ELSEVIER

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/cace





Optimal design of a local renewable electricity supply system for power-intensive production processes with demand response

Sonja H.M. Germscheid ^{a,b}, Benedikt Nilges ^c, Niklas von der Assen ^{c,d}, Alexander Mitsos ^{d,a,e}, Manuel Dahmen ^{a,*}

- ^a Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research, Energy Systems Engineering (IEK-10), Jülich 52425, Germany
- ^b RWTH Aachen University, Aachen 52062, Germany
- c RWTH Aachen University, Institute of Technical Thermodynamics (LTT), Aachen 52062, Germany
- d JARA-ENERGY, Aachen 52056, Germany
- e RWTH Aachen University, Process Systems Engineering (AVT.SVT), Aachen 52074, Germany

ARTICLE INFO

Keywords: Integrated design and scheduling Stochastic programming Demand response Local electricity supply system Renewable energy

ABSTRACT

This work studies synergies arising from combining industrial demand response and local renewable electricity supply. To this end, we optimize the design of a local electricity generation and storage system with an integrated demand response scheduling of a continuous power-intensive production process in a multi-stage problem. We optimize both total annualized cost and global warming impact and consider local photovoltaic and wind electricity generation, an electric battery, and electricity trading on day-ahead and intraday market. We find that installing a battery can reduce emissions and enable large trading volumes on the electricity markets, but significantly increases cost. Economically and ecologically-optimal operation of the process and battery are driven primarily by the electricity price and grid emission factor, respectively, rather than locally generated electricity. A parameter study reveals that cost savings from the local system and flexibilizing the process behave almost additively.

1. Introduction

Renewable electricity has a varying supply that leads to timevarying electricity prices on the electricity markets. The time-varying prices can incentivize flexible industrial processes to adapt their momentary production rate and, thus, power consumption in a demand response (DR) scheduling, which can reduce operational cost and is considered electricity grid balancing (Daryanian et al., 1989; Zhang and Grossmann, 2016; Burre et al., 2020; Mitsos et al., 2018). DR savings can be improved by participating in multiple short-term electricity markets, see, e.g., Leo et al. (2021), Dalle Ave et al. (2019), Simkoff and Baldea (2020), Liu et al. (2016), Pandžić et al. (2013), Kwon et al. (2017), Golmohamadi and Keypour (2018), Nolzen et al. (2022), Germscheid et al. (2022, 2023), Schäfer et al. (2019) and Varelmann et al. (2022). Furthermore, flexible operation should be accounted for at design stage in order to determine optimal investment decisions for both the production processes itself, see, e.g., Mitra et al. (2014), Teichgraeber and Brandt (2020), Steimel and Engell (2015), Seo et al. (2023) and Leenders et al. (2019), and for its local energy supply system, see, e.g., Yunt et al. (2008), Zhang et al. (2019), Voll et al.

(2013), Baumgärtner et al. (2019), Langiu et al. (2022), Bahl et al. (2017) and Fleschutz et al. (2023).

In local energy supply systems, integrated design and scheduling has already been used to optimize on-site renewable electricity generation and storage systems. In the corresponding studies, the considered systems satisfy a fixed demand profile but can offer flexibility by combining different electricity generation technologies, see, e.g., Zhang et al. (2019), Bahl et al. (2017), Fleschutz et al. (2023) and Baumgärtner et al. (2019). Furthermore, combining on-site renewable electricity generation and storage systems with flexible production processes can reduce both production cost and CO2 emissions, which has been shown for, e.g., a water electrolyzer in combination with Power-to-X processes (Mucci et al., 2023), ammonia and nitric acid production (Wang et al., 2020), ammonia generation (Allman and Daoutidis, 2018), and methanol production (Martín, 2016). Further power-intensive, flexible production processes could benefit from the combination with on-site renewable electricity supply, e.g., the chlor-alkali electrolysis (Brée et al., 2019), seawater desalination (Ghobeity and Mitsos, 2010), or air separation (Ierapetritou et al., 2002). However, to the best of our knowledge, a generalized assessment about synergies arising from

E-mail address: m.dahmen@fz-juelich.de (M. Dahmen).

Corresponding author.

combining on-site electricity supply systems and DR-capable processes has not been conducted vet.

In our prior work (Germscheid et al., 2022), we conducted a DR potential assessment of power-intensive production processes by means of the generalized process model introduced by Schäfer et al. (2020). The generalized process model can represent a wide range of continuous production processes by means of few key process characteristics, i.e., oversizing, minimal part load, ramping limitations, and production storage capacity. We analyzed the benefit of participating simultaneously in both the day-ahead (DA) and the intraday (ID) spot electricity market, but neglected potential electricity provision by onsite renewable electricity generation and storage (Germscheid et al., 2022).

In this article, we extend our prior work (Germscheid et al., 2022) by integrating the scheduling of the generalized production process into the design optimization of a local electricity generation and storage system. In the resulting multi-stage approach, we optimize the design of the local renewable electricity supply system considering photovoltaic (PV) power, wind power, and an electric battery for a location in Germany. On the lower stages, we optimize the DR scheduling of both the energy system and the process, together with the electricity market participation. We consider both economic and ecologic design objectives. i.e., we optimize with respect to the total annualized cost (TAC) and the global warming impact (GWI), respectively. We study the influence of different degrees of process flexibility on the optimal design of the energy system and the resulting ecologic and economic savings. Similar to our prior work (Germscheid et al., 2022), we consider simultaneous market participation in both the DA and ID electricity market to analyze the benefit of considering multiple electricity markets in an integrated design and scheduling problem.

The remainder of the article is structured as follows: Section 2.1 explains the structure of the integrated design and scheduling problem. We specify the objectives in Section 2.2 and the operational constraints in Section 2.3. The scenarios and the model parameters are specified in Sections 2.4 and 2.5, respectively. We discuss the optimal energy system design for a reference process in Section 3.1, the dependency between process parameters and potential savings in Section 3.2, and the benefit of considering simultaneous DA and ID market participation at design stage in Section 3.3. In Section 4, we conclude our work.

2. Methods

2.1. Structure of the integrated design and scheduling problem

Integrated design and scheduling problems are often set up as twostage stochastic problems (Birge and Louveaux, 2011) with the design decisions on the first stage and scheduling decisions and operational constraints on the second stage, see, e.g., Yunt et al. (2008), Zhang et al. (2019), Langiu et al. (2022), Mitra et al. (2014), Teichgraeber and Brandt (2020), Steimel and Engell (2015), Seo et al. (2023) and Bahl et al. (2018). In this work, we determine the optimal design of a local electricity supply system for a flexible industrial production process. We account for simultaneous DA and ID market participation in the design and scheduling problem by the three-stage structure shown in Fig. 1. In the first stage, the design decisions for the energy system are made, i.e., photovoltaic (PV), wind power, and electric battery capacities are to be determined. The DA trading decisions are taken the day before the operation when the ID price and renewable electricity generation are still uncertain. Thus, we consider the DA decisions on the second stage and ID trading and operational decisions on the third stage. In particular, the operation of the flexible process is adapted on the third stage in response to realizations of the ID price, renewable electricity production, and the momentary emission factor of the grid electricity. Note that we consider a time-varying average grid emission factor similar to Baumgärtner et al. (2019) and Nilges et al.

(2023) and that the emission factor is uncertain a day before the actual consumption.

Similar to our prior work (Germscheid et al., 2022), we consider hourly DA purchases and quarter-hourly ID purchases and sales and assume a one-day scheduling horizon. In addition, we allow selling electricity from the local generation and storage system on the DA market. For simplicity, we assume that throughout any quarter-hour time slice, renewable electricity generation is constant.

In the following, we omit a distinct notation for second- and thirdstage parameters and variables for better readability. In particular, we consider DA trading decisions q_{DA,s_3} and DA price c_{DA,s_3} on the third stage instead of the second stage and guarantee equality on the second stage by means of non-anticipativity constraints:

$$c_{\text{DA}, s_3} = c_{\text{DA}, \hat{s}_3} \quad \text{if} \quad f(s_3) = f(\hat{s}_3) \quad \forall (s, \hat{s}) \in \mathbb{S}_3 \times \mathbb{S}_3,$$
 (1)

$$q_{\mathrm{DA}, s_3} = q_{\mathrm{DA}, \hat{s}_3}$$
 if $f(s_3) = f(\hat{s}_3)$ $\forall (s, \hat{s}) \in \mathbb{S}_3 \times \mathbb{S}_3$ (2)

Here, $f: \mathbb{S}_3 \to \mathbb{S}_2$ maps a node on the third stage of the decision tree, i.e., $s_3 \in \mathbb{S}_3$, to the respective node on the second stage, i.e., $s_2 \in \mathbb{S}_2$. In the following, we refer to $s \in \mathbb{S}$ instead of $s_3 \in \mathbb{S}_3$ for conciseness and we use s for indexing the scenarios, i.e., paths in the decision tree.

