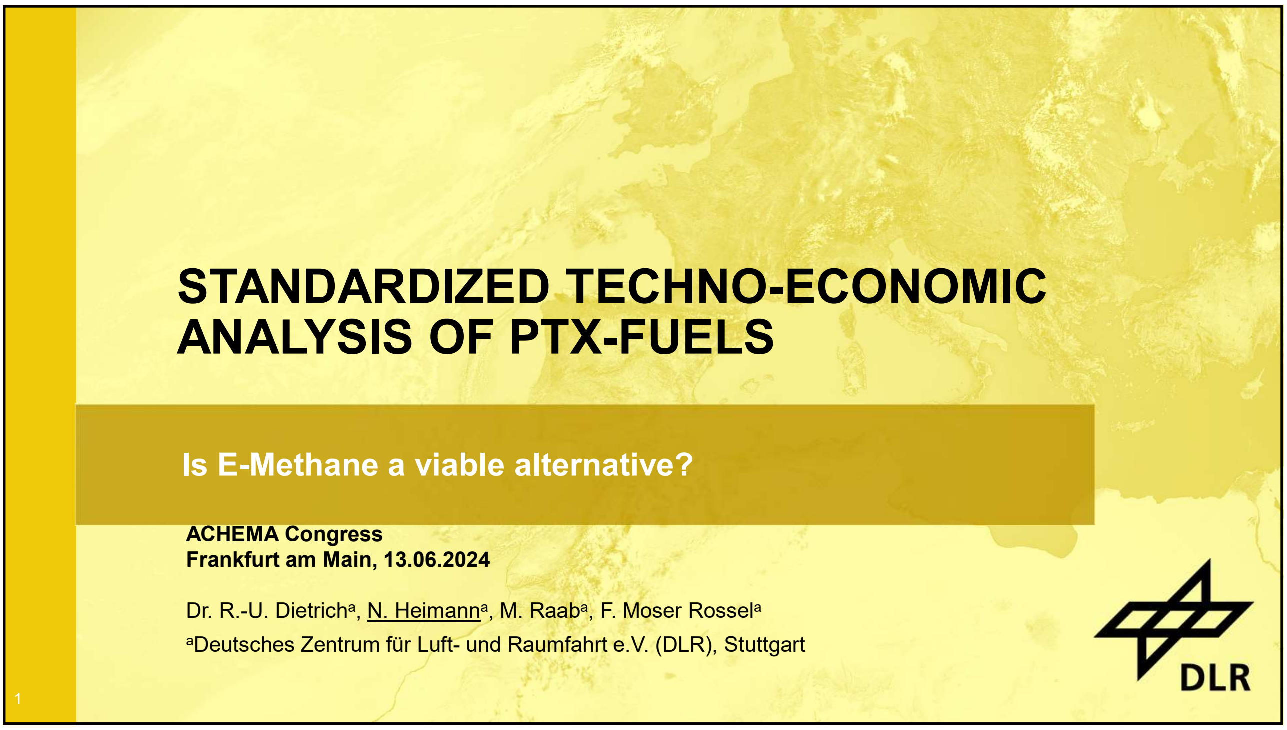
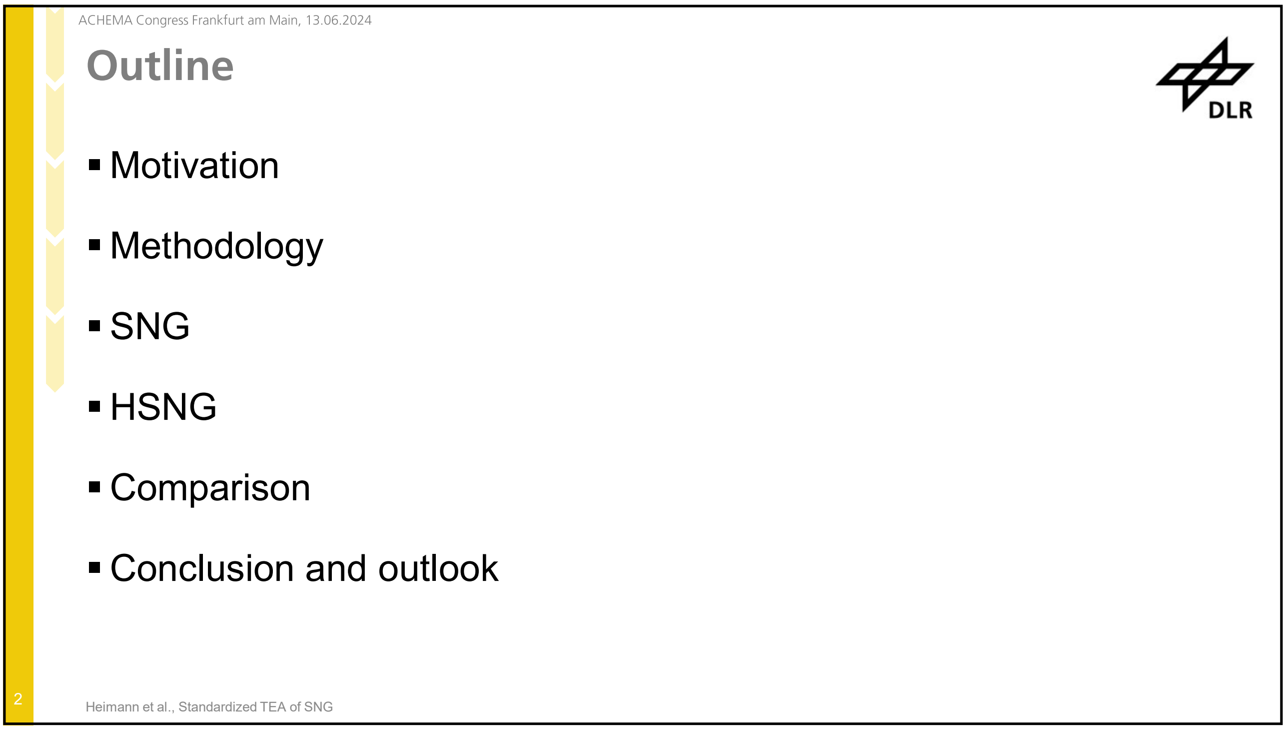


STANDARDIZED TECHNO-ECONOMIC ANALYSIS OF PTX-FUELS

Is E-Methane a viable alternative?

