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

11th FSC International Conference

Eurogress Aachen, 23 May 2023

Yoga Rahmat, Simon Maier, Moritz Raab, Francisco Moser, Ralph-Uwe Dietrich

German Aerospace Center (DLR), Institute of Engineering Thermodynamics

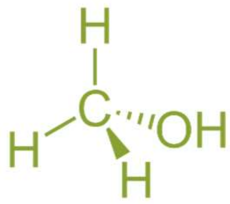
DLR

Outline

- Motivation
- Methodology
- Process description
- Results
- Conclusion

Motivation

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



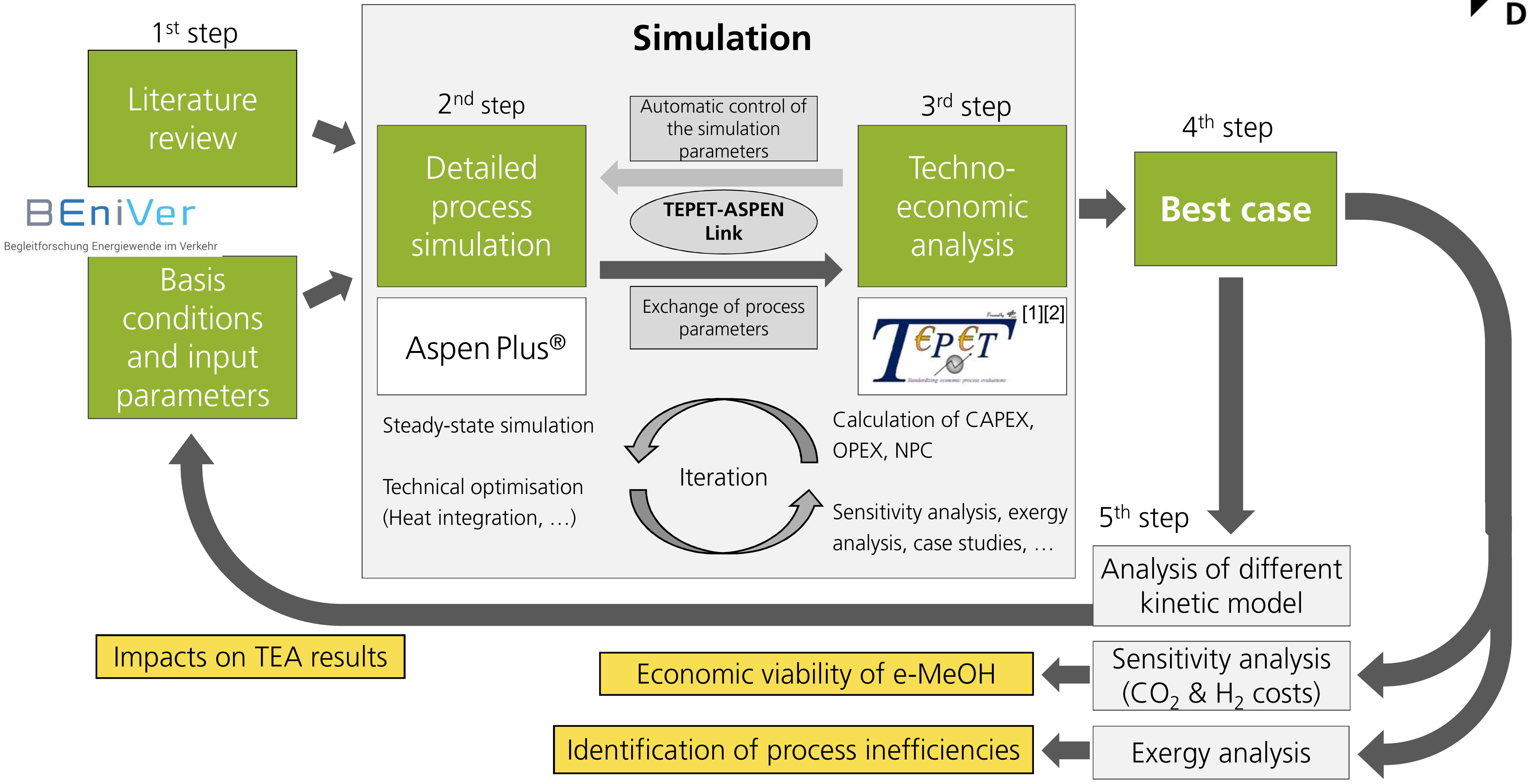
✔ Vol. energy density 50 % of gasoline[3]
✔ Basic chemical (157 million t a^{-1})[4]
✔ Raw material for MtK (SAF), DME, OME, MtG, etc.
⚠ Cold start problem in ICE
⚠ Water soluble

<u>Goals:</u>

- Techno-economic analysis of e-methanol production from German electricity grid and renewable electricity in northern and southern Germany
- Investigation of the recommended reactor design configuration
- Techno-economic comparison of different kinetic models
- Identification of process inefficiencies through an exergy analysis

[1] European Climate Law (europa.eu)
[2] Jedamzik et al. (2020) Energiewende in deutschland: Definition & Ziele 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] Methanol production capacity globally 2030 | Statista

Methodology



[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

Methodology
Kinetic models

Reactions[1]

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

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

$$CO + 2H_2 \rightleftharpoons CH_3OH \quad \Delta H_o = -91.0\,\frac{kJ}{mol} \quad (3)$$

Vanden Bussche and Froment (VDB)[2]*
Only CO_2 hydrogenation + RWGS
Reactions (1) and (2)

Graaf, Stamhuis and Beenackers (GRF)[3]
Both CO and CO_2 hydrogenation + RWGS
Reactions (1), (2) and (3)

Impacts of kinetics selection on TEA results?

