Supplementary Information (SI) for Energy & Environmental Science.

Supplementary Information: Transition pathways to electrified chemical production within sector-coupled national energy systems

Patricia Mayer[a], Florian Joseph Baader[a], David Yang Shu[a], Ludger Leenders[a], Christian Zibunas[b], Stefano Moret[a], and André Bardow*[a]

[a]*Energy & Process Systems Engineering, Department of Mechanical and Process Engineering, ETH Zürich, Switzerland*
[b]*Institute of Technical Thermodynamics, RWTH Aachen University, Germany*

Contents

1 Chemical industry process data

In this section, we provide data for the processes included in our chemical industry model. We provide specific data where publicly available. Process flow data is provided in Supplementary Table 1. The functional unit for each process is indicated by the flow with the value of 1. Negative flows indicate process inputs. IHS refers to the IHS Process Economics Program [1] which provides process flows and economic data for chemical facilities. Supplementary Table 2 provides the temperature (T) ranges for low, medium, and high T heat from Baumgärtner et al.[2].

Supplementary Table 3 provides data on process costs and net GHG emissions calculated as CO_2-eq following the IPCC GWP-100 methodology [3]. The costs and emissions are reported per process functional unit reported in Supplementary Table 1. Flows, costs, and emissions differentiated by year indicate a projected technological evolution throughout the transition pathway. Investment costs are annualized using the methodology in Baumgärtner et al.[2], using an interest rate of 5% and payback period of 30 years for the chemical facilities.

---

*corresponding author: abardow@ethz.ch

Supplementary Table 1: Process data for chemical industry model

Product	**Process**	**Flows**			
ammonia	Haber-Bosch	ammonia	1	tonne/hr	[4]
		electricity	-0.74	MW	
		H_2	-0.18	tonne/hr	
		nitrogen	-0.82	tonne/hr	
		cooling water	-155.14	tonne/hr	
	steam methane[1] reforming (SMR)	IHS			[1]
benzene[2] toluene[2] xylene (mixed)[2]	methanol-to-aromatics	IHS			[1]
	solvent extraction from pyrolysis gasoline	IHS			[1]
carbon dioxide (CO_2)	point source capture (from processes with footnote[1])	CO_2 (100 bar)	1	tonne/hr	[5]
		CO_2 (1 bar)	-1	tonne/hr	
		electricity	-0.1	MW	
		heat (high T)[3]	-0.003	MW	
	direct air capture[4]	CO_2 (100 bar)	1	tonne/hr	[6]
		electricity (*2016*)	-0.81	MW	
		heat (low T)[3]	-3.3	MW	
		electricity (*2020*)	-0.78	MW	
		heat (low T)[3]	-3.0	MW	
		electricity (*2025*)	-0.75	MW	
		heat (low T)[3]	-2.8	MW	
		electricity (*2030*)	-0.73	MW	
		heat (low T)[3]	-2.5	MW	
		electricity (*2035*)	-0.70	MW	
		heat (low T)[3]	-2.3	MW	
		electricity (*2040*)	-0.67	MW	
		heat (low T)[3]	-2.0	MW	
		electricity (*2045*)	-0.64	MW	
		heat (low T)[3]	-1.76	MW	
carbon monoxide (CO)	reverse water-gas shift[1]	CO	1	tonne/hr	[7]
		water	0.64	tonne/hr	
		CO_2 (1 bar)	0.075	tonne/hr	
		electricity	-0.3	MW	
		heat (high T)[3]	-0.6	MW	
		H_2	-0.08	tonne/hr	
		CO_2 (100 bar)	-1.65	tonne/hr	

cooling water	imports	cooling water	1	tonne/hr	
ethylene[5] propylene[5]	methanol-to-olefins UOP/hydro	IHS			[1]
	steam cracking of naphtha	IHS			[1]
heat (high T)	resistance heater	heat (high T)[3]	1	MW	[7]
		electricity	-1	MW	
		silicon carbide	$-9.3 \cdot 10^{-7}$	tonne/hr	
	H_2 boiler	heat (high T)[3]	1	MW	*own calculation*[6]
		H_2	-0.03	tonne/hr	
hydrogen (H_2)	PEM electrolysis	H_2	1	tonne/hr	[2]
		electricity (*2016*)	-49.8	MW	
		electricity (*2020*)	-48.3	MW	
		electricity (*2025*)	-47.0	MW	
		electricity (*2030*)	-45.7	MW	
		electricity (*2035*)	-44.5	MW	
		electricity (*2040*)	-43.4	MW	
		electricity (*2045*)	-42.3	MW	
	steam methane[1] reforming (SMR)	IHS			[1]
	imports	H_2	1	tonne/hr	
methane	carbon capture and utilization	methane	1	tonne/hr	[8, 9]
		electricity	-0.97	MW	
		H_2	-0.51	tonne/hr	
		CO_2	-2.78	tonne/hr	
	imports	methane	1	tonne/hr	
methanol	carbon capture and utilization	methanol	1	tonne/hr	[10]
		electricity	-0.018	MW	
		heat (medium T)[3]	-0.44	MW	
		H_2	-0.2	tonne/hr	
		CO_2	-1.46	tonne/hr	
	from synthesis gas	IHS			[1]
naphtha	imports	naphtha	1	tonne/hr	
nitrogen	air separation by pressure-swing adsorption	IHS			[1]
pyrolysis gas	steam cracking of naphtha	IHS			[1]
steam	natural gas boiler	IHS			[1]
	electrode boiler	IHS			[1]
silicon carbide	imports	silicon carbide	1	tonne/hr	

synthesis gas (2:1)	steam methane reforming with H_2 skimming	IHS			[1]
	steam methane reforming with CO_2 import	IHS			[1]
	partial oxidation of methane	IHS			[1]
	mixing of CO and H_2	synthesis gas	1	tonne/hr	[7]
		CO	-0.875	tonne/hr	
		H_2	-0.125	tonne/hr	

Supplementary Table 2: Temperature levels for low, medium, and high temperature heat [2].

	Temperature range [°C]
low temperature heat	< 100
medium temperature heat	100 - 400
high temperature heat	> 400

---

[1] Process produces concentrated CO_2 at 1 bar for industrial point source capture.

[2] Aromatics process data was divided among the individual chemicals, benzene, toluene, and xylene, based on mass allocation.

[3] Temperature ranges for low, medium, and high temperature (T) heat are provided in Supplementary Table 2.

[4] Process flows are linearly interpolated between the values given by Deutz and Bardow [6] for 'today', as 2016, and 'future', as 2050, as in Yang Shu et al. [11].

[5] Olefins process data was divided among the individual chemicals, ethylene and propylene, based on mass allocation.

[6] Assume 95% efficiency from hydrogen LHV (120 MJ/kg H_2) to MW heat

Supplementary Table 3: Cost and emission data for chemical industry model

Product	**Process**	**Costs**				**Emissions**[1]	
ammonia	Haber-Bosch	CAPEX	3300	$\frac{\text{k€}}{\text{tonne/hr}}$	[12]	0	
		OPEX	8.25[2]	$\frac{\text{€}}{\text{tonne}}$			
	steam methane reforming (SMR)	IHS			[1]		
benzene[3] toluene[3] xylene (mixed)[3]	methanol-to-aromatics	IHS			[1]		
	solvent extraction from pyrolysis gasoline	IHS			[1]		
carbon dioxide	point source capture	CAPEX	119	$\frac{\text{k€}}{\text{tonne/hr}}$	[13]	0	
		OPEX	0.43	$\frac{\text{€}}{\text{tonne}}$			
	direct air capture[4]	CAPEX (*2016/20*)	5840	$\frac{\text{k€}}{\text{tonne/hr}}$	[14]	-960	[6]
		OPEX (fixed)[5]	4	%			
		CAPEX (*2025*)	4272			-966	
		CAPEX (*2030*)	2704			-971	
		CAPEX (*2035*)	2300			-976	
		CAPEX (*2040*)	1896			-980	
		CAPEX (*2045*)	1744			-984	
carbon monoxide	reverse water-gas shift	IHS			[1][6]	8	
cooling water	imports	IHS			[1]	ecoinvent 3.6	[15]
ethylene[3] propylene[3]	methanol-to-olefins UOP/hydro	IHS			[1]		
	steam cracking of naphtha	IHS			[1]		
heat (high T)[7]	resistance heater	CAPEX	8,670	$\frac{\text{k€}}{\text{MW}}$	[16]	$1 \cdot 10^{-3}$	
		OPEX	2	$\frac{\text{€}}{\text{MWh}}$			
	H_2 boiler	*assume same costs and emissions as resistance heater*					
hydrogen (H_2)	PEM electrolysis	CAPEX (*2016*)	39,797	$\frac{\text{k€}}{\text{tonne/hr}}$	[2]	0	
		OPEX (fixed)	696	$\frac{\text{k€}}{\text{tonne/hr}\cdot\text{yr}}$			
		CAPEX (*2020*)	36,460	$\frac{\text{k€}}{\text{tonne/hr}}$			
		OPEX (fixed)	681	$\frac{\text{k€}}{\text{tonne/hr}\cdot\text{yr}}$			
		CAPEX (*2025*)	35,454	$\frac{\text{k€}}{\text{tonne/hr}}$			
		OPEX (fixed)	615	$\frac{\text{k€}}{\text{tonne/hr}\cdot\text{yr}}$			
		CAPEX (*2030*)	30,324	$\frac{\text{k€}}{\text{tonne/hr}}$			
		OPEX (fixed)	507	$\frac{\text{k€}}{\text{tonne/hr}\cdot\text{yr}}$			
		CAPEX (*2035*)	25,166	$\frac{\text{k€}}{\text{tonne/hr}}$			
		OPEX (fixed)	449	$\frac{\text{k€}}{\text{tonne/hr}\cdot\text{yr}}$			
		CAPEX (*2040*)	20,271	$\frac{\text{k€}}{\text{tonne/hr}}$			
		OPEX (fixed)	350	$\frac{\text{k€}}{\text{tonne/hr}\cdot\text{yr}}$			
		CAPEX (*2045*)	16,233	$\frac{\text{k€}}{\text{tonne/hr}}$			
		OPEX (fixed)	299	$\frac{\text{k€}}{\text{tonne/hr}\cdot\text{yr}}$			
	steam methane reforming (SMR)	IHS			[1]		
	imports	OPEX[8]	$1 \cdot 10^5$	$\frac{\text{k€}}{\text{tonne}}$		ecoinvent 3.5	[17]