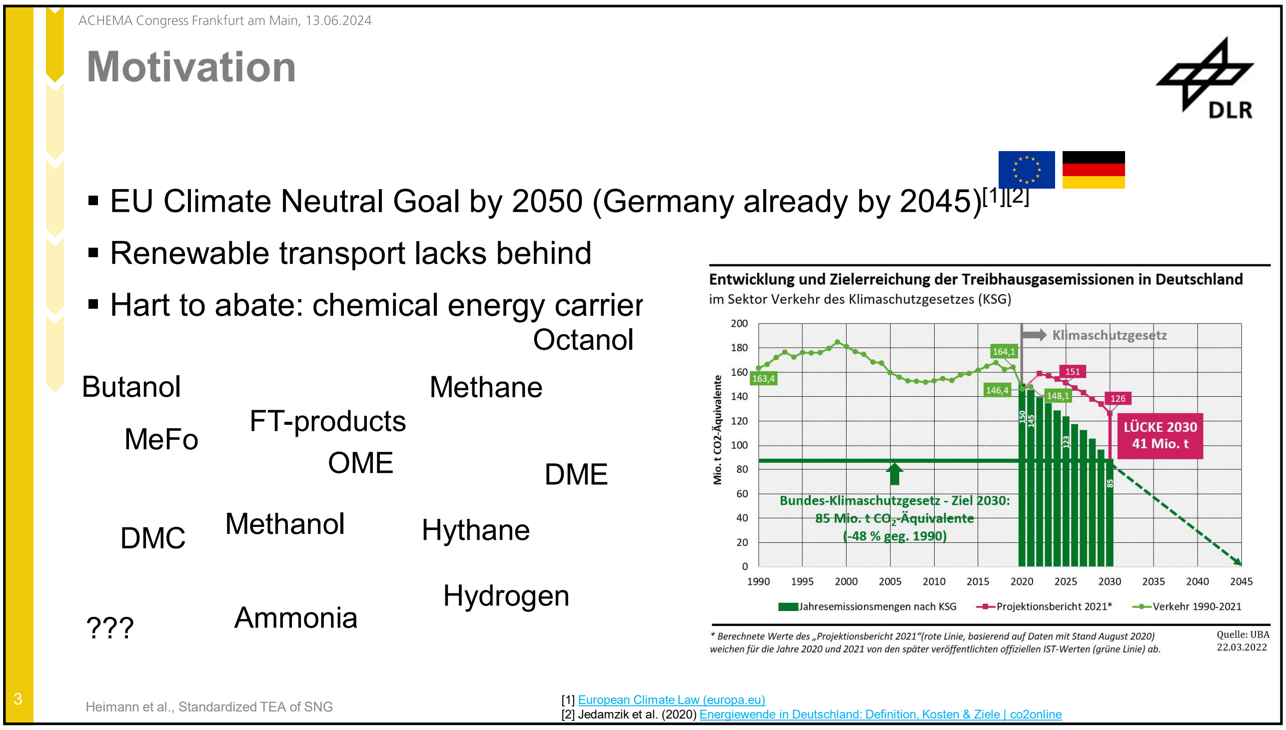
ACHEMA Congress
Frankfurt am Main, 13.06.2024

Dr. R.-U. Dietrich[a], N. Heimann[a], M. Raab[a], F. Moser Rossel[a]
[a]Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Stuttgart



Outline

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



Motivation

DLR

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

Octanol

Butanol

Methane

FT-products

MeFo

OME

DME

DMC

Methanol

Hythane

Hydrogen

???

Ammonia

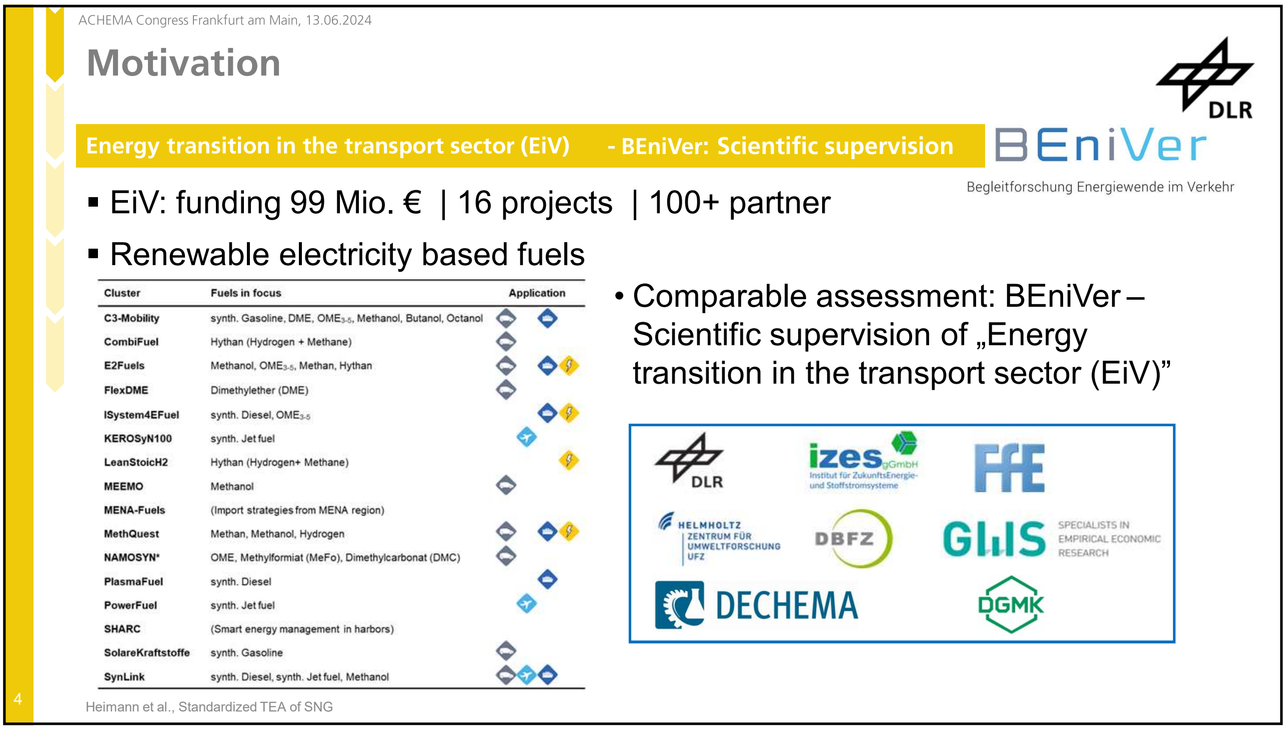
Entwicklung und Zielerreichung der Treibhausgasemissionen in Deutschland

