

# Decarbonizing integrated chlor-alkali and vinyl chloride monomer production: Reducing the cost with industrial flexibility

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## ABSTRACT

Industrial demand response will become increasingly important in power grids with high shares of variable renewables, yet the existing knowledge on how the industrial electricity demand and flexibility will change with the decarbonization of chemical processes is limited. Here we develop a mixed-integer linear optimization model, which we use to compare the cost and flexibility of the most relevant decarbonization options for the combined chlor-alkali electrolysis (CAE) and vinyl chloride monomer (VCM) production process. We combine product and energy storage to enable the full flexibility potential of the decarbonized process. Our results show that flexible operation of the CAE process is deemed technically possible but limited by internal process dependencies due to decarbonization of the VCM production. Combining energy and product storage for demand response enables up to 4% operational cost reduction by shifting loads during peak price hours. High overcapacity of PEM electrolyzers is required to release the full flexibility potential in the hydrogen based decarbonization option, while the less flexible direct electrification option shows a potential for OPEX reduction. Full decarbonization of the combined CAE and VCM process without increasing operational cost significantly appears difficult. Our study emphasizes demand response through product and energy storages as a viable pathway for minimizing the added cost, and also enables a significant reduction of electric demand in high-price hours.

## 1. Introduction

According to the IEA [1], the demand for flexibility in electricity systems will more than double by 2030 due to a higher share of variable renewable electricity (VRE) production. Global renewable electricity generation is expected to increase from 28% in 2021 to 43–49% in 2030. Increased flexibility on the end-user side will be required to balance electricity production and demand, with industrial demand response being a potentially important provider of flexibility to the power grid.

Industrial electricity demand is expected to account for one third of the growth in electricity demand by 2030, with a total growth of more than 2000 TWh. This is caused by both an increase in production and the electrification of fossil processes. In addition, hydrogen production by electrolysis is expected to make a significant impact on the electricity demand [1]. With the decarbonization of industry and an increasing fraction of VRE in the electricity system, demand response in industrial applications is receiving more attention.

In addition to contributing with balancing services in the power system, demand response can reduce grid congestions and the cost of industrial operations. Moving electricity consumption from periods of high prices to periods of low prices decreases the average paid electricity price for the consumer. Increasing demand in low-price hours may also reduce VRE curtailment and enable higher penetration of VRE electricity in electricity systems.

### 1.1. Previous literature

Several articles have covered the status of demand response research, most of them focusing on the residential and commercial sector, typically in a smart grid context [2]. Söder et al. [3] reviewed the potential for demand-side flexibility in Northern Europe, finding that the industrial potential for flexibility is high in the Nordic countries. In the same work, they estimated the current demand response potential from industry in Norway to be up to 6.3% of peak demand. In Kirkerud et al. [4], the potential for demand response in the future Nordic energy system was investigated using a bottom up energy system optimization.

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## Nomenclature

### Parameters

$c_t^{el}$	Electricity spot price	€/MWh
$c^{em}$	CO <sub>2</sub> emission tax	€/ton <sub>CO<sub>2</sub></sub>
$c^{H_2,b}$	Blue hydrogen price	€/MWh
$c^{LC}$	Load change cost	€/Full load change
$c^{ng}$	Natural gas price	€/MWh
$E^{stor,H_2,max}$	Maximum capacity of hydrogen storage	MWh
$m^{cr,VCM}$	VCM production rate	ton/hr
$m^{stor,EDC,max}$	Storage capacity of EDC	ton
$n^{DC,nom}$	Nominal molar flow of DC	mol/hr
$p^{CAE,nom}$	Nominal power demand of CAE	MWh/h
$p^{PEM,nom}$	PEM nominal capacity	MWh/h
$p^{SOEC,nom}$	SOEC nominal capacity	MWh/h
$\alpha^{CAE,min}$	Lower limit of CAE	%
$\alpha^{DC,max}$	Upper limit of DC	%
$\alpha^{DC,min}$	Lower limit of DC	%
$\alpha^{PEM,min}$	Lower limit of PEM	%
$\alpha^{SOEC,min}$	Lower limit of SOEC	%
$\delta^{CAE}$	Maximum ramping of CAE	%
$\delta^{DC}$	Maximum ramping of DC	%
$\eta_s^{cr}$	Cracker efficiency	%
$\eta_s^{PEM}$	PEM efficiency	%
$\eta^{SOEC}$	SOEC efficiency	%
$\eta^{tr}$	Power transformer efficiency	%

$\theta^{CAE}$	Electricity intensity of CAE	MWh/ton <sub>Cl<sub>2</sub></sub>
$\theta^{cr}$	Heat demand of cracker	MWh/ton
$\theta^{SOEC}$	Heat demand of SOEC	MWh <sub>th</sub> /MWh <sub>H<sub>2</sub>,LHV</sub>
$\theta^{stor,H_2}$	Electricity demand of hydrogen compression,	MWh <sub>el</sub> /MWh <sub>H<sub>2</sub>,LHV</sub>
$\phi^{ng}$	CO <sub>2</sub> intensity of natural gas	ton/MWh <sub>LHV</sub>

### Variables

$b$	Binary variable for activation of electrolyzers, [0;1]	
$C$	Costs	€
$e$	CO <sub>2</sub> emissions	ton
$E$	Energy	MWh
$\dot{E}$	Energy flow	MWh/h
$LC$	Load change, 0-1	
$m$	Mass	ton
$\dot{m}$	Mass flow	ton/hr
$n$	Mol	kmol
$\dot{n}$	Molar flow	kmol/hr
$P$	Electricity	MWh/h
$Q$	Heat flow	MWh/h

### Indices

$s$	Cracker type, Electric/Thermal	
$t$	Time	Hour

tion model, including both households and industry. They included load shedding alternatives in the ferrous metals, aluminium, silicon and pulp and paper industries, and load shifting in the pulp and paper industry. Most of the required demand response in the energy system was in the study found to be provided by households, due to the high cost of industrial load shedding. However, future electrified industrial demands were not included in the study, and neither was the load shifting potential of other sectors such as the chemical or mineral industry.

Although industrial demand response has been identified as a possible important future provider of demand response, little of the potential is so far exploited. Leinauer et al. [5] investigates which obstacles prevent industrial actors to take part in demand response programmes by interviewing 16 energy experts from different companies. They divide the industrial flexibility into three categories: 1) temporal load shifting, e.g., through storage; 2) load shedding, by not undertaking planned activities; and 3) fuel switching, by temporarily replacing electric demands with other energy carriers. They also find that in particular a lack of financial incentives or benefits from demand response are insufficient for companies to invest in the implementation of demand response possibilities. One important example presented is the conflict between grid fees and demand response markets. While grid fees typically encourage a flat consumption profile, electricity spot markets and other flexibility markets specifically encourage load shifting with potentially higher peaks.

The importance of shifting loads according to spot prices were investigated by Finn and Fitzpatrick [6]. They found that demand response could enable a 10% decrease in the average paid electricity price for an industrial actor in Ireland, which also increased the amount of demand derived from wind energy by 5.8%. They found that peak time reduction had little effect on wind uptake, while shifting demand to low-price hours had a significant impact, arguing that variable electricity prices incentivize demand shifting in favour of higher renewable energy uptake. Similar findings were presented by Ruggles et al. [7], where hydrogen production by electrolysis is shown to provide significant reduction in VRE curtailment in energy systems with high amounts of wind and solar. Industrial loads have a high potential for providing demand response services as the power demand of each actor is

typically much higher than other end-users. Activating the demand response potential of large end-users is therefore important in meeting the ongoing changes in the power grid.

In the work of Paulus and Borggreffe [8], the potential for demand response in German energy-intensive industries was investigated. They found that industrial demand response may be able to provide around 50% of the required tertiary balancing market reserves. However, to maximize their return on investment, numerous processes need to operate near their maximum capacity due to the substantial capital costs associated with the equipment. High utilization rates of the process equipment makes load reductions with subsequent overproduction to catch up with the nominal production rate challenging. Paulus and Borggreffe [8] therefore also found that the cost of activating the industrial reserves were mostly so high that other alternatives were chosen first, especially for the industrial processes with no potential for catching up with temporarily reduced production rates. Among the large-scale energy intensive processes with significant technical demand response potential, the chlor-alkali electrolysis (CAE) and the electric arc furnaces used for large scale steel production were identified as promising. In addition to chlorine and steel production, cement [9,10], wood and pulp [8], and aluminium production [11] are also typically identified as possessing a high potential for demand response. However, the detailed technical potential for demand response of future industrial electric demands has been sparsely analyzed.