*basis for this study

[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] Graaf et al. (1988) Kinetics of low-pressure methanol synthesis

Methodology
Key Performance Indicator (KPI)

Energetic efficiencies:

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

$$\eta_{\mathrm{H_2}tF} = \frac{LHV_{\mathrm{MeOH}} \cdot \dot{n}_{\mathrm{MeOH}}}{LHV_{\mathrm{H_2}} \cdot \dot{n}_{\mathrm{H_2}}}$$

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

Exergy balance:

$$\dot{E} = \dot{E}^{PH} + \dot{E}^{CH}$$

$$\dot{E}^{PH} = (\dot{H} - \dot{H}_0) - T_0(\dot{S} - \dot{S}_0)$$

$$\dot{E}^{CH} = \dot{m} \cdot \overline{e}^{CH} = \dot{m} \cdot (\sum x_k \overline{e}_k^{CH} + \overline{R} T_0 \sum x_k ln x_k)$$

$$\dot{E}_F = \dot{E}_P + \dot{E}_D + \dot{E}_L$$

Exergetic efficiencies:

$$\varepsilon_{PtF} = \frac{\dot{E}_{MeOH}}{\dot{E}_{net,elec} + \dot{E}_{net,heat}}$$

$$\varepsilon_{PtX} = \frac{\dot{E}_{MeOH} + \dot{E}_{HPS}}{\dot{E}_{net,elec} + \dot{E}_{net,heat}}$$

$$\varepsilon_{Process-to-X} = \frac{\dot{E}_{MeOH} + \dot{E}_{HPS}}{\dot{E}_{\mathrm{H_2}} + \dot{E}_{\mathrm{CO_2}} + \dot{E}_{elec,plant}}$$

Methodology
Economic analysis – Basis conditions, OPEX & NPC

Basis conditions[1]	
Base year	2018
Basis currency	€
Full-load hours	$8000\,h\,a^{-1}$
Plant lifetime (y)	20 a
Interest rate (IR)	5 %
Plant location	Germany

German labor costs ✓ $41\ €\ h^{-1}$

Year	Cost Case	CO_2 $[€\,t^{-1}]$	H_2 $[€\,kg^{-1}]$	Electricity $[€\,MWh_{el}^{-1}]$
2018 [1]	min.	68.95	4.74	55.72
	max.	73.13	6.43	87.27

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

$$NPC\left(\frac{€/\$}{t}\right) = \frac{ACC + \sum OPEX_{dir} + \sum OPEX_{ind} + h_{labour} \cdot c_{labour}}{\dot{m}_{fuel}}$$ [1]

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

See next slide!

$$FCI_i = EC_i \times \sum CAPEX\ cost\ factors$$ [2]

[1] Heimann et al. (2023b) Standardisierung der ökonomischen und ökologischen Analyse der herstellungspfade von PtX-Prozessen in Deutschland
[2] Peters et al. (2002) *Design and Economics for Chemical Engineers*. Europe: McGraw-Hill Education.

Methodology

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**	**$Year_{ref}$**	
Lurgi reactor, D_{tube} 2 in.*	0	156.03	11910	Number of tube [-]	$	2002	[1]**
Lurgi reactor, D_{tube} 1½ in.*	0	83.83	8532	Number of tube [-]	$	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]

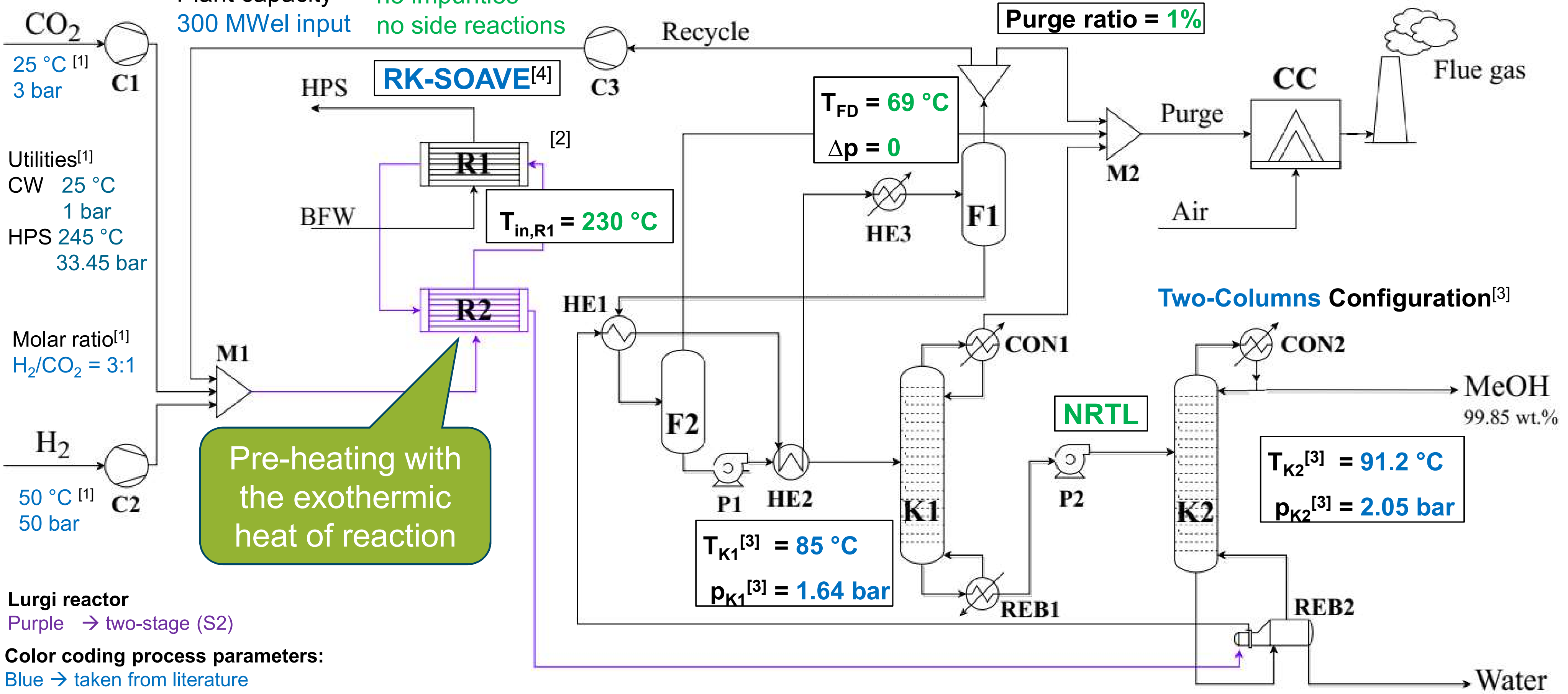
*stainless steel as the material construction
**with own reformulation