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

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



Motivation

DLR

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

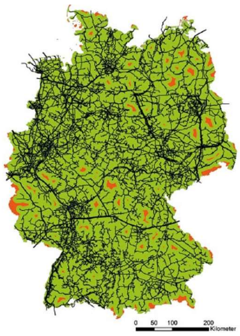
Cluster	Fuels in focus	Application
C3-Mobility	synth. Gasoline, DME, OME_{3-5}, Methanol, Butanol, Octanol	🚗 🚢
CombiFuel	Hythan (Hydrogen + Methane)	🚗
E2Fuels	Methanol, OME_{3-5}, Methan, Hythan	🚗 🚢 ⚡
FlexDME	Dimethylether (DME)	🚗
ISystem4EFuel	synth. Diesel, OME_{3-5}	🚢 ⚡
KEROSyN100	synth. Jet fuel	✈
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

Image: Avenir LNG

Source: Wolfgang Jargstorff / Fotolia.com

Image: Daimler

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

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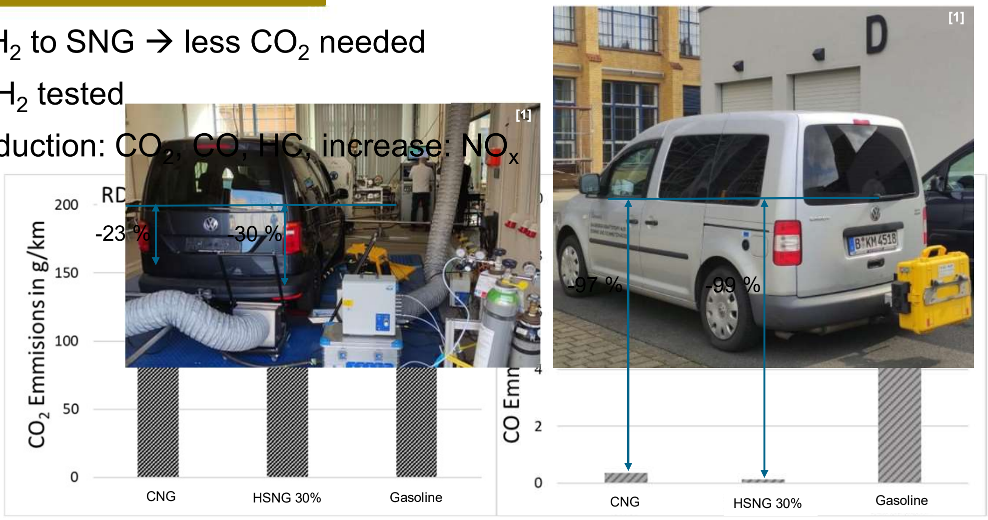
Motivation: HSNG

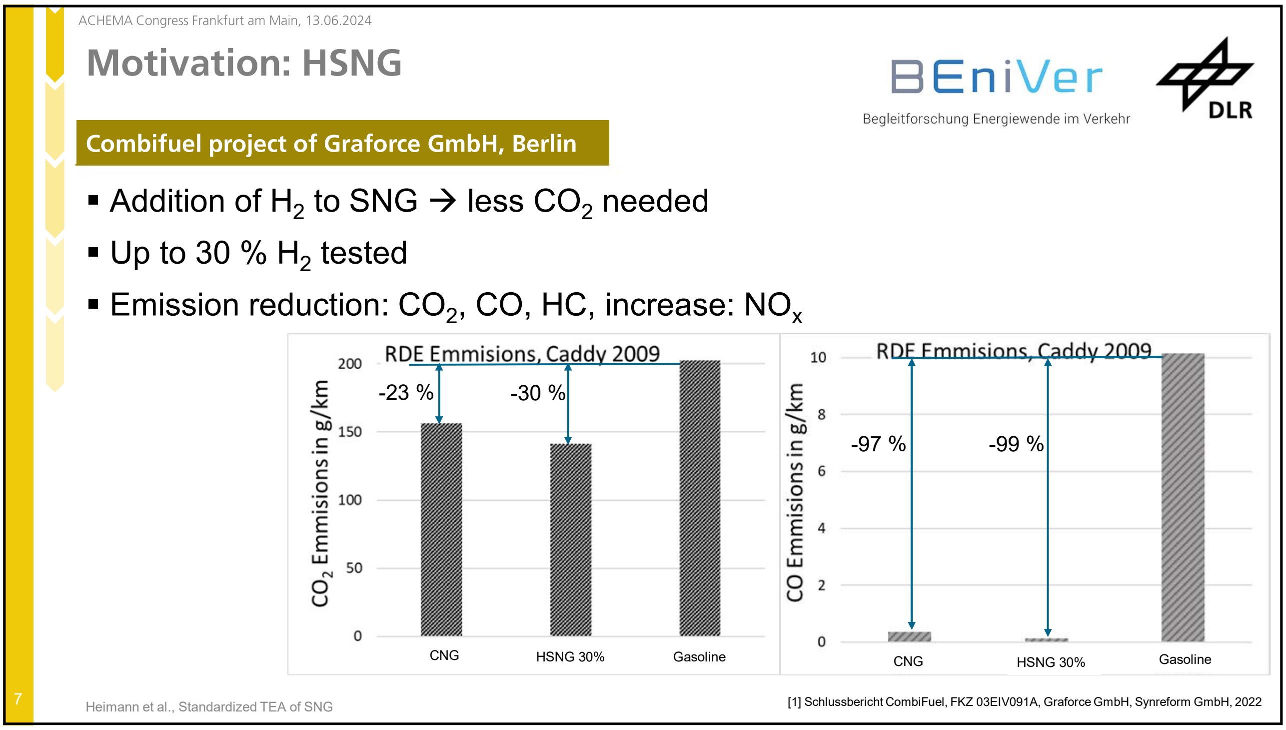
BEniVer
Begleitforschung Energiewende im Verkehr

