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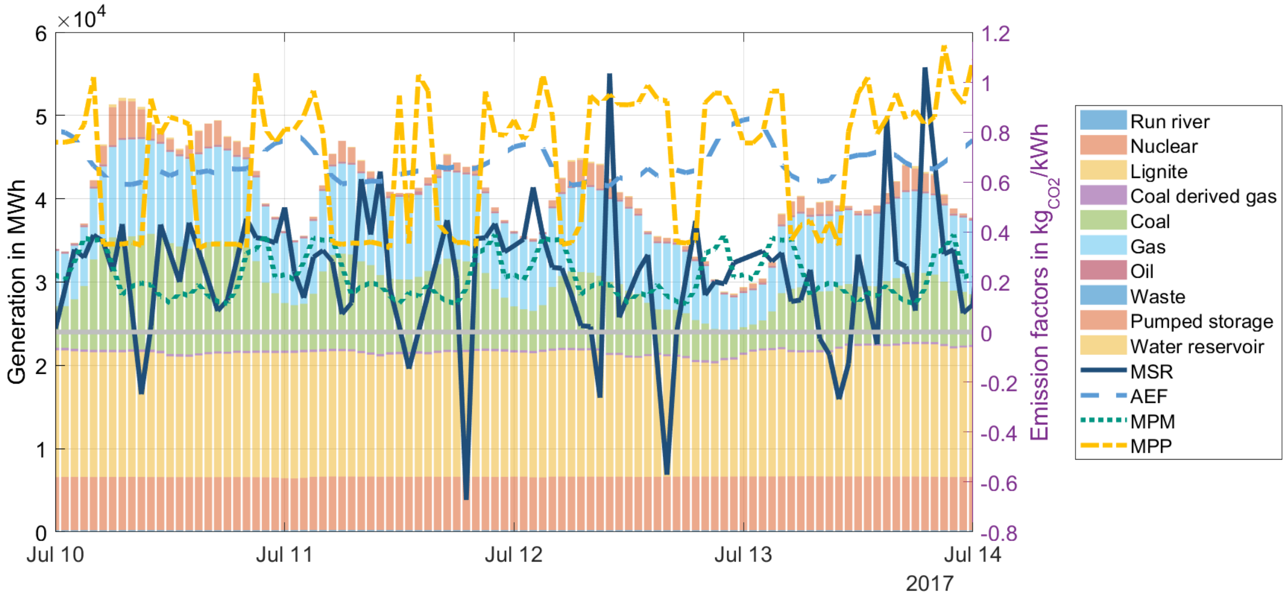

Comparing empirical and model-based approaches for calculating dynamic grid emission factors: An application to CO_2-minimizing storage dispatch in Germany

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As one possibility to increase flexibility, battery storage systems (BSS) will play a key role in the decarbonization of the energy system. The emissions-intensity of grid electricity becomes more important as these BSSs are more widely employed. In this paper, we introduce a novel data basis for the determination of the energy system's CO_2 emissions, which is a match between the ENTSO-E database and the EUTL databases. We further postulate four different dynamic emission factors (EF) to determine the hourly CO_2 emissions caused through a change in electricity demand: the average emission factor (AEF), the marginal power mix (MPM), the marginal system response (MSR) and an energy-model-derived marginal power plant (MPP). For generic and battery storage systems, a linear optimization on two levels optimizes the economic and environmental storage dispatch for a set of 50 small and medium enterprises in Germany. The four different emission factors have different signaling effects. The AEF leads to the lowest CO_2 reduction and allows for roughly two daily cycles. The other EFs show a higher volatility, which leads to a higher utilization of the storage system from 3.4 to 5.4 daily cycles. The minimum mean value for CO_2 abatement costs over all 50 companies is 14.13 $€/t_{CO2}$.

