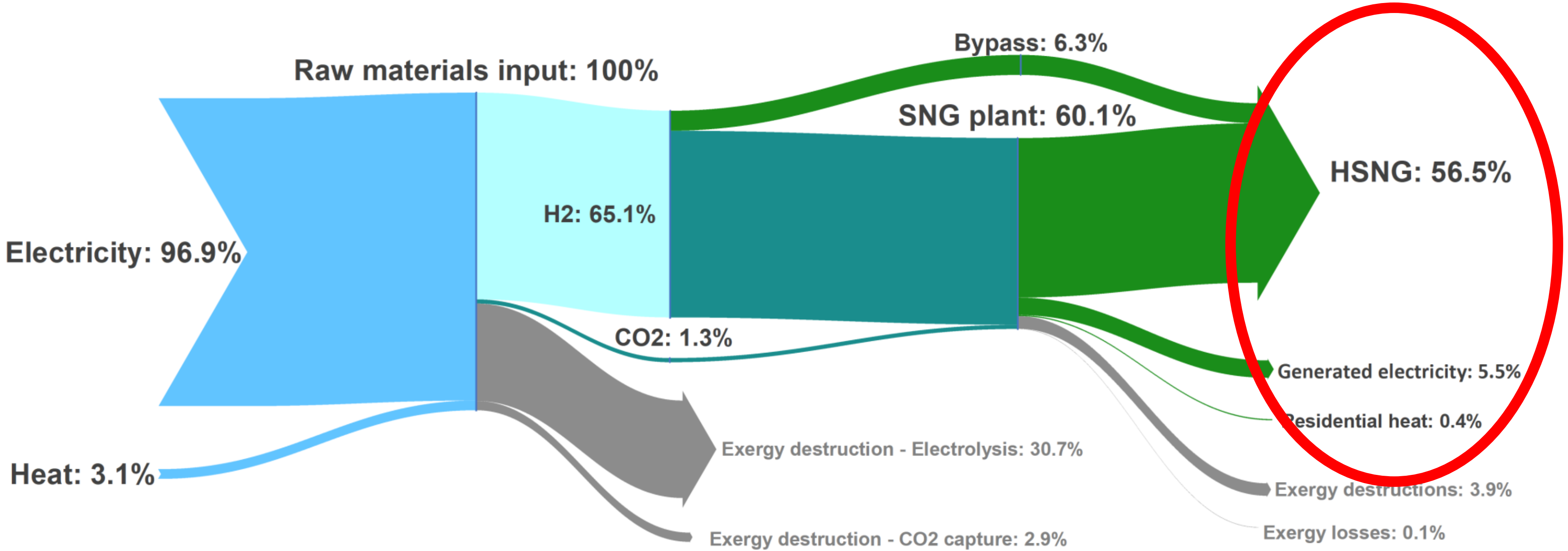
$\eta_{H_2tF} = 89\ \%$

$\eta_{PtF} = 58\ \%^{*}$

HSNG production exergy flow

62,4 % of exergy used

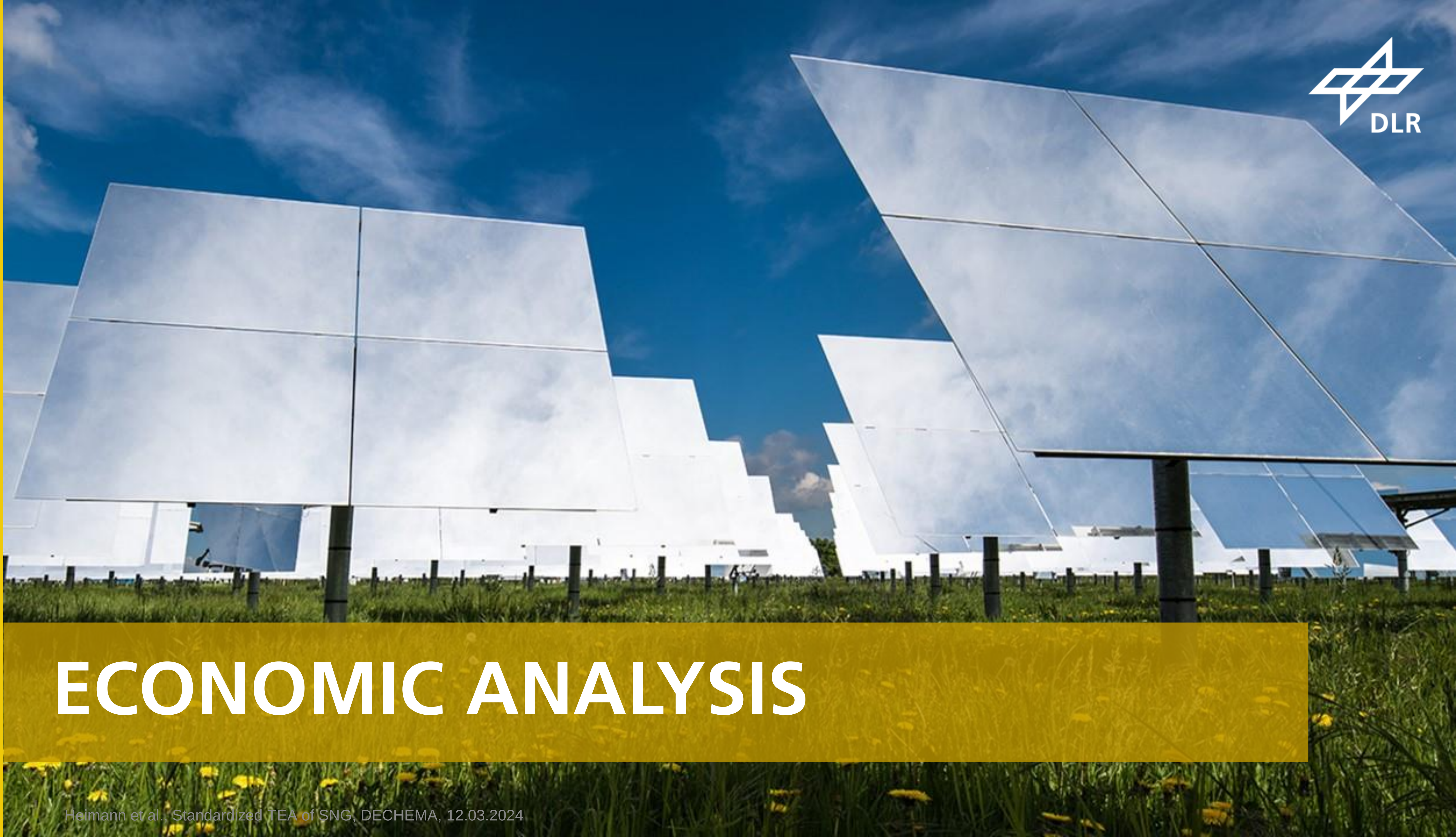
(SNG: 61,9 %)



*Electrolysis combined efficiency 69.2 % P_{el}/LHV: assumed: 1/3 PEM, AEL, SOEC each[1-3]

- 1.1 % more power to fuel than SNG
- 5.5 % reused in steam-cycle (compared to 6.1 %)