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



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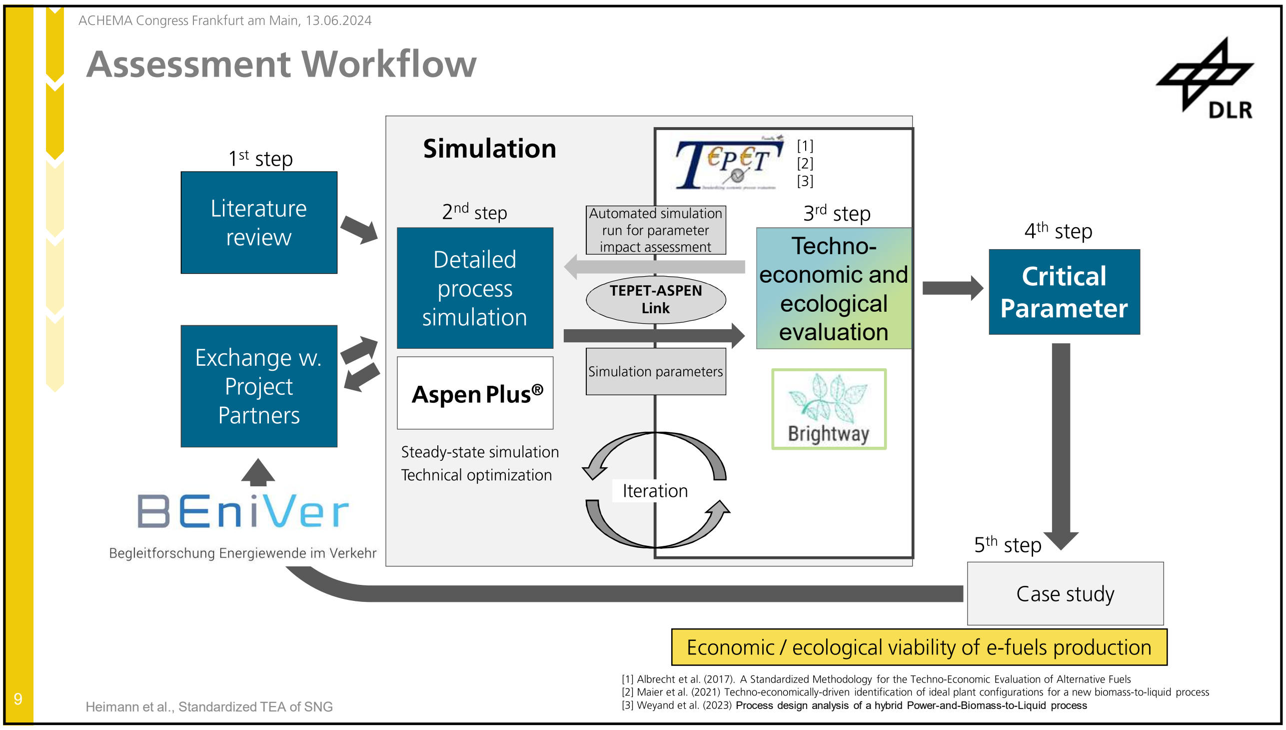
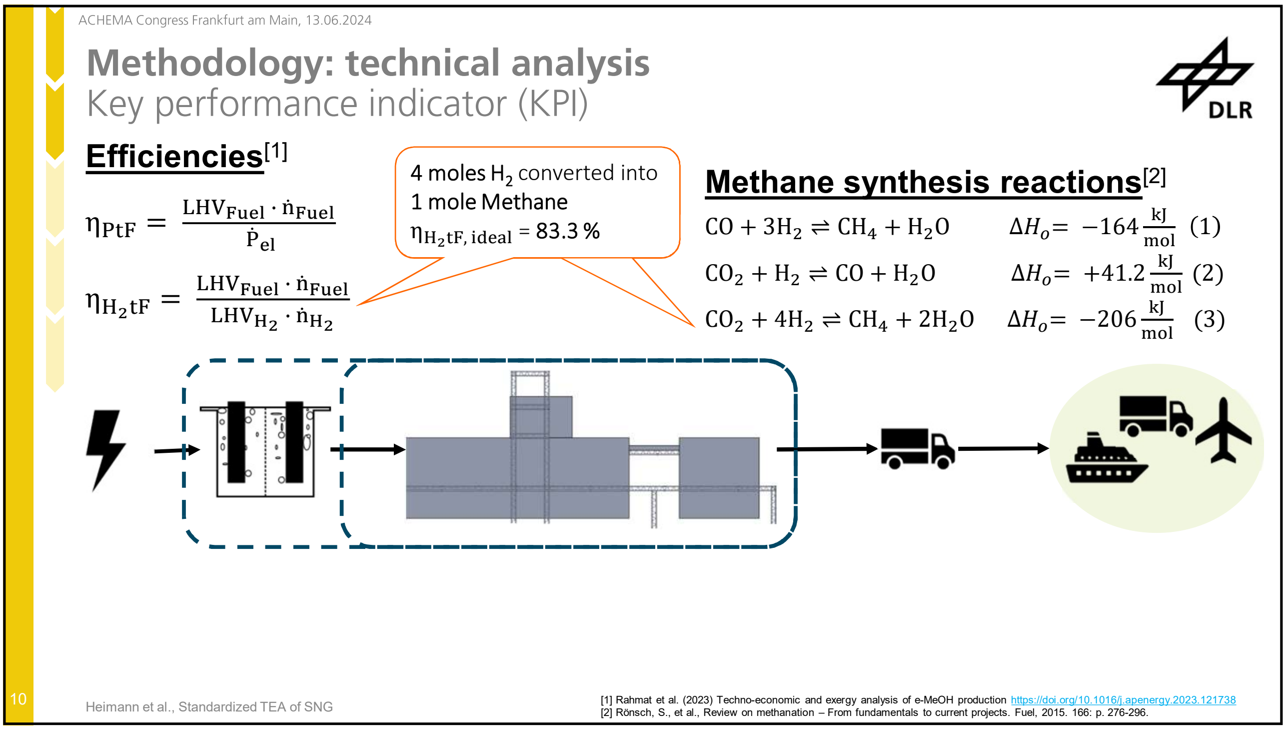
[1] Schlussbericht CombiFuel, FKZ 03EIV091A, Graforce GmbH, Synreform GmbH, 2022

METHODOLOGY



Assessment Workflow

[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)

Efficiencies[1]

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

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

4 moles H_2 converted into
1 mole Methane
$\eta_{\mathrm{H_2tF,\,ideal}}$ = 83.3 %

Methane synthesis reactions[2]

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

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

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

[1] Rahmat et al. (2023) Techno-economic and exergy analysis of e-MeOH production https://doi.org/10.1016/j.apenergy.2023.121738
[2] 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]

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

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

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

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

$$,\quad n,i,k\ \in\mathbb{N}$$

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

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 (2024), submitted.

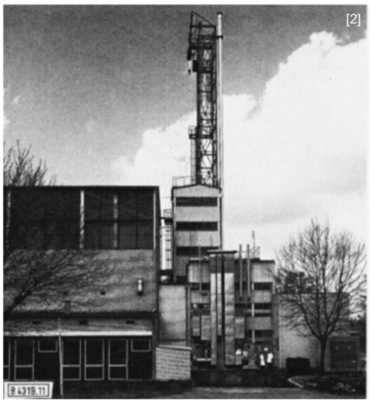
SNG

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

Assumptions in the simulation:

- No impurities
- No side reactions

Advanced TREMP™-process [1]


[2]

[1] Topsøe, H., From coal to clean energy. 2011
[2] Harms, H., B. Höhlein, and A. Skov, 1980, Methanisierung kohlenmonoxidreicher Gase beim Energie-Transport.
[3] Heimann, N. et al., 2024, Standardized TEA of sCNG and HCNG, to be submitted