The chemical industry is one of the largest industrial sectors, and in Chen et al. [12], decarbonized methanol production is investigated with regards to how the size of hydrogen storage for both energy and product purposes is affected by variable power prices from high VRE penetration. They find that utilizing storages in this chemical process may reduce the required VRE production capacity in a 100% renewable electricity system. In the chemical industry, the CAE process is one of the most electricity-intensive processes in the world. In Germany, CAE accounted for 4.3 % of the total industrial electricity consumption in 2017, and Brée et al. [13] compared various options for demand-side management in standalone chlorine production. They investigated different chlorine production processes, including the standard CAE process, both oversized and combined with a battery energy storage

system. They found that oversizing the standard process provides the shortest payout times in the various scenarios, and that combining with a battery for flexibility provision is not cost-effective. They also found that the results were very sensitive to energy prices, both with regards to electricity prices and hydrogen prices. Klaucke et al. [14] investigated the flexibility potential of different parts of the chlorine value chain. They found that combining the CAE process with subsequent vinyl chloride monomer (VCM) production enabled a process design with “excellent and good potential for flexibilisation”, with only a few adjustments necessary. VCM is an intermediate product, where most of it is further refined into polyvinyl chloride (PVC) and used for plastic products all over the world. In a further study, they found that the volatility of the power prices is of high importance in enabling the economic viability of demand response in the process [15]. The integrated CAE and VCM production process can store intermediates as chlorine or ethylene dichloride (EDC), with EDC being favourable due to the toxicity of chlorine [16]. Hence, the storage of intermediate EDC enables the flexibility of the process and the power demand, without affecting the production rate of VCM.

Richstein and Hosseinioun [17] used a mixed-integer linear optimization model to investigate the cost savings potential from flexible operation of the CAE when storing EDC as an intermediate. They investigated how network tariffs impact the flexibility provision in both day-ahead markets and reserve markets. With an overcapacity of the electrolyzer of 25%, they found an electricity cost savings potential of nearly 20% with flexible operation. However, the study did not include operational limitations in subsequent processes, such as the direct chlorination (DC) process, which limits the realizable flexibility in operation of CAE to around 5% [18]. At overcapacities of 6.25%, Richstein and Hosseinioun [17] found more moderate electricity cost savings of 5% to 7%. Hoffmann et al. [19] and Hofmann et al. [16] used an approach similar to that used by Richstein and Hosseinioun [17], but with restricted overcapacities caused by technical limitations. Both found the reduction in electricity costs of flexible operation of CAE to be in the range of 3% to 5% for a 5% overcapacity in the electrolyzer. The cost reduction potential is very tightly linked to the storage capacity of EDC and also the degradation cost of the CAE membranes.

## 1.2. Contribution

None of the above reviewed studies have investigated in which way decarbonization of the EDC cracker will affect the overall energy demand or the flexibility of the combined CAE and VCM process. While chlorine production using CAE is based on electricity, the subsequent thermal cracking of EDC to form VCM in furnaces at over 400 °C for 10-20 seconds is currently based primarily on natural gas [20,21]. In a combined CAE and VCM process, the thermal cracking is typically heated by the combustion of a combination of natural gas and hydrogen, which is a by-product of the CAE [22]. This creates a dependence between the CAE and the cracker, which may affect the flexibility of the process in the case of decarbonization of the cracker. The decarbonization options for the cracker process include fuel replacement (electrification or using hydrogen [23]), new cracker technologies and combinations thereof. As hydrogen burners or electric cracking furnaces have been shown to be the two most promising options known today [20], we explore both these options in depth. Hydrogen for the cracker can be produced by electrolysis of water (green hydrogen) or through natural gas reforming with CCS (blue hydrogen). Increasingly varying electricity prices and the decreasing cost of electrolyzers [24] represent an opportunity for leveraging hours of low electricity price to produce green hydrogen. Using this hydrogen to replace natural gas in periods of low electricity prices could thus potentially lower energy costs and emissions from the process. Polymer electrolyte membrane (PEM) electrolyzers have shown advantageous characteristics for providing load balancing services in electricity grids with high shares of VRE, due to part-load operation possibilities and fast response rates [25].

How the decarbonization of the thermal cracker affects the demand response potential of the CAE, and which new technical limitations occur, has to the authors’ knowledge not been investigated. Therefore, to determine the optimal combination of energy and product storage, it is necessary to evaluate the impact of combining flexible assets, such as CAE, hydrogen production and combinations of energy and product storage. As the CAE produces hydrogen used in the cracker, a combination of product and energy storage will be required to enable the CAE flexibility potential presented by the previously mentioned studies in a decarbonized process. To this end, case-specific investigations of electrolysis operation in industrial applications are required to find the real potential for the reduction of energy costs through demand response. The documented knowledge regarding how different decarbonization options to replace natural gas based heating may change the electricity demand, and hence, and its effect on the power grid, is also limited.

To explore the opportunities for decarbonization, product and energy storage and process flexibility, we develop a cost minimization model for the annual operational costs of the combined CAE and VCM process with storage potentials. We include both hydrogen fuelled cracking and direct electric cracking as decarbonization alternatives, investigating the differences in total energy demand, electricity demand, operational cost, and peak electric demand. We include blue hydrogen and green hydrogen produced by PEM or solid oxide electrolytic cells (SOEC). We then investigate the realistic potential for cost savings when implementing the demand response potential of the combined CAE and PEM operation, and how these technologies will react to variations in energy prices. We define flexibility in the same way as Leinauer et al. [5] and focus on flexibility enabled by the categories 1) and 3), namely load shifting or shedding of electric demands without reducing the production volume of the final product.

To this end, the novel contributions of this work can be summarized as follows: (1) an investigation of the operational cost of alternative decarbonization strategies for the thermal cracker of VCM production; and (2) the quantification of how the combination of product and energy storage in the VCM production enables increased demand response potential of the process.

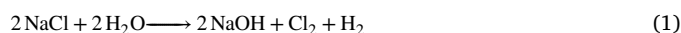
The remainder of this article is structured as follows. Section 2 presents the chemical process, and the capacities and parameters used in the study. In Section 3, the optimization model is presented, together with the energy and emission prices used in the study. The results from the optimization model are presented in Section 4, while a discussion of the most important findings in light of the issues raised in the introduction is presented in Section 5. Finally, Section 6 presents the conclusion of the work.

## 2. Process description

In this section, the integrated chlorine and VCM production process is described. VCM is most frequently produced from chlorine (Cl<sub>2</sub>) and ethene (C<sub>2</sub>H<sub>4</sub>), with EDC (C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>) being an intermediate product before VCM is produced through thermal cracking of EDC in furnaces [18]. First, the overall chemical reactions are described, before more specific details and limitations are presented.

### 2.1. Chemical process

The integrated chlorine and VCM production process consists of four main sections: CAE, oxychlorination (OXC), direct chlorination and the cracker section. Chlorine is produced in the CAE section, from the electrolysis of sodium chloride (NaCl) brine, with hydrogen and NaOH as by-products.



Chlorine (Cl<sub>2</sub>) from the CAE is used for the direct chlorination of ethene, producing EDC (C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>).

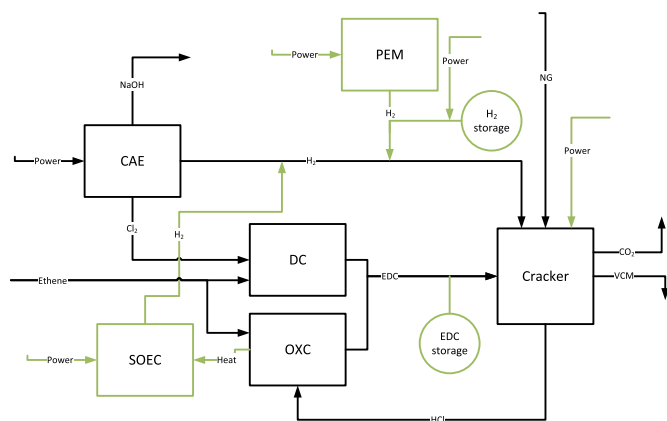


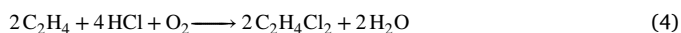
Fig. 1. The standard integrated chlorine and VCM process in black with the investigated modifications in this study to enable decarbonization or flexibility in green.



EDC from direct chlorination and oxychlorination is decomposed during thermal cracking into VCM ( $\text{C}_2\text{H}_3\text{Cl}$ ), which is the final product of this process.



During thermal cracking, hydrochloric acid (HCl) is formed and recirculated to the oxychlorination section, in which ethene and hydrochloric acid form additional EDC, used in the same thermal cracking section.



