#### PROCESS SYSTEMS ENGINEERING





# Do investments in flexibility enhance sustainability? A simulative study considering the German electricity sector

Pascal Schäfer<sup>1</sup> | Torben M. Daun<sup>1</sup> | Alexander Mitsos<sup>1,2,3</sup> |

<sup>1</sup>RWTH Aachen University, AVT - Aachener Verfahrenstechnik. Process Systems Engineering, Aachen, Germany

<sup>2</sup>JARA-ENERGY, Aachen, Germany

<sup>3</sup>Forschungszentrum Jülich, Energy Systems Engineering (IEK-10), Jülich, Germany

#### Correspondence

Alexander Mitsos, AVT - Aachener Verfahrenstechnik, Process Systems Engineering, RWTH Aachen University, 52056 Aachen, Germany. Email: amitsos@alum.mit.edu

#### Funding information

Bundesministerium für Bildung und Forschung

### **Abstract**

Current research concerning industrial demand side management primarily focuses on monetary aspects. Herein, we extend this perspective by assessing whether economically driven measures increasing the flexibility also result in reduced contributions to the residual load. For this purpose, we conduct a simulative study using historic and projected time series for the German electricity sector. First, Fourier analysis are performed to show that the main oscillation in the electricity price time series has a period length of 12 hr, whereas the renewable generation is primarily characterized by an oscillation with a period length of 24 hr. Second, a generic process model with capabilities for load shiftings is used to evaluate how the fluctuation patterns can be exploited via scheduling optimizations. Most importantly, our results demonstrate that prevalent price fluctuations prevent adequate monetary incentives for providing storage capacities for bridging up to 24 hr, which are desired for reducing the residual load.

#### **KEYWORDS**

demand side management, load shifting, renewable electricity, residual load, time-variable electricity prices

#### INTRODUCTION

In order to reduce the greenhouse gas emissions of the electricity sector, in many industrial nations, conventional power plants are steadily substituted by a generation from renewable sources. For instance, in the first 6 months of 2019, almost half of the net electricity generation in Germany originated from renewable sources-mostly wind and solar. However, the electricity generation by wind farms and photovoltaics is characterized by a strong volatile nature, thus representing a severe challenge for the energy system. In order to address this challenge, flexibility measures are required addressing both the supply and the demand side.<sup>2-5</sup> In this context, process and energy systems engineering can contribute by providing a systematic decision support between alternatives.<sup>6</sup> Considering the storage of surplus energy or the production of e-fuels, extensive studies have therefore been

carried out to quantify environmental impacts and identify the most sustainable of various technological alternatives. 7-10

In contrast, when considering the industrial load flexibility, referred to as industrial demand side management (DSM), the research focus shifts to an almost exclusively economic perspective, mostly addressing monetary entrepreneurial benefits from an active electricity market participation. 11 As the provision of industrial flexibility is in an inherent conflict with utilization rates, 12 industrial DSM is then interpreted as an enterprise-wide optimization problem. 13,14 Using mathematical programming, potential economic benefits from DSM have been identified for important energy-intense processes. Here, the majority of works focuses on air separation as application case. 15-24 However, other processes are well-investigated as well, such as chlor-alkali electrolysis, 25-30 electric arc steelmaking,31-34 aluminum electrolysis,35,36 cement,17,37 seawater desalination, 38-40 and pulp.41

This is an open access article under the terms of the Creative Commons Attribution License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

© 2020 The Authors. AIChE Journal published by Wiley Periodicals LLC on behalf of American Institute of Chemical Engineers.

wileyonlinelibrary.com/journal/aic AIChE J. 2020;66:e17010.

First few approaches exist assessing the environmental impacts of DSM activities in response to price signals, mostly focusing on specific processes. Finn and Fitzpatrick consider, for example, different industrial consumers in Ireland and find a positive correlation between cost savings and wind power consumption.<sup>42</sup> Going one-step further, hourly changing electricity mixes also offer an optimization potential for the schedule, such as minimizing the greenhouse gas emissions that are associated with the generation of the purchased electricity.<sup>43</sup> Focusing on a cement plant in the United Kingdom, Summerbell et al compare production schedules optimized for electricity costs and CO<sub>2</sub> emissions, finding synergetic effects (i.e., an optimization for cost savings also reduces the CO<sub>2</sub> emissions and vice versa).<sup>44</sup> Likewise, Kelley et al consider scheduling alternatives for air separation units using data for California in 2017.<sup>45</sup> Therein, the authors also find mostly synergetic effects. However, in specific periods, the environmentally optimized schedules lead to increased costs compared to the reference case. Trade-offs like these are accounted for by Baumgärtner et al, who present Pareto curves for the design of a utility system considering total annualized costs and global warming impacts as objectives. 46

However, there is still a significant research gap concerning a systematic bi-objective assessment of measures increasing the flexibility potential on the demand side. In particular, this includes the question if economically driven measures, that is, measures that enhance the exploitation of fluctuating electricity prices, promote the penetration of renewables by allowing to consume electricity primarily in periods with a high renewable share. We address this gap by assessing if the current pricing at the electricity markets sets incentives for investments in increased flexibility that are suitable for reducing the environmental impacts of the electricity consumption, which we measure by the contribution to the integral residual load. In our computational study, we focus on the German electricity sector as a prototype of a system characterized by a high share of intermittent renewable electricity generation. The study uses both historic electricity time series data from 2017 as well as publicly available projected time series data for 2030.<sup>47</sup> In a first step, we conduct a quantitative characterization of the timevariable input data sets using frequency and correlation analysis. Afterward, we investigate the effects of the different characteristics of the time series on process scheduling. For this purpose, we perform singleand bi-objective optimizations of the production schedule with regard to both electricity costs and residual load contribution using a generic process model. In this model, we introduce a general formulation for DSM activities allowing for load shiftings, including temporary shutdowns. Furthermore, we investigate numerous parametrizations of the generic process model considering varying average utilization rates, storage capacities, ramping limits, and off-design efficiency losses. Thereby, we cover the vast majority of DSM-relevant processes, which allows for generalizable conclusions not limited to a specific application. Finally, by analyzing the results of the scheduling optimizations, we systematically identify measures increasing the flexibility potential, which are driven by the economic perspective and those driven by the environmental perspective, and discuss potential contradictions.

The remainder of this article is structured as follows: first, we introduce and discuss the data basis for assessing the potential

economic and environmental benefits from DSM. Afterward, we present the generic process model with the considered DSM activities. In the subsequent section, we give a quantitative analysis of the timevariable input series. The results of the numerical optimization studies are presented thereafter. Finally, conclusion is drawn, emphasizing the need for modifications in the electricity market.

#### 2 | SCHEDULING OBJECTIVES

Nowadays, the German electricity market as well as many others is characterized by a time-variable electricity supply satisfying a (mostly) inelastic electricity demand. This induces time-variable fluctuations in both the electricity mix and the electricity price due to different operating costs of the power generation technologies. These fluctuations can be exploited by optimizing the electricity consumption accordingly. In this section, we introduce two objective functions for the optimization—one for the economic perspective and one for the environmental one—and briefly discuss their interrelation.

### 2.1 | Economic perspective

From an entrepreneurial perspective, the primary objective of DSM is to minimize the costs for electricity purchase by preferably consuming electricity in hours with low prices whilst respecting all requirements, for example, obeying operating limits, satisfying demands, and so forth. We herein focus on hourly changing spot prices at the day-ahead market due to its large trading volumes, although recent studies identify larger economic benefits if participating in real-time markets, as more distinct price peaks occur there. <sup>48,49</sup> For ease of presentation, we herein assume that the entire electricity is purchased at the day-ahead spot market. The economic objective for optimization thus equals the total electricity costs  $C = \sum_t c_t \cdot P_t$ , with  $c_t$  denoting the instantaneous spot market price in hour t and  $P_t$  the power consumption.