[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

Process Description
e-MeOH plant with Lurgi reactor concept

Plant capacity[1]
300 MWel input

no impurities
no side reactions



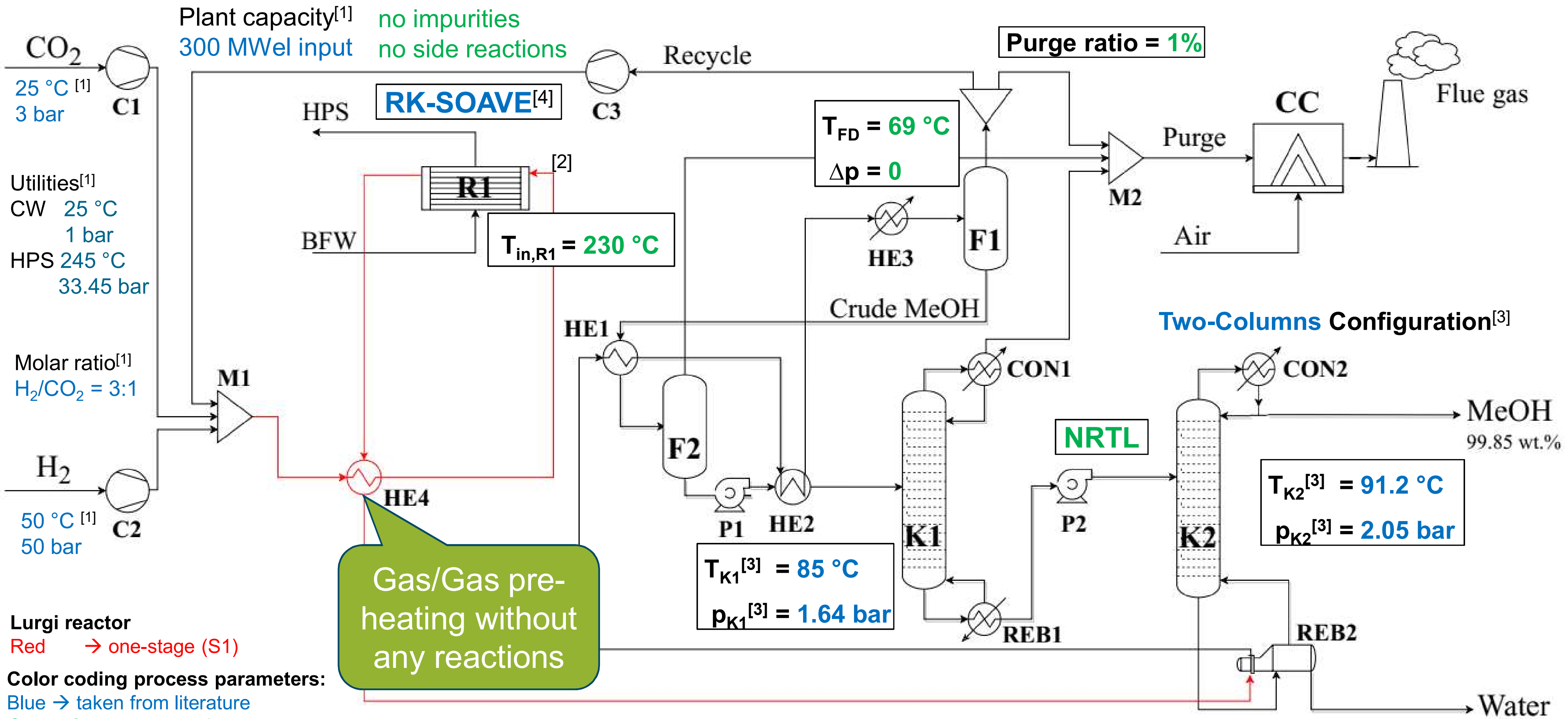
Lurgi reactor
Purple → two-stage (S2)