2.2. Objectives

We consider the total annualized cost (TAC) and the global warming impact (GWI) as economic and ecologic objective, respectively.

The TAC is defined as

$$TAC = CAPEX + OPEX_{el} + OPEX_{Grid},$$
 (3)

with $CAPEX = \sum_{i \in \{PV, W, B\}} \left(\frac{(\gamma_1 + 1)^{\gamma_{2,i}} \gamma_1}{(\gamma_1 + 1)^{\gamma_{2,i}} - 1} CAPEX_i^0 Q_i + \gamma_{3,i} Q_i \right),$ (4)

$$OPEX_{el} = 365 \sum_{s=0}^{\infty} \pi_s (4 \Delta t \ c_{DA,s} \cdot q_{DA,s} + \Delta t \ c_{ID,s} \cdot q_{ID,s}), \tag{5}$$

$$OPEX_{Grid} = 365 \sum_{s \in \mathbb{S}} \pi_s \sum_{t=1}^{T} OPEX_{Grid,s,t},$$
 (6)

$$OPEX_{Grid,s,t} \ge c_{Fee} \Delta t \left(q_{DA.s, \lfloor \frac{t-1}{2} \rfloor + 1} + q_{ID,s,t} \right), \tag{7}$$

$$OPEX_{Grid s.t} \ge 0. \tag{8}$$

In Eq. (3), we compute the TAC as the sum of investment cost, CAPEX, and operational cost, OPEX. According to current legislation in Germany (Status 2023), the grid fee has to be paid in addition to the market price for electricity removed from the electricity grid (Bundesministerium der Justiz der Bundesrepublik Deutschland, 2022). Thus, we consider both annual operational cost from electricity procurement, OPEX_{el} , as well as annual grid fee cost, OPEX_{Grid} . Eq. (4) specifies the investment cost of the local electricity generation and storage system considering photovoltaic (PV), wind power (W), and electric battery (B). Similar to Baumgärtner et al. (2019), we calculate the annualized CAPEX based on the total investment cost CAPEX, the present value factor with interest rate γ_1 and life time $\gamma_{2,i}$ (Broverman, 2010), a maintenance factor $\gamma_{3,i}$, and the installed capacity of the respective technology Q_i . Note that in contrast to Baumgärtner et al. (2019), we consider a component-specific life time $\gamma_{2,i}$. Eq. (5) defines the electricity cost OPEX_{al} by the purchases and sales on hourly DA and quarter-hourly ID electricity market $q_{\mathrm{DA,s}}$ and $q_{\mathrm{ID,s}}$, the DA and ID electricity price $c_{\mathrm{DA,s}}$ and $c_{\mathrm{ID,s}}$, the time step size $\Delta t = 0.25$ h, and the probability π_s of scenario s. In Eq. (6), the grid cost OPEX_{Grid} is derived from the sum of the grid cost $OPEX_{Grid,s,t}$ of each scenario s and time step t with a total of 96 time steps for the one-day scheduling horizon, i.e, T = 96. Eq. (7) and Eq. (8) constitute lower bounds for OPEX_{Grid.s.t}, which ensure that OPEX_{Grid.s.t} is equal to zero in case of electricity injection into the grid and greater or equal to the grid fee with the grid fee cost c_{Fee} in case of electricity removal from the grid. OPEX_{Grid.s.t} is equal to the respective lower limit, i.e., zero or the grid

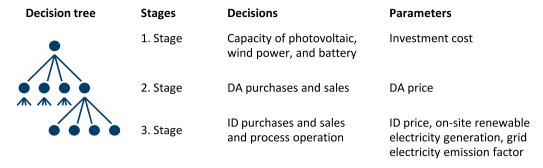


Fig. 1. Structure of the integrated design and scheduling problem: The problem structure allows optimizing the design of the local electricity generation and storage system while considering simultaneous DA and ID market participation and process DR. The decision tree models the chronological sequence of decisions. Each branch represents the realization of an uncertain parameter and each node represents a decision point.

fee, when minimizing the TAC. Note that in $OPEX_{Grid,s,t}$, $q_{ID,s,t}$ varies quarter-hourly and $q_{DA,s,t}$ varies hourly.

The expected annual GWI is computed as:

$$GWI = 365 \sum_{s \in \mathbb{S}} \pi_s \sum_{t=1}^{T} \left(GWI_{s,t}^{el} \Delta t \left(q_{DA,s, \lfloor \frac{t-1}{4} \rfloor + 1} + q_{ID,s,t} \right) \right)$$

$$+ \sum_{i \in \{PV,W,B\}} \frac{GWI^{i}Q_{i}}{\gamma_{2,i}}$$

$$(9)$$

Eq. (9) considers the quarter-hourly average GWI of the electricity from the grid GWI^{el}, the GWI of the installed PV, wind power, and battery capacity, i.e., GWIPV, GWIW, and GWIB, and their respective life time γ_{2i} in years. Consequently, the total annual GWI depends on hourly and quarter-hourly purchases and sales from the DA and ID market $q_{\mathrm{DA,s,t}}$ and $q_{\mathrm{ID,s,t}}$, respectively, and the installed PV, wind, and battery capacities, i.e., Q^{PV}, Q^W, and Q^B, respectively. Note that we allow for a GWI credit, i.e., negative GWI, in case of electricity sales accounting for an avoided emission burden (Horne et al., 2009).

2.3. Operational constraints

In the following, we shortly describe the generalized process model from our prior work (Schäfer et al., 2020; Germscheid et al., 2022) and discuss the operational constraints specific to the local energy system and the electricity trading.

The generalized process model (Schäfer et al., 2020) relies on few key parameters to describe the DR capabilities. In this work, we consider the key characteristics oversizing, minimal part load, product storage capacity with cyclic storage constraints, and ramping limitation. Note that without efficiency losses, the production rate of the process scales directly with the process power intake. For a detailed explanation of the generalized process model, including the model equations, we refer to Germscheid et al. (2022).

In the electricity generation and storage system, we consider the DA and ID purchases and sales $q_{DA.s.t}$ and $q_{ID.s.t}$, respectively, with positive values corresponding to purchases. In addition, we consider that the electricity purchases, PV power $q_{\text{PV},s,t}$, wind power $q_{\text{W},s,t}$, and battery charge and discharge $q_{\text{in},s,t}$ and $q_{\text{out},s,t}$ are equal to the power intake $p_{s,t}$ of the production process by the energy balance:

$$p_{s,t} = q_{\text{DA},s,\lfloor \frac{t-1}{t} \rfloor + 1} + q_{\text{ID},s,t} + q_{\text{PV},s,t} + q_{\text{W},s,t} - q_{\text{in},s,t} + q_{\text{out},s,t}$$
(10)

Additionally, we consider operational constraints similar to Baumgärtner et al. (2019):

$$q_{\text{PV},s,t} = \bar{q}_{\text{PV},s,t} \ Q_{\text{PV}},\tag{11}$$

$$q_{\mathbf{W},s,t} = \bar{q}_{\mathbf{W},s,t} \ Q_{\mathbf{W}},\tag{12}$$

$$0 \le q_{\text{in},s,t} \le Q_{\text{B}}/\tau,\tag{13}$$

$$0 \le q_{\text{out},s,t} \le Q_{\text{B}}/\tau,\tag{14}$$

$$0 \le SOC_{s,t} \le Q_{\mathsf{B}},\tag{15}$$

$$SOC_{s,t+1} = SOC_{s,t} + (\eta^{\text{in}}q_{\text{in},s,t} - \frac{q_{\text{out},s,t}}{n^{\text{out}}})\Delta t, \tag{16}$$

$$SOC_{s,1} = SOC_{s,T+1} \tag{17}$$

Here, Eq. (11) and Eq. (12) define the PV and wind power generation, $q_{\text{PV},s,t}$ and $q_{\text{W},s,t}$, by multiplying the relative power output, $\bar{q}_{\text{PV},s,t}$ and $\bar{q}_{W,s,t}$, with the installed PV and wind capacity, Q_{PV} and Q_{W} , respectively. Eq. (13) and Eq. (14) constrain the battery charge and discharge, i.e., $q_{\text{in},s,t}$ and $q_{\text{out},s,t}$, respectively, by the installed battery capacity Q_{B} and the allowed charging and discharging rate τ . Eq. (15) constrains the state of charge $SOC_{s,t}$ by the installed battery capacity $Q_{\rm B}$. Eq. (16) relates charging and discharging with respective efficiency losses $\eta^{\rm in}$ and η^{out} and the state of charge. Additionally, we consider the cyclic constraint, Eq. (17), requiring that the state of charge is the same at the beginning and at the end of the scheduling horizon.