The German day-ahead market applies a uniform pricing, that is, the market clearing price in each hour is determined by the intersection of the supply and the demand curve. Assuming a perfectly competitive market, the supply curve is the aggregated marginal cost curve of all power suppliers. Consequently, for given hourly demand curves and a given pool of suppliers with known marginal costs, the so-called marginal power plant would then solely determine the spot electricity price  $c_t$ . Therefore, in periods with a high share of renewable electricity generation, which is associated with negligible marginal cost (and in Germany also feed-in support), spot prices are low.  $c_t$ 

#### 2.2 | Environmental perspective

The described price setting procedure essentially leads to timevariable electricity mixes depending on the instantaneous electricity demand and the realized generation from intermittent renewable sources. Consequently, there is an analogous environmental optimization opportunity by preferably consuming electricity in those hours where the electricity generation is associated with low environmental impacts. In the previous literature referred to in the introduction, the environmental objective has mostly been quantified by accounting for different impacts of the individual electricity generation technologies on climate change, targeting the exploitation of time-variable carbon footprints for the electricity consumption.

As an alternative, we herein measure whether electricity is primarily consumed in hours with a high renewable generation by introducing the hourly residual load share  $r_t$ , which is the quotient of the instantaneous residual load and the network-wide electricity consumption. Thus,  $r_t$  gives the percentage of the entire network-wide electricity consumption that needs to be satisfied by a nonrenewable generation. Note that  $r_t \le 1$  thus holds and that  $r_t < 0$  is also possible, indicating hours with a surplus of renewable energy, which should certainly be preferred. A suitable environmental objective then reads  $R = \sum_t r_t \cdot P_t$  if assuming that the purchased electricity has the same mix as traded at the market, giving the individual contribution to the integral residual load, that is, the part of the total individual electricity consumption that needs to be satisfied by a nonrenewable generation.

We emphasize that the proposed environmental objective is not meant for a detailed life cycle analysis but should rather provide a tangible measure for the reduction in the consumption of fossil-produced electricity in favor of renewable electricity with a compact mathematical form comparable to that of the economic one. Moreover, using this measure omits an existing optimization potential between different fossil energy sources, which we do not intend to address in this study. In particular, we thereby prevent favoring periods with a high share of generation from gas-fired plants, which on the one hand involve less emissions than coal-fired plants, but on the other hand, commonly only contribute to the electricity mix in periods with a very low renewable generation due to their high operating costs.

# 2.3 | Data basis

We consider yearly time series for both  $c_t$  and  $r_t$ , that is,  $t \in \{1, ..., T=8760\}$  and investigate both the current and a projected future scenario for the German electricity sector. The first data set contains historic time series from 2017 and is provided by Agora Energiewende (www.agora-energiewende.de/). The 2030 data set is provided by Forschungsgesellschaft für Energiewende (www.ffegmbh.de/) and has been obtained in the project MONA 2030<sup>47</sup> by system simulations assuming a continued increase in installed renewable electricity generation capacities by  $\sim$ 70% compared to 2015. All used time series data are provided in the Supplementary Material.

#### 3 | GENERIC PROCESS MODEL

To evaluate the benefits from DSM, we consider a generic process that is able to vary its electricity consumption and store products. Processes like these act as virtual batteries, that is, load increases act

similarly to charging and load reductions to discharging a battery storage from the perspective of the electricity grid. 52,53 We remark however that these virtual batteries can obviously not have net feeding into the grid at any point in time. Moreover, we require that all load reductions have to be caught up, that is, we confine to load shiftings and not allow for load shedding, and so forth (cf. the classification by Gellings<sup>54</sup>). Depending on the considered process, the ability to shift loads is, however, limited by different constraints. To allow for a systematic treatment, we first introduce an idealized base case, referred to as ideal storage-type customer, and discuss ranges for the process parameters. Afterward, we present two extensions to account for off-design efficiency losses and enable temporary shutdowns of the process. Model equations are only briefly covered herein; instead, the focus is set on the underlying assumptions. Actual mathematical formulations have been extensively discussed in the relevant literature.

#### 3.1 | Ideal storage-type customer

The mathematical model of the ideal storage-type customer, which we consider as a base case, is given in the early work of Daryanian et al<sup>55</sup> and describes an idealized process with flexible power uptake and opportunities for product storage. Essentially, the model relies on two assumptions:

- (a) The production rate is proportional to the power consumption irrespective of the operating point. Note that in the battery analogy, this assumption leads to an ideal behavior in a sense that neither charging nor discharging is associated with any losses.
- (b) The total production of the process must remain constant, equaling that of a constant operation at the nominal production rate.

The ability of the process to shift loads is further limited by its operating range, its storage capacities, and ramping constraints.

#### 3.1.1 | Plant capacity and average utilization rate

The power consumption of the considered process is limited by lower and upper bounds. Beside the size of the flexibility range, the average utilization rate  $\overline{UR}$  (%), giving the ratio between the nominal and the maximum power consumption, is of crucial importance. Note that energy-intense processes are commonly sized for UR≈1 to minimize capital costs. This represents a main hindrance for load shiftings, <sup>56</sup> as missed production can hardly be caught up. For instance, for the chlor-alkali capacities in Germany, an average utilization rate of >90% is found, limiting the potential of DSM.<sup>57</sup> Thus, we herein consider a process with a representative average utilization rate  $\overline{UR}$  = 95% and a flexibility range of 50-100%, but investigate benefits from oversizing facilities, that is, reducing average utilization rates. In the simulative study, we consider oversizings by up to 20%, that is, average utilization rates  $\overline{\textit{UR}}$  = 79...95%. Obviously, oversizing of production facilities is usually in conflict with total annualized costs, requiring integrated optimizations in practice.<sup>29</sup>

# 3.1.2 | Storage capacities

To account for storage opportunities, the process model considers a simple buffer tank which is filled by the instantaneous production and continuously emptied by the nominal production, which can be interpreted as a constant demand that needs to be met. Note that several real processes are indeed characterized by seasonal fluctuations in the demand that might interact with the provision of load flexibility. The consideration of such aspects is, however, beyond the scope of this manuscript. The stored amount increases in case of overproduction and decreases in case of underproduction. We do not consider losses during storage. The stored amount is limited between zero and a maximum storage capacity. In order to avoid emptying the tank throughout the year, we force both the initial and the final tank level to 50%. Moreover, we allow for a systematic comparison between processes of different scales by using the time, up to which the production rate at the design operating point can be maintained with a completely filled storage tank, as a measure for the storage capacity, denoted by  $S^{max}$  (hr). In the parameter studies, we consider a wide range of storage capacities between  $S^{max} = 3...48$  hr. Note that in contrast to an oversizing of the actual production facilities, a retrofit of storage capacities is possible in many settings. 18

#### 3.1.3 | Ramping limits

Finally, the flexibility of a process can be limited by imposing a maximum change between two successive operating points. In particular, such ramping constraints are required to ensure that transitions between two operating points can be realized without violating requirements. Ramping constraints are commonly modeled using a set of linear equations. As we again target the comparability between processes of different scales, we herein impose a maximum on the change in utilization rates between consecutive hours, denoted by  $\Delta^{max}$  (%/hr). In the parameter studies, we investigate the influence of different ramping constraints by considering  $\Delta^{max} = 5...25\%$ /hr. Note that whereas adjustments of the average utilization rate by oversizing as well as of the storage capacities usually involve the installation of additional equipment, ramping constraints can be affected by changes in the operating philosophy beside modifications in the process design.  $^{61}$ 

### 3.2 | Off-design efficiency losses

The assumption of a linear production characteristic made above assuming constant efficiencies might in some cases be a poor approximation of the reality. Instead, efficiency losses in case of off-design operation occur and have to be accounted for when assessing the potential of DSM.<sup>57</sup> In order to enable a systematic treatment, we introduce the following assumptions, leading to an extended storage-type customer model that can account for efficiency characteristics.

- (a) The electric efficiency, that is, the ratio between the production rate and the power consumption, is a function of the instantaneous utilization rate.
- (b) The highest electric efficiency is reached at the design operating point.
- (c) To account for off-design efficiency losses, we use a quadratic approximation of the generally nonlinear function, leading to a cubic function for calculating the production rate from the power consumption.