methane	carbon capture and utilization	CAPEX (*2016/2020*)	11,536	$\frac{\text{k€}}{\text{tonne/hr}}$	[18]	38	
		OPEX (fixed)[5]	3	%			
		CAPEX (*2025*)	10,811	$\frac{\text{k€}}{\text{tonne/hr}}$			
		CAPEX (*2030*)	10,086	$\frac{\text{k€}}{\text{tonne/hr}}$			
		CAPEX (*2035*)	9,493	$\frac{\text{k€}}{\text{tonne/hr}}$			
		CAPEX (*2040*)	8,899	$\frac{\text{k€}}{\text{tonne/hr}}$			
		CAPEX (*2045*)	8,305	$\frac{\text{k€}}{\text{tonne/hr}}$			
	imports	OPEX	0.5	$\frac{\text{k€}}{\text{tonne}}$	[2]	ecoinvent 3.5	[17]
methanol[3]	carbon capture and utilization	IHS			[1]	1460	
	from synthesis gas	IHS			[1]		
naphtha	imports	OPEX	0.44	$\frac{\text{k€}}{\text{tonne}}$	[19]	ecoinvent 3.6	[15]
nitrogen	air separation by pressure-swing adsorption	IHS			[1]		
pyrolysis gas	steam cracking of naphtha	IHS			[1]		
steam	natural gas boiler	IHS			[1]		
	electrode boiler	IHS			[1]		
silicon carbide	imports	IHS			[1]	ecoinvent 3.6	[15]
synthesis gas (2:1)	steam methane reforming with H_2 skimming	IHS			[1]		
	steam methane reforming with CO_2 import	IHS			[1]		
	partial oxidation of methane	IHS			[1]		
	mixing of CO and H_2[9]	CAPEX	0	$\frac{\text{k€}}{\text{tonne/hr}}$		1.2	
		OPEX	0	$\frac{\text{€}}{\text{tonne}}$			

---

[1] Refers to process operational emissions in $[\frac{\text{kg CO}_2\text{-eq}}{\text{process functional unit}}]$. Life cycle operational emissions of process inputs that are modelled separately (i.e. H_2) are also considered separately. Except for direct air capture, which includes the life cycle impacts of the adsorbent, process operational emissions are calculated by closing the atom balance around process flows, as done by Meys et al.[7].

[2] Assume 2% O&M factor and 8000 full-load hours.

[3] Emissions include end-of-life emissions assuming complete combustion into CO_2, as done by Zibunas et al.[20].

[4] Intermediate years 2025, 2035, and 2045 are linearly interpolated using the data from Fasihi et al. [14].

[5] % for OPEX calculation refers to % of CAPEX per year.

[6] Own calculation derived from conventional CO production [1]. Take ratio of mass output per mass CO for conventional process, r_{conv}, and for reverse water-gas shift (rWGS) process, r_{rWGS}, and calculate scaling factor as $(\frac{r_{\text{rWGS}}}{r_{\text{conv}}})^{0.6}$. Scaling factor is used on conventional process costs to derive costs for rWGS process.

[7] CAPEX taken from [16], as investment cost for electric cracker. OPEX assumes 0.2% of the yearly CAPEX as the largest OPEX cost contributor is electricity which is accounted for separately.

[8] We place a high price penalty on imported green H_2 such that the system prioritizes domestic energy resources.

[9] Mixing cost neglected, as by Zibunas et al.[20].

2 Energy system model modifications

In this section, we provide the modifications made to the original German energy system model from Baumgärtner et al. [2]. Supplementary Table 4 provides modifications to the annual exogenous high temperature heat demand, which is distributed evenly for every hour. Of the exogenous heat demands, changes were made only for high temperature heat because chemical process heat requirements for conventional production were modelled as high temperature. Supplementary Table 5 provides modifications to the annual exogenous electricity demand. The chemical industry electricity demand is assumed constant for every hour and is subtracted from the original hourly profile from [2]. Supplementary Table 6 provides modifications to the exogenous emissions targets.

Supplementary Table 4: Chemical industry high temperature (T) heat demands subtracted from the exogenous demands from Baumgärtner et al.[2].

	High T Heat [TWh/yr]
Baumgärtner et al.[2]	**273**
Chemical Processing [2]	-59
Net exogenous demand	214

Supplementary Table 5: Chemical industry electricity demands subtracted from the exogenous demands from Baumgärtner et al.[2].

	Electricity [TWh/yr]
Baumgärtner et al.[2]	**550**
Mechanical energy [21]	-35.6
Process cooling [21]	-1.8
Net exogenous demand	512.6

Supplementary Table 6: Modified exogenous emission targets in $\mathrm{Mt}_{\mathrm{CO_2\text{-}eq}}$/yr.

	2016	2020	2025	2030	2035	2040	2045
Baumgärtner et al.[2]	**690**	**617**	**526**	**435**	**362**	**290**	**217**
Updated reduction targets[1] [22]	700	571	441	337	219	102	0
Process emissions [23]	+7	+7	+7	+4	+4	+4	+0
Chemical use-phase emissions[2]	+35	+35	+35	+12	+12	+12	+0
Net emission targets	742	613	483	354	236	118	0

---

[1] Historical emissions were updated using the BMU 2021 report [23] rather than BMU 2018 used in [2].

[2] Use-phase emissions calculated based on complete combustion of the carbon-containing chemicals to CO_2, with a 65% reduction by 2030 and net-zero by 2045.

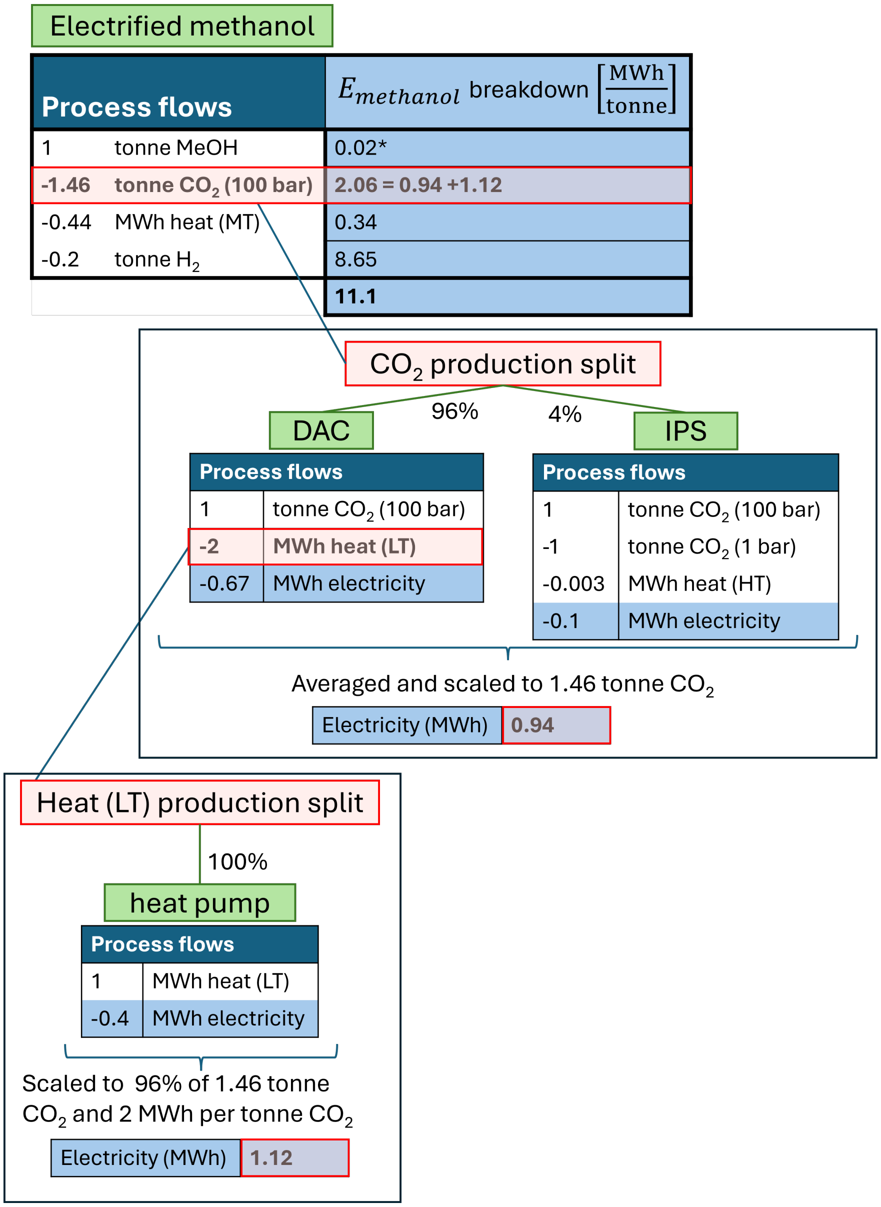
3 Underlying supply chain modelling for the *Cost-Avoided*

To calculate the electricity demands ($E_{i,t}$), operating costs ($C_{i,t}^{op,elec}$, $C_{i,t}^{op,fossil}$) and emissions ($e_{i,t}^{CO_2,elec}$, $e_{i,t}^{CO_2,fossil}$) for the *Cost-Avoided*, we consider both the direct process and the underlying supply chains of the process material and energy inputs (Supplementary Figure 1). In considering the underlying supply chains, we assume 100% allocation to a process's reference product. For example, H_2 as a by-product from synthesis gas production would not contribute to the electricity, operating costs, and emissions of an electrified process that utilizes that H_2 because everything is allocated to the synthesis gas.