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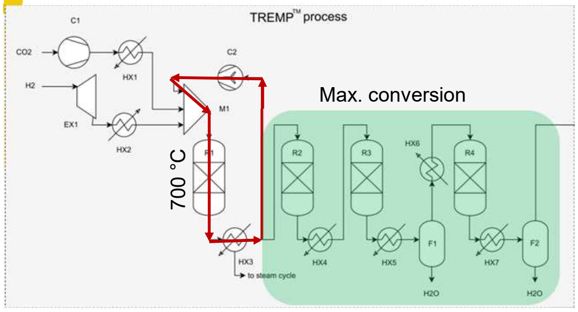
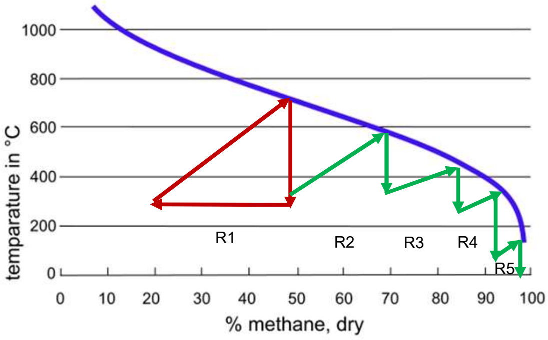


Max. conversion

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



[1] Topsøe, H., From coal to clean energy. 2011
[2] Harms, H., B. Höhlein, and A. Skov, 1980, Methanisierung kohlenmonoxidreicher Gase beim Energie-Transport.
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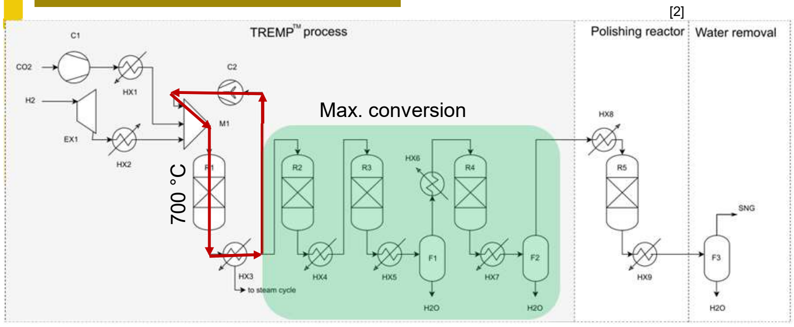

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[1] Topsøe, H., From coal to clean energy. 2011
[2] Harms, H., B. Höhlein, and A. Skov, 1980, Methanisierung kohlenmonoxidreicher Gase beim Energie-Transport.
[3] Heimann, N. et al., 2024, Standardized TEA of sCNG and HCNG, to be submitted

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

Catalysis

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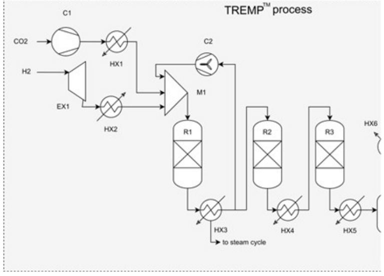
Advanced TREMP™-process [1]



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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DLR

KPI / efficiencies

$\eta_{PtF} = 57\ \%^*$

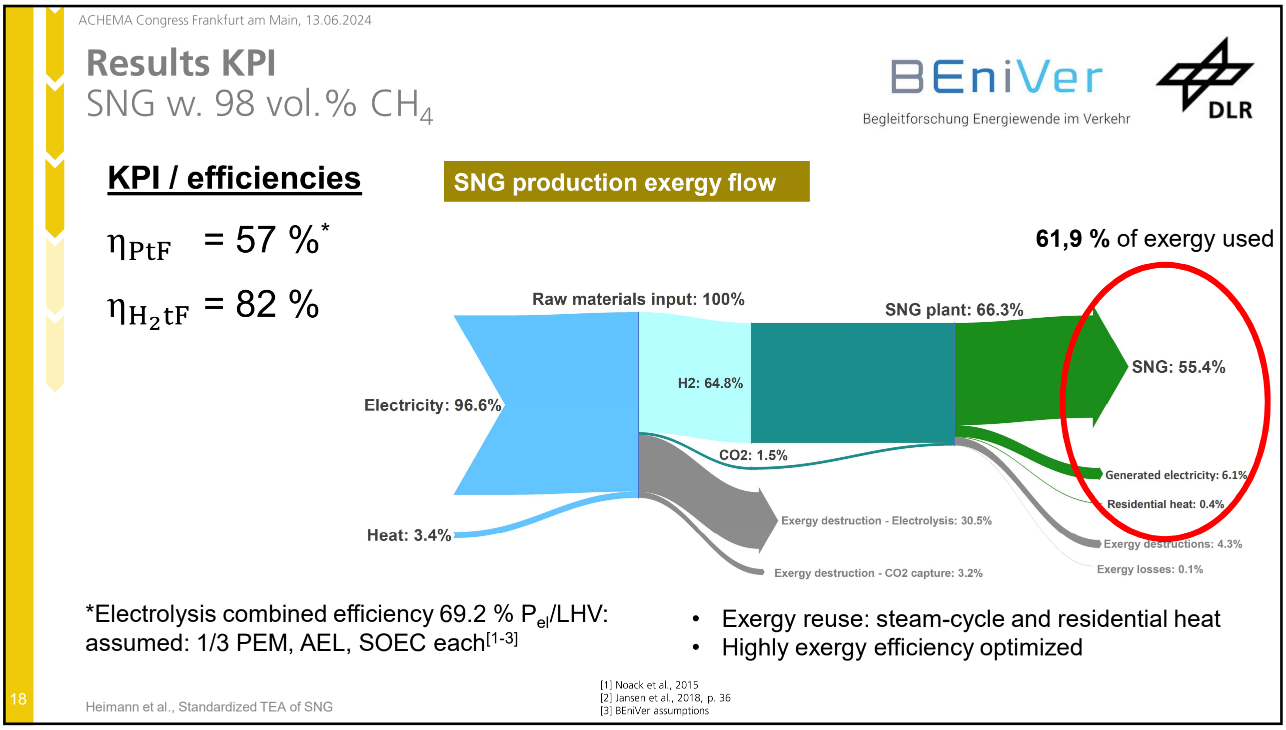
$\eta_{H_2tF} = 82\ \%$ $\eta_{H_2tF,ideal} = 83.3\ \%$

*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 SNG



Results KPI
SNG w. 98 vol.% CH_4

BEniVer
Begleitforschung Energiewende im Verkehr
DLR

KPI / efficiencies

$\eta_{PtF} = 57\ \%^*$

$\eta_{H_2tF} = 82\ \%$

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]