Following assumptions (b) and (c), the entire characteristic is defined by one parameter, denoted  $\zeta$  (%), giving the relative loss in electric efficiency at the lowest utilization rate (50%) compared to the electric efficiency at nominal operation. Considering the large variety of processes in the DSM-relevant literature, we evaluate a range of potential parameters  $\zeta$  = 0...33%. Using the battery analogy, we thereby account for losses during charging and discharging. Moreover, we highlight that under the aforementioned assumptions, the constraint on satisfying the integral production target involves that any load shifting, that is, any temporary off-design operation, increases the total electricity consumption.

In order to enable the use of efficient mixed-integer linear programming solvers, the cubic relation for calculating the production rate is approximated using a piecewise-linear continuous approximation. More precisely, we apply linear segmentation<sup>62</sup> using six intervals with individual slopes and intercepts. Interval bounds are found by minimizing the error between the cubic function and the piecewise linearization.

#### 3.3 | Shutdowns

In order to circumvent price peaks, it can be beneficial to shut down the entire process for a certain period. Herein, we focus on shutdowns that allow for fast warm-starts after a limited downtime. For modeling these opportunities, we make use of the following assumptions:

- (a) During the downtime, no product is produced and negligible electricity is consumed.
- (b) Shutdowns are only possible if the process is operated at its lower operating bound. Thereby, we prohibit abrupt shutdowns from high utilization rates that might stress the equipment disproportionately.
- (c) Warm-starts, that is, start-ups after downtimes, are only possible within a specified period.

Herein, we also study the influence of a varying maximum downtime, denoted by  $\tau^{max}$  (hr), on the different objective functions. To capture the highly different characteristics of the numerous DSM-relevant processes, we apply  $\tau^{max} = 0...12$  hr.

Modeling of shutdowns relies on the introduction of binary variables indicating operating modes and transitions.<sup>59,63,64</sup> Constraints on the maximum downtime can then be established using a set of

linear inequalities. <sup>17,65</sup> Note that modeling the opportunities for shutdowns under the given assumptions further involves an adjustment of the ramping constraints introduced above, which can be found in the literature. <sup>28</sup>

### 3.4 | Implementation and numerical optimization

We implement the scheduling optimization problem applying the generic process model described above in GAMS version 26.1.0 (GAMS Development Corp.). Therein, we use an hourly discretization and consider the entire year. Moreover, we consider a constant product demand that corresponds to an average utilization rate of 95% for the nonoversized process. GAMS implementations of the three versions of the generic process model ((a) ideal storage-type customer, (b) extended storage type customer accounting for efficiency losses, and (c) ideal storage-type customer with shutdown opportunities) can be found in the Supplementary Material. The resulting (MI)LPs are solved using CPLEX version 12.8 (IBM Corp.). Default solver settings are applied. Pareto curves when conducting bi-objective optimizations are identified using an  $\varepsilon$ -constraint method, furnishing 15 equidistant Pareto optima.

#### 4 | ANALYSIS OF THE TIME SERIES

The input time series for evaluating the considered objective functions, that is, the series of electricity prices and residual load shares, show different characteristics as will be explained in the following. The results presented in this section allow for qualitatively anticipating the observations we make during the scheduling optimizations and facilitate the interpretation thereof in the next section.

# 4.1 | Quantitative characterization

Table 1 gives quantitative descriptors for all considered time series. All values are normalized to the respective means to make the series comparable. As we confine to the discussion of relative improvements through DSM activities in the remainder of the manuscript by comparing to a constant production, that is, with averaged input data, the normalization appears reasonable for interpreting the results. As can

**TABLE 1** Quantitative descriptors for the four time series. All value are normalized to the mean

	Electricity price (-)		Residual load share (–)	
	2017	2030	2017	2030
Mean	1.00	1.00	1.00	1.00
Minimum	-2.43	0.00	0.19	-2.03
Maximum	4.78	2.68	1.46	2.37
SD	0.52	0.35	0.24	0.86

be seen, electricity prices in the historic 2017 time series show a very broad distribution compared to the residual load shares, as measured by both the range and the SD. Consequently, higher relative optimization potentials from the economic perspective are expected compared to the environmental one. Comparing the 2017 to the 2030 time series, one finds that the distribution of electricity prices becomes narrower, whereas the distribution of residual load shares becomes broader with even a larger range and SD than the prices. Consequently, identified relative economic optimization potentials are expected to decrease, whereas environmental ones are expected to increase. The latter conclusion can be explained by an increasing penetration of electricity generation from intermittent renewable sources assumed for 2030. From this perspective, the narrowing of the distribution of electricity prices seems counterintuitive. However, we presume that this observation stems from the assumptions behind the time series simulation for 2030. More precisely, projected prices are bounded by the minimal (zero without feed-in support) and maximal marginal cost of the power plant fleet when assuming a perfectly competitive market. Possible market behavior going beyond this assumption, which is apparently present in 2017 and causes more distinct price peaks and troughs, is not included in the 2030 price series. Besides, we emphasize that absolute price spreads in 2030 are still higher than in 2017.

#### 4.2 | Correlation analysis

Considering bi-objective optimizations, that is, trade-offs in simultaneous fulfilling both objectives, the correlation between the time series of electricity prices and residual load shares is crucial. Thus, in Figure 1, we show scatterplots containing the pairs  $(c_t, r_t)$  for every hour in 2017 and 2030, respectively. In both cases, an S-curve can be observed indicating a positive correlation. The intensity of the correlation can be quantitatively assessed using correlation coefficients. Here, the use of Spearman's rank coefficient  $\rho$  is highly informative, as it represents a measure for the monotonicity of a correlation. More precisely, if one finds a strictly monotone function (represented by  $\rho$  = 1), the bi-objective perspective on DSM would be redundant, that is, the Pareto curve would become a point. For the 2017 time series, we find  $\rho$  = 0.64, whereas for 2030, we find  $\rho$  = 0.76. Thus, for both 2017 and 2030, monotone trends can be observed. However, there is also a potential for balancing trade-offs between the two objectives, which we expect to become particularly important in the presence of efficiency losses.

### 4.3 | Frequency analysis

Further details concerning fluctuation patterns in the considered time series can be gained by frequency analysis. For this purpose, we conduct discrete Fourier transforms. The resulting spectra are depicted in Figure 2. Our analysis focuses on fluctuations on an hourly-to-daily scale, which is typically considered in DSM due to, in general, limited

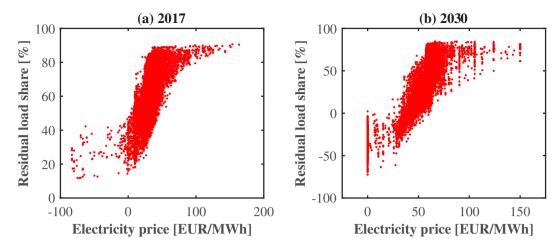
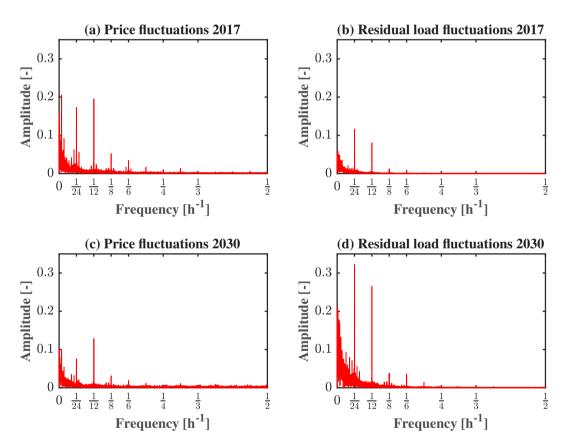


FIGURE 1 Scatterplots for both the historic and the projected time series [Color figure can be viewed at wileyonlinelibrary.com]



**FIGURE 2** Frequency spectra of the fluctuation patterns of the considered normalized time series obtained by discrete Fourier transform [Color figure can be viewed at wileyonlinelibrary.com]

storage capacities. Note that the lower frequencies are nevertheless of interest for different technologies addressing, for example, seasonal storage. <sup>66</sup>

Confining to the DSM-relevant frequency components, one finds the most important frequency components at  $\frac{1}{24}$  and  $\frac{1}{12}$  hr $^{-1}$ . In other words, all time series are characterized by the superposition of two sine waves, one with period length of 1 day (day–night fluctuations) and one with period length of half a day (intraday fluctuations).