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

[1] Heimann et al. (2023b) Standardisierung der ökonomischen und ökologischen Analyse der herstellungspfade von PtX-Prozessen in Deutschland
[2] Metallgesellschaft AG (1996) – EP 0 790 226 B1
[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

Process Description
e-MeOH plant with Lurgi reactor concept

DLR



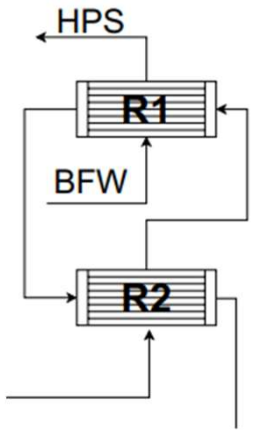
Lurgi reactor
Red → one-stage (S1)

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

[1] Heimann et al. (2023b) Standardisierung der ökonomischen und ökologischen Analyse der herstellungspfade von PtX-Prozessen in Deutschland
[2] Metallgesellschaft AG (1996) – EP 0 790 226 B1
[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

Process Description
Reactor fixed parameters and design variations

AspenPlus® model: RPlug



Pressure drop[2]: Ergun's equation

$T_{in,R1}$ = 230 °C

D_{shell}[5] = 120 in.

L_{tube}[4] = 5 m

N_{tube}[6] = $f(N_{reactor}, D_{tube})$

Size ratio R2/R1[1] = 1

Catalyst[2] $Cu/ZnO/Al_2O_3$

Bulk density[2] = 1065 kg m^{-3}

Diameter[2] = 5.5 mm

Lifespan[4] = 3 years

Dilution Factor[3] = 15 %

Config.[1]= two-stage (**S2**) & one-stage (**S1**)

p[1] = **80** bar & **60** bar

D_{tube}[3] = 2 in. OD **(LD)** & 1½ in. OD **(SD)**

NRP = **1**, **3** & **5**
(R1 in parallel)