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

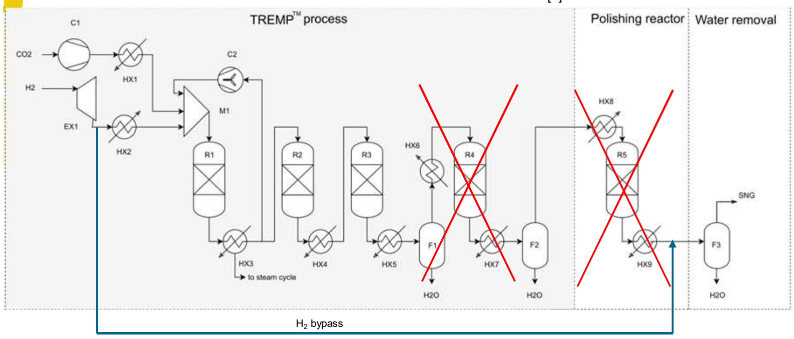
Heimann et al., Standardized TEA of SNG

HSNG-30

Large scale HSNG production

HSNG w. 30 vol.% H_2

Adapted TREMP™ process [2]



- 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, N. et al., 2024, Standardized TEA of sCNG and HCNG, to be submitted

Large scale e-Hythane production (HSNG-30)

KPI / efficiencies

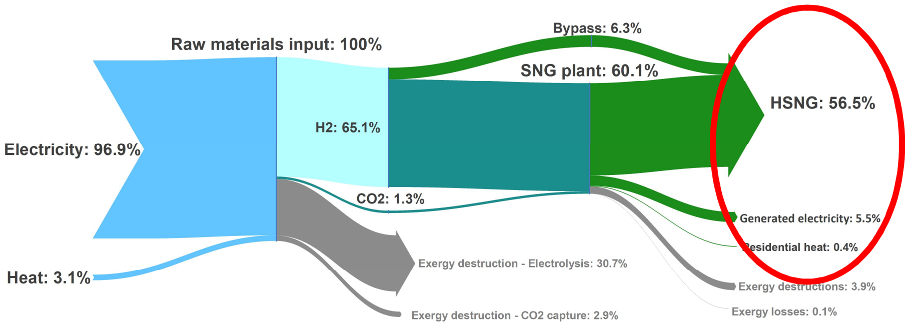
$\eta_{\mathrm{PtF}} = 58\ \%^{*}$

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

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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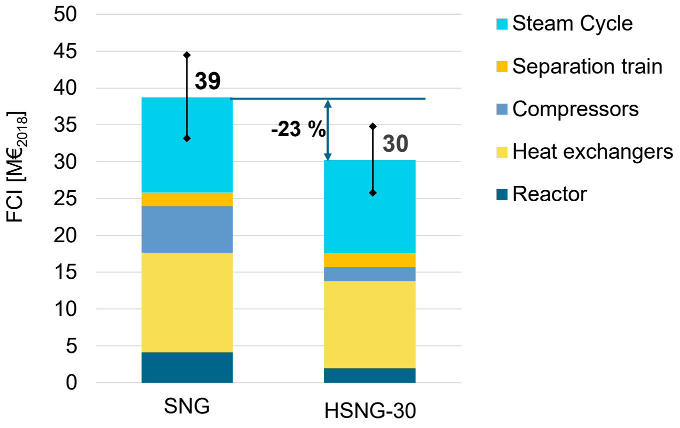
DLR



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

Results: Net Production Costs
electrolyzer excluded

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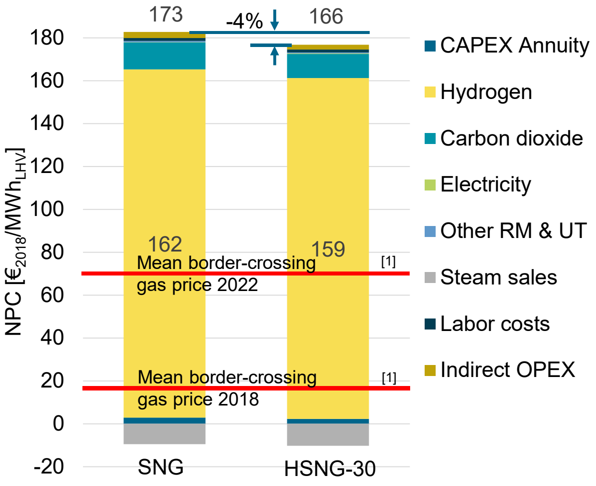
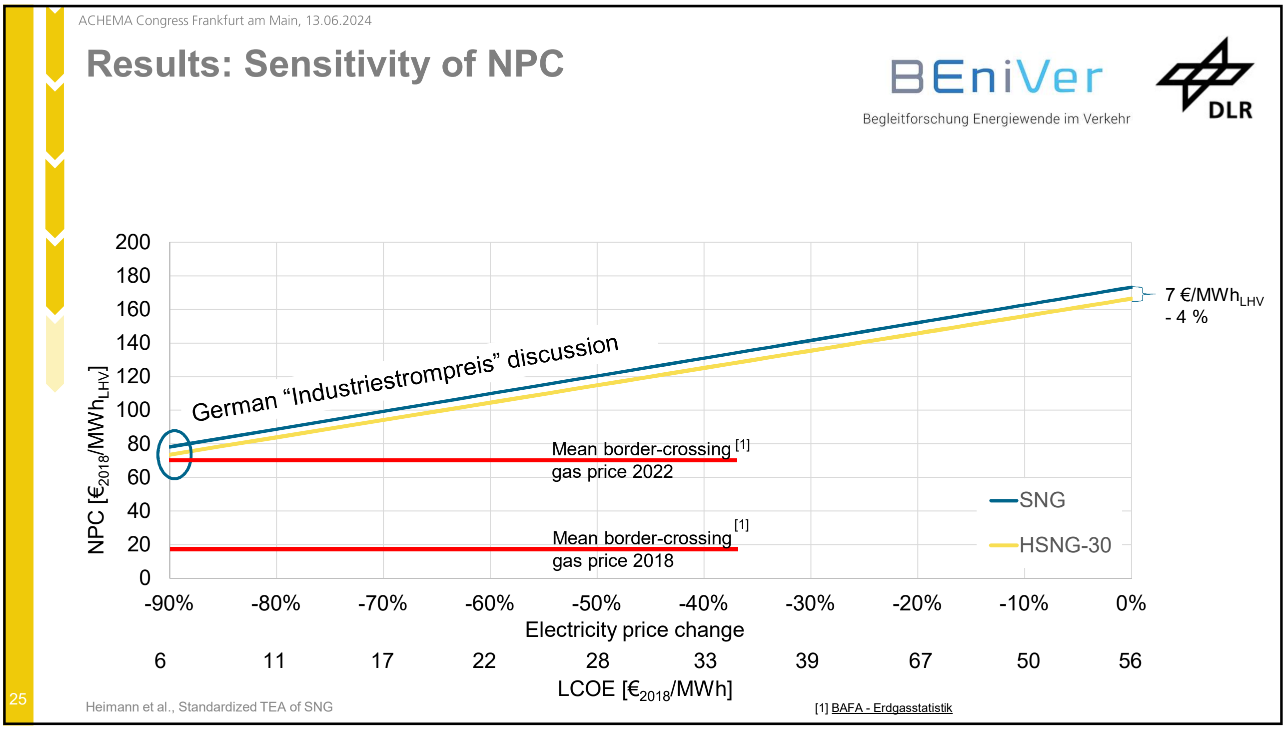