To enable flexibility in the process, storage of intermediates is necessary. EDC can be easily stored as a liquid in tanks, enabling flexible operation of the CAE and direct chlorination processes [18]. The complete molar balances used in the modelling for the same process steps, including the EDC storage, are described in the work by Hofmann et al. [16].

The energy-intensive steps of the process are the CAE and the thermal cracking section. While the CAE uses electricity to operate the electrolysis, the thermal cracker uses hydrogen from the CAE and natural gas in a burner to obtain the required temperatures for the cracking of EDC at around  $500^\circ\text{C}$  [26]. To reduce on-site  $\text{CO}_2$  emissions, the options are CCS, electrification of the cracker, or replacement of the natural gas fraction in the cracker with hydrogen. In the present study, the direct electrification and hydrogen options are investigated. All investigated modifications to the existing standard process are indicated in green in Fig. 1 as compared to the standard process in black.

## 2.2. System configuration

We have investigated an integrated CAE and VCM production process with a production rate of 60 tonnes VCM per hour. Ethylene is provided from a nearby process plant, and electricity is provided from the regional power grid.

### 2.2.1. Chlor-alkali electrolysis

CAE is in most cases based on the membrane technology, in which the membrane degrades over time, and at an increasing rate with load changes. Few studies have investigated the effect of load changes, but from a theoretical calculation, Hofmann et al. [16] derived a cost of load change per full load cycle of €5000. The electricity demand of the CAE to produce one tonne of chlorine is 2.58 MWh [14], and in this work it is assumed to be constant at all loads. In the work by Weigert et al. [27], the load ramping rate of a real plant was used to verify an

operational model, in which a load ramp of 0.08 MW/s, representing 0.1% of full load, was used. In this work, the full ramp rate of one hour of operation therefore exceeds 100% of the load. The main operational limit of the CAE is therefore the minimum operational limit at 66% of nominal load [19].

### 2.2.2. Direct chlorination

In the direct chlorination step, ethene is chlorinated to EDC under temperatures of  $85$  to  $200^\circ\text{C}$ . The minimum load of operation of the direct chlorination process has been found to be 70%, limiting the process significantly in flexible operation [18]. In this work, the range of operation of the direct chlorination process has therefore been limited to 75 to 105% [19].

### 2.2.3. Oxychlorination

Combining the direct chlorination, thermal cracking and oxychlorination provides the so-called balanced process for production of VCM. In the oxychlorination section, HCl from the thermal cracker reacts with ethene to form EDC. Oxychlorination typically occurs under  $180$  to  $550^\circ\text{C}$  and is an exothermic process. Cooling is required in the process to avoid temperature spikes, and hence, catalyst deactivation as well as EDC condensation [28,29]. The exact temperature of the condensation of EDC depends on its partial pressure, and hence, the process parameters. It may also be possible to utilize the chemical reaction heat as a waste heat potential. We have limited the waste heat potential to the condensation of EDC, assuming it to appear at temperatures high enough to produce steam at  $150^\circ\text{C}$ , which is required in the SOEC process. The cooling demand of EDC after the oxychlorination is 320 kJ/kg, equivalent to the heat of vaporization of EDC [30]. This heat is in this work regarded as available waste heat for the SOEC electrolyzer process [29].

### 2.2.4. Cracker

In the thermal cracker, EDC is heated up to around  $400^\circ\text{C}$  to  $500^\circ\text{C}$ , starting the cracking reactions forming VCM and HCl. The energy demand of the process is covered by combustion processes, consuming around 0.91 MWh/tonne VCM [21]. More than half of the heat demand is covered by the combustion of hydrogen from the CAE, while the deficit is covered by the combustion of natural gas [26]. The possibilities for the decarbonization of the thermal cracker are either replacing the natural gas with hydrogen, or replacing the entire cracker with an electrified one. In this work, it is assumed that replacing natural gas by hydrogen requires only minor modifications. An electrified cracker is assumed to have an efficiency of 98.5%, an improvement on the assumed 93.5% of the gas fired cracker [31]. The cracker is assumed to require constant operation, as the performance of the cracking process is sensitive to temperature changes. As the energy demand of the cracker is covered to a significant extent by the hydrogen by-product of the CAE, the constant operational demand of the cracker limits the potential for flexibility in the CAE operation. With decreased CAE operation, there will be a deficit in energy input to the cracker, which will require this demand to be covered by other sources.

### 2.2.5. PEM and hydrogen storage

The electricity based production of hydrogen with PEM electrolyzers has in several studies been identified as a potential technology to balance variable power production. PEM electrolyzers have favorable power response attributes, enabling them to go from standby to full operation in less than 3 seconds. They have also been found to degrade faster at full load than at variable loads [25]. In this work, it is assumed that variable operation does not speed up the degradation process, and therefore no degradation cost is included. The operational limit of standard PEM electrolyzers is typically a minimum of 10% with an electricity demand of 50.4 MWh/tonne hydrogen, delivered at 30 bar [32]. This equals an efficiency of 66% from electricity to  $\text{H}_{2,LHV}$ . In

addition, a transformer is required with an assumed efficiency of 95% [33].

Hydrogen storage is assumed to be in tanks at 200 bar, giving an electricity demand for compression from 30 bar of 0.659 MWh/ton.

### 2.2.6. Solid oxide electrolytic cells

Solid Oxide Electrolytic Cells are an alternative electrolyzer technology, based on using steam in the electrolysis process instead of liquid water as used in PEM electrolyzers. This gives the advantage of higher electrical efficiencies, and in cases where waste heat can be used to produce steam for the process, the overall performance can become very efficient. In practical applications of SOECs, a steam demand of 331 kg/h per MW electric at 150 °C and 6.5 bar is used. Assuming the heat demand is equal to the heat of vaporization at the given pressure, this equals 0.23 MWh<sub>th</sub>/MWh<sub>H<sub>2</sub>,LHV</sub>. The electrical system efficiency is 84% from electricity to H<sub>2</sub>,LHV, produced at 1 bar [34]. The process can operate down to a 5% load [35].

## 3. Method

This section describes the developed model used to investigate the cost optimal operation of the integrated chlorine and VCM production process, as presented in Section 2 and the scenarios and parameters used in the study.

### 3.1. Model description

The optimization model is formulated as a deterministic, mixed-integer linear problem for a one-year horizon, using an hourly resolution to obtain the cost optimal operation for that year, considering energy, emissions and possible load change costs related to degradation. The specific modelling of different components is described in Appendix A and they are connected with energy, molar or mass balances representing the relations shown in Fig. 1. The molar and mass balances of the specific components are described in detail by Hofmann et al. [16].

The model hence optimizes the process operation required to meet the constant product demand, specified as an input parameter. Including intermediate product and energy storage makes the process able to provide flexibility, enabling the production to provide demand response in the form of shifted electricity consumption. The system is built up as similar as possible to a standard state-of-the-art VCM production process, however with the possibility of flexible operation within the defined limits presented in Section 2. The main parameters used for investigation in this study are hence the energy storage capacities, and the capacity of the electrolyzers for decarbonizing the cracker energy demand.

#### 3.1.1. Objective function

The objective function described in Equation (5) minimizes the costs related to energy, emissions and load change costs for the combined CAE and VCM production process. Energy costs include electricity, natural gas and the cost of blue hydrogen supply. Emissions are in this case the emissions from the natural gas used in the cracker. The load change cost is the cost of a full load change of the CAE.

$$\min C^{\text{total}} = C^{\text{el}} + C^{\text{ng}} + C^{\text{H}_2, \text{b}} + C^{\text{em}} + C^{\text{LCC}} \quad (5)$$

$$C^{\text{el}} = \sum_t (P_t^{\text{tot}} * c_t^{\text{el}}) \quad (6)$$

$$C^{\text{ng}} = \sum_t (\dot{E}_t^{\text{ng}} * c^{\text{ng}}) \quad (7)$$

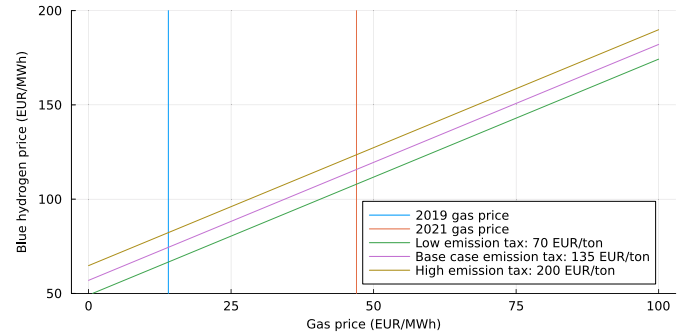
$$C^{\text{H}_2, \text{b}} = \sum_t (\dot{E}_t^{\text{H}_2, \text{b}} * c^{\text{H}_2, \text{b}}) \quad (8)$$

$$C^{\text{em}} = \sum_t (e_t * c^{\text{em}}) \quad (9)$$

**Table 1**

Energy prices in 2019 and 2021, respectively.