Case naming : **Config. – p – D_{tube} – NRP**

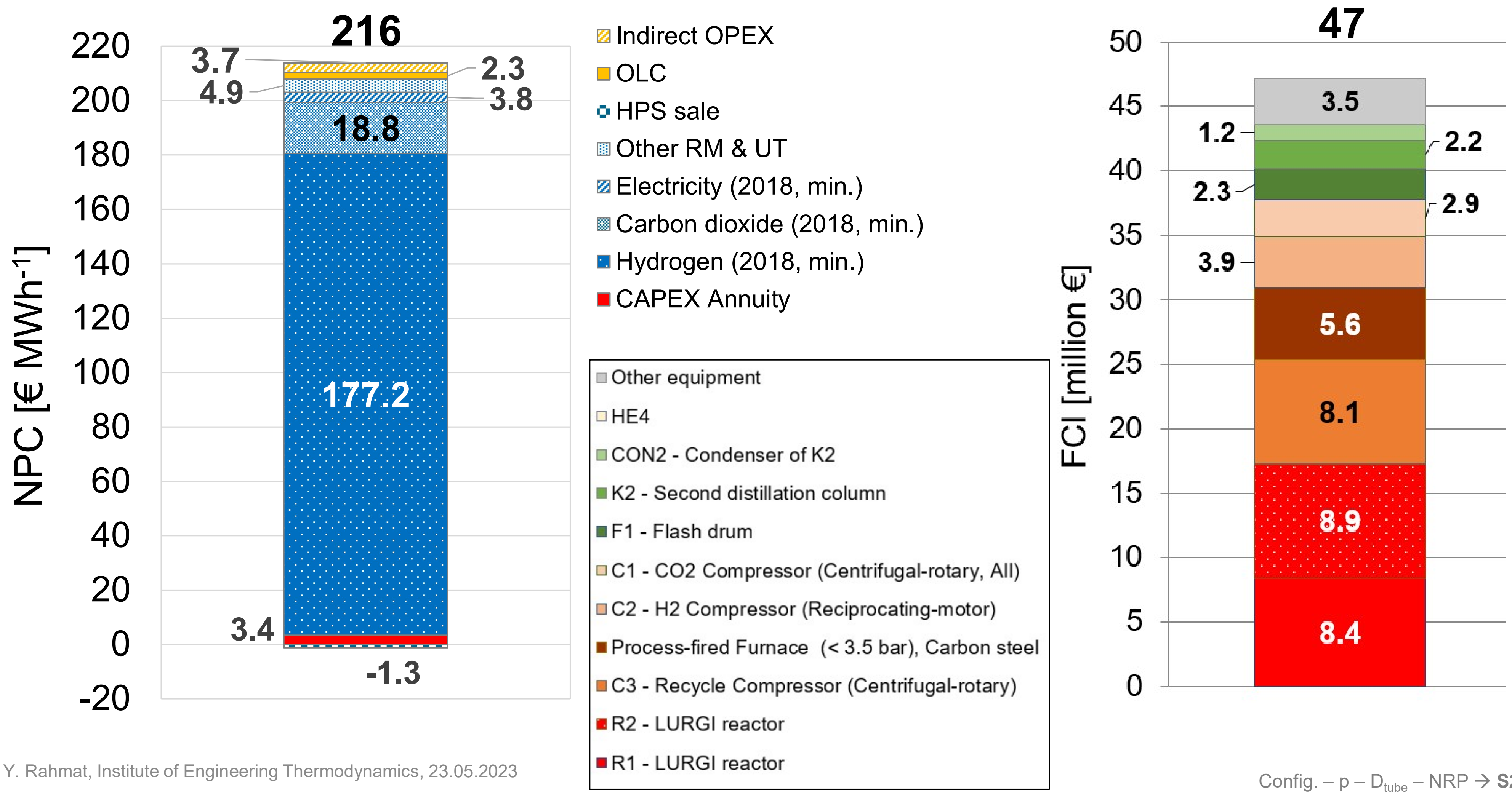
Base case : **S2-80-LD-1**

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

[1] Metallgesellschaft AG (1996) – EP 0 790 226 B1
[2] Van-Dal and Bouallou (2013) Design and simulation of a methanol plant plant from CO_2 hydrogenation
[3] Doraiswamy and Sharma (1984) Heterogenous reactions: Analysis examples and reactor design
[4] Bartholomew and Farrauto (2006) Fundamentals of Industrial Catalytic Processes, 2. Ed.
[5] Serth and Lestina (2014) Process Heat Transfer: Principles, Applications and Rules of Thumb
[6] Rase (1990) Fixed-Bed Reactor Design and Diagnostics: Principles, Applications and Rules of Thumb