Point-source CO_2 emissions are released from fossil-based processes (i.e. ammonia and hydrogen via steam-methane reforming) assuming a pressure of 1 bar (Table Supplementary Table 1). These emissions can then be compressed to 100 bar for use as feedstock in CCU-based electrified chemical processes. We allocate these point-source emissions to the CCU-based processes rather than to the fossil-based processes since the CCU-based processes should account for the underlying emissions of the CO_2 feed [24]. Our allocation assumption, however, underestimates the emissions from fossil-based processes when the point-source emissions are not utilized downstream, consequently decreasing the *Cost-Avoided* from electrified production under these circumstances. This phenomenon can be seen in the ammonia portion of the load-duration curve presented in the main paper (Figure 5, MIDDLE). Due to our allocation assumption, the *Cost-Avoided* from electrified ammonia production is underestimated for the portion of fossil-based ammonia that produces point-source CO_2 in excess of what is needed to meet the CCU-based methanol demand. As a result, there is a tranche of ammonia production that is prioritized over high-temperature heat electrified production but that is shown to have a lower *Cost-Avoided* in the merit order curve (Figure 5, BOTTOM, dashed red line). This phenomenon can also be seen in the results for our sensitivity on the HT heat cost assumptions (Supplementary Section 5). This scenario electrifies only methanol and a portion of ammonia in excess of the fossil-based ammonia that produces the necessary point-source CO_2 to meet the electrified methanol demand (Supplementary Figure 11).

In addition to our allocation assumption regarding point-source emissions, we consider 100 bar CO_2 flows into a process as negative emissions, and out of a process as positive emissions. We also account for a process's modelled CO_2-eq operational emissions to properly account for the carbon flows in the underlying supply chain of an electrified process.

In Supplementary Figure 1 we show an example of how the underlying CO_2 supply chain is considered in the electricity demand of methanol ($E_{methanol}$). This procedure applies to all the process flows, and to all the flows in the processes of the underlying supply chain. The top table shows the material and energy flows involved in the production of 1 tonne methanol, and their corresponding contributions to the electricity demand of methanol of 11.1 $\frac{\text{MWh}}{\text{tonne methanol}}$. The direct process electricity demand is listed next to the 1 tonne of methanol. In the middle part of the figure, we zoom into the production mix of CO_2, showing that 96% is produced via direct air capture (DAC) and 4% from industrial point sources. We calculate a weighted average of the electricity demands using the production split, and scale this weighted electricity demand by 1.46 $\frac{\text{tonne CO}_2}{\text{tonne methanol}}$ to obtain 0.94 $\frac{\text{MWh}}{\text{tonne methanol}}$ attributed to CO_2 production. In the bottom part of the figure, we zoom into the production of low temperature (LT) heat needed for DAC, which is 100% produced via heat pumps. We take the electricity demand per MWh of LT heat, and scale it to 96% of the 1.46 $\frac{\text{tonne CO}_2}{\text{tonne methanol}}$ multiplied by 2 $\frac{\text{MWh LT heat}}{\text{tonne CO}_2}$ to obtain 1.12 $\frac{\text{MWh}}{\text{tonne methanol}}$ attributed to heat production for the CO_2 supply chain. With this example, we show how the 2.06 $\frac{\text{MWh}}{\text{tonne methanol}}$ attributed to the CO_2 process flow is calculated.



Process flows		$E_{methanol}$ breakdown $\left[\frac{\text{MWh}}{\text{tonne}}\right]$
1	tonne MeOH	0.02*
-1.46	**tonne CO$_2$ (100 bar)**	**2.06 = 0.94 +1.12**
-0.44	MWh heat (MT)	0.34
-0.2	tonne H$_2$	8.65
		11.1

DAC

Process flows	
1	tonne CO$_2$ (100 bar)
-2	MWh heat (LT)
-0.67	MWh electricity

IPS

Process flows	
1	tonne CO$_2$ (100 bar)
-1	tonne CO$_2$ (1 bar)
-0.003	MWh heat (HT)
-0.1	MWh electricity

Electricity (MWh)	0.94

heat pump

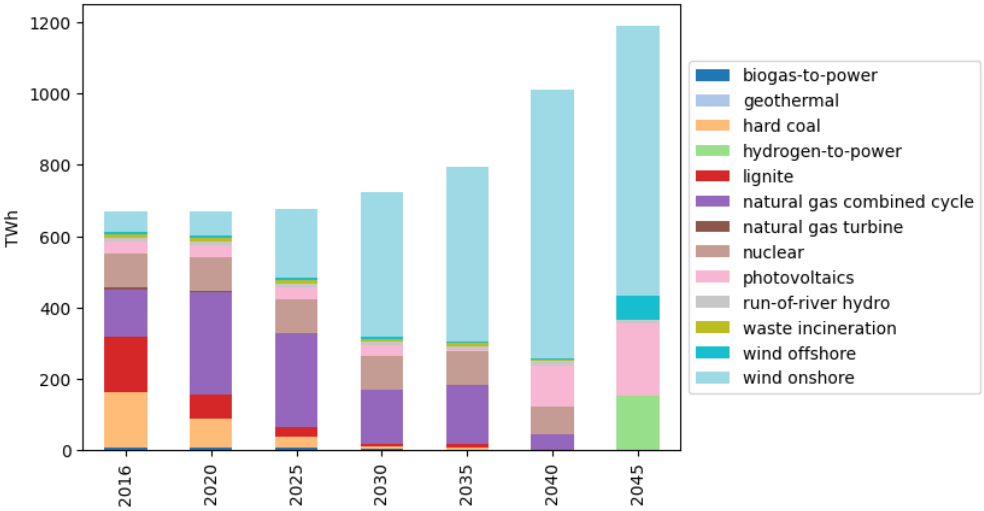
Process flows	
1	MWh heat (LT)
-0.4	MWh electricity

Electricity (MWh)	1.12

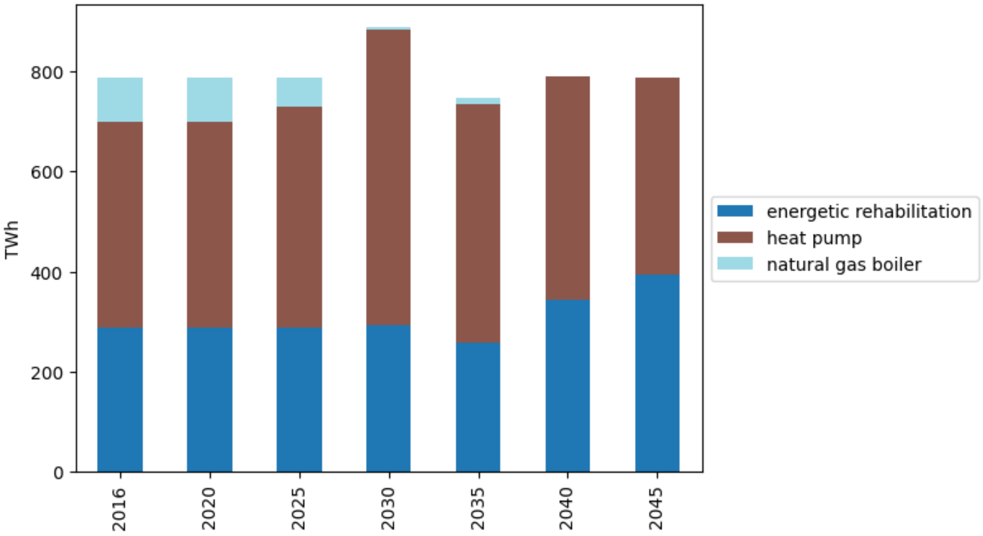
Supplementary Figure 1: Depiction of underlying CO$_2$ supply chain consideration in the calculation of methanol's electrified production electricity demand, $E_{methanol}$. Other process flows follow the same procedure for calculation of their contribution to $E_{methanol}$. The operating costs ($C^{op,elec}_{methanol}$, $C^{op,fossil}_{methanol}$) and emissions ($e^{CO_2,elec}_{methanol}$, $e^{CO_2,fossil}_{methanol}$) are also calculated in the same manner. The process flows are taken from the year 2040, and the production mix as the aggregate production mix from 2040. **TOP**: Material and energy process flows that go into production of 1 tonne electrified methanol, and the electricity demands associated with a given flow. **MIDDLE**: Zoom into CO$_2$ production mix between direct air capture (DAC) and industrial point source (IPS), showing how the electricity requirements are averaged across the production mix and scaled to the methanol feed requirement. **BOTTOM**: Zoom into low temperature (LT) heat production mix, showing how the electricity demands are scaled to the methanol CO$_2$ feed requirement and to the portion produced via DAC. We note that while here we show a static example of the underlying supply chain, the supply chain varies for every hour. *direct electricity demand of electrified methanol production.