Noticeably and independently from the considered year, in case of the residual load share, the day-night fluctuation is more distinct, leading to a temporal course with typically one local minimum per day, which matches the peak in generation from photovoltaics at noon. In contrast, in case of the electricity price, the intraday fluctuation is more distinct, which leads to typically two local maxima a day, that occur around 8:00 a.m. and 8:00 p.m., respectively. This two-peak-behavior directly follows from the market clearing procedure

itself, considering that the peak in generation from photovoltaics at noon is superimposed with a daily flat plateau in the network-wide electricity consumption between 8:00 a.m. and 8:00 p.m. That is, at the beginning and the end of this plateau, a high demand meets a comparably low supply from photovoltaics. In contrast, at the center of the plateau, that is, at noon, there is much more supply from photovoltaics at low marginal costs and thus less conventional electricity generation at higher marginal costs is required to meet the demand, involving temporary daily price troughs. We again highlight that the different fluctuation patterns can be observed irrespective of the considered year, indicating that these are not caused by imperfect market behavior. Moreover, we observe that components with frequencies above  $\frac{1}{4}$ ... $\frac{1}{4}$ hr<sup>-1</sup> show a larger contribution to the spectra of the electricity prices than to the spectra of the residual load shares. This corresponds to the existence of very short-term price spreads, whereas there are no spreads to be exploited on a similar scale with regard to a reduction of the contribution to the residual load. Together, these findings represent an indication that some measures increasing the flexibility potential might influence the economic and the environmental objective in a different manner. In particular, whereas the exploitation of day-night fluctuations is possible even for processes with limited capabilities for load changes, the exploitation of short-term spreads certainly requires a high plant agility, that is, loose ramping constraints. Consequently, we expect mostly economic and almost no environmental incentives for loosening ramping constraints. Finally, we note that Figure 2 also illustrates the trend of increasing fluctuations of the residual load shares and decreasing relative fluctuations of prices in the projected time series.

# 5 | SCHEDULING OPTIMIZATIONS USING THE GENERIC PROCESS MODEL

In this section, we evaluate to what extent different measures increasing the flexibility potential can enhance the exploitation of the above described characteristics of the input time series. Optimization results are herein discussed in detail for the historic time series from 2017. Afterward, a brief presentation of the key insights from using the projected time series for 2030 is given. Note that throughout this section, all objective values are relative to a stationary operation for comparison purpose.

# 5.1 | Effect of average utilization rates on Pareto curves

First, we analyze the impact of different average utilization rates on bi-objective optimizations by varying the oversizing of the process, that is, by decreasing the average utilization rate below its reference value  $\overline{UR} = 95\%$  when considering the ideal storage-type customer model described above. Furthermore, we also identify an optimized average utilization rate by treating it as an additional optimization variable. Pareto curves given in Figure 3 correspond to different process

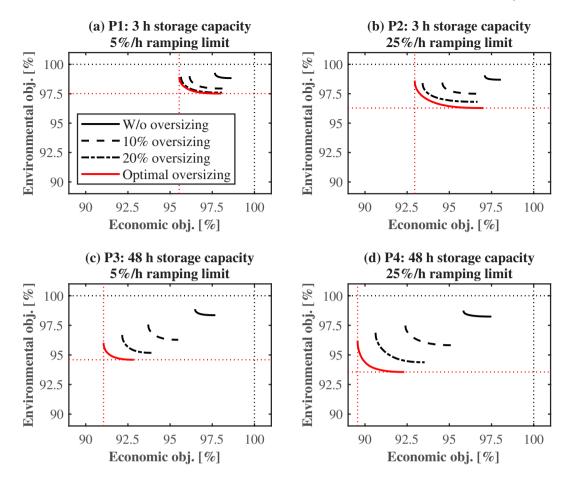
variants, spanning a range for various storage capacities  $S^{max}$  and ramping limits  $\Delta^{max}$ .

- P1—a variant with a low storage capacity  $S^{max} = 3$  hr and a limited load shifting capability due to severe ramping limits  $\Delta^{max} = 5\%$ /hr. Consequently, the flexibility potential of this variant is expected to be substantially restricted.
- P2—a variant with a low storage capacity  $S^{max} = 3$  hr, but strongly loosened ramping limits  $\Delta^{max} = 25\%$ /hr. Compared to P1, the flexibility potential of the variant is higher.
- P3—a variant with a limited load shifting capability due to severe ramping limits  $\Delta^{max} = 5\%$ /hr, but with a significantly increased storage capacity  $S^{max} = 48$  hr. Again, there is a higher flexibility potential than for P1. Note that a comparison with P2 is not intended here.
- P4—a variant with both an increased storage capacity  $S^{max}$  = 48 hr and loosened ramping limits  $\Delta^{max}$  = 25%/hr, hence exhibiting the largest flexibility potential of all variants.

Figure 3 confirms the anticipated larger saving potentials in the economic objective compared to the environmental one (cf. Table 1). Concerning an assessment of trade-offs between the objectives, the most important result is that for the idealized case without efficiency losses, there are mostly synergetic effects between economic and environmental objectives when conducting optimizations of the production schedule. In particular, in none of the considered cases, an optimization for a single objective leads to a deterioration of the other compared to a stationary operation. Nevertheless, one sees that there is a nonnegligible space for balancing between the objectives. More precisely, optimizations for a single objective leave a substantial saving potential in the second objective of up to 3-4% unexploited. Summarizing, in case of near-ideal processes, that is, with negligible efficiency losses, optimizations of the production schedule for economic performance, which are likely conducted from an entrepreneurial perspective, lead to improved environmental objectives, but do not exploit the full environmental potential.

Furthermore, one finds a crucial importance of average utilization rates in Figure 3. If these are too high, almost no saving potentials can be exploited, leading to incentives for oversizing production facilities. Decreasing the average utilization rate evenly affects the economic and the environmental objective, so that Pareto curves are almost parallel to each other for a fixed process variant. Along the same lines, we find a nearly constant optimal average utilization rate along the corresponding Pareto curve. These findings are very important, as we can conclude that the average utilization rate that is favored from an economic perspective and thus highly relevant for investment decisions, is also favored from an environmental perspective.

Finally, comparing the variants P1...P4, there is a strong dependence of both the achievable savings as well as the shape of the Pareto curves on the parametrization of the process. Whereas the first finding is an obvious result of the different flexibility potentials of the variants as discussed at the beginning of the subsection, the second finding is not as intuitive. For instance, we find that process variants with loosened ramping constraints exhibit Pareto curves, which extend over larger ranges of objective values and thus indicate more distinct trade-offs between the objectives. Moreover, in Figure 3b,



**FIGURE 3** Pareto curves for different parametrizations of the ideal storage-type customer model. The solid black curve is the reference with an average utilization rate  $\overline{UR} = 95\%$ . The dashed curve corresponds to 10% oversizing compared to the reference (i.e.,  $\overline{UR} = 86\%$ ), the dashed-dotted curve to 20% (i.e.,  $\overline{UR} = 79\%$ ). The red solid line depicts the Pareto curve for an optimal average utilization rate. Thin dotted lines are depicted for orientation. The intersection of dotted black lines corresponds to a stationary operation; the intersection of dotted red lines gives the utopia point of the red Pareto curve. Used parametrizations are: (a)  $S^{max} = 3$  hr and  $\Delta^{max} = 5\%$ , (b)  $S^{max} = 3$  hr and  $\Delta^{max} = 25\%$ /hr, (c)  $S^{max} = 48$  hr and  $\Delta^{max} = 25\%$ /hr, and (d)  $S^{max} = 48$  hr and  $\Delta^{max} = 25\%$ /hr [Color figure can be viewed at wileyonlinelibrary.com]