We consider trading electricity on both DA and ID market while making use of the local energy system:

$$-q_{\text{PV},s,t} - q_{\text{W},s,t} - Q_{\text{B}}/\tau \le q_{\text{DA},s,|\frac{t-1}{\tau}|+1},\tag{18}$$

$$-q_{\text{PV},s,t} - q_{\text{W},s,t} - SOC_{s,t}/\Delta t \le q_{\text{DA},s} |_{t=1}^{t=1}|_{t=1},$$
 (19)

$$-q_{\mathrm{DA},s,|\frac{t-1}{t}|+1} - q_{\mathrm{PV},s,t} - q_{\mathrm{W},s,t} - Q_{\mathrm{B}}/\tau \le q_{\mathrm{ID},s,t},\tag{20}$$

$$-q_{\text{DA},s,\lfloor \frac{t-1}{t} \rfloor + 1} - q_{\text{PV},s,t} - q_{\text{W},s,t} - SOC_{s,t}/\Delta t \le q_{\text{ID},s,t}, \tag{21}$$

$$q_{\text{DA,s,}|\frac{t-1}{L}|+1} \le P_{\text{nom}}(1+\theta_{\text{max}}) + Q_{\text{B}}/\tau,$$
 (22)

$$q_{\text{DA},s,\lfloor\frac{t-1}{t}\rfloor+1} \le P_{\text{nom}}(1+\theta_{\text{max}}) + \frac{Q_{\text{B}} - SOC_{s,t}}{At},$$
 (23)

$$q_{\text{ID s},t} \le P_{\text{nom}}(1 + \theta_{\text{max}}) + Q_{\text{R}}/\tau, \tag{24}$$

$$q_{\text{ID},s,t} \le P_{\text{nom}}(1 + \theta_{\text{max}}) + Q_{\text{B}}/\tau,$$

$$q_{\text{ID},s,t} \le P_{\text{nom}}(1 + \theta_{\text{max}}) + \frac{Q_{\text{B}} - SOC_{s,t}}{\Delta t}$$

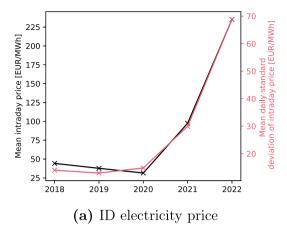
$$(24)$$

Here, Eqs. (18)-(21) constrain DA and ID sales by produced PV and wind power, the current state of charge, and maximum discharging capabilities of the installed battery. Similar to our prior work (Germscheid et al., 2022), Eqs. (20) and (21) allow selling previously purchased DA electricity on the ID market. Eqs. (22)-(25) constrain DA and ID purchases by the maximum power consumption of the production process and the battery. The maximum consumption of the process is defined by the nominal consumption P_{nom} and the process oversizing θ_{max} . The maximum consumption of the battery is given by the state of charge and the charging capabilities of the battery.

2.4. Time series

In the following, we specify the time series representing realizations of uncertain parameters in the assessment and refer to them as scenarios in this context.

We base our scenarios for the electricity price, wind power generation, PV power generation, and grid emission factor on historical



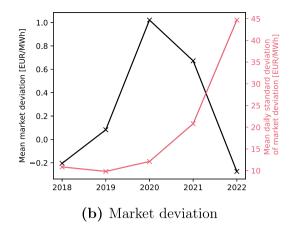


Fig. 2. Mean and mean daily standard deviation of ID electricity price (a) and market deviation (b), i.e., the price difference between the DA and the ID price.

time series. Specifically, for the electricity price, we use data from the German DA and ID spot market (Fraunhofer Institute for Solar Energy Systems ISE, 2023), assuming that the consumer can purchase and sell electricity at DA market-clearing price and ID index price. We refer to Germscheid et al. (2022) for a detailed explanation about these assumptions. Fig. 2 shows the annual mean and the annual mean daily standard deviation of the ID electricity market price and the market deviation, i.e., the difference between the DA and the ID price. The corresponding figure for the DA price shows similar characteristics as the one of the ID price and can be found in Section 1 of the supporting material. Fig. 2(a) reveals a price decrease in 2020 that can be attributed to the initial phase of the COVID-19 pandemic (Halbrügge et al., 2021) and an increase of mean and standard deviation in 2021 and 2022 due to the conflict in the Ukraine (Haucap and Meinhof, 2022). Fig. 2(b) reveals that in 2020 and 2021, the mean ID price was slightly larger than the mean DA price as indicated by the positive market deviation. Moreover, the standard deviation of the market deviation has significantly increased in 2021 and 2022.

DR scheduling optimization necessitates electricity price time series rather than an average annual electricity price. Long-term German electricity price forecasting is challenging, e.g., due to the conflict in Ukraine and the German energy transition. The time series for 2030 derived by the project MONA 2030 (Forschungsstelle für Energiewirtschaft e. V., 2017) used in Schäfer et al. (2020) and the prices for 2050 reported in Hecking et al. (2018) are outdated. For our assessment, we require a time series of both DA and ID prices for which, to the best of our knowledge, no forecasts exists. Therefore, we pragmatically consider the time series of the years 2020, 2021, and 2022 in our analysis, assuming that these represent scenarios for low, medium, and high future electricity prices.

To compute the corresponding historical wind and PV power time series, we use weather data for Aachen, Germany, from the German weather service (Deutscher Wetterdienst, 2023; Gutzmann and Motl, 2023). Specifically, we pre-process the measured wind speed, global radiation, and diffuse radiation similar to Bahl et al. (2017) and obtain the relative PV and wind power generation as discussed in detail in Section 2 of the supporting material. Section 1 of the supporting material shows the mean and the standard deviation of the historical wind speed and solar irradiance that stay within rather narrow ranges, with 2020 as a windier year and 2022 as a sunnier year.

Following Baumgärtner et al. (2019) and Nilges et al. (2023), we determine the average emission factor of electricity from the German grid for every time step, i.e., $GWI_{s,t}^{el}$ used in Eq. (9), by considering the momentary mix of power sources and their respective emission factors based on data of Bundesnetzagentur|smard.de (2023) and the ecoinvent database (Wernet et al., 2016), respectively.

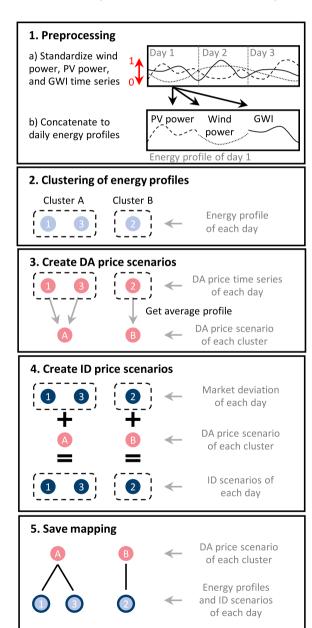


Fig. 3. Approach to determine scenarios based on historical time series data: The colored dots refer to the multi-dimensional data points that represent (concatenated) time series data.

Table 1

Degrees of freedom: The number of degrees of freedom depends on the number of clusters n_c , the number of quarter-hourly time steps T, and the number of scenarios $|\mathbb{S}|$, with T=96 and $|\mathbb{S}|=365$ in our case. The operational degrees of freedom concern the charging and discharging of the battery. Note that other optimization variables, e.g., power intake, PV power, and wind power, are not degrees of freedom, but can be determined from equality constraints.

	Degrees of freedom	Explanation
Design	3	Capacities of PV, wind power, and battery
DA market	$n_c \cdot T/4$	DA electricity purchases and sales
ID market	$ S \cdot T$	ID electricity purchases and sales
Operation	$2 \cdot S \cdot T$	Battery charging and discharging rate

Table 2
Parameters of the generalized process model: Process oversizing, minimal part load, and ramping limit are given related to the nominal power intake. The product storage capacity refers to the time necessary to fill an empty product storage considering production at nominal power intake.