4 Sector-specific transition pathway results

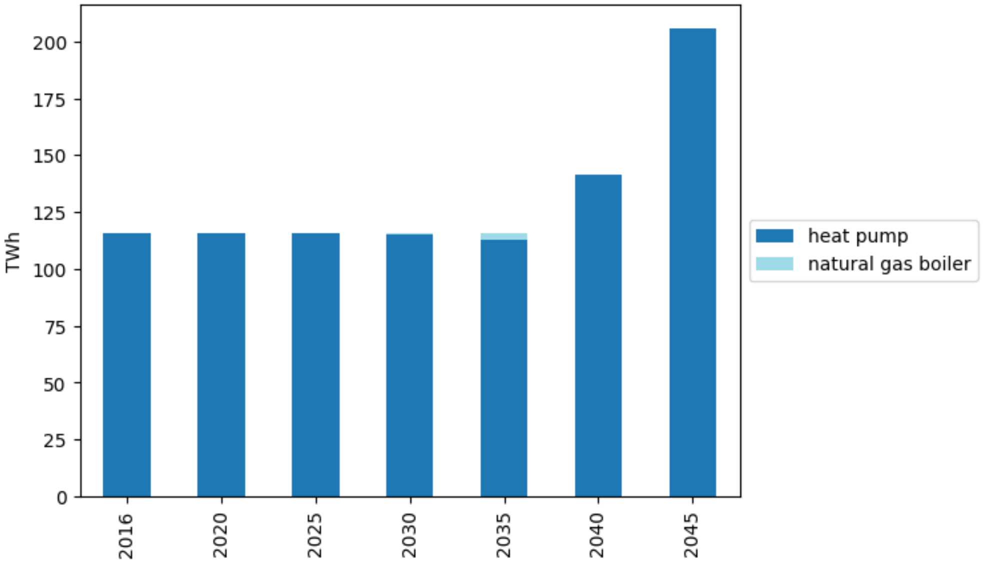
In this section, we present the transition pathwas results for the individual energy sectors: electricity (Supplementary Figure 2), residential heat (Supplementary Figure 3), low (Supplementary Figure 4), medium (Supplementary Figure 6), and high (Supplementary Figure 7) temperature industrial heat, and mobility (Supplementary Figure 5).



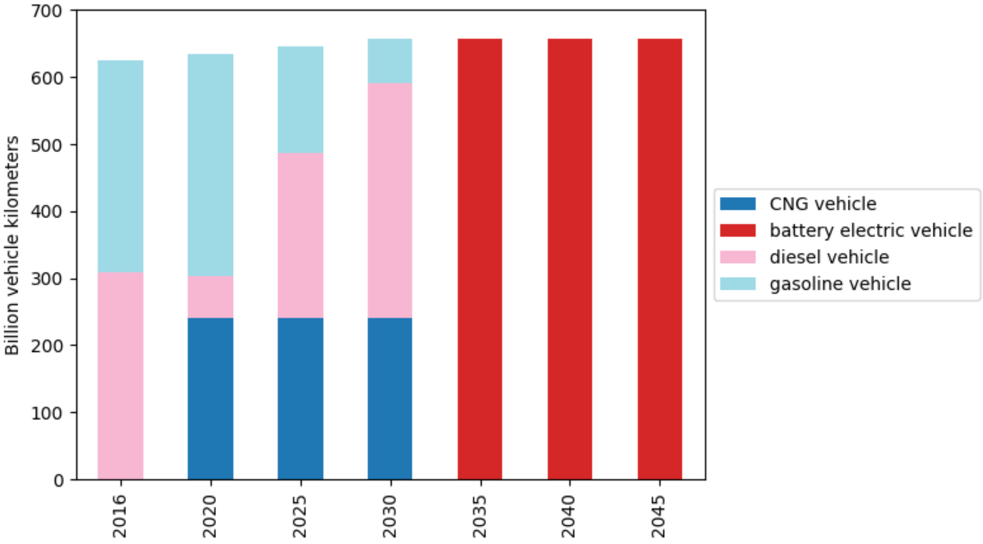
Supplementary Figure 2: Electricity production mix transition pathway. A nuclear phase-out is exogenously imposed by 2045, as shown by the resulting production mix in that year.



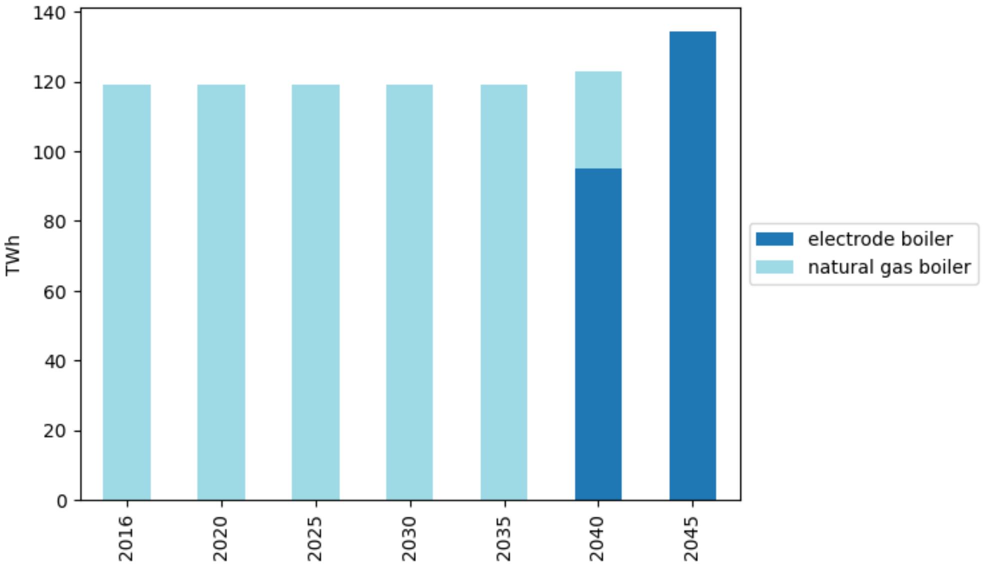
Supplementary Figure 3: Residential heat production mix transition pathway. Varying aggregate production arises from time series aggregation. Energetic rehabilitation refers to building renovations with improved thermal insulation. We introduce an exogenous constraint limiting the heat provision from energetic rehabilitation to a maximum of 50%, as in Baumgärtner et al. [2].



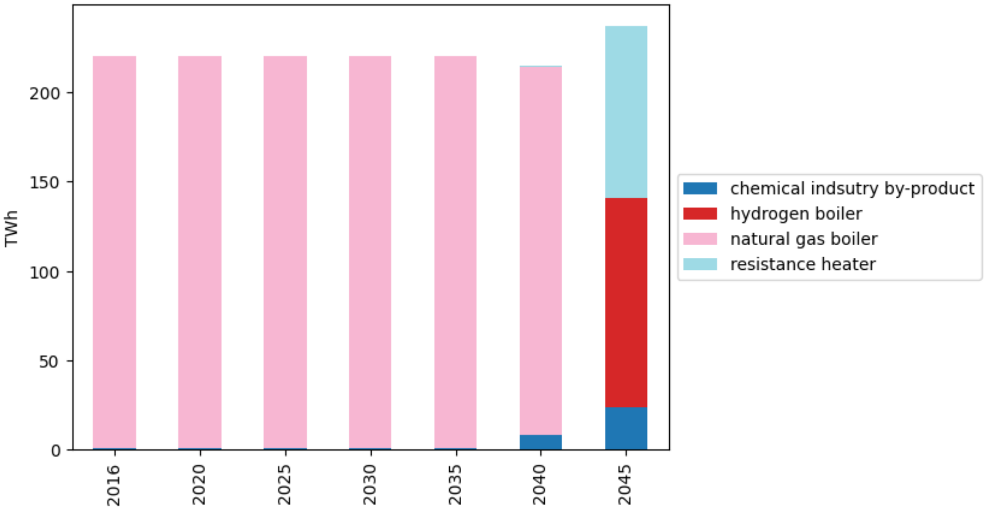
Supplementary Figure 4: Low temperature (LT) industrial heat production mix transition pathway. Our cost-optimal results how that heat pumps should comprise 100% of LT heat production since 2016. Natural gas boilers are introduced in 2035 due to the increased electricity demand from the mobility fleet transition to electric vehicles, which reduces the renewable electricity available for heat pumps.



Supplementary Figure 5: Mobility production mix transition pathway. The transition of the mobility sector occurs in a single investment period in 2035 due to the existing vehicle fleet reaching the end of its lifetime, and the foresight to the net-zero emissions target in 2045 influencing the decision to invest in electric vehicles rather than reinvest in fossil fuel vehicles. CNG: compressed natural gas.



Supplementary Figure 6: Medium temperature (MT) industrial heat production mix transition pathway. An increase in methanol production as an intermediate for electrified olefins and aromatics leads to an increase in MT heat production in 2040 and 2045.



Supplementary Figure 7: High temperature (HT) industrial heat production mix transition pathway. Only 0.5% of HT heat is produced via resistance heaters in 2040. In 2045, all HT heat transitions away from natural gas boilers due to the exogenous net-zero emissions constraint. The late transition of high temperature heat to electrified technologies is driven by the high capital cost assumptions for resistance heaters and hydrogen boilers. Results considering optimistic cost assumptions are presented in Section 5

.