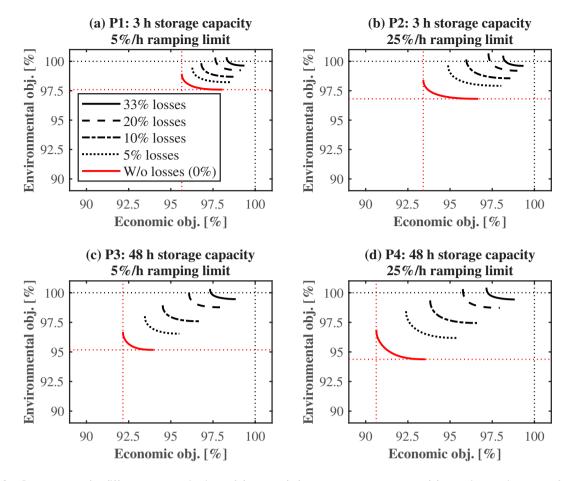
the anchor points of the Pareto curves with lower average utilization rate do not always dominate the corresponding anchor points at higher average utilization rates, as is the case for all other variants. These findings indicate that measures adjusting the storage capacities and those adjusting ramping limits affect economic and environmental objectives in DSM in a different manner, which has been anticipated based on the spectra in Figure 2 and will be discussed in more detail in the following.

# 5.2 | Influence of off-design efficiency losses on Pareto curves

Before analyzing the influence of storage capacities and ramping limits, we first study the effect of off-design efficiency losses. For this purpose, bi-objective optimizations using the process variants introduced above are repeated using a fixed oversizing of 20% (i.e.,  $\overline{UR}$  = 79%). In contrast, we now vary the intensity of the off-design efficiency losses. Comparing the Pareto curves under consideration of

off-design efficiency losses in Figure 4 to their respective references without losses, one finds a significant influence of the loss intensity on the achievable savings through an almost parallel shifting of the Pareto curves. For instance, when considering rather low losses of 10% at the lower operating bound, the saving potential in both objectives for all process variants is reduced by 30...50%. Moreover, high loss intensities bear a severe risk that optimizations for economic objectives, which still yield promising cost savings, lead to an impaired environmental performance. In particular, applying the contribution to the residual load as environmental objective as done in this work, an optimal spot market participation can lead to a net increase in the environmental objective. Most likely, if applying other objectives, for example, the carbon footprint of the electricity consumption, similar observations will be made.

We furthermore remark that the findings presented above, that is, that increased storage capacities and loosened ramping constraints do not affect economic and environmental objectives evenly, are crucial for assessing the risk of a net increase in the environmental objective. In particular, in case of processes with low storage capacities and



**FIGURE 4** Pareto curves for different parametrizations of the extended storage-type customer model assuming varying curves for quadratic efficiency losses and using a fixed oversizing of 20% (i.e., average utilization rate  $\overline{UR}$  = 79%). The solid red curve is the reference without losses. The dashed curve corresponds to 5%, the dashed-dotted line to 10%, the dashed line to 20%, and the solid line to 33% losses at the lower operating bounds compared to the reference. Thin dotted lines are depicted for orientation. The intersection of dotted black lines corresponds to a stationary operation; the intersection of dotted red lines gives the utopia point of the red Pareto curve. Used parametrizations are:

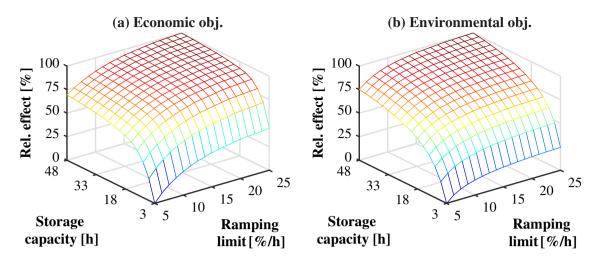
(a)  $S^{max} = 3$  hr and  $\Delta^{max} = 5\%$ , (b)  $S^{max} = 3$  hr and  $\Delta^{max} = 25\%$ /hr, (c)  $S^{max} = 48$  hr and  $\Delta^{max} = 5\%$ /hr, and (d)  $S^{max} = 48$  hr and  $\Delta^{max} = 25\%$ /hr [Color figure can be viewed at wileyonlinelibrary.com]

a high load shifting agility (i.e., P2), economic optimizations are more likely to lead to an increase in the environmental objective even for large low-loss operating ranges. In spite of that, our results indicate that the presence of off-design efficiency losses is not significant for the intended bi-objective assessment of measures increasing the flexibility potential, as we find rather even influences on the two objectives represented by nearly parallel Pareto curves.

# 5.3 | Parameter study for storage and ramping constraints

As discussed in the previous subsection, it is sufficient to consider an ideal process without off-design efficiency losses for studying the influence of storage capacities and ramping limits on the economic and environmental objectives. We therefore conduct a detailed parameter study on their influences on the results of single-objective optimizations using a fixed average utilization rate  $\overline{UR}$  = 79 %, which corresponds to an oversizing of 20% compared to the reference and

thus enables promising saving potentials. In Figure 5, both objectives exhibit only weak gradients at the upper bounds of the considered parameter ranges, indicating only minor additional improvements from increasing storage capacities to above  $S^{max} = 48$  hr and loosening ramping limits to more than  $\Delta^{max} = 25\%$ /hr. In fact, when discarding both storage and ramping constraints, the additional improvements are substantial smaller than what can be achieved by exhausting the parameter ranges from Figure 5. Thereby, our results indicate low additional economic and environmental values of providing seasonal storage capacities in the order of several hundreds of hours. Furthermore, it can be clearly seen that the two process parameters do not affect the two objectives evenly, representing a noticeable difference to the average utilization rate. In particular, we find that the influence of loosening ramping constraints, that is, increasing a process's agility, is much more distinct in case of the economic objective. For instance, comparing a process with low storage capacities and limited load shifting capabilities (P1 with  $S^{max} = 3$  hr and  $\Delta^{max} = 5\%$ /hr) to a process with substantial storage capacities and loose ramping limits (P4 with  $S^{max}$  = 48 hr and  $\Delta^{max}$  = 25%/hr), one finds improvements in



**FIGURE 5** Parameter study for single-objective optimizations assuming an oversizing of 20% compared to the reference with average utilization rate  $\overline{UR}$  = 95%. The relative effect, that is, the additional savings, from increasing the storage capacity  $S^{max}$  and loosening the ramping constraints  $\Delta^{max}$  is scaled between its minimum ( $S^{max}$  = 3 hr,  $\Delta^{max}$  = 5%/hr) and maximum ( $S^{max}$  = 48 hr,  $S^{max}$  = 25%/hr) [Color figure can be viewed at wileyonlinelibrary.com]

economic and environmental savings of factors 2.15 and 2.34, respectively. In case of the economic objective,  $\sim\!\!44\%$  of this improvement can be obtained by only loosening the ramping constraints while maintaining low storage capacities (P2), whereas this value is only  $\sim\!\!24\%$  for the environmental objective. If in contrast only increasing storage capacities while maintaining the severe ramping limits (P3), one achieves  $\sim\!\!69\%$  of the maximum improvement in the economic objective, but even  $\sim\!\!75\%$  of the maximum improvement in the environmental one.

Presumably, this behavior is caused by the different fluctuation patterns of the input time series, which are analyzed above by means of discrete Fourier transform (cf. Figure 2). Apparently, the different spectra require different process capabilities for an exploitation. More precisely, the identified electricity price spreads on short time scales (period lengths below 6 hr) can only be exploited by processes with substantial load shifting capabilities, that is, loose ramping limits. As spreads in the residual load share on a similar scale are much less distinct, the impact of loosening ramping constraints is less significant in case of the environmental objective. Following this argumentation, the very low sensitivity of the environmental objective to ramping limits above 10...15% is not surprising. Along the same lines, the differences in the spectra of the input time series also explain the course of the sensitivity of the objectives to storage limits. More precisely, the very distinct frequency component with period length of 12 hr in the price time series requires comparably low storage capacities for exploitation, resulting in high sensitivities of the economic objective in this range. As the frequency component with period length of 24 hr is less distinct, the sensitivity drastically decreases at higher storage capacities. As in case of the environmental objective, the frequency component with period length of 24 hr is the dominant one, this behavior does not occur.