	2019	2021
Electricity price (avg) [EUR/MWh]	38.7	75.1
- Std.dev.	8.0	47.2
Gas price [EUR/MWh]	14.0	47.0



**Fig. 2.** Blue hydrogen price as a function of gas price for the base case scenario and a low and high sensitivity. 2019 and 2021 gas prices are indicated with vertical lines.

**Table 2**

Resulting blue hydrogen prices in 2019 and 2021.

	2019	2021
Blue hydrogen price [EUR/MWh]	74.4	115.7

$$C^{\text{LCC}} = \sum_t ((LC^{\text{up}} + LC^{\text{down}}) * c^{\text{LC}}) \quad (10)$$

#### 3.1.2. Load change costs of CAE

The load change costs are based on the work by Hofmann et al. [16]. The relation in Equation (10), together with Equation (11), minimizes the number of load changes to the cost optimal minimum, where  $LC$  is a number between 0 and 1, indicating the relative load change of the maximum available load change.

$$\frac{P_t^{\text{CAE}} - P_{t-1}^{\text{CAE}}}{P^{\text{CAE, nom}} (1 - \alpha^{\text{CAE, min}})} = (LC_t^{\text{CAE, up}} - LC_t^{\text{CAE, down}}) \quad (11)$$

### 3.2. Energy and emission prices

In this study, the energy prices described in Table 1 are used for the evaluation and comparison of cost optimality. The prices are based on the hourly electricity prices from the Norwegian price area NO2 as obtained from Nord Pool [36] for 2019 and 2021, as well as the yearly average natural gas prices from the TTF trading point for natural gas for the same years [37]. The emission taxes are based on the 2030 forecast of the Announced Pledges scenario in the World Energy Outlook 2022 [1], in which an emission tax of 135 EUR/tonne in advanced economies is predicted for 2030. The energy prices of 2021 are used in most of the following investigations, unless otherwise specified.

One option for the decarbonization of the process is to import hydrogen from an external market. The low carbon hydrogen in the market may in theory originate from both electrolysis (green) or from fossil fuels with CCS (blue). We have considered a market consisting of blue hydrogen, where the price calculation is based on the work by Oni et al. [38]. The price is based on the sensitivity towards carbon price and gas prices for blue hydrogen produced from autothermal reforming with CCS. As seen in Fig. 2, derived from Oni et al. [38], the sensitivity is clearly highest towards the gas price, compared with the emission tax. The resulting market hydrogen prices used in this work are presented in Table 2.

**Table 3**  
Presentation of the cases included in Sections 4.1 to 4.4.

	Not flexible	Flexible
<b>Not decarbonized</b>	Section 4.1	Section 4.2
	Base case	PEM
	No storage	SOEC
<b>Fully decarbonized</b>	Section 4.3	Section 4.4
	PEM	PEM
	SOEC	Hydrogen storage
	Electrified	EDC storage
	Blue hydrogen	
	No storage	

**Table 4**  
Resulting energy demands from cost optimal operation of the standard operation of an integrated CAE and VCM process.

Process	Electric [MWh/h]	Thermal [MWh/h]
Chlor-Alkali-Electrolysis	87.8	
Cracker total		56.6
- Covered by hydrogen from CAE		32.2
- Net demand (covered by NG)		24.4

## 4. Results

The results are presented in five sections. We first investigate the energy demand and operational costs of the process in the base case as it is operated traditionally (Section 4.1), or partially decarbonized (Section 4.2). In the following Sections 4.3 and 4.4, the fully decarbonized process is investigated, first without flexibility potential, then with storages to enable process flexibility. In Section 4.5, the main results from the previous sections are compared.

The outline of the results is presented in Table 3, while the specific flexibility cases are presented in Table 6.

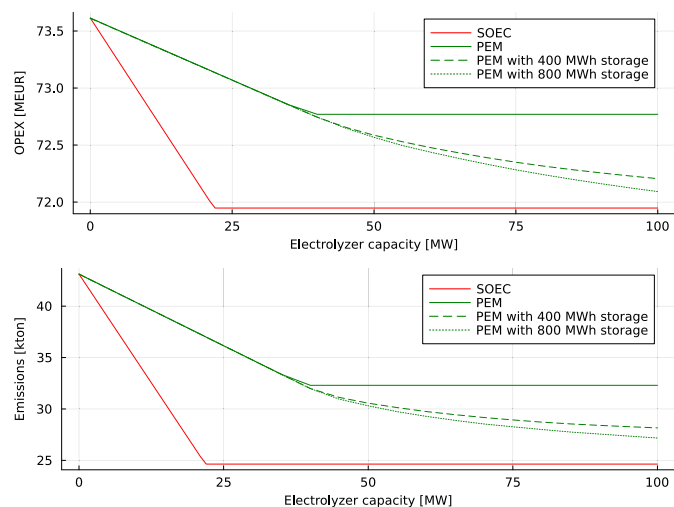
The model is implemented in the optimization modelling language JuMP [39] and is solved using Gurobi [40]. The model was run on a laptop computer with an Intel(R) Core(TM) i7-8665U processor with CPU at 1.90 GHz, and 32.0 GB installed memory. In the current application, the model consists of 403 000 continuous variables and 17 520 binary variables, and has a total run time of between 1 s in the base case to around 120 s in the more complex cases with storages and load shifting. In cases with increasing complexity beyond what is investigated in this work, it would be possible to reduce computational time by reducing the timesteps, or by assuming a fully linear operation of the components which include a binary term in the current application.

### 4.1. Energy demands and energy balance of the integrated chlorine and VCM production process

In this section, the results from the optimization model described in Section 3 for the energy demands of a standard operated integrated CAE and VCM production process are presented. As seen in Table 4, the highest part of the energy demand is related to the CAE process, which is a pure electric demand. The EDC cracking section has a fuel demand of 56.6 MWh/h, which is covered by 32.2 MWh/h H<sub>2</sub> from the CAE process, while the remaining 24.4 MWh/h is covered by import of natural gas. This fraction is in the same range as reported by Karlsen [26]. Hence, to decarbonize the VCM production process, the 24.4 MWh/h of natural gas must be replaced by a zero-emission energy carrier.

### 4.2. Cost and emission reduction potential by fuel-switching from natural gas to green hydrogen

In this section, the potential for cost and emission reduction by utilizing variable electricity prices to produce hydrogen as a fuel switching



**Fig. 3.** OPEX and CO<sub>2</sub> emissions changes for increasing electrolyzer capacity in the cases of SOEC and PEM electrolyzers. The PEM case also includes the option of hydrogen storage with two different capacities.

alternative to natural gas in the cracker is investigated. Two different technologies are investigated: the PEM and SOEC electrolyzers, and the results from the cost-optimization model are presented in the following sections.

#### 4.2.1. OPEX and emission reduction with PEM electrolysis

The total OPEX is only reduced by 1.2% with PEM electrolyzers compared with the standard process today, while CO<sub>2</sub> emissions are reduced by up to 25%. As seen in Fig. 3, the utilized capacity of PEM electrolyzers stagnates at slightly below 40 MW, unless the option of hydrogen storage is available. The PEM covers the full cracker heating demand at 38.8 MW capacity, and up to this capacity, the full hydrogen production is utilized at the same time in the cracker to replace natural gas. Including hydrogen storage increases the range of the PEM electrolyzers, as the overcapacity can be utilized to store hydrogen produced during low electricity price hours for later use. Considering the CAPEX of installation of PEM electrolyzers being in the range of 1000 EUR/kW [25], an installation of 40 MW PEM would cost approx. 40 MEUR. As indicated in Fig. 3, the annual savings in OPEX would be approx. 1 MEUR, resulting in an exceedingly long payback period.