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Abstract

As one possibility to increase flexibility, battery storage systems (BSS) will play a key role in the decarbonization of the energy system. The emissions-intensity of grid electricity becomes more important as these BSSs are more widely employed. In this paper, we introduce a novel data basis for the determination of the energy system's CO_2-emissions, which is a match between the ENTSO-E database and the EUTL databases. We further postulate four different dynamic emission factors (EF) to determine the hourly CO_2-emissions caused through a change in electricity demand: the average emission factor (AEF), the marginal power mix (MPM), the marginal system response (MSR) and an energy-model-derived marginal power plant (MPP). For generic and battery storage systems, a linear optimization on two levels optimizes the economic and environmental storage dispatch for a set of 50 small and medium enterprises in Germany. The four different emission factors have different signaling effects. The AEF leads to the lowest CO_2-reduction and allows for roughly two daily cycles. The other EFs show a higher volatility, which leads to a higher utilization of the storage system from 3.4 to 5.4 daily cycles. The minimum mean value for CO_2-abatement costs over all 50 companies is 14.13 €$/t_{CO_2}$.

Keywords: Dynamic emission factor, Empirical emission factors, CO2-minimizing dispatch, Energy storage system, German industry, CO2-emissions

1. Introduction

In light of global decarbonization efforts, flexibility becomes increasingly important in energy systems [1]. Energy storage systems (ESS) in industry can contribute to the needed flexibility in two ways: First, they allow for a time variable consumption of electricity in good adaptation to volatile supply of renewable energies [2, 3]. Thus, ensuring both security of supply and price stability for consumers. Second, they enable consumers to reduce their carbon footprint with respect to electricity drawn from the grid, if the carbon intensity is sufficiently signalled. The high and volatile load profile in industry is a key premise for a profitable utilization of flexible storage systems [4].

Simultaneously, in energy systems where the power plant fleet comprises a variety of technologies, the CO_2-emissions change considerably over the course of one day [5, 6]. This holds true for average system emissions in one hour as well as for the marginal power plant, which responds to an incremental increase in electricity demand. ESSs offer a great potential to reduce the CO_2-footprint of energy intensive industry and CO_2-emissions of the energy system as they can charge/discharge in hours of low/high emissions.

Identifying these hours and incentivizing storage providers to utilize their flexibility potential to reduce greenhouse gas (GHG) emissions is no trivial task. Due to the missing internalization of cost, which are related to GHG emissions, market prices in most power markets do not reflect GHG intensity of the respective marginal technology. Hence a clear price signal is missing to incentivize CO_2-reducing charging or discharging behaviour. This problem can be solved by hourly emission factors (EFs), which signal CO_2-intensity to storage operators.

A number of researchers study dynamic CO_2-EFs. Most researchers apply dynamic EFs to evaluate charging strategies of electrical vehicles (EVs). Axsen et al. [7] consider the owner's behavior on CO_2-emissions in California. Jansen et al. [8] extend their study on EV-emissions onto the western grid of the U.S. Kintner-Meyer et al. [9] assess the technological load shifting potential of EVs in the U.S. while Stephan and Sullivan [10] study the impact of night time charging and Tamayao et al. [11] analyse the life cycle emissions for EVs on the U.S. market. As one of the fewer publications, Jochem et al. [12] focus on the impact of EVs on the German energy system. One important result of these studies is that considering times of low emissions for the charging strategies reduces the overall CO_2-emissions substantially. The applied average and marginal EFs are results of different energy system models, which study the reaction of the energy system to different scenarios. Few studies consider the dynamic influence of emissions on the operation of stationary storage technologies. Hittinger and Azevedo [13] studied the impact of bulk central energy storage systems on the emissions of the U.S. energy system; Arciniegas and Hittinger [14] build up on this research and implement a multi-objective optimization of the storage operation considering economic and ecologic factors. Section 2 presents an extensive discussion on existing literature and identifies the following deficiencies in the literature on dynamic EFs and energy storage systems:

- No study derives dynamic EFs for the German energy system based on empirical data.
- No study investigates the environmental dispatch of ESS in industry.

In this study, we develop four different EFs, three based on empirical data and one model-based, to understand the average and marginal emissions of an energy system. The application to the German energy system is a novelty in the literature. We use these EFs to analyse the CO_2-emission abatement potential for 50 small to medium sized companies. An additional novel contribution is the development of a two-step approach based on Braeuer et al. [15], in which we first identify the optimal investment and dispatch of an EES from an economic perspective (*economic dispatch*) followed by the second step, in which the storage system is utilized to minimize the CO_2-intensity of the electricity drawn from the grid (*environmental dispatch*). This energy storage model (ESM) is formulated as a linear optimization model with perfect foresight. Thus,

CO_2-abatement costs for the different companies can be formalized and used by decision-makers to compare the ESS to other reduction measures at their disposal.