5 Sensitivity on high-temperature heat cost assumptions

Our base scenario presented in the main paper assumes high costs for high-temperature (HT) resistance heaters and H_2 boilers (Supplementary Table 3) due to the low TRL for large-scale industrial deployment. Here, we present the results for a scenario with optimistic cost assumptions for HT heat technologies (Supplementary Table 7). For HT resistance heaters, we assume the same costs as for medium-temperature heat electrode boilers. For H_2 boilers, we assume the same costs as for natural gas boilers. The cost values are taken from Baumgärtner et al. [2].

Our results show that under optimistic cost assumptions for HT heat technologies, 62% of HT heat is produced via resistance heaters in 2040 as opposed to only 0.5% in the base scenario (Supplementary Figure 8). The energy system invests in resistance heater capacity to meet 100% of the HT heat demand and in electrified chemical production capacities for a portion of the chemical industry that has a higher *Cost-Avoided* than the HT heat sector. This portion includes 100% of the hourly methanol demand and 16% of the hourly ammonia demand. Electrification of the remaining ammonia demand and the olefins, which are electrified in the base scenario, is pushed to 2045.

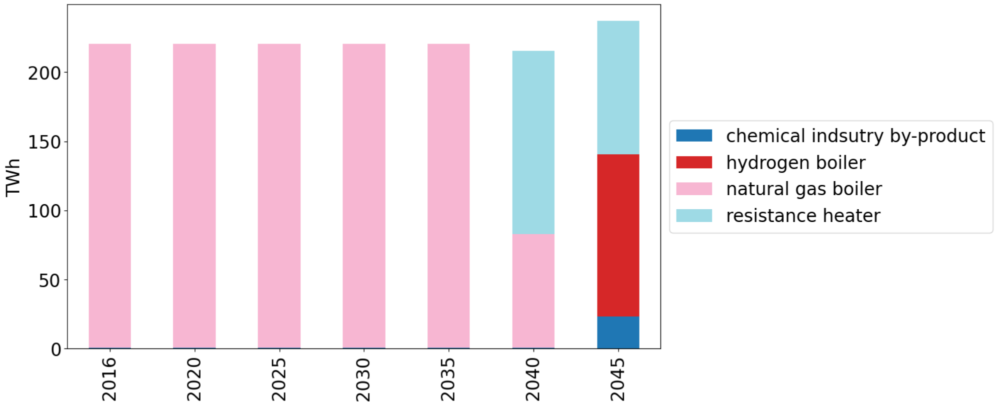
Fossil-based ammonia produces point-source CO_2 used to meet the electrified, CCU-based, methanol demand. This downstream utilization of the CO_2 removes the emissions accounting from the fossil-based production, which decreases the *Cost-Avoided* for this share of ammonia production (Supplementary Section 3). Once the methanol demand is fulfilled, however, the CO_2 is released to the environment, increasing the *Cost-Avoided*. Due to this distinction between the *Cost-Avoided* of ammonia production depending on the downstream utilization of the point-source CO_2 emissions, we still see some electrified ammonia deployed in 2040. Still, even though the electrified olefins and a portion of electrified ammonia production are pushed to 2045 under this optimistic cost scenario (Supplementary Figure 9), methanol and ammonia begin their transitions in 2040 (Supplementary Figure 10). This finding emphasizes the alignment between the transitions of the chemical industry and the HT heat sector, and highlights the prioritization of methanol and ammonia among chemicals for electrification.

Under optimistic cost assumptions, we see diminished flexibility provision from the chemical industry to the energy system in 2040 and increased flexibility from the MT and HT heat sectors (Supplementary Figure 11). In 80% of the hours in the year, all of the electrified chemicals installed capacities are used, showing less benefit from diversifying and over-sizing the chemical industry than in our base results. However, it must be noted that due to our system set-up, we are not able to capture any flexibility provision from a transitioning chemical industry beyond 2040 since we force the chemical industry to fully electrify by 2045. In actuality, the chemical industry will likely not fully electrify but will rather be comprised of a mix of sustainable production options together with electrification, such as biomass, recycling, and carbon capture and storage. Once this mix is available, it can enable flexibility through diversification and over-capacities regardless of when the chemical industry's transition occurs relative to the other energy sectors. Furthermore, our results indicate that flexibility can also arise from other energy sectors that integrate electrified technologies with more dispatchable alternatives.

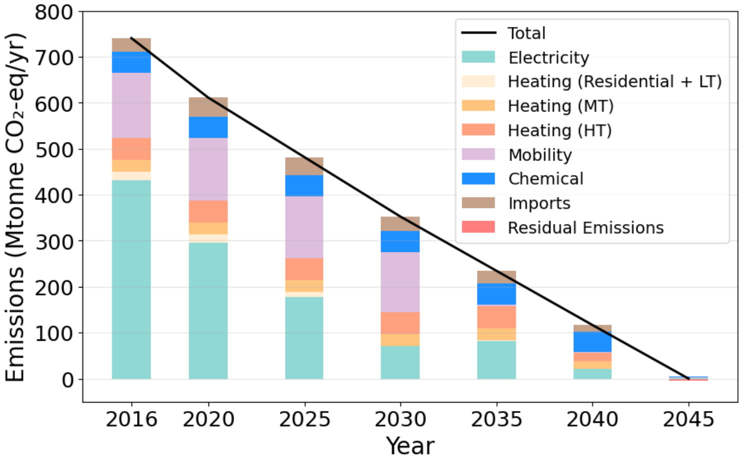
In summary, our scenario with optimistic cost assumptions for HT resistance heaters and H_2 boilers shows that the HT heat sector transitions before the bulk of the chemical industry. Still, methanol and ammonia begin their transitions alongside the HT heat sector, highlighting their priority for electrification within the chemical industry. Finally, although the flexibility provision from a transitioning chemical industry is weakened under this optimistic cost scenario, we see increased flexibility from a transitioning HT heat sector. This finding shows the broader benefit of over-sizing and diversifying production options across the energy system.

Supplementary Table 7: High-temperature heat technology cost assumptions for optimistic scenario.

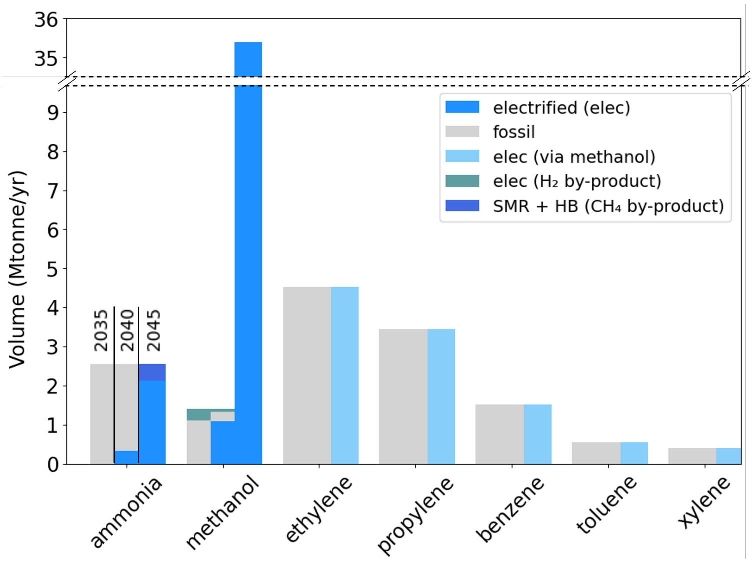
Process	CAPEX [$\frac{k€}{MW}$]	OPEX (fixed) [$\frac{k€}{MW \cdot yr}$]
resistance heater	238	4.7
H_2 boiler	175	3.5



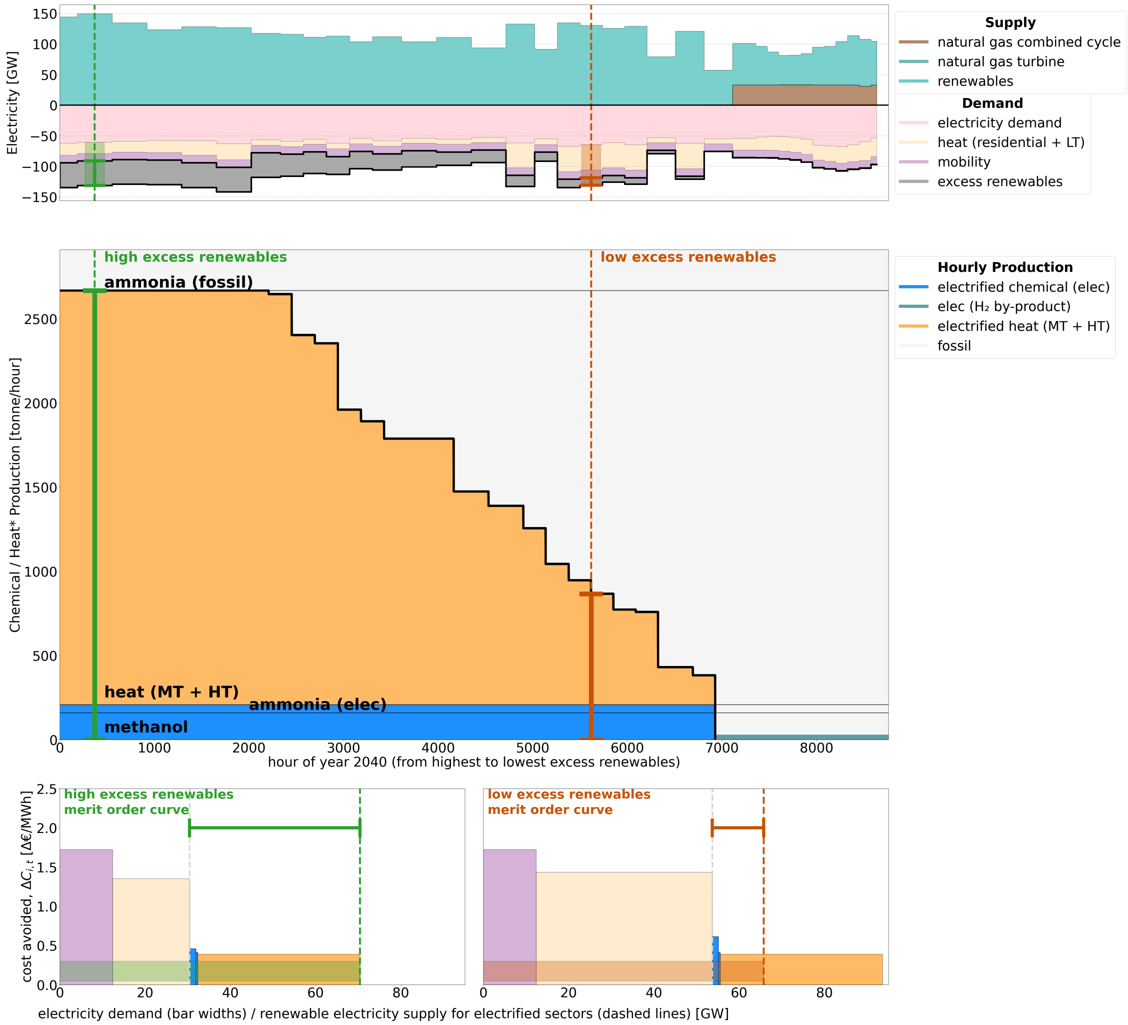
Supplementary Figure 8: High temperature (HT) industrial heat production mix transition pathway under optimistic cost assumptions for resistance heaters and H_2 boilers. 62% of HT heat is produced via resistance heaters in 2040, as opposed to only 0.5% in the base scenario.