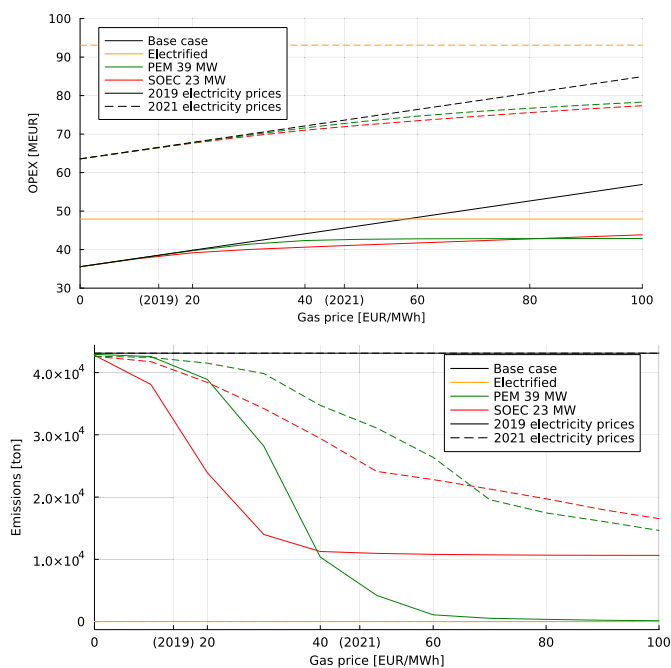
#### 4.2.2. OPEX and emission reduction with SOEC electrolysis

The utilization of waste heat from the oxychlorination process increases the electric efficiency of the hydrogen production compared to the PEM electrolysis, enabling OPEX savings of up to 2.3% and CO<sub>2</sub> emission savings of up to 43% in the case of SOEC hydrogen production. However, due to limitations in the maximum available waste heat from the oxychlorination, the maximum capacity of the SOEC is 21.9 MW, as seen in Fig. 3. Even so, the value of utilizing the available waste heat from the oxychlorination section to increase the electrolyzer efficiency is clearly seen in the figure, lowering the cost compared with PEM electrolysis.

#### 4.2.3. The energy price impact on cost optimal emission reduction

As the process mainly uses electricity, also in the base case, the operating expenses are significantly more sensitive to changes in the electricity price, compared to gas prices. In Fig. 4, the OPEX of the base case is increasing linear to the gas price, but the increase due to the change in electricity prices from 2019 to 2021 dominates the changes in OPEX. As there is no flexibility in the base case process, the CO<sub>2</sub> emissions are constant in all variations of energy prices.

The electrolyzer alternatives (PEM and SOEC) without hydrogen storage show nearly equal OPEX for all gas price variations. The SOEC



**Fig. 4.** Change in OPEX and CO<sub>2</sub> emissions for the different cases as a function of the gas prices. Solid lines are for the electricity prices in 2019, while dashed lines are for electricity prices in 2021. The 2019 and 2021 gas prices are indicated on the x-axis.

alternative gives slightly lower OPEX at low gas prices, while PEM gives lower OPEX at higher gas prices. This is due to the limitations in the waste heat availability of the SOEC, while the PEM utilizes the production capacity for longer periods in high price scenarios to avoid using expensive natural gas. The same effects are seen for the CO<sub>2</sub> emissions in the cost optimal operation of the electrolyzer alternatives. SOEC gives a larger decrease in emissions in low gas price scenarios, but is limited to a certain maximum emission reduction around 75%. PEM is able to reduce the emissions towards zero at higher gas prices, but even in the case of 2019 electricity prices, this first happens when gas prices are higher than 80 EUR/MWh.

At 2019 electricity prices and gas prices above 20 EUR/MWh, the electrolyzer alternatives prove more cost efficient than the base case operation. At 2021 electricity prices, the gas price needs to increase to beyond approx. 40 EUR/MWh for the same to happen.

The electrified cracker alternative is also included in Fig. 4. This is the most expensive alternative in all scenarios, except at high gas prices and low electricity prices, where the operational expenses of the base case exceed the electrified cracker. This alternative is further explored in Section 4.3.

#### 4.3. Cost-optimal operation of decarbonized CAE and VCM production process

In the following section, the alternatives for the full decarbonization of the cracker process are assessed, presenting the change in OPEX and energy demands of the different alternatives. 2021 energy prices are used in all the following investigations.

We consider an electrified or hydrogen fuelled cracker as alternatives for fully decarbonizing the process. The hydrogen can be provided by onsite electrolysis or imported from an external blue hydrogen market at a given price, as described in Section 3.2. In the case where onsite electrolysis is insufficient (SOEC case), hydrogen is bought externally to cover the remaining demand. In Table 5, the resulting nominal capacities under constant operation of the different decarbonization alternatives are presented.

**Table 5**  
Resulting energy import demand in cost-optimal operation of the fully decarbonized alternatives.

	Electricity import	Gas import (H <sub>2</sub> )
Electrified	53.2 MW	0
PEM	38.8 MW	0
SOEC	21.9 MW	6.0 MW
Blue hydrogen	0	24.4 MW



**Fig. 5.** OPEX and energy demands of the different cases under cost-optimal operation, including an option where hydrogen from the CAE is sold externally. Negative values indicate energy export. Green is electricity, dark blue is natural gas, while light blue is blue hydrogen.

The direct electrification of the cracker is, as seen in Table 5, the option with the highest electricity demand. It is also the option with highest operating expenses, net energy import, and peak demand, as seen in Fig. 5. In the base case, the cracker heating demand is covered by nearly 60% self-produced hydrogen from the CAE, and an electrified cracker would not be able to utilize the hydrogen for internal demands. Although an electric cracker has a higher efficiency than the existing one, the energy import would therefore increase by around 26%. However, there could be an option to export and sell the hydrogen produced in the CAE. This would reduce the OPEX by 18% compared to the base case and even reduce the net energy import of the process. As also seen in Fig. 5, the hydrogen sales option gives the lowest net energy import and OPEX of all cases.

The options including on-site hydrogen production from electrolysis are the PEM and SOEC options. The OPEX of these alternatives are quite similar, with the SOEC being slightly more cost-effective. However, the SOEC requires 5% of the total energy imported as hydrogen from an external source to cover the full cracker demand. Even so, the increased efficiency of the SOEC lowers both energy import and electric peak demand compared to both the PEM option and the electrified cracker without hydrogen sales, with only a 7% cost increase compared to the base case.

The final investigated option is the one where all natural gas is replaced by blue hydrogen imported from an external market. This is presumably the alternative with the lowest cost of investment, and the OPEX is in the same range as the on-site hydrogen production alternatives, increasing by 12% from the base case. However, it relies on the availability of hydrogen import and will require infrastructure for fuel and storage. With the energy import and electric peak demand also being among the lowest cases, this alternative presents a cost-efficient and viable path to rapid decarbonization of the industrial process.

**Table 6**  
Flexibility options in the fully decarbonized CAE and VCM process utilizing PEM electrolyzers. Capacity increase is relative to the nominal capacities as described in Tables 4 and 5.

	Process		Storage		OPEX	
	CAE [%]	PEM [%]	EDC [hr]	H <sub>2</sub> [hr]	[MEUR]	[%]
Nominal	100	100	0	0	83.3	100
CAE flexibility	105	105	24	0	83.1	99.8
PEM flexibility	105	105	0	24	82.3	98.8
Combined flexibility	105	105	24	24	81.8	98.2
Full flexibility	105	131	24	24	80.8	96.9

#### 4.4. Demand response potential of combining product and energy storage

In the following section, the possibility of operating the process flexibly is investigated. Flexibility is provided by ramping up or down different parts of the process, using storage to enable a constant production rate. As explained in Section 1, both the CAE process with EDC storage and PEM electrolyzer flexibility have been extensively studied in other works. Consequently, this section will focus on comparing the two options with regard to flexibility in the integrated chlorine and VCM production processes, thereby combining the flexibility of the two options.

##### 4.4.1. Cases

A set of cases are defined to investigate the effect of the flexibility of each separate process, as well as the combination of all. As described in Section 3, the CAE has a limit of reducing the load to 75% of nominal capacity, while the subsequent direct chlorination process has lower and upper limits of 75% and 105% of nominal capacity. The upper limit of capacity increase of the CAE is therefore limited by the direct chlorination process to a maximum of 5% overcapacity. For comparison, the overcapacity of both PEM and CAE is set to 5% in three of the investigated cases.

The cracker depends on sufficient hydrogen input delivered by either the CAE or the PEM, or both. This limits the potential for power reduction of the CAE process, as it is the main source of hydrogen for the cracker. To exploit the full flexibility potential of the CAE process, going down to 75% of nominal operation, an oversizing of the PEM electrolyzer to 51 MW is required to replace all the hydrogen from CAE. A fourth case is therefore included, in which the PEM electrolyzer has an overcapacity of 31%.

The cases are presented in Table 6, together with the nominal process without flexibility, and the resulting OPEX. The advantage of including both energy and product flexibility is seen, as the cost savings of the *Combined flexibility* case (1.8%) exceeds the sum of cost savings of the two separate *CAE* (0.2%) and *PEM flexibility* (1.2%) cases. The cost savings of all cases are quite moderate compared with the nominal process, which operates at a constant rate regardless of electricity price variations. The effect of variations in storage capacity is further investigated in Fig. 8.