- NPC reduction for Hythan30 compared to SNG: ➔ 4 %
- Less H_2 needed
- >8 fold natural gas price

Heimann et al., Standardized TEA of SNG

[1] BAFA - Erdgasstatistik



Results: Sensitivity of NPC

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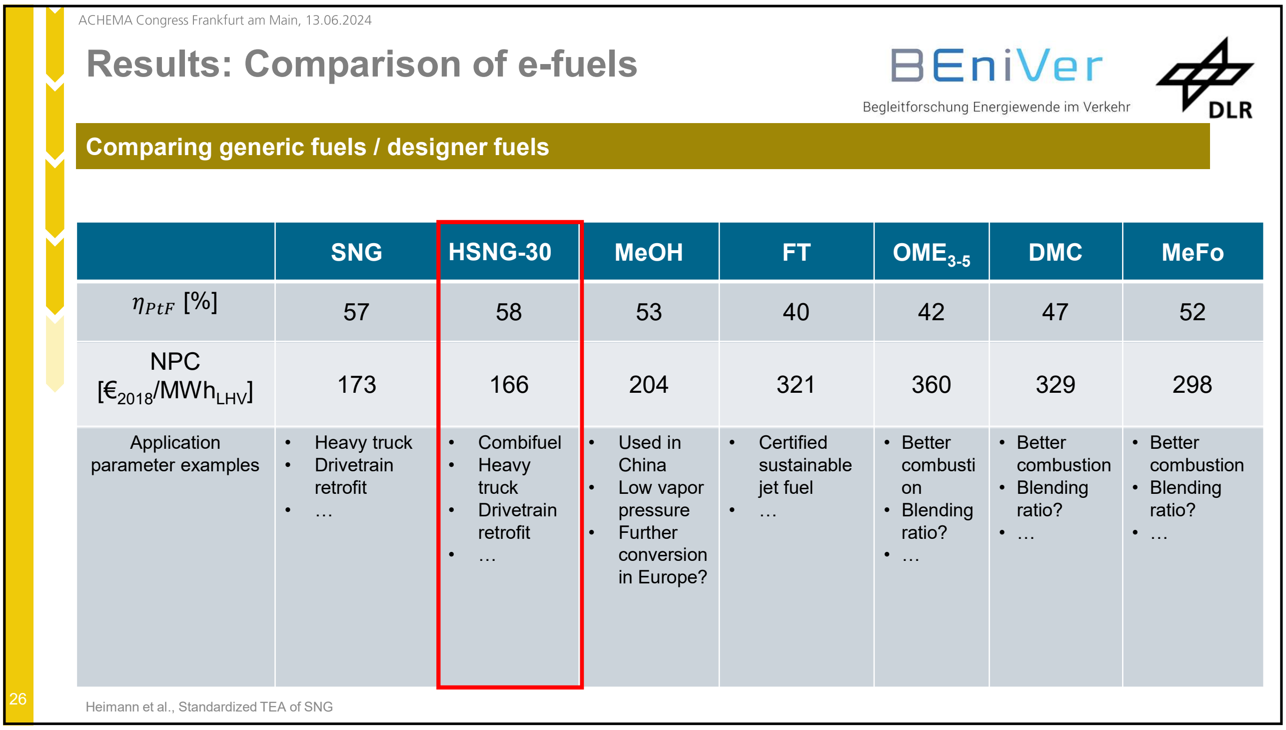
Heimann et al., Standardized TEA of SNG

[1] BAFA - Erdgasstatistik



Results: Comparison of e-fuels

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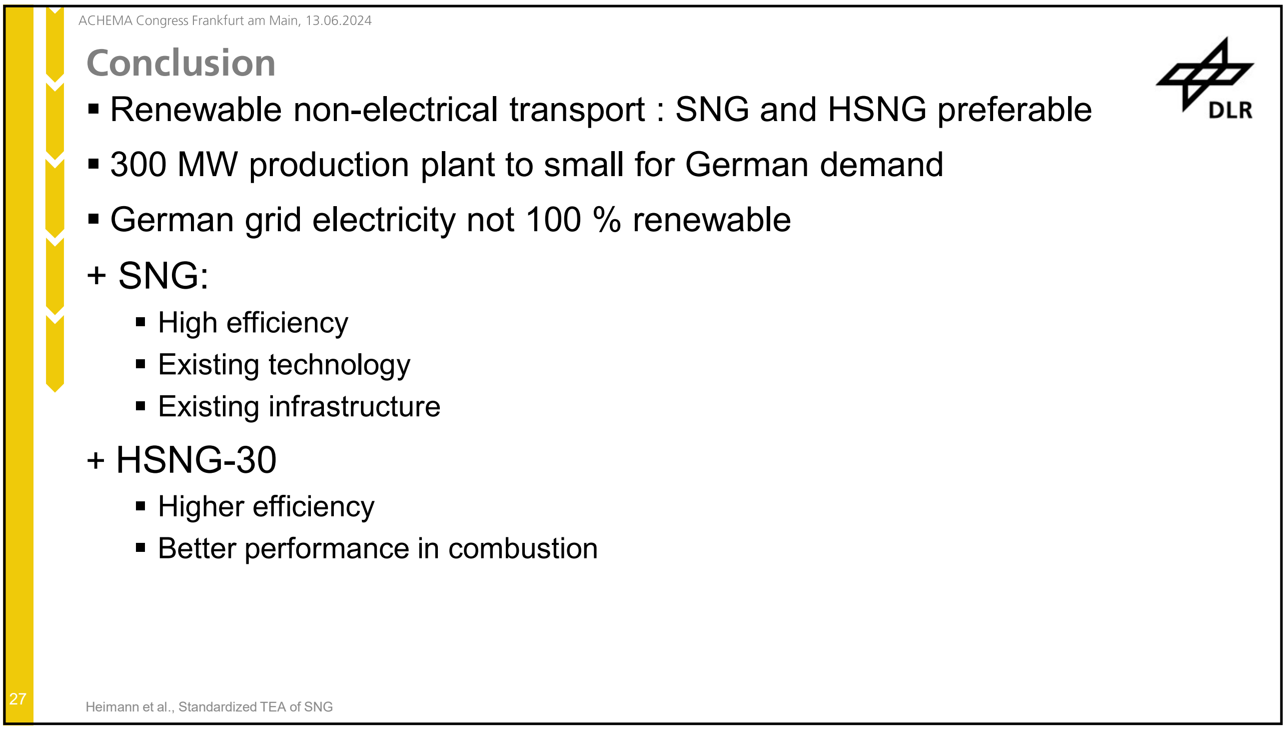
Comparing generic fuels / designer fuels