Supplementary Figure 9: CO_2-eq emissions, in million tonnes, of the integrated energy system and chemical industry model by sector. With the optimistic cost assumptions, high-temperature (HT) heat transitions in 2040, rather than 2045, pushing the majority of the chemical industry to transition last in 2045. MT: medium temperature, LT: low temperature.



Supplementary Figure 10: Transition of chemical production from 2035 to 2045. Years prior to 2035 have the same production mix as 2035 and are therefore excluded from the figure. With the optimistic cost assumptions, chemicals still begin their transition to electrified production in 2040. However, only methanol and some ammonia are produced electrically in 2040, while the olefins and the bulk of ammonia transition in 2045. elec (via methanol) refers to the methanol-to-olefins and methanol-to-aromatics processes. elec (H_2 by-product) refers to methanol produced via CCU using by-product H_2 from synthesis gas production and CO_2 from chemical industry point sources. SMR + HB (CH_4 by-product) refers to ammonia produced via steam methane reforming + Haber-Bosch using by-product CH_4 from other electrified processes.



Supplementary Figure 11: TOP: electricity supply and demand for each hour in the year 2040. The hours are ordered from highest to lowest excess renewables after full electrification of the electricity, residential and low-temperature (LT) heat, and mobility sectors. Due to the time series aggregation, the hours repeat themselves, causing the steps in the figure. Electricity storage is excluded from the figure. With the optimistic cost assumptions, electricity consumption for high-temperature heat increases, decreasing the availability for electrified chemicals. **MIDDLE**: load-duration curve for the year 2040, with the hourly breakdown of electrified vs. fossil-based production for medium and high-temperature (MT + HT) heat and for chemicals with electrified capacities. The hours are in the same order as in the electricity balance plot (top figure). Ammonia is split into its electrified (elec) and fossil-based portions due to the different *Cost-Avoided* for each portion (Supplementary Section 5). In hours with high excess renewables (dashed green line), all chemicals and heat are produced via their electrified process up to the installed capacities. In hours with low excess renewables (dashed red line), only a portion of heat is electrified while all chemical electrified capacities are operated. This behavior is explained by the merit order curves created by the *Cost-Avoided* and the electricity demand of each electrified product (bottom figure). **BOTTOM**: merit order curves of electrified products in the sector-coupled energy system. Each curve corresponds to a separate hour, identified by the red and green dashed lines crossing the top and middle figures. The red and green dashed lines show the hourly renewable electricity supplied for the electrified energy sectors. Everything to the left of the intersection between an hour's renewable electricity supply and the merit order curve is produced electrically for that hour. Mobility, residential heat, and LT heat are fully electrified in every hour (dashed gray lines). The excess renewables (red and green brackets) are then used for electrification of chemicals and MT + HT heat. *Heat production is shown in tonne natural gas equivalents using a heating value of 15.4 $\frac{\text{MWh}}{\text{tonne}}$.

6 Large-scale sensitivity analysis on cost assumptions

To evaluate the sensitivity of the chemical industry's transition to cost increases, we perform two sensitivity analyses: In the first analysis, we evaluate a scenario with 10-year lifetimes for electrified chemical production technologies since shorter lifetimes have been identified as a key challenge in the development of these technologies [25]. We find that the energy system still invests in underutilized capacities for methanol, ammonia, and the olefins in the transition period despite the higher CAPEX. The transitions of ammonia and methanol are not affected by the higher CAPEX, while 29% of the electrified olefins installed capacity is delayed until 2045. Of the chemicals that begin transitioning in 2040, olefins have the lowest *Cost-Avoided* and are the most sensitive to CAPEX increases due to the need for methanol as a feedstock. However, despite the decrease in installed capacity, the underutilization phenomenon remains. Electrified olefins capacities have an overall yearly utilization of 39% (before 47%). From the energy system perspective, investments in underutilized capacities are still beneficial despite the higher CAPEX.

In the second sensitivity, we evaluate 512 scenarios varying the 1) CAPEX and OPEX of direct air capture (DAC), 2) CAPEX of electrolyzers, 3) CAPEX and OPEX of point source CO_2 capture, 4) and CAPEX of electrified methanol technologies (Supplementary Table 8). We assume uniform distributions for our cost assumptions and generate the 512 scenarios using a Sobol sampling design of experiments. Our results confirm that electrified capacities for methanol and ammonia are always built and underutilized regardless of cost increases (Supplementary Figure 12). This result highlights the robustness of the system-wide benefits enabled by an oversized and diversified chemical industry.

Our results also reiterate the sensitivity of the olefins transition to CAPEX increases, particularly to the CAPEX of DAC and of electrolyzers (Supplementary Figure 12 and Supplementary Figure 13). Sufficiently high CAPEX for these technologies can fully delay the olefins transition to 2045. As the olefins transition shifts to 2045, the methanol feedstock demand diminishes, decreasing the installed capacity of electrified methanol. Furthermore, as the DAC CAPEX increases, the CO_2 feedstock sourcing for electrified methanol shifts to point source capture from fossil-based ammonia production. This effect decreases the installed capacity of electrified ammonia. Nonetheless, the consistent deployment and underutilization of electrified methanol and ammonia capacities reinforces the value of flexibility from an oversized and diversified chemical industry.

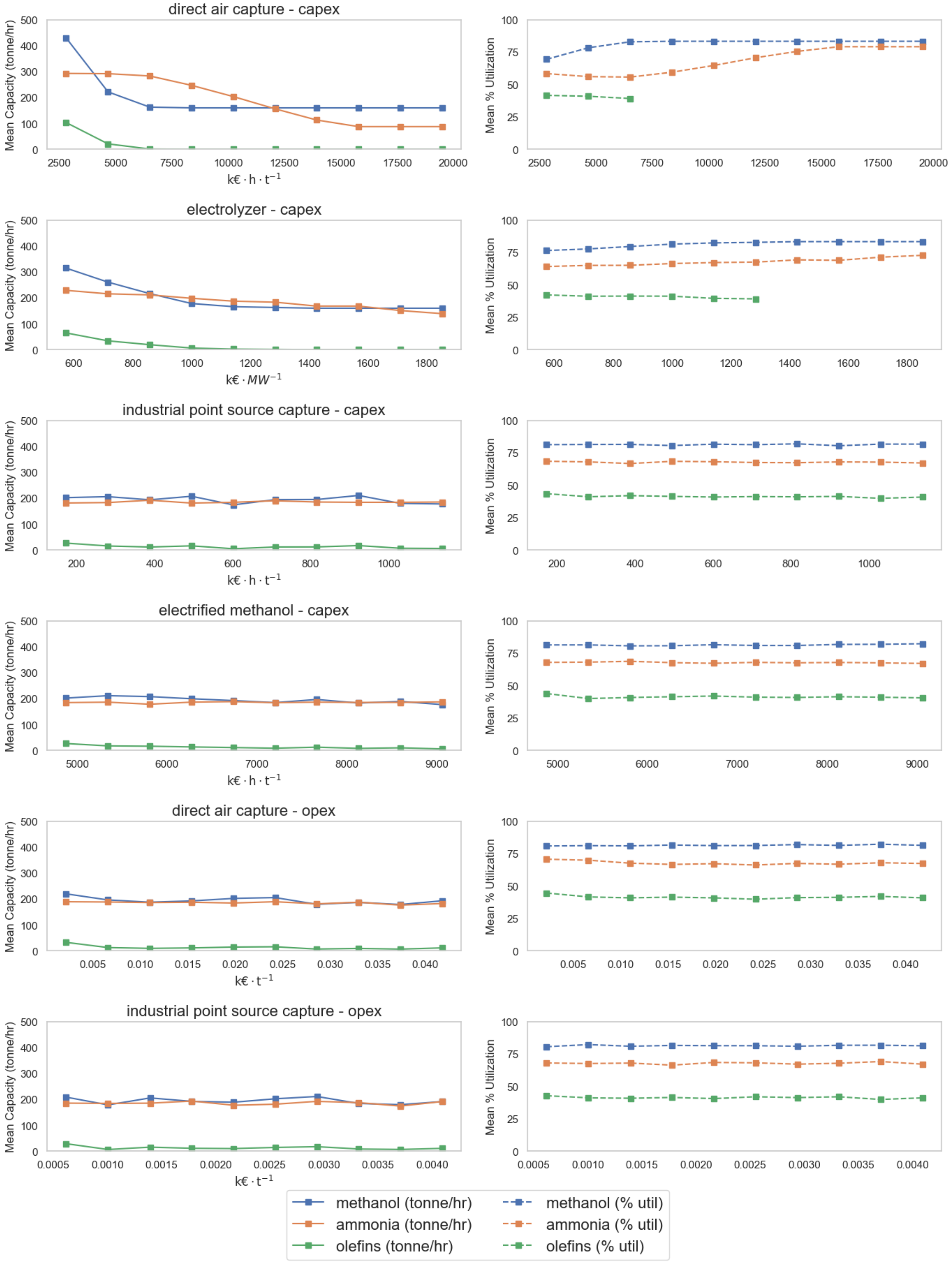
As a further analysis, we train a decision tree on the results of the second sensitivity analysis (Supplementary Figure 13). The results clearly demonstrate the predominant effect of DAC and electrolyzer CAPEX on the olefins transition over the other cost assumptions. Once again, we see that CAPEX beyond certain thresholds for these technologies completely shifts the olefins transition to 2045. Furthermore, methanol and ammonia always have some share of electrified production, illustrating the robustness of an accelerated transition to electrified chemical production regardless of cost.