Parameter	Reference values
Nominal power intake	2.74 MW
Process oversizing	20%
Minimal part load	50%
Product storage capacity	3 h
Ramping limit	25%/h

We determine the scenarios and the mapping between second and third stage of the optimization problem based on a clustering as depicted in Fig. 3. First, we preprocess the data by standardizing the wind and PV power time series and the GWI time series using the z-score (Mohamad and Usman, 2013) and concatenating the daily profiles of wind power, PV power, and GWI time series to daily energy profiles. Next, we apply k-means clustering using the scikit-learn module in Python (Pedregosa et al., 2011) treating each daily energy profile as a multi-dimensional data point. This leads to a clustering of similar energy profiles. We transfer the obtained clustering to the DA price and market deviation time series and create an average DA profile as DA price scenario for each cluster. We add the market deviations from all constituents of a respective cluster to the average DA price scenario to obtain ID price scenarios. Note that using the market deviation allows accounting for the inter-market correlation similar to our prior work (Germscheid et al., 2022). Finally, we use the mapping resulting from the clustering to connect the second and third stage of the optimization problem. Note that on the second stage, the probability of the DA realizations depends on the cluster size. In contrast, the realizations on the third stage are equi-probable, i.e., $\pi_s = 1/|S|$, as the clustering is used on the third stage to establish the mapping but not for data reduction. We show in Section 3 of the supporting material that the within-cluster sum-of-squares does not allow deriving an obvious decision on a suitable number of clusters for the given data. For our application, we look for a compromise between the number of clusters and number of scenarios per cluster. Pragmatically, we consider 20 clusters, which leads to roughly 18 scenarios per cluster on average. We will discuss the impact of clustering on the results in Section 3.3.

2.5. Model specifications and evaluation

Table 1 specifies the degrees of freedom of the integrated design and scheduling problem.

Table 2 lists reference parameters of the generalized process that we also used in our prior work (Germscheid et al., 2022). Note that the reference parameters are similar to the chlor-alkali electrolysis (Germscheid et al., 2022) with the exception of stricter ramping limitations of the considered reference process. This stricter limitation allows analyzing the impact of ramping restrictions on the potential savings of the integrated design and scheduling in the parameter study in Section 3.2.

Table 3
Component-specific life time, investment and maintenance cost for Germany based on Hecking et al. (2018).

	Lifetime $\gamma_{2,i}$	$CAPEX_i^0$	Annual maintenance cost $\gamma_{2,i}$
Roof-top PV	25 a	927 EUR/kWp	17 EUR/kWp
Onshore wind	25 a	1113 EUR/kWp	13 EUR/kWp
Battery	15 a	550 EUR/kWh	20 EUR/kWh

We consider the parameters given in Table 3 for the CAPEX. Similar to Sass et al. (2020), we consider an interest rate $\gamma_1 = 8\%$. In Section 4 of the supporting material, we list the resulting annual PV and wind electricity generation cost, showing that wind power has lower production cost than PV due to a higher average utilization rate. For the GWI of the electricity generation and storage system, we use data of the ecoinvent database 3.9.1 (Wernet et al., 2016) that we specify in Section 4 of the supporting material for reproducibility. For the battery, we consider a charging and discharging rate of 4 h (Tesla, 2023), i.e., $\tau = 4$ h, and a round-trip efficiency of 90% (Hecking et al., 2018), i.e., $\sqrt{\eta_{in}}$ = $\sqrt{\eta_{\text{out}}} = \sqrt{0.9}$. Moreover, we consider the average grid fee cost of 2022 for industrial consumers in Germany, i.e., $c_{\rm Fee} = 29.6$ EUR/MWh (Bundesnetzagentur und Bundeskartellamt, 2022). Furthermore, we choose the nominal capacity of the power-intensive production process such that the process is classified as an industrial consumer, i.e., 24 GWh per year (Bundesnetzagentur und Bundeskartellamt, 2022), which allows the process operator to benefit from lower grid fees compared to non-industrial consumers (Bundesnetzagentur und Bundeskartellamt, 2022).

We expect the maximum allowed capacities of the energy system to have an impact on the optimization results. Pragmatically, we first restrict the admissible capacities for wind power and PV by the nominal power intake, i.e., $Q_{\rm W}^{\rm max}=Q_{\rm PV}^{\rm max}=P_{\rm nom}$. We choose the admissible battery size such that the maximum discharge rate corresponds to the nominal power intake of the production process, i.e., $P_{\rm nom}=Q_{\rm B}^{\rm max}/\tau$. In Section 3.2, we then analyze the impact of the maximum allowed energy system capacities on the TAC in detail.

We implement the model in Pyomo (Hart et al., 2011) and use the solver Gurobi 9.5.0 (Gurobi Optimization, LLC, 2020) with default settings on an Intel Core i7-9700 processor and 32 GB RAM. We formulate the multi-stage problem by means of its deterministic equivalent.

3. Results

In the following, we analyze the synergies between the local energy system and the flexible production process and the benefit of considering simultaneous market participation at design stage. To this end, we first consider market participation only in the ID market and discuss the optimal design and savings of the local energy system (Section 3.1) as well as the impact of the process flexibility on the potential savings (Section 3.2). Note that we select the ID market instead of the DA market, as the ID market allows adapting the electricity procurement in response to realization of the uncertainty in the renewable electricity supply. We then show the difference between single and simultaneous market participation and discuss the energy system design in the context of DR scheduling with simultaneous DA and ID market participation (Section 3.3).

3.1. Design and operation for single market participation

In the following, we evaluate the energy system design considering only the ID market for the reference process defined in Table 2.

Fig. 4 shows Pareto-optimal energy system designs based on the time series for 2020, 2021, and 2022. In three cases, the ecologic and economic objectives lead to competing solutions. Interestingly, the TAC-optimal solutions do not contain a battery, as potential savings from operating the battery do not outweigh the battery investment

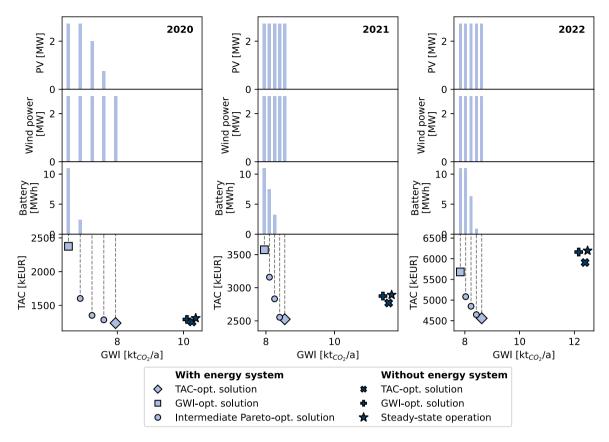


Fig. 4. Energy system design for ID market-only participation: Pareto-optimal solutions are given for 2020 (left), 2021 (center), and 2022 (right). For each year, the TAC-optimal, the GWI-optimal, and three intermediate Pareto-optimal solutions are shown, which are equi-distant with respect to GWI. GWI and TAC (lower part) are given with vertical gray dashed lines pointing to the respective optimal capacities of the local electricity supply system (upper three parts). Additionally, the TAC- and GWI-optimal DR as well as the steady-state operation without a local energy system are given for comparison.

cost. High electricity prices in 2021 and 2022 incentivize both onsite wind and PV electricity generation in the TAC-optimal solutions, whereas only wind electricity generation is used in 2020. The preference for wind can be explained by the higher average utilization rate (see Section 4 of the supporting material). In contrast, battery, PV, and wind generation capacities are built at maximum capacity for all GWI-optimal solutions, irrespective of the year studied. However, integrating a battery leads to a large increase in TAC with only a small improvement in GWI, as can be seen from the shape of the Pareto front.