	SNG	HSNG-30	MeOH	FT	OME_{3-5}	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? • …

Heimann et al., Standardized TEA of SNG

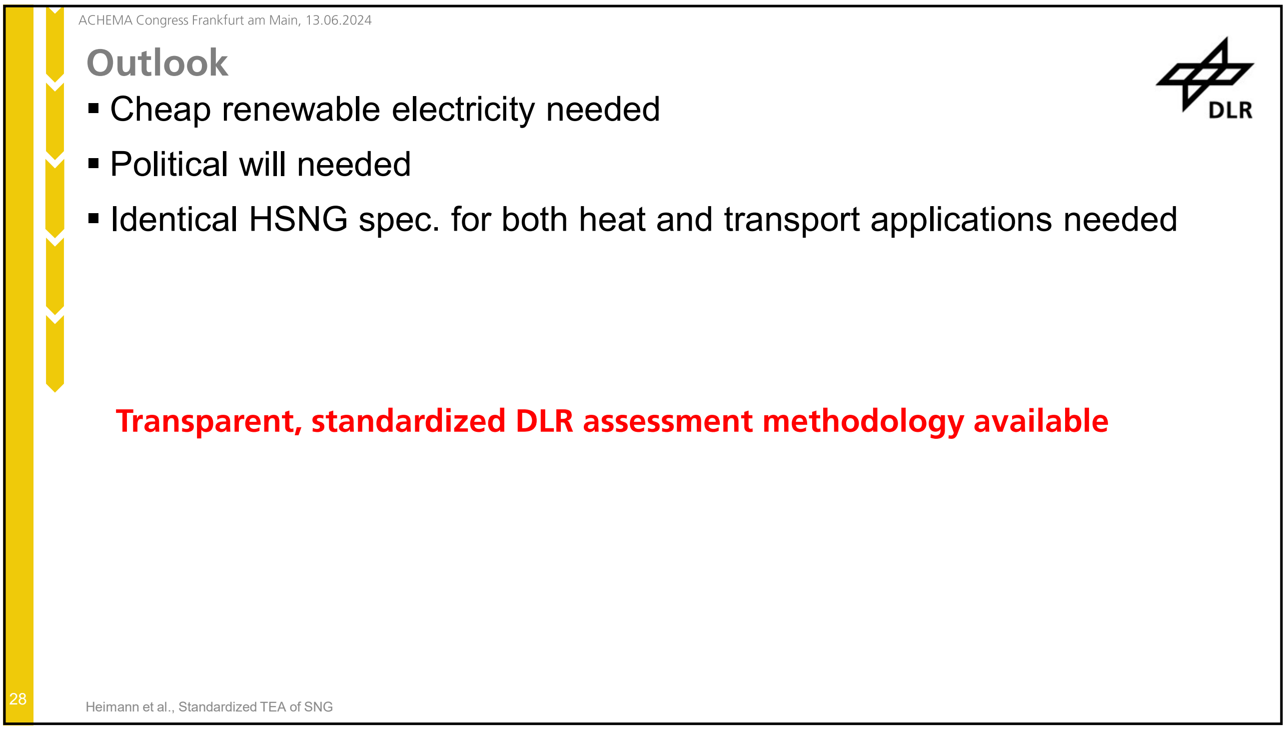


Conclusion

- 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

+ HSNG-30
  - Higher efficiency
  - Better performance in combustion



Outlook

- Cheap renewable electricity needed
- Political will needed
- Identical HSNG spec. for both heat and transport applications needed

Transparent, standardized DLR assessment methodology available

To be published

Example Results:

Based on renewable H_2 production cost of 3.28 €/kg in Namibia[1]

	Unit	LH_2	LOHC – H12-BT	LNG	MeOH	NH_3	FT - diesel
Production rate	$t\,h^{-1}$	29.5	469.6	59.6	145.0	158.5	84
η_{PtF}	$\%\ (GW_{LHV,F}\ GW_{el}^{-1})$	60.6	55.4	57.3	54.7	53.6	43.3
η_{HtF}	$\%\ (GW_{LHV,F}\ GW_{LHV,H}^{-1})$	98.4	97.3	82.8	80.1	81.8	63.9
P demand	$GW_{el}\ GW_{LHV,F}^{-1}$	1.65	1.80	1.74	1.83	1.86	2.31
η_c	%	-	-	98.5	95.2	-	95.5
NPC	$€_{2021}\ kg^{-1}$	5.00	3.55	2.05	1.10	0.71	3.37
	$€_{2021}\ MWh_{LHV,F}^{-1}$	150	107.4	147.6	198.6	137.6	306.5
Fossil sales price	$€_{2021}\ MWh_{LHV,F}^{-1}$	43.1 – 56.5[2]	43.1 – 56.5[2]	43.34[3]	77.2[4]	86.2[5]	69.0[6]
Renewable/fossil	**(energy related) [-]**	2.7-3.5	1.9-2.5	3.4	2.6	1.7	4.4
Transport cost	$€_{2021}\ MWh_{LHV,F}^{-1}$	8.4	6.6	5.9	3.9	5.3	5.0
Regasification cost	$€_{2021}\ MWh_{LHV,F}^{-1}$	9.0	26.7	5.4	-	-	-
Specific FCI	$€_{2021}\ kW_{LHV,F}^{-1}$	1,365	874	656	475	347	799
OPEX	$M€_{2021}\ a^{-1}$	1,035	230	1,059	1,084	786	1,123

[1] Encyclopedia of Electrochemical Power Sources, 2nd Edition, in publication
[2] https://www.iea.org/data-and-statistics/charts/global-average-levelised-cost-of-hydrogen-production-by-energy-source-and-technology-2019-and-2050
[3] IGU World LNG report - 2022 Edition
[4] Methanol Price|Methanol Institute|www.methanol.org (Rotterdam)
[5] Mineral Commodity Summaries 2022 - Nitrogen (usgs.gov)
[6] Spritpreis-Entwicklung: Benzin- und Dieselpreise seit 1950 (adac.de) (German market prices minus taxes)

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THANK YOU FOR YOUR ATTENTION!

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