Supplementary Table 8: Parameter ranges for the sensitivity analysis on cost assumptions. The nominal value corresponds to the value used in the main paper. Our sensitivity analysis evaluates the effect of increases for all cost assumptions. We assume uniform distributions for all parameters and evaluate a total of 512 scenarios using a Sobol sampling design of experiments.

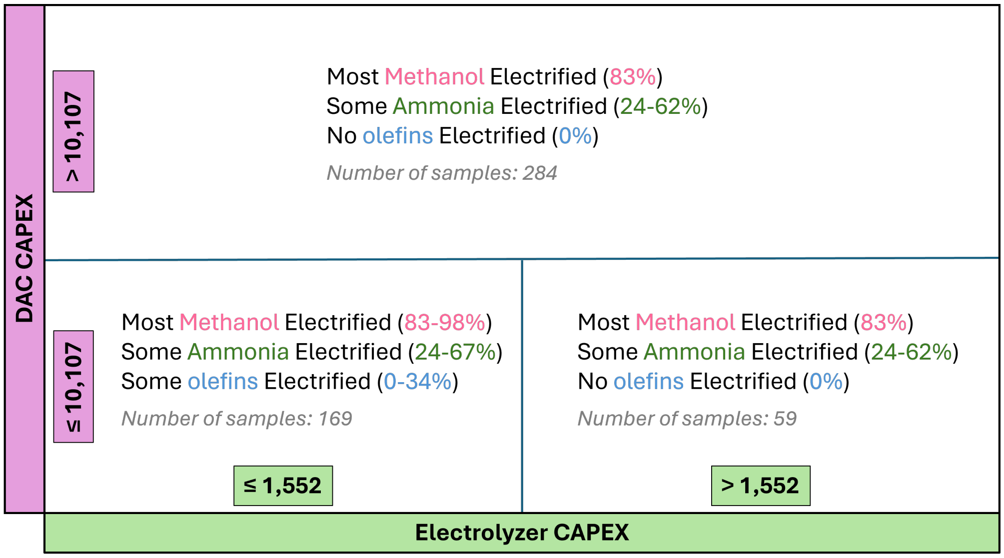
Parameter	**Nominal value**	**Max value**	**Unit**
Direct air capture - CAPEX	1,896 [14]	20,457 [26]	€/(kg/hr)
Electrolyzer - CAPEX	467 [2]	1,926 [27]	€/kW
Industrial point-source capture - CAPEX	119.3 [12]	1,993*	€/(kg/hr)
Electrified methanol - CAPEX	IHS [1]	Double IHS**	€/(kg/hr)
Direct air capture - OPEX	0 [14]	0.0447 [28]	€/kg
Industrial point-source capture - OPEX	0.00043 [12]	0.0043*	€/kg

*Assuming a factor of 10 as an upper bound

**Assuming supply chain costs double the capex as an upper bound. IHS data is proprietary and cannot be shared.


direct air capture - capex
electrolyzer - capex
industrial point source capture - capex
electrified methanol - capex
direct air capture - opex
industrial point source capture - opex
Mean Capacity (tonne/hr)
Mean % Utilization
0
100
200
300
400
500
0
25
50
75
100
2500
5000
7500
10000
12500
15000
17500
20000
k€ · h · t^{-1}
600
800
1000
1200
1400
1600
1800
k€ · MW^{-1}
200
400
600
800
1000
k€ · h · t^{-1}
5000
6000
7000
8000
9000
k€ · h · t^{-1}
0.005
0.010
0.015
0.020
0.025
0.030
0.035
0.040
k€ · t^{-1}
0.0005
0.0010
0.0015
0.0020
0.0025
0.0030
0.0035
0.0040
k€ · t^{-1}
methanol (tonne/hr)
ammonia (tonne/hr)
olefins (tonne/hr)
methanol (% util)
ammonia (% util)
olefins (% util)

Supplementary Figure 12: Sensitivities of electrified installed capacities (left) and of utilization rates of the electrified installed capacities (right) for various CAPEX and OPEX assumptions (rows) (Supplementary Table 8). The parameter ranges for the CAPEX and OPEX assumptions are divided into 12 equally sized bins resulting in an average of $512/12 \approx 42.7$ scenarios per bin. The points on the curves correspond to the bin means. Missing points in the % utilization curves indicate bins with no installed capacities. The methanol installed capacity includes the methanol needed as feedstock for electrified olefins. This explains why as olefins installed capacity decreases, the electrified methanol utilization increases. Installed capacities of electrified methanol and ammonia are always deployed regardless of cost increases, while electrified olefins can be fully delayed to 2045 depending on the CAPEX of direct air capture and of electrolyzers.



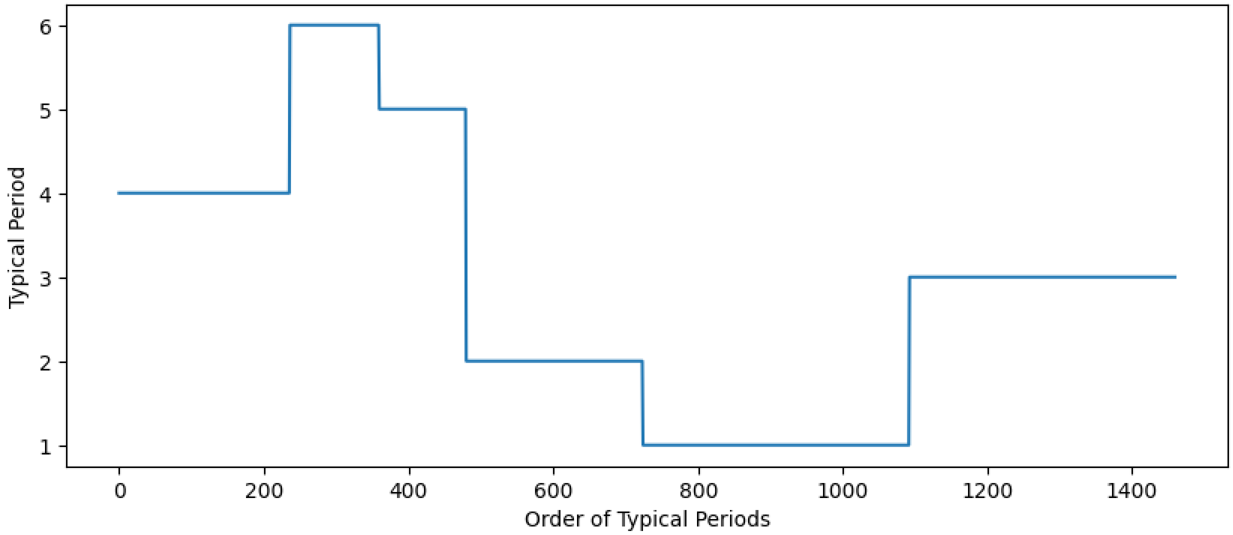
Supplementary Figure 13: Decision tree showing the key cost assumptions driving variability in the chemical industry transition. The percentages refer to the electrified share of a chemical's total production in the year 2040, with the ranges indicating the variation across the samples within each leaf node of the decision tree. The results show that sufficiently high direct air capture (DAC) and electrolyzer CAPEX can drive the olefins percentage electrified to 0% in 2040, indicating a delayed transition to 2045. Furthermore, the methanol and ammonia percentage electrified always remain above 80% and 20% respectively, illustrating the robustness of an accelerated transition in 2040 regardless of cost increases.