Fig. 4 reveals that for 2022, the two designs with the lowest GWI have identical PV, wind power, and battery capacities but have notable differences in TAC and GWI, indicating different operating strategies. Fig. 5 shows the operation for an exemplary day given a fixed energy system design and confirms these findings. In particular, the electricity price and grid emission factor (Fig. 5(a)) set different incentives for TAC-optimal and GWI-optimal operation of the process (Fig. 5(c)) and the battery (Fig. 5(d)). Note that an alignment of electricity price and grid emission factor could be achieved by increasing renewable energy penetration in the grid as well as a sufficiently high CO2 price (Nilges et al., 2024). In case of a high renewable energy penetration in the grid, the benefit of on-site renewable generation would decrease. However, on-site generation would still be advantageous as it partially avoids grid fee cost and electricity losses due to long-distance transmission, reduces the need to expand the electricity grid, and helps avoiding the emissions and costs associated to grid expansion.

Fig. 5(c) additionally shows the process operation without a local energy system, revealing a similar DR schedule as for a process with a local system. Similarly, Fig. 5(d) shows the battery operation with and without local renewable electricity generation revealing a similar operating pattern with only minor differences. We attribute this behavior to

the time-varying incentives for DR at the operational level, i.e., the electricity price and the grid emission factor. The incentives predominantly influence the operation of the process and the local energy system, while on-site generated electricity has a minor influence.

Fig. 4 suggests that the difference between steady-state operation and DR without local energy system remains rather similar. In contrast, the difference between DR without energy system and DR with a local energy system increases each year in particular with respect to the TAC. Table 4 compares ecologic and economic savings, i.e., savings with respect to the GWI and cost, respectively, resulting from DR and the local energy system and confirms these findings. The absolute economic savings from DR in comparison to steady-state operation increase due to the increasing standard deviation of the electricity price (Fig. 2(a)). The relative and absolute economic savings resulting from the energy system increase due to the increasing grid electricity cost. In particular, the savings increase significantly from 1.4% in 2020 to 22.8% in 2022. Looking at the GWI-optimal solution, the ecologic savings resulting from the energy system are much larger than the savings from DR in comparison to steady-state operation. Furthermore, the ecologic savings are somewhat similar in all years, i.e., between 30.3% and 35.6%, and the variance can be attributed to the natural variability of PV and wind power production and the varying grid emission factor.

3.2. Parameter study of process flexibility and energy system capacity

In the following, we analyze the impact of process flexibility and admissible energy system capacities on TAC and GWI.

For a parameter study on the process flexibility, we fix all process parameters to their respective reference values as defined in Table 2 and vary one process parameter at a time between the value corresponding to an inflexible process and the value corresponding to twice

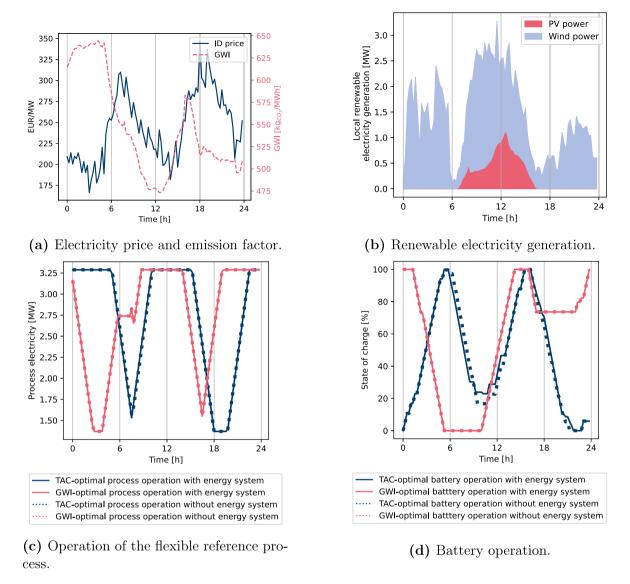


Fig. 5. Process and energy system operation for an exemplary day in 2022 (ID-only market participation): An energy system design with maximum admissible PV, wind power, and battery capacities is considered. The operation is shown for the ID electricity price and emission factor (a) and the renewable electricity generation (b). The process operation determines the electricity consumption (c). The battery operation determines the state of charge (d).

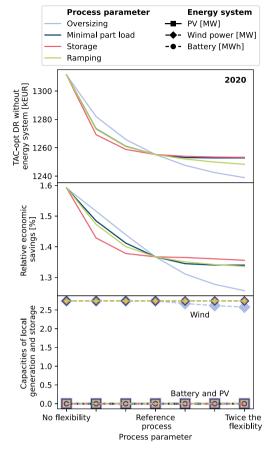
the flexibility of the process parameter. Fig. 6 shows the impact of varying degrees of process flexibility on the TAC-optimal DR without a local energy system, the economic savings enabled by a local energy system, and the optimal capacities of the local electricity generation and storage. Fig. 6(a) (top) shows exemplary for 2020 that without a local energy system, the flexible process particularly benefits from oversizing. Behaviors for 2021 and 2022 are similar and thus the corresponding figures are omitted. The results confirm the findings of our prior work (Germscheid et al., 2022), where we considered price data of 2019. Furthermore, Fig. 6(a) (bottom) shows the optimal capacities of the energy system components and reveals that the optimal wind capacity for 2020 slightly decreases with a high degree of process oversizing. Thus, process flexibility can impact the optimal energy system capacity. Corresponding figures for 2021 and 2022 are omitted, as no impact of the process flexibility on the resulting optimal designs can be found.

Fig. 6 reveals that the range of the economic savings due to a local energy system for any given year is rather narrow, i.e., varying the process flexibility does not impact the relative savings in a strong manner. Even though the range is small, varying the process oversizing has the largest leverage on the savings in comparison to the other

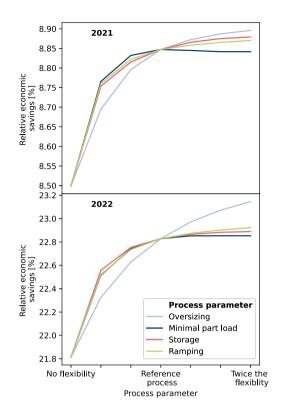
process parameters. Interestingly, the impact of the process parameters may differ depending on the investigated year, as higher process flexibility actually leads to lower relative savings in 2020 (Fig. 6(a), center) whereas higher relative savings are recorded for 2021 and 2022 (Fig. 6(b)). However, an analysis of the cost contributions shows exemplary for varying oversizing that the absolute TAC monotonously decreases, irrespective of the case with or without a local energy system (see Section 5 of the supporting material).

Fig. 7 shows the optimal TAC for varying admissible energy system size and process oversizing, the latter having the largest flexibility leverage for the economic savings. Specifically, we vary the maximum allowed energy system capacities, i.e., $Q_{\rm W}^{\rm max}$, $Q_{\rm PV}^{\rm max}$, and $Q_{\rm B}^{\rm max}$, by a joint scaling factor. Corresponding optimal capacities of the energy system can be found in Section 5 of the supporting material. For 2020, process oversizing has a larger leverage on the TAC than local electricity generation and storage. Furthermore, the TAC remains constant for scaling factors larger than one, as a cost-optimal maximum of the wind power capacity is attained (see Section 5 of the supporting material). For 2021 and 2022, it can be seen that local electricity generation and storage is more economically attractive than process flexibility.

Interestingly, the absolute savings of the TAC-optimal solution enabled by a higher process flexibility and by a larger energy system



(a) TAC-optimal solutions for 2020.



(b) Relative economic savings due to a local energy system for 2021 and 2022

Fig. 6. Economic impact of different degrees of process flexibility: The TAC-optimal cost of DR without energy system (a, top), the savings due to a local energy system (a, center), and optimal energy system design (a, bottom) for 2020 are shown. Furthermore, the savings due to a local energy system are shown for 2021 (b, top) and 2022 (b, bottom).

Table 4Economic and ecologic savings due to DR and local electricity generation and storage. The savings are compared for the TAC-optimal solutions (upper part) and the GWI-optimal solutions (lower part). Single market participation in the ID market is considered.

2022				
4.6%				
288				
DR with energy system vs. DR without energy system				
22.8%				
1349				
2.6%				
0.3				
DR with energy system vs. DR without energy system				
6 35.6%				
4.3				

behave roughly additively, which is shown exemplary for 2022 in Fig. 7. Section 5 of the supporting material shows the relative difference between the optimal TAC and the estimated TAC, the latter being defined as the sum of the absolute savings from process flexiblization and installation of a local energy system. The difference being rather small, i.e., less than 0.5%, means that a quick first approximate economic

assessment can be performed by considering the savings from DR and the cost savings from a local energy system independently.