[1] Noack et al., 2015
[2] Jansen et al., 2018, p. 36
[3] BEniVer assumptions



ECONOMIC ANALYSIS

Results: Fixed Capital Investment

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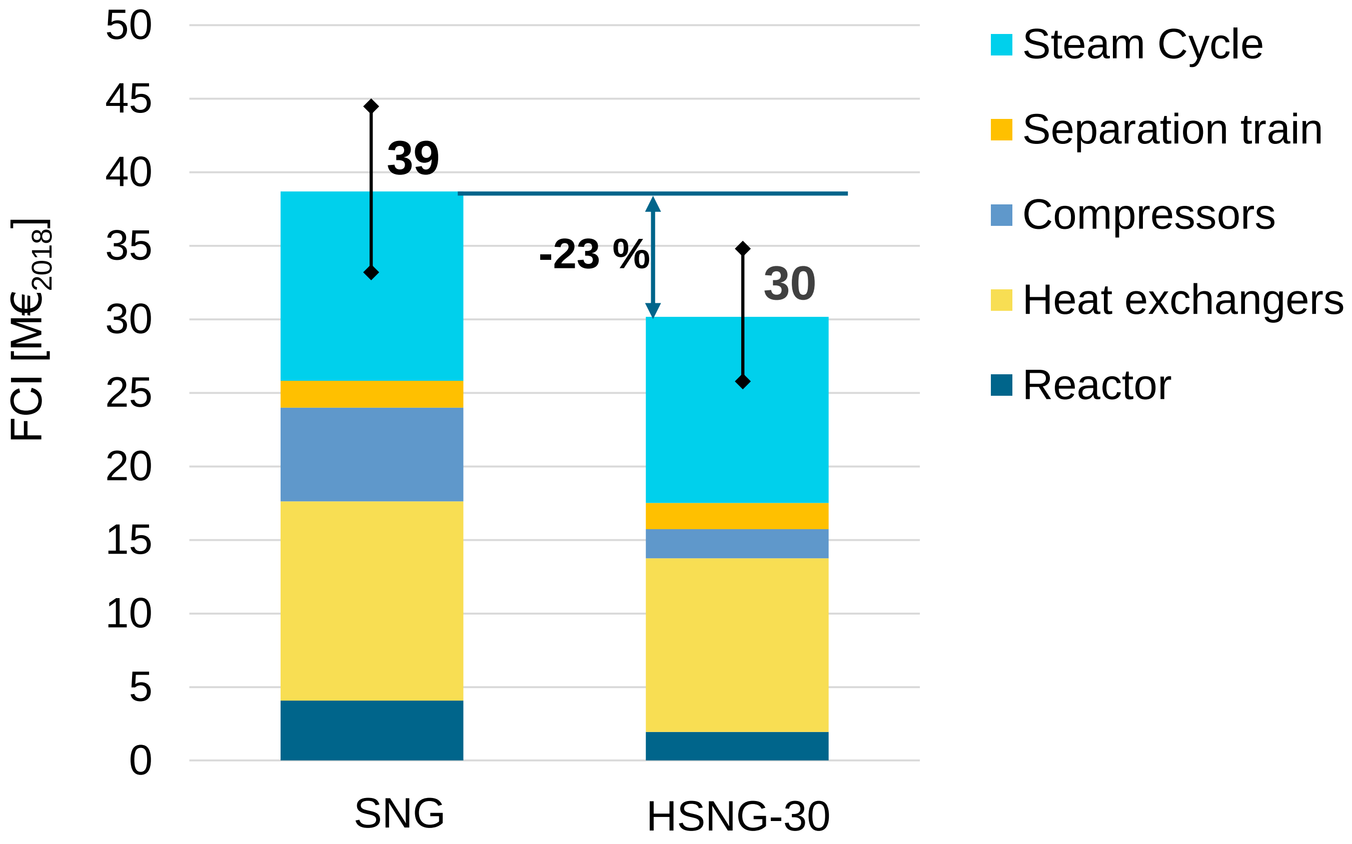