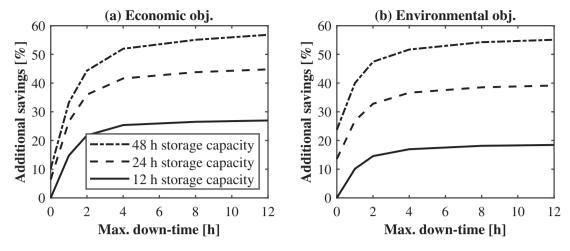
With regard to a bi-objective assessment of different measures increasing the flexibility potential, the findings presented in this subsection are highly relevant, as they unveil a systematic problem:

current price time series set promising monetary incentives for increasing a process's load shifting capabilities, although this will not noticeably affect the process's ability to contribute to a reduction of the residual load. Even more severely, there are no monetary incentives for increasing a process's storage capacities up to the level that would be favored from an environmental perspective.

#### 5.4 | Improvements from shutdown opportunities

Finally, we assess possible improvements from temporary shutdowns by performing single-objective optimizations. For this purpose, we consider an ideal process without efficiency losses using a fixed oversizing of 20% (i.e.,  $\overline{UR} = 79$  %) and a fixed ramping constraint of  $\Delta^{max}$  = 10%/hr. In the study, we vary both the storage capacity  $S^{max}$ and the maximum downtime  $\tau^{max}$ . As can be seen in Figure 6, temporary shutdowns are incentivized from both the economic and the environmental perspective, as they allow for avoiding peak hours in electricity prices as well as residual load shares. Nevertheless, differences between the two objectives are apparent. In particular, we find that the additional savings through temporary shutdowns are substantially more distinct from the economic perspective and predominate the benefits from a further increase in the storage capacities. For instance, when considering a storage capacity of 12 hr as a reference, savings enabled by shutting down the process for only 1 hr are more than twice as high as the savings from doubling the storage capacities without shutdown opportunities and still 50% higher than from quadrupling the storage capacities. Similar observations however cannot be made for the environmental objective. Here, the benefits from increasing storage capacities are more important.

As discussed above, the reason for the described differences in the behavior lies in the different fluctuation patterns of the electricity price and the residual load share time series. In particular, electricity price spreads occur on faster time scales, leading to a higher "value"



**FIGURE 6** Analysis of additional savings in economic (a) and environmental (b) objectives enabled by temporary shutdowns as a function of the maximum downtime  $\tau^{max}$ . A fixed oversizing of 20% (i.e., average utilization rate  $\overline{UR}$  = 79%) is used and a ramping constraint of  $\Delta^{max}$  = 10%/hr is imposed. Line styles indicate the storage capacity  $S^{max}$ . Solid lines:  $S^{max}$  = 12 h, dashed lines:  $S^{max}$  = 24 hr, dashed-dotted lines:  $S^{max}$  = 48 hr. Values are scaled to the savings in the reference case with  $S^{max}$  = 12 hr and without shutdowns. Calculations are conducted for  $\tau^{max}$  = 0.1.2.4.8.12 hr

of short downtimes of few hours compared to further increased storage capacities that are not required for short-term buffering. For the contribution to the residual load in contrast, the frequency components with large period lengths correspond to the only important spreads, explaining the higher importance of storage. Note that the differences in the influence on economic and environmental objectives are not as distinct for temporary shutdowns as for loosened ramping constraints, that hardly affect environmental savings (cf. Figure 5). This finding stems from the fact that shutdowns also widen the operating range, which is equally beneficial from both the economic and the environmental perspective as can be seen in Figure 3.

# 5.5 Key insights from the 2030 study using the projected time series

In this subsection, we only qualitatively describe the key observations from the scheduling optimizations considering the projected time series for 2030 and omit a detailed presentation of quantitative results. Corresponding figures can, however, be found in the Supplementary Material. In particular, we are herein interested in the question whether the drawn conclusions will remain valid in the future, where electricity markets will be characterized by an even stronger penetration of generation from intermittent renewable sources. Furthermore, the considered setting also allows for assessing whether imperfectly competitive market behavior, which characterizes the historic 2017 price time series but not the projected 2030 time series, distorts the observations.

Comparing the results for 2030 with those for 2017, the most noticeable difference is that the relative saving potentials are now larger for the environmental objective as anticipated by comparing the widths of the distributions (cf. Table 1). Note that this also has a considerable effect on the shape of the Pareto curves. These differences become most recognizable when considering off-design efficiency losses. Here, optimizations for the environmental objective now bear a risk of increasing costs and not vice versa as in 2017. Furthermore, the Pareto curves seem to shrink, which is in good agreement with the higher correlation coefficient in 2030 (cf. Figure 1). Note that both effects are likely a consequence of decreasing relative economic saving potentials in 2030. However, as discussed above. these can at least partially be explained by an assumed ideally competitive market avoiding extreme price peaks. In this work, we do not intend to draw a final conclusion whether an increase in the renewable generation will cause an increase in relative price spreads in addition to the inevitable rise in both average prices and absolute spreads. In contrast, we strongly emphasize that these findings do not affect the prioritization of different possible measures increasing the flexibility potential and should thus be discussed elsewhere.

The observations made in the previous subsections are indeed still visible when considering the projected time series for 2030, although they appear slightly weakened. We thus conclude that parts of the high-frequency electricity price fluctuations that set incentives for loosening ramping constraints and creating shutdown opportunities but not for increasing storage capacities, presumably stem from a nonideal market behavior. However, the statements made concerning uneven influences of different measures increasing the flexibility potential on the two objectives remain unaffected. In particular, this includes the finding that measures loosening ramping limits or allowing for temporary shutdowns are also in future significantly incentivized from an economic perspective, although they continue to exhibit only minor capabilities for improving the environmental objective. Consequently, our observations are primarily caused by the prevalent market mechanisms governing the price setting that impose the

differences in time scales for the fluctuations in electricity mixes and prices (cf. Figure 2) irrespective of the actual partially nonideal strategic behavior of market participants.

### 6 | CONCLUSION

We present a systematic assessment of measures increasing the flexibility potential with regard to both economic and environmental targets. Therein, the economic perspective is represented by achievable cost savings for the electricity purchase through the exploitation of day-ahead spot market price spreads, whereas environmental impacts are measured in a simplifying yet tangible manner by reductions in the contribution to the integral residual load through the exploitation of time-variable electricity mixes. We use a generic process model, which acts like a battery from a grid level perspective, comprising general formulations for DSM activities for load shiftings, including the possibility for temporary shutdowns, as well as for off-design efficiency loss characteristics. By varying the constituting process parameters, we consider the vast majority of DSM-relevant processes from literature, which allows for a systematic treatment not limited to a specific application.

Before conducting numeric optimizations, we first analyze the input time series to be exploited and find different contributions of certain frequency components to the spectra. In particular, the electricity price time series is characterized by fluctuations on shorter time scales below 1 day. In contrast to that, the share of renewable electricity generation is mostly characterized by a day-night fluctuation. This then leads to uneven influences of certain measures increasing the flexibility potential when performing bi-objective optimizations of the schedule. Most importantly, we find that measures loosening ramping limits or allowing for temporary shutdowns are significantly incentivized from an economic perspective, although they exhibit only minor capabilities for reducing the residual load. The latter is achieved much more effectively through substantially increased storage capacities, which are in turn not monetarily incentivized in an adequate manner. Measures optimizing the operating range of processeswhich are commonly designed for nearly full utilization—by oversizing existing production facilities, however, affect economic and environmental objectives evenly.