Fig. 8 shows the impact of varying degrees of process flexibility on the GWI-optimal solution exemplary for 2020. Figures for the other years show similar behavior and are therefore omitted. Fig. 8(a) shows the case of DR without a local energy system and reveals that the process oversizing and the product storage capacity have the largest impact on the GWI. This finding is consistent with the results of our prior work Schäfer et al. (2020), where we considered the residual load as ecologic objective instead of the GWI. Fig. 8(b) shows that process oversizing and product storage capacity have the largest leverage on the ecologic savings. Note that, in general, the degree of process flexibility has a rather low impact on the range of the ecologic savings.

3.3. Simultaneous market participation

Finally, we evaluate the benefit of considering simultaneous DA and ID market participation in the integrated design and scheduling problem. Table 5 compares the average wall-clock run times of the single and the simultaneous market participation. As expected, the single market participation is slightly faster than the simultaneous participation that additionally contains the DA trading decisions.

Table 6 lists the TAC-optimal designs for the reference process. Designs for 2020 and 2021 do not reveal differences to the case of ID-only market participation, i.e., the price differences between the markets in these years are not large enough to incentivize the installation of a battery. In contrast, a battery is built for the simultaneous market participation in 2022 as the battery offers trading capacity

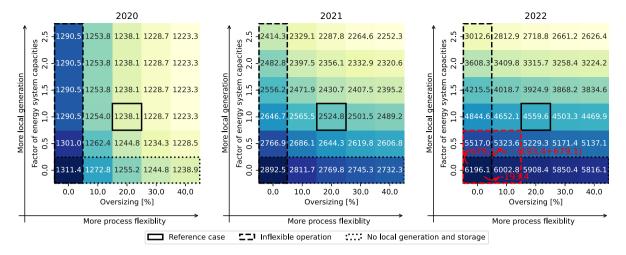
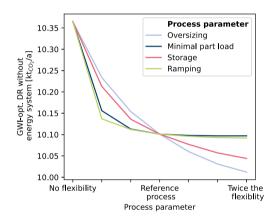
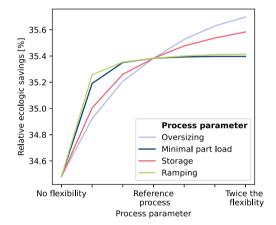


Fig. 7. Optimal TAC [EUR] with varying process oversizing and maximum admissible energy system capacity for 2020 (left), 2021 (center), and 2022 (right): For 2022, the approximately additive behavior of the absolute savings is shown exemplary in red.







(b) Relative ecologic savings due to a local energy system

Fig. 8. Ecologic impact of varying process flexibility for 2020: GWI-optimal DR without a local energy system (a) and relative savings due to installation of a local system (b) are shown.

Table 5

Run time comparison of single and simultaneous market participation: The stated wall-clock times of the integrated design and scheduling problem are the averages over 15 Pareto-optimal solutions (5 Pareto-optimal solutions per year). The solver Gurobi 9.5.0 (Gurobi Optimization, LLC, 2020) was used and the machine was equipped with an Intel Core i7-9700 processor and 32 GB RAM.

	Run time
Single market participation	21.8 s
Simultaneous market participation	29.6 s

for exploitation of large price differences between the DA and ID market. The Pareto-optimal energy system designs of 2022 vary with respect to the battery capacity for the simultaneous DA and ID market participation compared to the ID-only case and are shown in Section 6 of the supporting material.

Table 6 compares single and simultaneous market participation with respect to the electricity purchases and sales. It shows that for ID-only participation more electricity is purchased in 2020, compared to 2021 and 2022, which are years with larger optimal PV and wind power capacities. For the simultaneous participation in 2020, the majority of the electricity is purchased on the DA market due to the positive price difference (Fig. 2(b)). The combination of PV and wind enables higher DA sales in 2021. Moreover, total purchases and sales significantly

increase for the simultaneous participation in 2022 due to an increased trading capacity enabled by the battery.

Table 7 shows that the relative savings of simultaneous market participation compared to single market participation stay within a similar range, irrespective of the considered year. In contrast, the absolute savings increase each year due to the increased variance of the market deviation (Fig. 2(b)). Table 7 reveals that both the absolute and relative savings of simultaneous market participation increase with both process flexibilization and the integration of local electricity generation and storage.

Table 8 shows the contributions of cost savings for the year 2022 considering TAC-optimal simultaneous market participation. Here, an inflexible process without an energy system is modified by separately adding a battery, renewable electricity generation, and process flexiblization. Table 8 reveals that the main cost savings result from the on-site electricity generation followed by process flexiblization. The integration of a battery accounts only for a small fraction of the savings. Note that similar to ID-only participation (Section 3.2), summing up the absolute savings from battery installation, renewable electricity generation, and flexiblization, separately, allows for a good overall savings estimate.

Similar to Section 3.2, we vary the degree of process flexibility. Fig. 9 shows the impact of process flexibility on the optimal battery

Table 6

System capacities and electricity trading amounts for ID-only participation (upper part) and simultaneous DA and ID market participation (lower part): In all cases, TAC-optimal DR of the reference process (Table 2) with a local energy system is considered. The stated values of the ID-only participation correspond to the TAC-optimal solution from Fig. 4.

0			
	2020	2021	2022
ID-only participation	I		
PV capacity	-	2.74 MW	2.74 MW
Wind capacity	2.74 MW	2.74 MW	2.74 MW
Battery capacity	-	-	-
Total purchases	17,316 MWh	16,008 MWh	14,776 MWh
Total sales	62 MWh	203 MWh	357 MWh
Simultaneous market	t participation		
PV capacity	_	2.74 MW	2.74 MW
Wind capacity	2.74 MW	2.74 MW	2.74 MW
Battery capacity	-	-	5.31 MWh
DA purchases	18,582 MWh	16,389 MWh	18,874 MWh
ID purchases	6796 MWh	7442 MWh	12,944 MWh
Total purchases	25,378 MWh	23,831 MWh	31,818 MWh
DA sales	452 MWh	954 MWh	5947 MWh
ID sales	7678 MWh	7080 MWh	11,083 MWh
Total sales	8130 MWh	8034 MWh	17,030 MWh

Table 7

The TAC savings from simultaneous market participation compared to single market participation for an inflexible process without an energy system (top), a flexible process without an energy system (center), and a flexible process with an energy system

(bottom). The flexible process is the reference process (Table 2).

	2020	2021	2022	
Inflexible process without energy system				
Relative savings Absolute savings	3.0% 39.3 kEUR	2.0% 57.4 kEUR	2.0% 122.7 kEUR	
Flexible process without energy system				
Relative savings Absolute savings	3.8% 47.1 kEUR	2.5% 68.9 kEUR	2.5% 147.2 kEUR	
Flexible process with energy system				
Relative savings Absolute savings	3.9% 47.9 kEUR	2.9% 72.8 kEUR	4.4% 198.7 kEUR	

Table 8
Savings contributions of simultaneous market participation in the TAC-optimal case for 2022: The savings are related to the inflexible process without an energy system (first row). The battery capacity of the inflexible process with the battery (third row) is identical to the flexible process with an energy system (second row).

	TAC	Savings
Inflexible process without energy system	6073.5 kEUR	_
Flexible process with energy system	4360.9 kEUR	1712.6 kEUR
Inflexible process with battery	6044.7 kEUR	28.8 kEUR
Inflexible process with wind and PV power	4702.5 kEUR	1371.0 kEUR
Flexible process without energy system	5761.2 kEUR	312.3 kEUR

capacity for 2022. An analysis of the optimal capacities of PV and wind power is omitted as these quantities do not vary in response to a varying degree of process flexibility. It can be noted that larger batteries are built for less flexible processes, in particular for processes with part load and ramping restrictions. DR without energy system and economic savings of DR with an energy system behave similarly to the case of single market participation (Section 3.2), irrespective of the investigated year. Thus, respective figures are omitted.

Recall that we pragmatically consider 20 clusters for the assessment. In Section 6 of the supporting material, we show the results for 10 and 30 clusters. More clusters lead to higher savings enabled by the simultaneous market participation and a larger optimal battery capacity in 2022. In the supporting material, we show that the average standard deviation of the market deviation decreases with increasing number

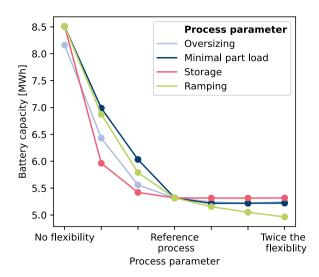


Fig. 9. TAC-optimal battery capacity for simultaneous market participation for 2022 with varying degree of process flexibility.

of clusters, which enables better positioning on the two markets in case of the simultaneous participation and, thus, increases savings and incentivizes a larger battery.