##### 4.4.2. Flexible operation and response to electricity prices

In Fig. 6, the operation of the process for three weeks in April 2021 is presented. The *CAE flexibility* case (top), where no hydrogen storage is available, is clearly not utilizing the full flexibility potential of the process. As the power demand of the PEM increases when CAE reduces the production rate, the total power demand only sees a slight reduction. In the *PEM case* with hydrogen storage, the results show increased flexibility, as the PEM process can be shut off completely without affecting the CAE process. However, when both flexibility options are combined, the power demand of both processes can be reduced simultaneously, increasing the potential for power reduction. This is even more visible in the *Full flexibility* case, with a 31% overcapacity of the PEM electrolyzer.

From Fig. 6 it can also be seen that the price responses of the CAE and the PEM show significantly different behaviour. While the PEM ex-

**Table 7**

Average paid electricity price in the flexible cases compared to the average paid electricity price in the nominal case without flexibility options.

Case	Avg. paid electricity price [EUR/MWh]
Nominal	75.10
CAE flexibility	74.92
PEM flexibility	74.18
Combined flexibility	73.53
Full flexibility	72.56

ploits differences in power price more or less from hour to hour, the CAE operates more on a day-to-day frequency, filling the EDC storage in longer periods of low average prices, to decrease the power demand on days of higher power prices. This is due to both the cost of the load change of the CAE process but also the fact that the CAE process can only reduce to 75% of nominal power and hence is unable to fully empty the 24 hr full capacity storage as fast as the hydrogen demand.

The power duration curves over the year for the total power demand in all cases are presented in Fig. 7. Power duration curves present the number of hours the electricity import is at a certain level. The base case, which does not include decarbonization, is included for comparison. As seen, the pure *CAE flexibility* case only provides a slight decrease in power demand compared to the *Nominal*, due to the limitations caused by the PEM, as seen in Fig. 6. This decrease is realized for approximately half the year, while the *PEM flexibility* case gives a larger reduction in power demand but only for around 500 hours of the year. The *Combined flexibility* shows some advantageous behaviour of both processes and, although the power demand is slightly higher for most of the year, the power demand reduction is significant for approximately 3000 hours, and drastically reduced for 500 hours. In the *Full flexibility* case, the process has a much lower power demand than all other cases for nearly 2000 hours of the year. In the standard process today, *Base case*, the power demand is just below 88 MW constantly. In the decarbonized cases presented here, the power demand is significantly higher for most of the year, but the power demand is reduced below the standard process in periods of high power prices due to the reduction in power demand from the flexibility in the CAE.

The flexible operation enables load shifting from periods of high power prices to periods of lower power prices. By comparing the average paid electricity price to the overall average electricity price for the period, the effect of load shifting can be seen. In Table 7, the average paid electricity price for the cases is presented compared to the non-flexible nominal case, where the average paid electricity price is also equal to the average electricity price over the year.

##### 4.4.3. Storage capacity sensitivity

Fig. 8 presents the relative reduction in OPEX compared with the same case without storage. For comparison, the case of CAE flexibility in a non-decarbonized setting is also presented, where natural gas provides flexibility to the cracker fuel demand as a replacement for hy-



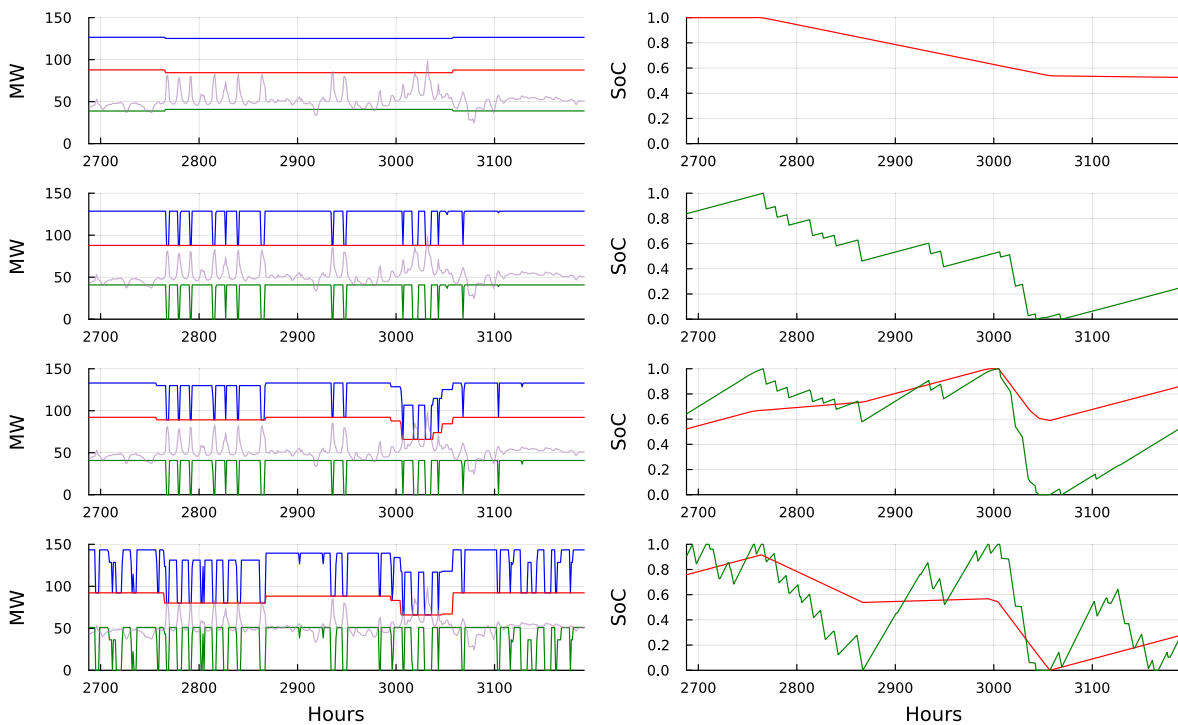


Fig. 6. Three weeks of operation of the processes and cases presented in Table 6. From top to bottom, the cases are as follows: CAE flexibility, PEM flexibility, Combined flexibility and Full flexibility. On the left is the power demand with PEM in green, CAE in red and total power demand in blue. The spot price is indicated in purple. To the right is the State of Charge (SoC) of storages, with red indicating the EDC storage and green being the hydrogen storage.

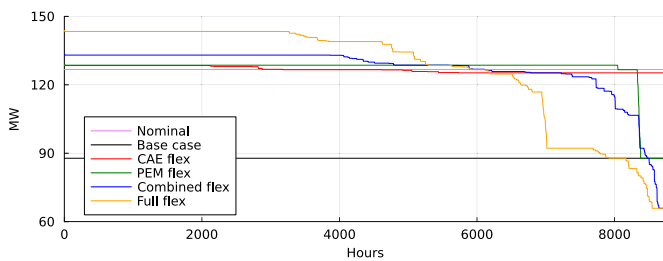


Fig. 7. Power duration curves presenting the number of hours where the total electricity import is at a certain value for the cases described in Table 6. The base case is included for comparison.

drogen from CAE. This is a case which comes with nearly no investment costs. As expected, the reduction in OPEX is smaller for the *CAE flexibility* case than for the other cases, with a reduction of around 0.25% at a EDC storage capacity of 24 hours. CAE flexibility alone, without any storage on the hydrogen side, provides little value, and only when combined with hydrogen flexibility can the EDC storage decrease the OPEX of the process. As seen, a combination of product and energy storage is required to enable the same potential for OPEX reduction as the non-decarbonized case, showing a potential OPEX decrease of nearly 2% with 24 hours of EDC and hydrogen storage. The results also indicate that the combination of PEM and CAE flexibility can increase the reduction in OPEX more than the sum of the two separate flexibility measures, showing significant advantages of coordinating the options. As expected, the *Full flexibility* case provides the largest decrease in OPEX at more than 3% with 24 hours capacity for both storages; however, this case would also demand the highest investment costs.