For the future, we recommend further developments of the model to increase the generalizability and hence the significance of the results, for example, by studying the interactions between seasonally varying product demands and the provision of load flexibility in detail. Along these lines, we are also interested in assessing the potentials of switching the energy sources. For instance, there are gas-fired but electrically boosted furnaces for glass production. Here, temporarily increasing/decreasing the electricity consumption might be motivated either by economic or environmental considerations that do not necessarily need to result in similar operating schemes. Finally, we see clear benefits if incorporating design aspects into the scheduling optimizations by considering annualized costs and environmental impacts, but at the same time, acknowledge that these will be highly

process-specific and in some cases also hard to quantify, particularly when assessing the environmental impacts.

Although our analysis suggests that comparable observations are likely when considering other countries, whose electricity markets apply similar pricing schemes and whose energy sectors are characterized by comparably high penetrations of intermittent renewable electricity sources as the German one, we recommend additional studies using both historic and projected future time series to validate the findings. Nevertheless, our results already give rise to the question whether adjustments in the market itself can overcome the described issues. In particular, these should aim at setting adequate monetary incentives for providing storage capacities that enable load shiftings on desired time scales in the order of 1 day. Here, it is worth investigating whether the desired balancing of day-night fluctuations should be considered as an ancillary service to the power grid and should thus be compensated in a more active manner. Along these lines, future research should also include a third perspective into the assessment of measures increasing the flexibility potential at the demand side: the stabilization of the grid. This will on the one hand include the provision of ancillary services for balancing short-term frequency fluctuations that certainly require large capacities that can be ramped up and down on time scales, which are substantially faster than spot market fluctuations. On the other hand, this will also include the remedy of regional network congestion, where the prioritization of measures is certainly also not obvious and will thus require systematic approaches. Concerning the latter, we are also particularly interested in extending the study toward market environments that account for network congestion in the price setting by applying nodal prices, as is done in several U.S. American electricity markets. In particular, this should address the question whether regional differences in the renewable electricity generation, which induce regional price signals due to limited transmission capacities, then also lead to different regional prioritizations of measures increasing the flexibility potential at the demand side.

# **ACKNOWLEDGMENTS**

The authors gratefully acknowledge the financial support of the Kopernikus project SynErgie by the Federal Ministry of Education and Research (BMBF) and the project supervision by the project management organization Projektträger Jülich. Moreover, the thank their colleagues from SynErgie Cluster IV for fruitful discussions. In particular, the authors are grateful to Serafin von Roon and Timo Kern from FfE for providing us with the time series data. Open access funding enabled and organized by Projekt DEAL.

#### ORCID

Pascal Schäfer https://orcid.org/0000-0002-3268-8976 Alexander Mitsos https://orcid.org/0000-0003-0335-6566

#### **REFERENCES**

 Burger B. Stromerzeugung in Deutschland im ersten Halbjahr 2019 https://www.ise.fraunhofer.de/content/dam/ise/de/documents/publ ications/studies/daten-zu-erneuerbaren-energien/ISE\_Stromerzeugu ng\_2019\_Halbjahr.pdf. 2019.

- Lund PD, Lindgren J, Mikkola J, Salpakari J. Review of energy system flexibility measures to enable high levels of variable renewable electricity. Renew Sustain Energy Rev. 2015;45:785-807.
- Brouwer AS, Broek M, Zappa W, Turkenburg WC, Faaij A. Least-cost options for integrating intermittent renewables in low-carbon power systems. Appl Energy. 2016;161:48-74.
- Alizadeh MI, Parsa MM, Amjady N, Siano P, Sheikh-El-Eslami MK. Flexibility in future power systems with high renewable penetration: a review. Renew Sustain Energy Rev. 2016;57:1186-1193.
- Kondziella H, Bruckner T. Flexibility requirements of renewable energy based electricity systems a review of research results and methodologies. Renew Sustain Energy Rev. 2016;53:10-22.
- Mitsos A, Asprion N, Floudas CA, et al. Challenges in process optimization for new feedstocks and energy sources. Comput Chem Eng. 2018;113:209-221.
- Sternberg A, Bardow A. Power-to-what?—environmental assessment of energy storage systems. Energ Environ Sci. 2015;8:389-400.
- Matzen M, Demirel Y. Methanol and dimethyl ether from renewable hydrogen and carbon dioxide: alternative fuels production and lifecycle assessment. J Clean Prod. 2016;139:1068-1077.
- Deutz S, Bongartz D, Heuser B, et al. Cleaner production of cleaner fuels: wind-to-wheel environmental assessment of CO2-based oxymethylene ether as a drop-in fuel. *Energ Environ Sci.* 2018;11:331-343.
- Koj JC, Wulf C, Zapp P. Environmental impacts of power-to-X systems—a review of technological and methodological choices in life cycle assessments. Renew Sustain Energy Rev. 2019;112:865-879.
- Dowling AW, Kumar R, Zavala VM. A multi-scale optimization framework for electricity market participation. Appl Energy. 2017;190: 147-164
- Paulus M, Borggrefe F. The potential of demand-side management in energy-intensive industries for electricity markets in Germany. Appl Energy. 2011:88:432-441.
- 13. Grossmann IE. Enterprise-wide optimization: a new frontier in process systems engineering. AIChE J. 2005;51:1846-1857.
- Zhang Q, Grossmann IE. Enterprise-wide optimization for industrial demand side management: fundamentals, advances, and perspectives. Chem Eng Res Des. 2016;116:114-131.
- Ierapetritou MG, Wu D, Vin J, Sweeney P, Chigirinskiy M. Cost minimization in an energy-intensive plant using mathematical programming approaches. *Ind Eng Chem Res.* 2002;41:5262-5277.
- Karwan MH, Keblis MF. Operations planning with real time pricing of a primary input. Comput Oper Res. 2007;34:848-867.
- Mitra S, Grossmann IE, Pinto JM, Arora N. Optimal production planning under time-sensitive electricity prices for continuous powerintensive processes. Comput Chem Eng. 2012;38:171-184.
- Mitra S, Pinto JM, Grossmann IE. Optimal multi-scale capacity planning for power-intensive continuous processes under time-sensitive electricity prices and demand uncertainty. Part I: modeling. Comput Chem Eng. 2014;65:89-101.
- Zhang Q, Grossmann IE, Heuberger CF, Sundaramoorthy A, Pinto JM. Air separation with cryogenic energy storage: optimal scheduling considering electric energy and reserve markets. AIChE J. 2015;61:1547-1558.
- Zhang Q, Sundaramoorthy A, Grossmann IE, Pinto JM. A discretetime scheduling model for continuous power-intensive process networks with various power contracts. Comput Chem Eng. 2016;84: 382-393.
- Zhang Q, Morari MF, Grossmann IE, Sundaramoorthy A, Pinto JM. An adjustable robust optimization approach to scheduling of continuous industrial processes providing interruptible load. *Comput Chem Eng.* 2016;86:106-119.
- Pattison RC, Touretzky CR, Johansson T, Harjunkoski I, Baldea M.
   Optimal process operations in fast-changing electricity markets:
   framework for scheduling with low-order dynamic models and an air
   separation application. *Ind Eng Chem Res.* 2016;55:4562-4584.