4. Conclusion

We assessed the optimal design of a local electricity generation and storage system for a generalized continuous, power-intensive production process that is capable of performing demand response and can act on both the day-ahead and intraday electricity market. In a three-stage stochastic problem, we optimized the capacities of photovoltaic power, wind power, and electric battery with an integrated demand response scheduling of the production process. Building on our prior work (Schäfer et al., 2020; Germscheid et al., 2022), we used a generalized process model with few flexibility-defining parameters, i.e., process oversizing, minimal part load, product storage, and ramping limitation. In a bi-objective optimization, we considered both economic and ecological objectives. We considered scenarios of low, intermediate, and high electricity prices for a plant location in Germany as well as a time-varying grid emission factor.

We find that batteries are mainly built to lower the global warming impact, however, leading to a significant increase in total annualized cost. Economically and ecologically-optimal operation of the process and battery primarily respond to the time-varying electricity price and grid emission factor, but only to a little extent to the on-site generation of renewable electricity. Varying the degree of process flexibility, we find a rather small impact on the achievable relative economic and ecologic savings that come with local electricity generation and storage. Moreover, we show that the absolute cost savings from flexibilizing the process and installing a local energy system are approximately additive. Comparing intraday-only and simultaneous day-ahead and intraday market participation, we find that the energy system designs are similar for the investigated scenarios, except when high price differences between the markets incentivize the installation of a battery. The costoptimal battery capacity significantly depends on the available process flexibility, enables large volumes for trading on the markets, but comes with only minor economic savings.

In our assessment, we pragmatically considered time series based on historic data of three years to understand the effects of low, medium, and high electricity prices. To account for long-term variability of prices and the long lifetime of both the process and the energy system equipment, our approach should be extended to consider multiple years by incorporating long-term time series forecasting, e.g., based on the

hourly day-ahead price forecasting of Ziel and Steinert (2018) and Gabrielli et al. (2022) that would need to be extended to also consider quarter-hourly intraday prices. Uncertainties associated to the forecasts and financial risks must be particularly accounted for, e.g., in a risk-averse optimization similar to Xuan et al. (2021) and Vieira et al. (2021). In order to use our approach to evaluate the potential of a local system for a specific process and location, the process characteristics must be known and respective local weather data is required.

CRediT authorship contribution statement

Sonja H.M. Germscheid: Writing – original draft, Visualization, Software, Methodology, Investigation, Data curation, Conceptualization. Benedikt Nilges: Writing – review & editing, Data curation. Niklas von der Assen: Writing – review & editing, Funding acquisition. Alexander Mitsos: Writing – review & editing, Supervision, Funding acquisition. Manuel Dahmen: Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization.

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

Data sharing not applicable to this article.

Acknowledgments

SG gratefully acknowledges the financial support of the Helmholtz Association of German Research Centers through program-oriented funding (POF) and the grant *Uncertainty Quantification – From Data to Reliable Knowledge (UQ)* (grant number: ZT-I-0029). AM and MD acknowledge funding from the Helmholtz Association of German Research Centers through program-oriented funding (POF). BN gratefully acknowledges the financial support of the Kopernikus project SynErgie (grant number 03SFK3L1-2) by the Federal Ministry of Education and Research (BMBF), Germany. This work was performed as part of the *Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE)*. We kindly thank Yifan Wang (RWTH Aachen University, Institute of Technical Thermodynamics) for providing the wind turbine performance curve developed by Bahl et al. (2017) which was used for pre-processing of the wind data.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.compchemeng.2024.108656.

References

- Allman, A., Daoutidis, P., 2018. Optimal scheduling for wind-powered ammonia generation: Effects of key design parameters. Chem. Eng. Res. Des. 131, 5–15.
- Bahl, B., Kümpel, A., Seele, H., Lampe, M., Bardow, A., 2017. Time-series aggregation for synthesis problems by bounding error in the objective function. Energy 135, 900–912.
- Bahl, B., Söhler, T., Hennen, M., Bardow, A., 2018. Typical periods for two-stage synthesis by time-series aggregation with bounded error in objective function. Front. Energy Res. 5 (January), 1–13.
- Baumgärtner, N., Delorme, R., Hennen, M., Bardow, A., 2019. Design of low-carbon utility systems: Exploiting time-dependent grid emissions for climate-friendly demand-side management. Appl. Energy 247 (April), 755–765.
- Birge, J.R., Louveaux, F., 2011. Introduction to stochastic programming. In: Analysis. In: Springer Series in Operations Research and Financial Engineering, Springer New York, New York, NY, p. 524.
- Brée, L.C., Perrey, K., Bulan, A., Mitsos, A., 2019. Demand side management and operational mode switching in chlorine production. AIChE J. 65 (7), 1–14.

- Broverman, S., 2010. Mathematics of Investment and Credit, fifth ed. ACTEX Publications. Inc..
- Bundesministerium der Justiz der Bundesrepublik Deutschland, 2022. Stromnetzentgeltverordnung vom 25. Juli 2005 (BGBl. I S. 2225), die zuletzt durch artikel 6 des gesetzes vom 20. Juli 2022 (BGBl. I S. 1237) geändert worden ist. https://www.gesetze-im-internet.de/stromnev/BJNR222500005b.html# BJNR222500005BJNG000500000 (accessed 12-09-2023).
- Bundesnetzagentur und Bundeskartellamt, 2022. Monitoringbericht 2022. https://www.bundesnetzagentur.de/DE/Fachthemen/ElektrizitaetundGas/Monitoringberichte/start.html (accessed 24-04-2023).
- Bundesnetzagentur|smard.de, 2023. SMARD strommarktdaten. https://www.smard.de/home (accessed 2023-10-10).
- Burre, J., Bongartz, D., Brée, L., Roh, K., Mitsos, A., 2020. Power-to-X: Between electricity storage, e-production, and demand side management. Chem. Ing. Tech. 92 (1–2), 74–84.
- Dalle Ave, G., Harjunkoski, I., Engell, S., 2019. A non-uniform grid approach for scheduling considering electricity load tracking and future load prediction. Comput. Chem. Eng. 129, 106506.
- Daryanian, B., Bohn, R.E., Tabors, R.D., 1989. Optimal demand-side response to electricity spot prices for storage-type customers. IEEE Trans. Power Syst. 4 (3), 897–903.
- Deutscher Wetterdienst, 2023. Open data. https://opendata.dwd.de/ (accessed 19-04-2023).
- Fleschutz, M., Bohlayer, M., Braun, M., Murphy, M.D., 2023. From prosumer to flexumer: Case study on the value of flexibility in decarbonizing the multi-energy system of a manufacturing company. Appl. Energy 347 (January), 121430.
- Forschungsstelle für Energiewirtschaft e. V., 2017. Merit Order Netz-Ausbau 2030 (MONA 2030). https://www.ffe.de/projekte/mona/ (accessed 2024-02-24).
- Fraunhofer Institute for Solar Energy Systems ISE, 2023. Energy charts. https://www.energy-charts.info (accessed 2023-08-06).
- Gabrielli, P., Wüthrich, M., Blume, S., Sansavini, G., 2022. Data-driven modeling for long-term electricity price forecasting. Energy 244, 123107.
- Germscheid, S.H.M., Mitsos, A., Dahmen, M., 2022. Demand response potential of industrial processes considering uncertain short-term electricity prices. AIChE J. 68 (11), e17828.
- Germscheid, S.H., Röben, F.T., Sun, H., Bardow, A., Mitsos, A., Dahmen, M., 2023.Demand response scheduling of copper production under short-term electricity price uncertainty. Comput. Chem. Eng. 178, 108394.
- Ghobeity, A., Mitsos, A., 2010. Optimal time-dependent operation of seawater reverse osmosis. Desalination 263, 76–88.
- Golmohamadi, H., Keypour, R., 2018. Stochastic optimization for retailers with distributed wind generation considering demand response. J. Mod. Power Syst. Clean Energy 6 (4), 733–748.
- Gurobi Optimization, LLC, 2020. Gurobi optimizer reference manual. http://www.gurobi.com (accessed 01-06-2021).
- Gutzmann, B., Motl, A., 2023. Wetterdienst. http://dx.doi.org/10.5281/zenodo. 7839066.
- Halbrügge, S., Schott, P., Weibelzahl, M., Buhl, H.U., Fridgen, G., Schöpf, M., 2021. How did the german and other European electricity systems react to the COVID-19 pandemic? Appl. Energy 285 (November 2020), 116370.
- Hart, W.E., Watson, J.-P., Woodruff, D.L., 2011. Pyomo: modeling and solving mathematical programs in python. Math. Program. Comput. 3 (3), 219–260.
- Haucap, J., Meinhof, J., 2022. Die strompreise der zukunft. Wirtschaftsdienst 102 (S1), 53–60.
- Hecking, H., Kruse, J., Hennes, O., Wildgrube, T., Lencz, D., Hintermayer, M., Gierkink, M., Lorenczik, J.P.D.S., 2018. Dena-leitstudie integrierte energiewende. https://shop.dena.de/fileadmin/denashop/media/Downloads_Dateien/esd/9262_dena-Leitstudie_Integrierte_Energiewende_Ergebnisbericht.pdf (accessed 19-04-2023).
- Horne, R.E., Grant, T., Verghese, K., 2009. Life Cycle Assessment: Principles, Practice and Prospects. Csiro Publishing, Collingwood, Australia.
- Ierapetritou, M.G., Wu, D., Vin, J., Sweeney, P., Chigirinskiy, M., 2002. Cost minimization in an energy-intensive plant using mathematical programming approaches. Ind. Eng. Chem. Res. 41 (21), 5262–5277.
- Kwon, S., Ntaimo, L., Gautam, N., 2017. Optimal day-ahead power procurement with renewable energy and demand response. IEEE Trans. Power Syst. 32 (5), 3924–3933.
- Langiu, M., Dahmen, M., Mitsos, A., 2022. Simultaneous optimization of design and operation of an air-cooled geothermal ORC under consideration of multiple operating points. Comput. Chem. Eng. 161, 107745.
- Leenders, L., Bahl, B., Lampe, M., Hennen, M., Bardow, A., 2019. Optimal design of integrated batch production and utility systems. Comput. Chem. Eng. 128, 496–511.
- Leo, E., Dalle Ave, G., Harjunkoski, I., Engell, S., 2021. Stochastic short-term integrated electricity procurement and production scheduling for a large consumer. Comput. Chem. Eng. 145, 107191.
- Liu, G., Xu, Y., Tomsovic, K., 2016. Bidding strategy for microgrid in day-ahead market based on hybrid stochastic/robust optimization. IEEE Trans. Smart Grid 7 (1), 227–237.
- Martín, M., 2016. Methodology for solar and wind energy chemical storage facilities design under uncertainty: Methanol production from CO2 and hydrogen. Comput. Chem. Eng. 92, 43–54.