7 Constrained ramping of chemical production facilities

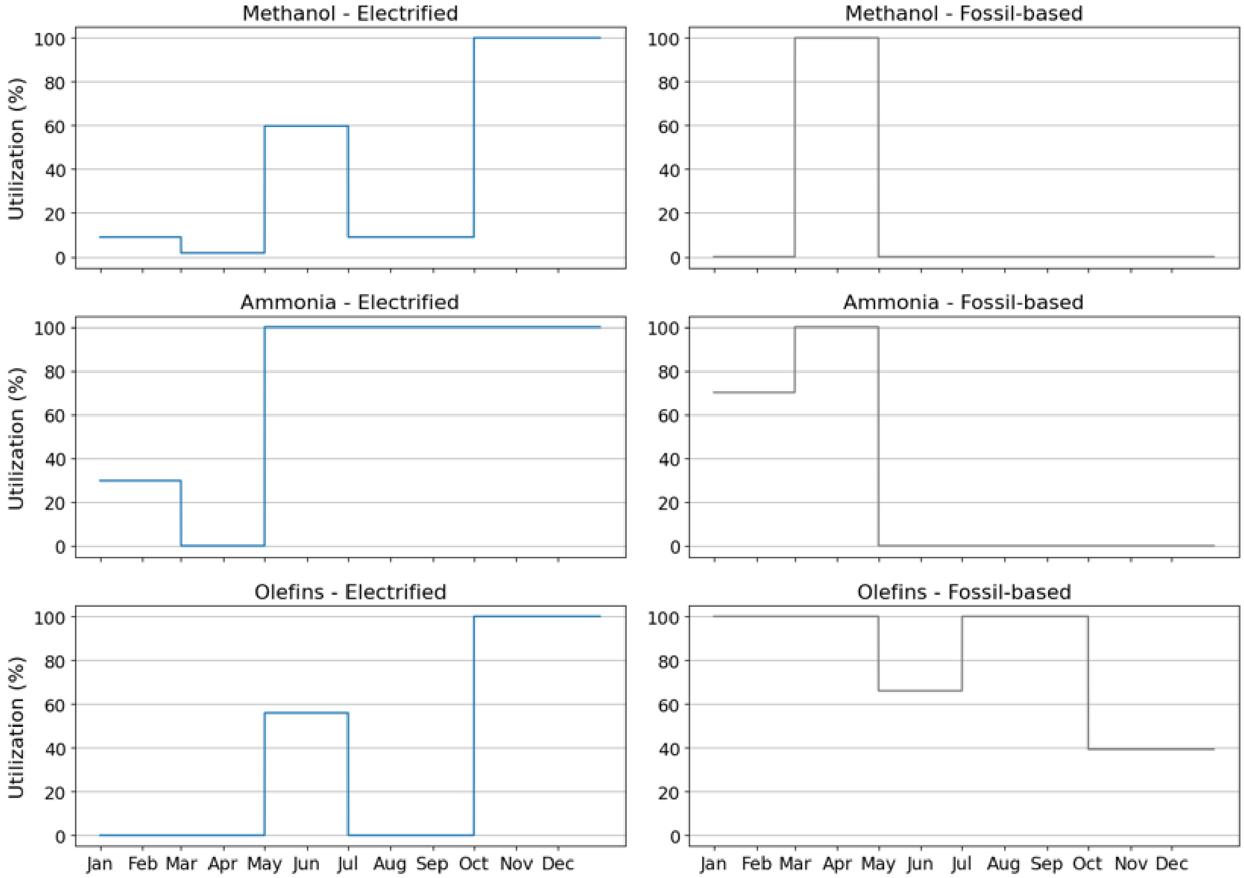
Our results demonstrate that dynamic operation of chemical production facilities in response to renewables availability provides valuable flexibility to the energy system. However, dynamically switching between production routes is incompatible with the real-world ramping limitations of chemical facilities, which often require weeks or even months to ramp up or down. To evaluate the effect of this real-world ramping limitation on the industry's transition, we evaluate a scenario with constrained facility ramping.

To implement this constraint, we take advantage of the results of our time-series aggregation (TSA), which already orders our 6 typical periods using a seasonal pattern (Supplementary Figure 14). Based on this structure, we impose a constraint that enforces constant chemical production within a typical period. Because of the consecutive placement of the typical periods in the TSA order, the constraint results in longer ramping between chemical production levels.

The resulting utilization profiles of the electrified and fossil-based production capacities in the year 2040 are shown in Supplementary Figure 15. These results show the constant chemical production levels across months or even seasons. Under this constraint, the energy system costs increase by only 0.1% in 2040. Hence, flexibility from a diversified and underutilized chemical industry retains its value even considering more realistic ramping rates, making the underutilized configuration viable for real-world implementation.



Supplementary Figure 14: Ordering of the typical periods throughout the year resulting from our time-series aggregation (TSA) of 6 typical periods of 6 hours each. Each number on the y-axis represents a distinct typical period, and the x-axis reflects their chronological assignment across the year. The resulting order captures the seasonality in the underlying data used for the TSA.



Supplementary Figure 15: Temporal profiles of electrified and fossil-based chemical production capacity utilization rates in the year 2040 considering longer facility ramping rates. The chemical industry still provides flexibility over monthly and seasonal time horizons, thus showing the value to the energy system under more realistic ramping assumptions. The methanol electrified capacity considers the methanol needed for olefins production. Therefore, the installed capacities of electrified and fossil-based methanol differ, and the sum of their utilization does not equal 100%. A 100% electrified methanol utilization includes methanol as feedstock for electrified olefins.

References

[1] IHS Markit, *Process Economics Program (PEP) Yearbook*, 2018.

[2] N. Baumgärtner, S. Deutz, C. Reinert, N. Nolzen, L. E. Kuepper, M. Hennen, D. E. Hollermann and A. Bardow, *Frontiers in Energy Research*, 2021, **9**, year.

[3] O. Edenhofer, *Climate change 2014: mitigation of climate change*, Cambridge University Press, 2015, vol. 3.

[4] P. Mayer, A. Ramirez, G. Pezzella, B. Winter, S. M. Sarathy, J. Gascon and A. Bardow, *IScience*, 2023, **26**, year.

[5] N. Von Der Assen, L. J. Muller, A. Steingrube, P. Voll and A. Bardow, *Environmental science & technology*, 2016, **50**, 1093–1101.

[6] S. Deutz and A. Bardow, *Nature Energy*, 2021, **6**, 203–213.

[7] R. Meys, A. Kätelhön, M. Bachmann, B. Winter, C. Zibunas, S. Suh and A. Bardow, *Science*, 2021, **374**, 71–76.

[8] B. Müller, K. Müller, D. Teichmann and W. Arlt, *Chemie Ingenieur Technik*, 2011, **11**, 2002–2013.

[9] M. De Saint Jean, P. Baurens and C. Bouallou, *International journal of hydrogen energy*, 2014, **39**, 17024–17039.

[10] M. D. M. Perez Fortes, E. Tzimas *et al.*, *Publications Office of the European Union*, 2016.

[11] D. Y. Shu, S. Deutz, B. A. Winter, N. Baumgärtner, L. Leenders and A. Bardow, *Renewable and Sustainable Energy Reviews*, 2023, **178**, 113246.

[12] Z. Cesaro, M. Ives, R. Nayak-Luke, M. Mason and R. Bañares-Alcántara, *Applied Energy*, 2021, **282**, 116009.

[13] J. Farla, C. Hendriks and K. Blok, *Carbon Dioxide Recovery From Industrial Processes. Climate Change*, 1995.

[14] M. Fasihi, O. Efimova and C. Breyer, *Journal of cleaner production*, 2019, **224**, 957–980.

[15] Ecoinvent, *Ecoinvent Data V. 3.6. Swiss Centre for Life Cycle Inventories*, 2020.

[16] R. Geres, A. Kohn, S. C. Lenz, F. Ausfelder, A. Bazzanella and A. Möller, *Roadmap Chemie 2050: Auf dem Weg zu einer treibhausgasneutralen chemischen Industrie in Deutschland: eine Studie von DECHEMA und FutureCamp für den VCI*, DECHEMA Gesellschaft für Chemische Technik und Biotechnologie eV, 2019.

[17] G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz and B. Weidema, *The International Journal of Life Cycle Assessment*, 2016, **21**, 1218–1230.

[18] Agora Energiewende and Agora Verkehrswende, *Study. Berlin: Agora Energiewende*, 2018.

[19] International Energy Agency, *World Energy Outlook 2018*, 2018.

[20] C. Zibunas, R. Meys, A. Kätelhön and A. Bardow, *Computers & Chemical Engineering*, 2022, **162**, 107798.

[21] J. Repenning, L. Emele, R. Blanck, H. Böttcher, G. Dehoust, H. Förster, B. Greiner, R. Harthan, K. Henneberg, H. Hermann *et al.*, 2015.

[22] Deutscher Bundestag, *Bundesgesetzblatt I*, 2021, **59**, 3905–7.

[23] Federal Ministry for the Environment, Nature Conservation and Nuclear Safety and www.bmu.de/en.

[24] L. J. Müller, A. Kätelhön, M. Bachmann, A. Zimmermann, A. Sternberg and A. Bardow, *Frontiers in Energy Research*, 2020, **8**, 15.

[25] D. S. Mallapragada, Y. Dvorkin, M. A. Modestino, D. V. Esposito, W. A. Smith, B.-M. Hodge, M. P. Harold, V. M. Donnelly, A. Nuz, C. Bloomquist *et al.*, *Joule*, 2023, **7**, 23–41.

[26] K. Sievert, T. S. Schmidt and B. Steffen, *Joule*, 2024, **8**, 979–999.

[27] G. Guidati and A. Marcucci, *Value of synthetic gases and fuels for the decarbonization of Switzerland (VADER)*, 2022.

[28] Sustainability in Business Lab, ETH Zürich, *Feasibility of a demonstrator for the carbon capture and storage value chain in CH with a waste-to-energy plant*, 2020.