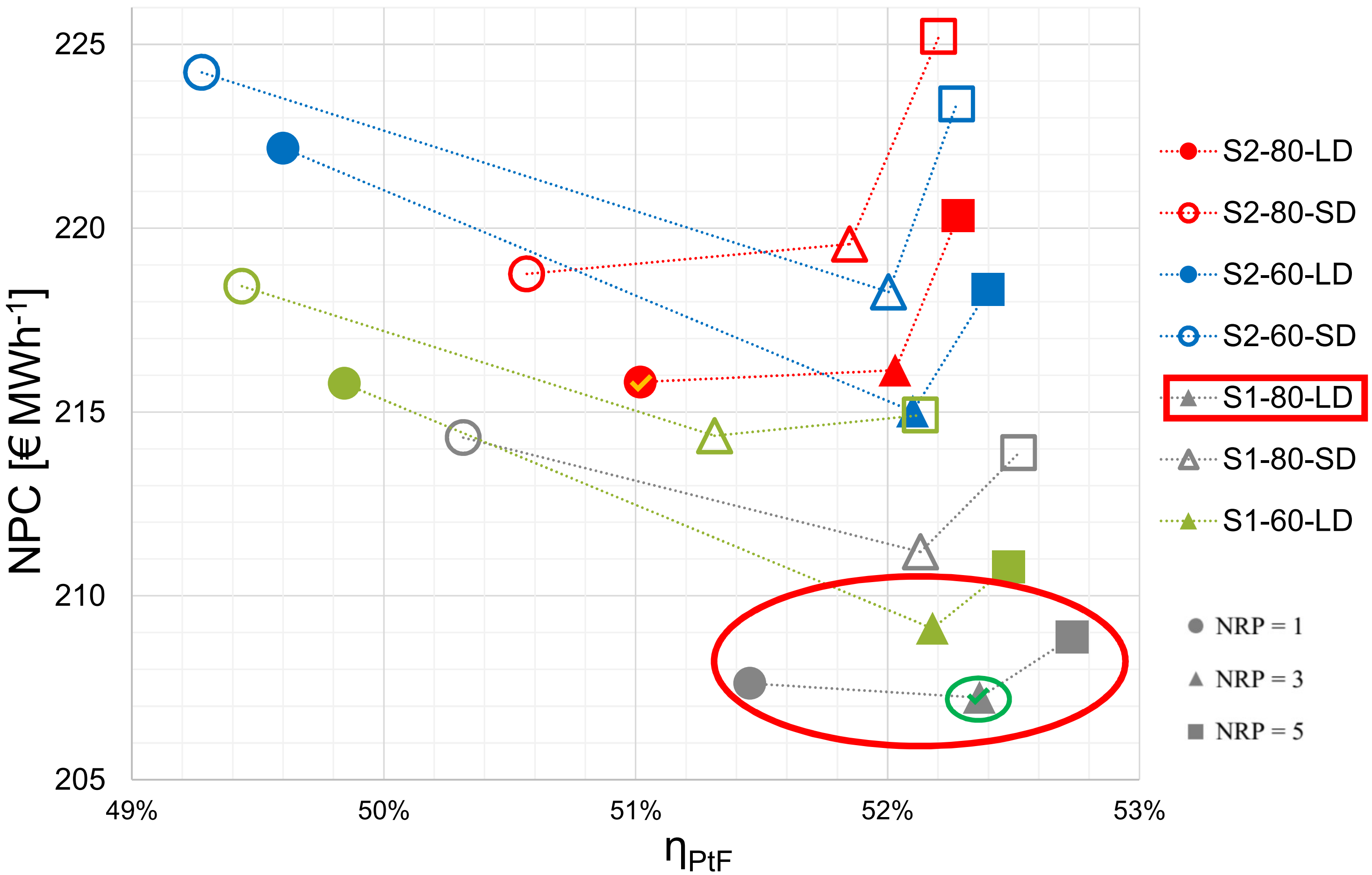
Results

Base case – NPC, OPEX, CAPEX



Config. – p – D_{tube} – NRP → **S2-80-LD-1**

Results
Techno-economic comparison NPC vs η_{PtF}



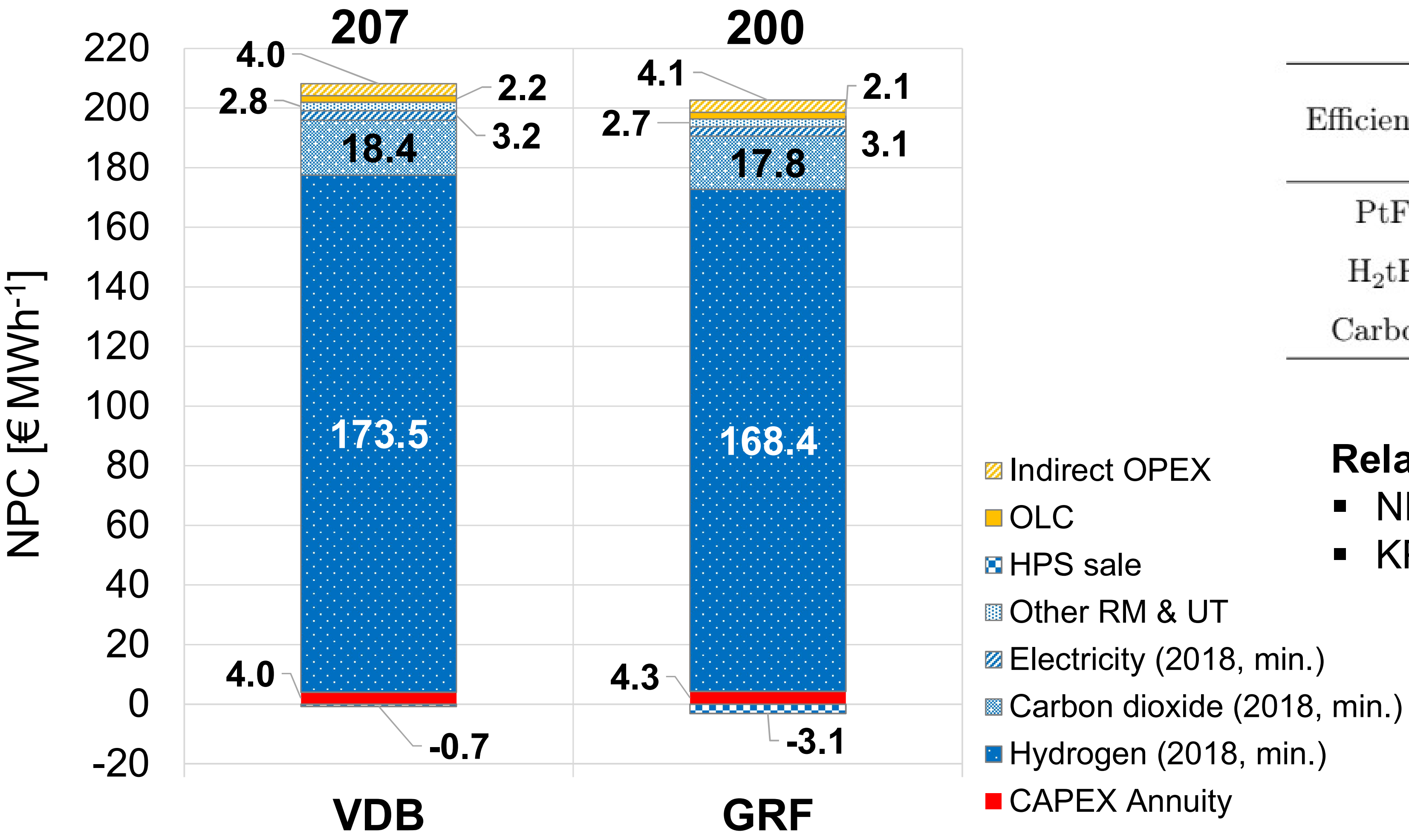
Best cases:

- One-stage ✔
- 80 bar ✔
- Larger diameter ✔
- NRP 3 ✔

Config. – p – D_{tube} – NRP → **S1-80-LD-3**

✔ Base case
✔ Best case

Results
Techno-economic comparison of VDB and GRF kinetics



Efficiencies	Kinetic model	
	VDB	GRF
PtF	52.4 %	54.7 %
H_2tF	81.5 %	83.9 %
Carbon	93.2 %	96.0 %

Relative difference:

- NPC = 2.3 %
- KPI < 2.8 %

Config. – p – D_{tube} – NRP → **S1-80-LD-3**

Results

Sensitivity analysis

NPC [€ MWh^{-1}]		H$_2$ costs [€ kg^{-1}]												
				2045				2030				2018		
CO_2 costs [€ t^{-1}]		1	1.5	2	2.5	3	3.5	4	4.5	5	5.5	6	6.5	7
	0	50	68	86	105	123	141	159	177	195	214	232	250	268
	20	55	73	92	110	128	146	164	182	201	219	237	255	273
MEA	40	61	79	97	115	133	151	170	188	206	224	242	260	279
MEA	60	66	84	102	120	139	157	175	193	211	229	248	266	284
MEA	80	71	89	108	126	144	162	180	198	217	235	253	271	289
MEA	100	76	95	113	131	149	167	185	204	222	240	258	276	295
MEA	120	82	100	118	136	154	173	191	209	227	245	263	282	300
DAC	200	103	121	139	157	176	194	212	230	248	266	285	303	321
DAC	300	129	148	166	184	202	220	238	257	275	293	311	329	347
DAC	400	156	174	192	210	228	247	265	283	301	319	338	356	374
DAC	500	182	200	219	237	255	273	291	309	328	346	364	382	400
DAC	600	209	227	245	263	281	300	318	336	354	372	390	409	427
DAC	700	235	253	271	290	308	326	344	362	380	399	417	435	453

Summary:

- NPC €⇗
- DAC €⇗
- Affordable electricity price needed
  H_2 = f(electricity)

Competitive if:

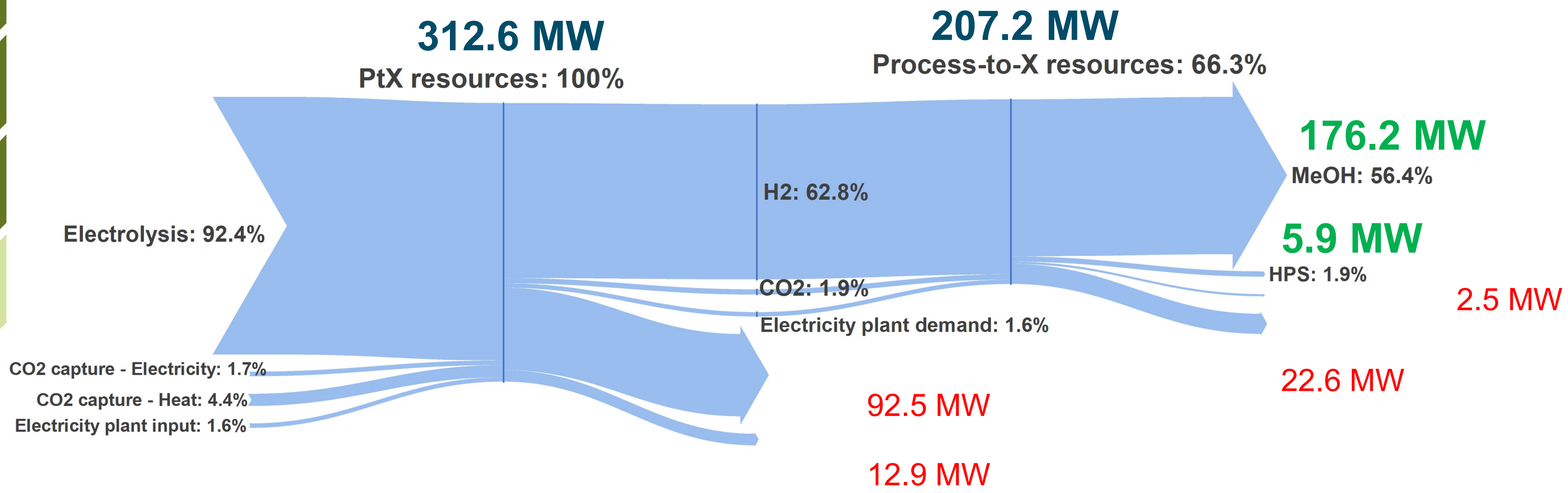
- H_2 < 2 € kg^{-1}
- CO_2 < 120 € t^{-1}

NPC Range [€ MWh^{-1}]	e-MeOH production	
< 109	Competitive	→ max. 150 % of current price level
109 - 181	Presumably competitive	→ max. 250 % of current price level
> 181	Not competitive	→ more than 250 % of current price level

★ Raw materials costs in 2018 (Heimann et al., 2022b)

● Raw materials costs in 2020 (Heimann et al., 2022a)

Results
Exergy analysis



Exergetic efficiencies

ε_{PtF} 56.4 %

ε_{PtX} 58.3 % (1.9 % from the generated HPS)