FCI reduction for Hythan30 compared to SNG ➔ 23 %

Significant reduction in compressors and reactors

Steam cycle, heat-exchangers remain significant FCI

Heimann et al., Standardized TEA of SNG, DECHEMA, 12.03.2024

Results: Net Production Costs

electrolyzer excluded

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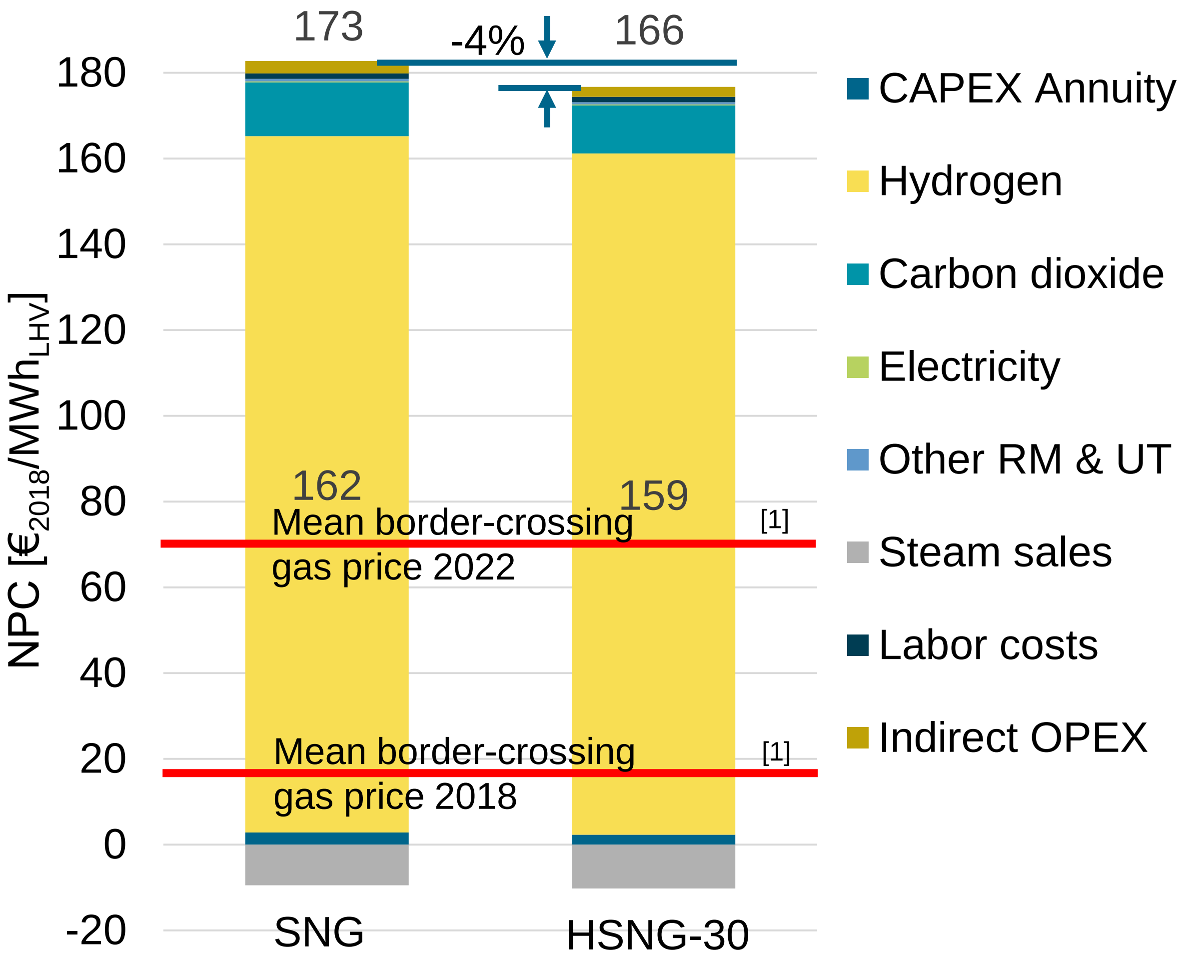

- NPC reduction for Hythan30 compared to SNG: ➔ 4 %
- Less H_2 needed
- >8 fold natural gas price