- Mitra, S., Pinto, J.M., Grossmann, I.E., 2014. Optimal multi-scale capacity planning for power-intensive continuous processes under time-sensitive electricity prices and demand uncertainty. part I: Modeling. Comput. Chem. Eng. 65, 89–101.
- Mitsos, A., Asprion, N., Floudas, C.A., Bortz, M., Baldea, M., Bonvin, D., Caspari, A., Schäfer, P., 2018. Challenges in process optimization for new feedstocks and energy sources. Comput. Chem. Eng. 113, 209–221.
- Mohamad, I.B., Usman, D., 2013. Standardization and its effects on k-means clustering algorithm. Res. J. Appl. Sci. Eng. Technol. 6 (17), 3299–3303.
- Mucci, S., Mitsos, A., Bongartz, D., 2023. Cost-optimal power-to-methanol: Flexible operation or intermediate storage? J. Energy Storage 72, 108614.
- Nilges, B., Burghardt, C., Roh, K., Reinert, C., von der Aßen, N., 2023. Comparative life cycle assessment of industrial demand-side management via operational optimization. Comput. Chem. Eng. 177 (March), 108323.
- Nilges, B., Reinert, C., von der Assen, N., 2024. Is demand-side management environmentally beneficial? Analyzing the greenhouse gas emissions due to load shifting in electric power systems. J. Clean. Prod. 434, 140062.
- Nolzen, N., Ganter, A., Baumgärtner, N., Leenders, L., Bardow, A., 2022. Where to market flexibility? Optimal participation of industrial energy systems in balancing-power, day-ahead, and continuous intraday electricity markets. arXiv: 2212.12507.
- Pandžić, H., Morales, J.M., Conejo, A.J., Kuzle, I., 2013. Offering model for a virtual power plant based on stochastic programming. Appl. Energy 105, 282–292.
- Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., Duchesnay, E., 2011. Scikit-learn: Machine learning in python. J. Mach. Learn. Res. 12, 2825–2830.
- Sass, S., Faulwasser, T., Hollermann, D.E., Kappatou, C.D., Sauer, D., Schütz, T., Shu, D.Y., Bardow, A., Gröll, L., Hagenmeyer, V., Müller, D., Mitsos, A., 2020. Model compendium, data, and optimization benchmarks for sector-coupled energy systems. Comput. Chem. Eng. 135, 106760.
- Schäfer, P., Daun, T.M., Mitsos, A., 2020. Do investments in flexibility enhance sustainability? A simulative study considering the german electricity sector. AIChE J. 66 (11), 1–14.
- Schäfer, P., Westerholt, H.G., Schweidtmann, A.M., Ilieva, S., Mitsos, A., 2019. Model-based bidding strategies on the primary balancing market for energy-intense processes. Comput. Chem. Eng. 120, 4–14.

- Seo, K., Retnanto, A.P., Martorell, J.L., Edgar, T.F., Stadtherr, M.A., Baldea, M., 2023. Simultaneous design and operational optimization for flexible carbon capture process using ionic liquids. Comput. Chem. Eng. 178, 108344.
- Simkoff, J.M., Baldea, M., 2020. Stochastic scheduling and control using datadriven nonlinear dynamic models: Application to demand response operation of a chlor-alkali plant. Ind. Eng. Chem. Res. 59 (21), 10031–10042.
- Steimel, J., Engell, S., 2015. Conceptual design and optimization of chemical processes under uncertainty by two-stage programming. Comput. Chem. Eng. 81, 200–217.
- Teichgraeber, H., Brandt, A.R., 2020. Optimal design of an electricity-intensive industrial facility subject to electricity price uncertainty: Stochastic optimization and scenario reduction. Chem. Eng. Res. Des. 163, 204–216.
- Tesla, 2023. Product details. https://www.tesla.com/megapack/design (accessed 2023-07-24).
- Varelmann, T., Erwes, N., Schäfer, P., Mitsos, A., 2022. Simultaneously optimizing bidding strategy in pay-as-bid-markets and production scheduling. Comput. Chem. Eng. 157, 107610.
- Vieira, M., Paulo, H., Pinto-Varela, T., Barbosa-Póvoa, A.P., 2021. Assessment of financial risk in the design and scheduling of multipurpose plants under demand uncertainty. Int. J. Prod. Res. 59 (20), 6125–6145.
- Voll, P., Klaffke, C., Hennen, M., Bardow, A., 2013. Automated superstructure-based synthesis and optimization of distributed energy supply systems. Energy 50 (1), 374–388.
- Wang, G., Mitsos, A., Marquardt, W., 2020. Renewable production of ammonia and nitric acid. AIChE J. 66 (6), 1-9.
- Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., Weidema, B., 2016. The ecoinvent database version 3 (part I): Overview and methodology. Int. J. Life Cycle Assess. 21 (9), 1218–1230.
- Xuan, A., Shen, X., Guo, Q., Sun, H., 2021. A conditional value-at-risk based planning model for integrated energy system with energy storage and renewables. Appl. Energy 294 (52007123), 116971.
- Yunt, M., Chachuat, B., Mitsos, A., Barton, P.I., 2008. Designing man-portable power generation systems for varying power demand. AIChE J. 54 (5), 1254–1269.
- Zhang, Q., Grossmann, I.E., 2016. Planning and scheduling for industrial demand side management: Advances and challenges. In: Alternative Energy Sources and Technologies. Springer International Publishing, pp. 383–414.
- Zhang, Q., Martín, M., Grossmann, I.E., 2019. Integrated design and operation of renewables-based fuels and power production networks. Comput. Chem. Eng. 122 (2), 80–92.
- Ziel, F., Steinert, R., 2018. Probabilistic mid- and long-term electricity price forecasting. Renew. Sustain. Energy Rev. 94, 251–266.