$\varepsilon_{Process\text{-}to\text{-}X}$ 87.9%

Config. – p – D_{tube} – NRP → **S1-80-LD-3**

Results

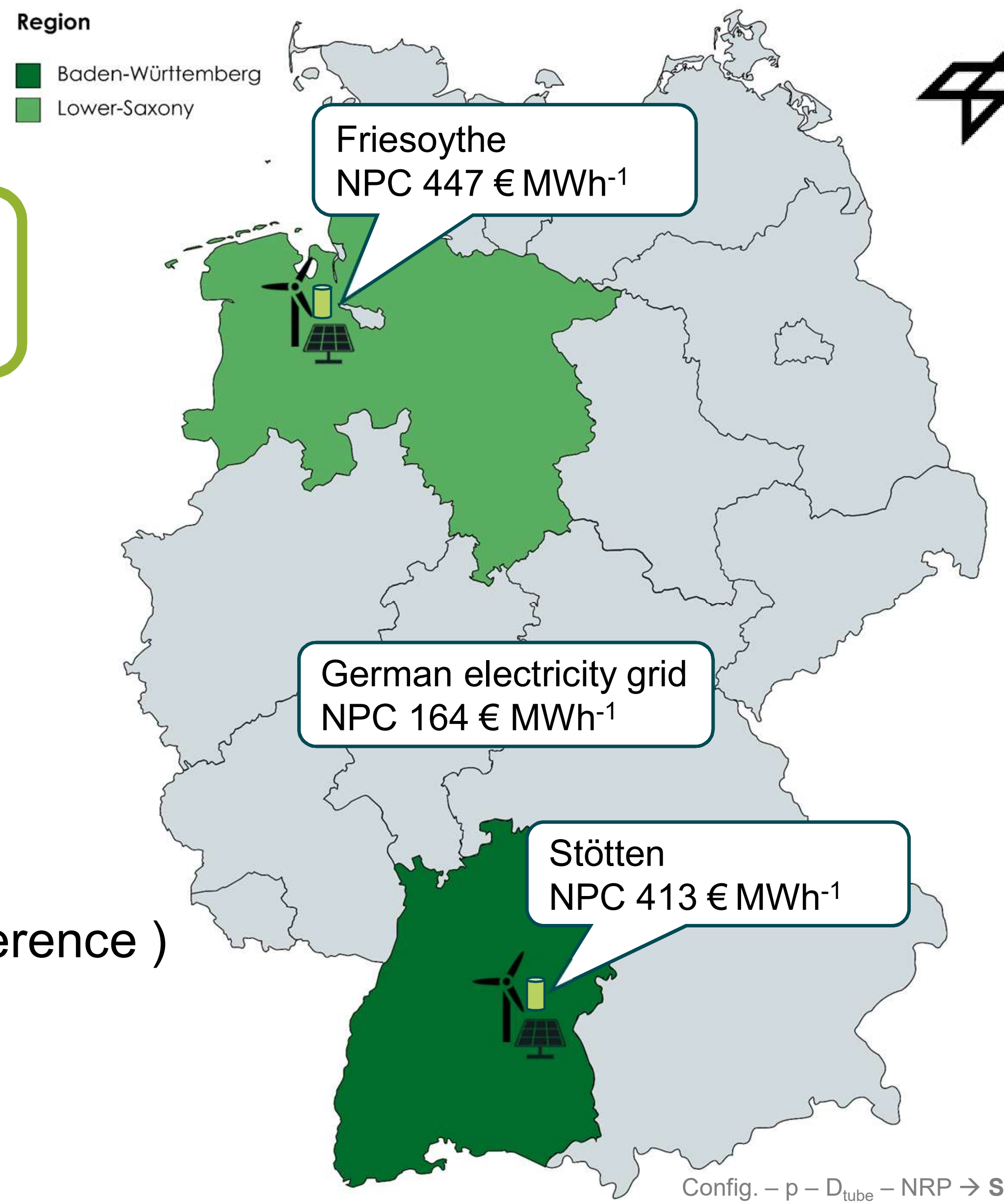
NPC using German renewable electricity

"Island solution"

Year	Cost Case	CO_2 [€ t^{-1}]	H_2 [€ kg^{-1}]	Electricity [€ MWh $_{el}{}^{-1}$]
2020 [1]	Grid	71.63	3.66	42.15
	Friesoythe	71.63	11.44	42.15
	Stötten	71.63	10.51	42.15

e-MeOH production:

- NPC ⇗⇗⇗
- PV/Wind potential[2][3] ⇘
- Southern > Northern (>10 % difference)
- CO_2 certification/incentives



[1] Heimann et al. (2023a) Synthetic natural gas and hythane production for german sustainable transport
[2] Wetter und Klima - Deutscher Wetterdienst - CDC (Climate Data Center) (dwd.de)
[3] Renewables.ninja

Config. – p – D_{tube} – NRP → **S1-80-LD-3**

Conclusion

- e-MeOH production was in detail techno-economically assessed (2 kinetics compared)
- Energetic efficiency η_{PtF} 52.4 % and η_{H2tF} 81.5 % can be achieved
  - Exothermic process, equilibrium-limited reactions, CO-based syngas is preferred, purge stream
- Cost driver is renewable H_2 which depends on the electricity costs
- NPC e-MeOH from German renewable electricity is 3 times higher than from German electricity grid in 2020
- NPC e-MeOH could be considered competitive if
  - H_2 costs < 2 € kg^{-1} (electrolysis technology development, affordable renewable electricity)
  - CO_2 costs < 120 € t^{-1} (MEA currently preferred over DAC, CO_2 certification/incentives)
- NPC is similar despite implementing two different kinetic models
- TEA methodology used for reactor configuration preference

THANK YOU FOR YOUR ATTENTION!

Yoga.Rahmat@dlr.de

Impressum

Thema: **Techno-economic analysis of e-methanol production under fixed operating conditions in Germany**
11th FSC International Conference, Eurogress Aachen

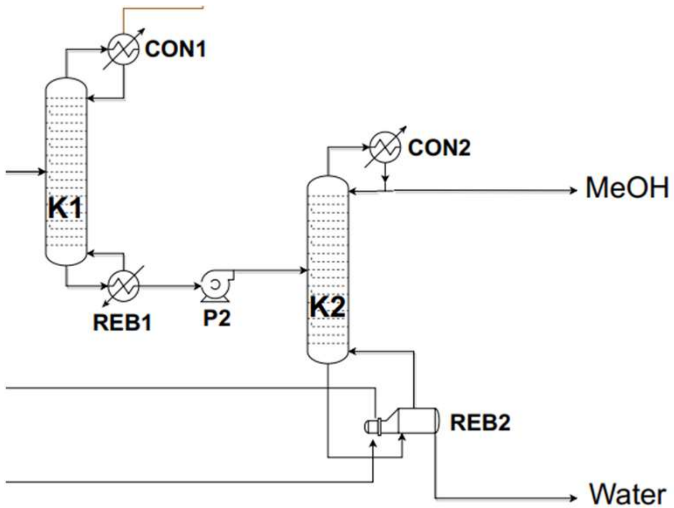
Datum: 23.05.2023

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

Institut: Technische Thermodynamik

Simulation – Purification sector
Columns

AspenPlus® model: RadFrac



Column design	K1	K2
Number of stages	10	28
Feed stage	5	14
Reflux ratio	1.5	0.9

Assumptions:
- Cooling water for cooling down all condensers
- Estimation of the number of stages and feed stage
- Stabilizer column (K1):
  - Number of stages ~2.1 min. stages
- MeOH/Water column (K2):
  - Number of stages ~1.1 min. stages