[1] BAFA - Erdgasstatistik

Results: Sensitivity of NPC

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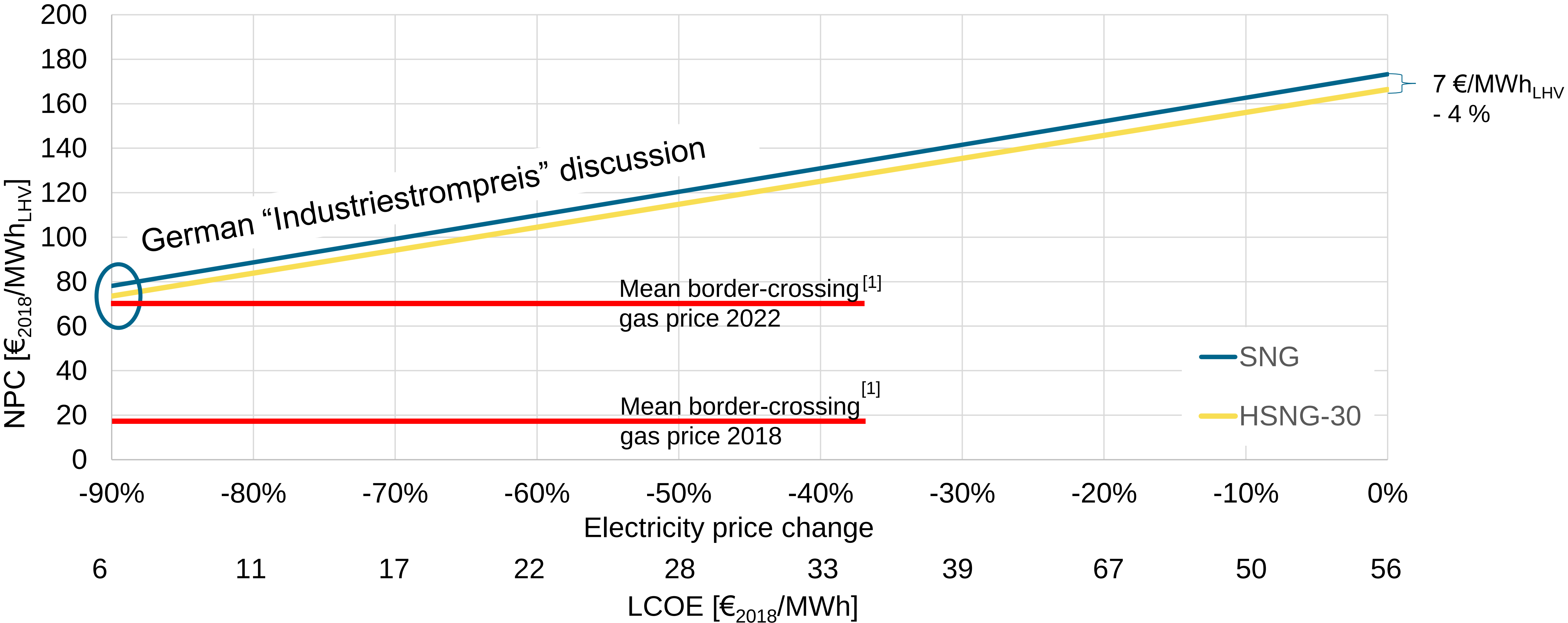

[1] BAFA - Erdgasstatistik

Results: Comparison of e-fuels

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Comparing generic fuels / designer fuels

	SNG	HSNG-30	MeOH	FT	$OME_{3\text{-}5}$	DMC	MeFo
η_{PtF} [%]	57	58	53	40	42	47	52
NPC [$€_{2018}$/MWh_{LHV}]	173	166	204	321	360	329	298
Application parameter examples	• Heavy truck • Drivetrain retrofit • …	• Combifuel • Heavy truck • Drivetrain retrofit • …	• Used in China • Low vapor pressure • Further conversion in Europe?	• Certified sustainable jet fuel • …	• Better combustion • Blending ratio? • …	• Better combustion • Blending ratio? • …	• Better combustion • Blending ratio? • …

HSNG-30: highest efficiency cheapest e-fuel of EiV
Ecological assessment still pending
Application assessment started

Heimann et al., Standardized TEA of SNG, DECHEMA, 12.03.2024

Conclusion

- Renewable non-electrical transport : SNG and HSNG preferable
- 300 MW production plant to small for German demand
- German grid electricity not 100 % renewable

+ SNG:
    - High efficiency
    - Existing technology
    - Existing infrastructure

+ Hythan
    - Higher efficiency
    - Better performance in combustion

Outlook

- Cheap renewable electricity needed
- Political will needed

➔Outlook: Identical HSNG spec. for both heat and transport applications

Transparent, standardized DLR assessment methodology available

THANK YOU FOR YOUR ATTENTION!

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