4.5. Summary of cases

In Fig. 9, the Base case from Section 4.2 is compared with the decarbonization option using PEM electrolyzers from Section 4.3 and

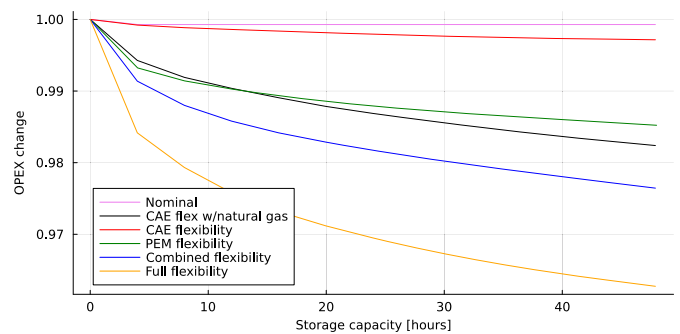


Fig. 8. Investigation of the value of EDC or hydrogen storage capacity in the cases of installed overcapacities in CAE and PEM, compared with the non-flexible case and the not-decarbonized case.

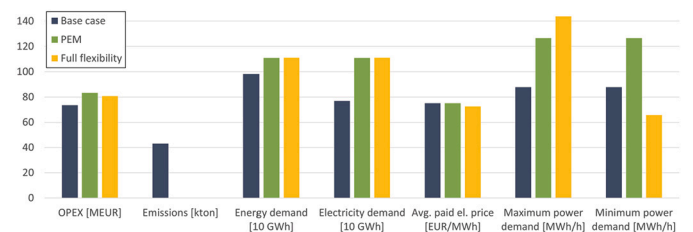


Fig. 9. Comparison of the base case with the decarbonized process, with and without process flexibility.

the decarbonized option including the Full flexibility demand response potential from Section 4.4. The results show that under cost-optimal operation, the OPEX increases by 10

## 5. Discussion

### 5.1. Cost-optimal operation of partly decarbonized VCM process

The results from the cost-optimization model show that utilizing electrolyzers to produce green hydrogen at a lower cost than natural gas has limited potential for energy cost savings. The OPEX was only slightly reduced compared with the fossil status quo alternative, however, with large investment demands. A large gap between the gas prices and the electricity price would be needed to motivate industries to switch from fossil-fuelled furnaces to hydrogen-based or electric alternatives solely on operational cost savings. Yet, although the cost decrease is very small, the emission reduction potential in using electrolyzers for replacement of natural gas is significant. For industries considering a change from natural gas based furnaces to hydrogen or electricity, low investment costs are, therefore, crucial. With an increasing share of VRE with low marginal costs in the grid, it is also likely that average electricity costs will decrease and decouple from gas prices in the future, incentivizing a switch to electricity in industrial energy systems.

### 5.2. Fully decarbonized VCM production

On the path to full decarbonization of industrial energy supply, demand response is one potential instrument to decrease energy costs. The results show that full decarbonization without demand response implementation gives a cost increase in all the investigated cases, unless it is possible to sell the surplus hydrogen from the CAE in an external market in the case of an electric cracker. The results of the electric cracker option are sensitive to both electricity and hydrogen prices, supporting the findings of Brée et al. [13], where the sensitivity to hydrogen prices was found to be important for the cost optimal flexible operation. Our analysis does not, however, include investment costs, which for an electrified cracker will be significant. Electric crackers are currently under development but are not ready at an industrial scale. There is also some uncertainty associated with the SOEC case, which depends on internal waste heat for steam production. The exact availability of waste heat can vary from plant to plant, depending on existing heat integration utilities. With higher waste heat availability, the SOEC case may become more cost-competitive, especially when compared with the PEM case. However, the SOEC operational flexibility and the scalability is limited, due to the dependency on the continuous oxychlorination and cracker processes, and waste heat availability. While electric crackers will have limited scalability as they are designed to fit the exact process, PEM electrolyzers scale easily, and may fit both larger or smaller process demands. However, it is also noteworthy that the decarbonization option based on blue hydrogen gives the lowest net energy import demand, lowest electricity peak demands and presumably lowest investment costs. Blue hydrogen may in this way be a highly relevant fast-track to decarbonization, possibly as a first step on the road to a fully decarbonized energy system. Overall, there is not one perfect solution, but a trade-off between energy efficiency, investment cost, operational costs and flexibility required to design a decarbonized system.

### 5.3. Demand response in combined CAE and VCM production

In the cases of increased capacity installation for use in demand response applications, an important finding is that the different flexible processes have direct mutual impact. The combination of both product and energy storage can provide flexibility to a higher degree than the sum of the two separate technologies. In the case of combined flexibility, the electricity demand can be reduced to a minimum when shutting down PEM operation completely, while at the same time reducing the CAE to a minimum. Total power demand can then be significantly reduced, and the duration curves in Fig. 7 show that total power demand is reduced to below the power demand of the not-decarbonized case.

This is an important finding from a grid point of view, as it indicates the possibility of utilizing industrial demand response for lowering power demand in hours of high power grid strain. Grid tariff structures have not been considered in this work but could be a point of further studies, as grid tariffs may be utilized to free up capacity in the grid in periods of high strain.

Although demand response shows potential for reducing power demand in peak price or peak demand hours, the operational cost savings for the industrial actor are moderate. In the most flexible of the investigated cases, with 5% overcapacity in the CAE, 31% in the PEM electrolyzers, and 48 hours of both product and energy storage, the overall OPEX is reduced by up to 4% from flexible operation. CAE and PEM flexibility shows potential at different time scales, and another case for further studies could be to investigate how a rolling horizon optimization based on energy price forecasts would affect the results. We have considered a deterministic model, in which the EDC storage, in particular, is charged over multiple days. In reality, the power price is only known for a maximum of 36 hours upfront, making charging and discharging of long-term storages more complex [41]. Another obstacle to obtaining the full potential of demand response is the implementation of the control system. Although the technical potential has been identified in this study, significant control mechanisms would be required to respond to price signals, such as the ones set by the electricity prices. The costs related to such changes to the production facility have not been considered in this work.

### 5.4. Policy and regulations

Even if large-scale industries do not utilize demand-side management today to reduce power demand at high price hours to a large extent [5], this work underpins that there is technical potential to do so. This potential will increase with electrolyzers being implemented in industries with heating demands. However, several industries typically have fixed-price contracts for parts or all of their electricity demand, removing the incentive to shift consumption to hours of low spot prices. As discussed in the Introduction, Finn and Fitzpatrick [6] found a significant correlation between shifting demand to low-price hours and decreased VRE curtailment. Exposing electricity-intensive industries to spot prices may, therefore, enable more VRE into the power grid in a shorter time, but it comes with a significant economic risk to industries with high sensitivity to electricity prices. These results are also in line with what was presented by Leinauer et al. [5], where they suggest to readjust taxes and levies for power purchase to increase financial incentives for demand response. Another alternative, which has not been investigated here, is to motivate industries to increase or decrease loads as a service to the power system in periods of instability with a significant financial benefit. This could be an interesting option, both in local systems with power grid constraints, on a higher system level when the electricity generation is in imbalance with the demand, or for reserve provision. Identifying the proper policies and regulations could hence enable a broader use of industrial demand response, establishing industry as a significant contributor to power system flexibility.

## 6. Conclusion

This study has investigated the decarbonization options and their potential for reducing operational costs through demand response for the integrated CAE and VCM production process. Utilizing hydrogen from electrolyzers only reduced the operational costs by 2.5% compared with the base case using natural gas only, posing challenges in achieving cost-parity with capital expenditures. Nevertheless, notable emission reductions of up to 43% were achieved.

In the case of a fully decarbonized process, the different possible paths to decarbonization showed significantly different characteristics. The SOEC and the blue hydrogen cases reduced electric peak demand and energy import, while direct electrification of the cracker reduced

OPEX and net energy import. PEM electrolyzers enabled a high degree of flexibility in the process with a 13% cost increase compared to the non-decarbonized base case.

An overcapacity of 31%, combined with large product and energy storages was required to fully exploit the potential of flexible operation of the chlor-alkali electrolysis, when decarbonized with PEM electrolyzers. Given that the necessary overcapacity and storage was available, it was possible to reduce the power demand below the base case for shorter periods. A decrease in OPEX by up to 4% in the best case was deemed possible.

Although industrial flexibility has been identified as important for balancing in electricity systems dominated by VRE, this study found that the economic viability in flexible operation is challenging. A technical potential to reduce peak demands by nearly 50% for shorter periods compared to non-flexible operation was found, which may enable a more rapid electrification of other energy demands, albeit at the cost of significant storage investments. Strategic implementation of policies and levies that promote flexible practices through mechanisms like dynamic grid tariffs, electricity spot prices or other measures could hence increase the pace of electrification and decarbonization of the industry.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

### Data availability

No data was used for the research described in the article.