- Kelley MT, Pattison RC, Baldick R, Baldea M. An MILP framework for optimizing demand response operation of air separation units. *Appl Energy*. 2018;222:951-966.
- Obermeier A, Windmeier C, Esche E, Repke J-U. A discrete-time scheduling model for power-intensive processes taking fatigue of equipment into consideration. *Chem Eng Sci.* 2019;195:904-920.
- 25. Babu CA, Ashok S. Peak load management in electrolytic process industries. *IEEE Trans Power Syst.* 2008;23:399-405.
- Wang X, El-Farra NH, Palazoglu A. Optimal scheduling of demand responsive industrial production with hybrid renewable energy systems. *Renew Energy*. 2017;100:53-64.
- Otashu JI, Baldea M. Demand response-oriented dynamic modeling and operational optimization of membrane-based chlor-alkali plants. Comput Chem Eng. 2019;121:396-408.
- Brée LC, Perrey K, Bulan A, Mitsos A. Demand side management and operational mode switching in chlorine production. AIChE J. 2019;65: e16352
- Roh K, Brée LC, Perrey K, Bulan A, Mitsos A. Flexible operation of switchable chlor-alkali electrolysis for demand side management. *Appl Energy*. 2019;255:113880.
- Otashu JI, Baldea M. Scheduling chemical processes for frequency regulation. Appl Energy. 2020;260:114125.
- Castro PM, Sun L, Harjunkoski I. Resource task network formulations for industrial demand side management of a steel plant. *Ind Eng Chem Res.* 2013;52:13046-13058.
- Zhang X, Hug G, Kolter Z, Harjunkoski I. Industrial demand response by steel plants with spinning reserve provision. North Am Power Symp (NAPS). 2015;1-6.
- Hadera H, Harjunkoski I, Sand G, Grossmann IE, Engell S. Optimization of steel production scheduling with complex time-sensitive electricity cost. Comput Chem Eng. 2015;76:117-136.
- Zhao S, Grossmann IE, Tang L. Integrated scheduling of rolling sector in steel production with consideration of energy consumption under time-of-use electricity prices. Comput Chem Eng. 2018;111:55-65.
- Zhang X, Hug G. Bidding strategy in energy and spinning reserve markets for aluminum smelters' demand response. 2015 IEEE Power Energy Society Innovative Smart Grid Technologies Conference (ISGT):1–5 2015.
- Schäfer P, Westerholt H, Schweidtmann AM, Ilieva S, Mitsos A. Model-based bidding strategies on the primary balancing market for energy-intense processes. Comput Chem Eng. 2019;120:4-14.
- Vujanic R, Mariéthoz S, Goulart P, Morari M. Robust integer optimization and scheduling problems for large electricity consumers. Am Control Conf (ACC). 2012;3108-3113.
- 38. Ghobeity A, Mitsos A. Optimal time-dependent operation of seawater reverse osmosis. *Desalination*. 2010;263:76-88.
- Williams CM, Ghobeity A, Pak AJ, Mitsos A. Simultaneous optimization of size and short-term operation for an RO plant. *Desalination*. 2012;301:42-52.
- Jiang A, Wang J, Biegler LT, Cheng W, Xing C, Jiang Z. Operational cost optimization of a full-scale SWRO system under multi-parameter variable conditions. *Desalination*. 2015;355:124-140.
- Hadera H, Ekström J, Sand G, Mäntysaari J, Harjunkoski I, Engell S. Integration of production scheduling and energy-cost optimization using mean value cross decomposition. Comput Chem Eng. 2019;129: 106436.
- 42. Finn P, Fitzpatrick C. Demand side management of industrial electricity consumption: promoting the use of renewable energy through real-time pricing. *Appl Energy*, 2014;113:11-21.
- Kopsakangas-Savolainen M, Mattinen MK, Manninen K, Nissinen A. Hourly-based greenhouse gas emissions of electricity cases demonstrating possibilities for households and companies to decrease their emissions. J Clean Prod. 2017;153:384-396.
- Summerbell DL, Khripko D, Barlow C, Hesselbach J. Cost and carbon reductions from industrial demand-side management: study of potential savings at a cement plant. *Appl Energy*. 2017;197:100-113.

- Kelley MT, Baldick R, Baldea M. Demand response operation of electricity-intensive chemical processes for reduced greenhouse gas emissions: application to an air separation unit. ACS Sustain Chem Eng. 2019;7:1909-1922.
- Baumgärtner N, Delorme R, Hennen M, Bardow A. Design of lowcarbon utility systems: exploiting time-dependent grid emissions for climate-friendly demand-side management. *Appl Energy*. 2019;247: 755-765.
- Kern T, Böing F, Roon S. Merit Order Netz-Ausbau 2030— Preiszeitreihe Basisszenario https://www.ffe.de/themen-und-methoden/speicher-und-netze/521-merit-order-netz-ausbau-2030-mona-2030. 2018.
- 48. Shao Y, Zavala VM. Space-time dynamics of electricity markets incentivize technology decentralization. *Comput Chem Eng.* 2019;127: 31-40
- Tsay C, Kumar A, Flores-Cerrillo J, Baldea M. Optimal demand response scheduling of an industrial air separation unit using datadriven dynamic models. Comput Chem Eng. 2019;126:22-34.
- 50. Kirschen DS, Strbac G. Fundamentals of Power System Economics. West Sussex, England: Wiley; 2004.
- Sensfuß F, Ragwitz M, Genoese M. The merit-order effect: a detailed analysis of the price effect of renewable electricity generation on spot market prices in Germany. *Energy Policy*. 2008;36: 3086-3094.
- Depree N, Düssel R, Patel P, Reek T. The virtual battery—operating an aluminium smelter with flexible energy input. In: Williams E, ed. 145th TMS Annual Meeting and Exhibition. Springer International Publishing; 2016 Light Metals:571–576.
- Otashu JI, Baldea M. Grid-level "battery" operation of chemical processes and demand-side participation in short-term electricity markets. Appl Energy. 2018;220:562-575.
- 54. Gellings CW. The concept of demand-side management for electric utilities. *Proc IEEE*. 1985;73:1468-1470.
- Daryanian B, Bohn RE, Tabors RD. Optimal demand-side response to electricity spot prices for storage-type customers. *IEEE Trans Power* Syst. 1989:4:897-903.
- Ausfelder F, Beilmann C, Bertau M, et al. Energy storage technologies as options to a secure energy supply. Chem Ing Tech. 2015;87:17-89.
- 57. Klaucke F, Karsten T, Holtrup F, et al. Demand response potenziale in der chemischen industrie. *Chem Ing Tech.* 2017;89:1133-1141.
- Baldea M, Harjunkoski I. Integrated production scheduling and process control: a systematic review. Comput Chem Eng. 2014;71: 377-390.

- 59. Mitra S, Sun L, Grossmann IE. Optimal scheduling of industrial combined heat and power plants under time-sensitive electricity prices. *Energy*, 2013;54:194-211.
- Schäfer P, Bering LF, Caspari A, Mhamdi A, Mitsos A. Nonlinear dynamic optimization for improved load-shifting agility of cryogenic air separation plants. In: Eden MR, Ierapetritou MG, Towler GP, eds. 13th International Symposium on Process Systems Engineering (PSE 2018).44 of Computer Aided Chemical Engineering Elsevier; 2018: 547–552.
- Cao Y, Swartz CLE, Baldea M, Blouin S. Optimization-based assessment of design limitations to air separation plant agility in demand response scenarios. *J Process Control*. 2015;33:37-48.
- Floudas CA. Nonlinear and Mixed-Integer Optimization: Fundamentals and Applications (Topics in Chemical Engineering). Oxford, England: Oxford University Press; 1995.
- Sahinidis NV, Grossmann IE. Reformulation of multiperiod MILP models for planning and scheduling of chemical processes. Comput Chem Eng. 1991;15:255-272.
- Erdirik-Dogan M, Grossmann IE. Simultaneous planning and scheduling of single-stage multi-product continuous plants with parallel lines. Comput Chem Eng. 2008;32:2664-2683.
- Simoglou CK, Biskas PN, Bakirtzis AG. Optimal self-scheduling of a thermal producer in short-term electricity markets by MILP. *IEEE Trans Power Syst.* 2010;25:1965-1977.
- Burre J, Bongartz D, Brée LC, Roh K, Mitsos A. Power-to-X: between electricity storage, e-production, and demand side management. Chem Ing Tech. 2020;92:74-84.
- 67. Seo K, Edgar TF, Baldea M. Optimal demand response operation of electric boosting glass furnaces. *Appl Energy*. 2020;269:115077.

#### SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.

How to cite this article: Schäfer P, Daun TM, Mitsos A. Do investments in flexibility enhance sustainability? A simulative study considering the German electricity sector. *AIChE J*. 2020;66:e17010. https://doi.org/10.1002/aic.17010