### Acknowledgement

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## Appendix A. Detailed model description

### A.0.1. Chlor-alkali electrolysis

The CAE process power demand is described as a relation between the chlorine production rate and the power demand per tonne of chlorine ( $\theta$ ). It is limited by the minimum operation of the CAE ( $\alpha$ ), as well as the ramping rate ( $\delta$ ).

$$P_t^{\text{CAE}} = \dot{m}_t^{\text{CAE,Cl}_2} * \theta^{\text{CAE}} \quad (\text{A.1})$$

$$\dot{m}_t^{\text{CAE,Cl}_2} = \dot{n}_t^{\text{CAE,Cl}_2} * M^{\text{Cl}_2} \quad (\text{A.2})$$

$$\dot{n}_t^{\text{CAE,Cl}_2} = \dot{n}_t^{\text{CAE,H}_2} \quad (\text{A.3})$$

$$\dot{m}_t^{\text{CAE,H}_2} = \dot{n}_t^{\text{CAE,H}_2} * M^{\text{H}_2} \quad (\text{A.4})$$

$$\dot{E}_t^{\text{CAE,H}_2} = \dot{m}_t^{\text{CAE,H}_2} * \text{LHV}^{\text{H}_2} \quad (\text{A.5})$$

$$P_t^{\text{CAE}} \geq \alpha^{\text{CAE,min}} * P^{\text{CAE,nom}} \quad (\text{A.6})$$

$$P_t^{\text{CAE}} - P_{t-1}^{\text{CAE}} \leq (1 + \delta^{\text{CAE}}) * P^{\text{CAE,nom}} \quad (\text{A.7})$$

$$P_t^{\text{CAE}} - P_{t-1}^{\text{CAE}} \geq (1 - \delta^{\text{CAE}}) * P^{\text{CAE,nom}} \quad (\text{A.8})$$

### A.0.2. Direct chlorination

The direct chlorination process is also limited by ramping rates ( $\delta$ ) and operation limits ( $\alpha$ ).

$$\dot{n}_t^{\text{DC,EDC}} = \dot{n}_t^{\text{DC,Cl}_2} \quad (\text{A.9})$$

$$\dot{n}_t^{\text{DC,EDC}} - \dot{n}_{t-1}^{\text{DC,EDC}} \leq (1 + \delta^{\text{DC}}) * \dot{n}^{\text{DC,nom}} \quad (\text{A.10})$$

$$\dot{n}_t^{\text{DC,EDC}} - \dot{n}_{t-1}^{\text{DC,EDC}} \geq (1 - \delta^{\text{DC}}) * \dot{n}^{\text{DC,nom}} \quad (\text{A.11})$$

$$\dot{n}_t^{\text{DC,Cl}_2} \leq \alpha^{\text{DC,max}} * \dot{n}^{\text{DC,nom}} \quad (\text{A.12})$$

$$\alpha^{\text{DC,min}} * \dot{n}^{\text{DC,nom}} \leq \dot{n}_t^{\text{DC,Cl}_2} \quad (\text{A.13})$$

### A.0.3. Oxychlorination

The waste heat generated from the oxychlorination process is a product of the mass flow rate of EDC and the heat of evaporation of EDC at the temperatures and pressures given in Section 2, as the EDC is condensed from gas phase to liquid.

$$\dot{n}_t^{\text{OXC,EDC}} = \frac{\dot{n}^{\text{OXC,HCl}}}{2} \quad (\text{A.14})$$

$$Q_t^{\text{OXC,EDC}} = \dot{n}_t^{\text{OXC,EDC}} * M^{\text{EDC}} * h_{\text{evap}}^{\text{EDC}} \quad (\text{A.15})$$

### A.0.4. EDC storage

The storage level of the EDC storage is limited by the maximum capacity given in tonnes.

$$\dot{n}_t^{\text{stor,EDC}} = \dot{n}_{t-1}^{\text{stor,EDC}} + \dot{n}_t^{\text{stor,EDC,in}} - \dot{n}_t^{\text{stor,EDC,out}} \quad (\text{A.16})$$

$$\dot{n}_t^{\text{stor,EDC}} \leq \dot{n}_t^{\text{stor,EDC}} \quad (\text{A.17})$$

$$\dot{m}_t^{\text{stor,EDC}} = \dot{n}_t^{\text{stor,EDC}} * M^{\text{EDC}} \quad (\text{A.18})$$

$$\dot{m}_t^{\text{stor,EDC}} \leq \dot{m}^{\text{stor,EDC,max}} \quad (\text{A.19})$$

### A.0.5. Cracker

In the cracker, electric energy or thermal energy from the combustion of hydrogen or natural gas is used to elevate the temperature of EDC for cracking to VCM. The heat demand per tonne of VCM is described by the parameter  $\theta$ . The required energy input to the cracker is a relation between the heat demand and the cracker efficiency ( $\eta$ ), which is different between an electric cracker and a combustion based cracker. CO<sub>2</sub> emissions from the process are related to the combustion and emission intensity of natural gas ( $\phi$ ).

$$\dot{n}_t^{\text{cr,EDC}} = \dot{n}_t^{\text{cr,HCl}} \quad (\text{A.20})$$

$$\dot{m}_t^{\text{cr,EDC}} = \dot{n}_t^{\text{cr,EDC}} * M^{\text{EDC}} \quad (\text{A.21})$$

$$Q_t^{\text{cr}} = \dot{m}_t^{\text{cr,VCM}} * \theta^{\text{cr}} \quad (\text{A.22})$$

$$\dot{n}_t^{\text{cr,EDC}} = \dot{n}_t^{\text{cr,VCM}} \quad (\text{A.23})$$

$$\dot{m}_t^{\text{cr,VCM}} = \dot{n}_t^{\text{cr,VCM}} * M^{\text{VCM}} \quad (\text{A.24})$$

$$e_t^{\text{cr}} \geq \dot{E}_t^{\text{cr,ng}} * \phi^{\text{ng}} \quad (\text{A.25})$$

$$Q_t^{\text{cr}} = \eta_s^{\text{cr}} * \dot{E}_t^{\text{cr}} \quad (\text{A.26})$$

### A.0.6. PEM electrolyzers

The power demand of PEM electrolyzers is related to efficiencies of power transformers and the PEM stack ( $\eta$ ). As PEM electrolyzers are limited by a minimum operational limit ( $\alpha$ ), a binary variable ( $b$ ) is introduced.

$$\dot{E}_t^{\text{PEM,H}_2} = P_t^{\text{PEM}} * \eta^{\text{tr}} * \eta^{\text{PEM}} \quad (\text{A.27})$$

$$P_t^{\text{PEM}} \leq P^{\text{PEM,nom}} * b_t^{\text{PEM}} \quad (\text{A.28})$$

$$P_t^{\text{PEM}} \geq \alpha^{\text{PEM,min}} * P^{\text{PEM,nom}} * b_t^{\text{PEM}} \quad (\text{A.29})$$

### A.0.7. SOEC

The power demand of SOEC electrolyzers are calculated in the same way as the PEM electrolyzers. However, SOEC also requires a heat input, in this case available from the oxychlorination process and quantified by the heat demand,  $\theta$ .

$$\dot{E}_t^{\text{SOEC,H}_2} = P_t^{\text{SOEC}} * \eta^{\text{tr}} * \eta^{\text{SOEC}} \quad (\text{A.30})$$

$$P_t^{\text{SOEC}} \leq P^{\text{SOEC,nom}} * b_t^{\text{SOEC}} \quad (\text{A.31})$$

$$P_t^{\text{SOEC}} \geq \alpha^{\text{SOEC,min}} * P^{\text{SOEC,nom}} * b_t^{\text{SOEC}} \quad (\text{A.32})$$

$$\dot{E}_t^{\text{SOEC,H}_2} * \theta^{\text{SOEC}} = Q_t^{\text{SOEC}} \quad (\text{A.33})$$

### A.0.8. Hydrogen storage

The storage of hydrogen requires compressor work, calculated by the amount of energy required to compress from the electrolyzer delivery pressure to the storage pressure, per tonne of hydrogen ( $\theta$ ).

$$E_t^{\text{stor,H}_2} = E_{t-1}^{\text{stor,H}_2} + \dot{E}_t^{\text{stor,H}_2,\text{in}} - \dot{E}_t^{\text{stor,H}_2,\text{out}} \quad (\text{A.34})$$

$$E_1^{\text{stor,H}_2} \leq E_T^{\text{stor,H}_2} \quad (\text{A.35})$$

$$E_t^{\text{stor,H}_2} \leq E^{\text{stor,H}_2,\text{max}} \quad (\text{A.36})$$

$$P_t^{\text{stor,H}_2} = \frac{\dot{E}_t^{\text{stor,H}_2,\text{in}}}{\text{LHV}^{\text{H}_2}} * \theta^{\text{stor,H}_2} \quad (\text{A.37})$$

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