This paper formulates four different EFs in hourly resolution. The main focus is on CO_2-emissions. The empirical CO_2-EFs are derived by joining the transparency platform of the European Network of Transmission System Operators for Electricity (ENTSO-E) with the European Union Transaction Log (EUTL) database, linking power output to reported emissions. This is the final novel contribution to the literature. Additionally, EFs for other emissions, SO_2, NO_x and Dust, are derived from combining the ENTSO-E-database and the large combustion plants directive (LCPD) and shown in the Supplementary Information (SI) SI E. The empirical EFs are the average EF (*AEF*), the marginal system response (*MSR*) and the EF based on Hawkes [16] (*MPM*). These EFs are compared to a model-based marginal power plant (*MPP*). It is result of a European electricity market model(EEMM).

The key objectives of this paper are the following:

1. Derive dynamic EFs for the German energy system from empirical and model data
2. Investigate the effect of four different EFs on the environmental dispatch of the ESS
3. Evaluate the CO_2-reduction potential of ESSs for different industrial load profiles.

2. Literature review

No standardized method to assess the EF of a country's or region's power mix has been presented in the scientific literature. Yang [17] and Ryan et al. [18] give an overview of the different dimensions to consider when calculating EFs. Yang [17] divides these dimensions into scenario based (prospective) vs. system based (retrospective), aggregated vs. temporally explicit and average vs. marginal. Ryan et al. [18] present an algorithm to guide the practitioner's selection of the appropriate EF fitting to their specific use case. For this study, we only consider dynamic EFs. Static and aggregated EFs are not further investigated. To assess dynamic EFS, we identify three approaches mentioned in recent scientific publications:

1. marginal power mix (MPM)
2. marginal power plant (MPP)
3. average power mix (AEF).

For MPM, a linear regression model and historical data are used to compare the change in the generation to the change in CO_2-emissions of the electricity mix. The base definition of the MPM was first presented in [16] and [19]. The MPP approach determines the marginal power plant, which reacts to a marginal change in demand. Usually, it is a simulation or optimization model based approach. Tamayao et al. [11, p. 8846] differentiates between these two approaches as top-down respectively bottom-up methods. The AEF relates the total CO_2-emissions to the total energy generated. Spork et al. [20] present the method for a dynamic AEF applied to the Spanish electricity system. All three EFs can be disaggregated in different temporal resolutions. Furthermore, these approaches can be differentiated by their system boundaries. Tamayao et al. [11] divides them into consumption based EFs, which consider exchange over the system boundaries and production based EFs, which take only the inner system production units into account. Table A.4 summarizes the reviewed literature and SI A further reviews literature on MPM and MPP.

2.1. Comparison of the approaches

The MPM is based on empirical data. It depends strongly on the quality and accessibility of the data. The advantage of the MPM is that it does not need further assumptions regarding the pricing strategy of the power plants. A disadvantage is the lack of informative value for future scenarios. For the MPP, a variety of assumptions regarding inputs enable the incorporation of future developments into the model. At the same time, this makes the comparability of different model results difficult. For both approaches, the system boundaries need to be considered and it should be distinguished between a consumption based and a production based approach. Furthermore, many studies compare either EF to the AEF. While the AEF is seen as the intuitive approach, commonly applied to formulate political implications, Axsen et al. [7] raise the question if a marginal emission factor (MEF) or an AEF is the appropriate measure. They conclude, the appropriateness depends on how "new and existing electricity demand" is valued [7, p. 1621]. Yang [17] consider the AEF suitable to "assign the emissions to all electricity load" while MEF help "understand the change in total electricity emissions " with the increase in demand [17, p. 724]. Tamayao et al. [11] explicitly deem the AEF as "conceptually inappropriate for assessing" additional demand technologies. Ryan et al. [18] propose that the appropriate method to evaluate additional, dynamic electricity demand is the MPP. For all studies considered, the MPP or MPM always surpasses the AEF. Regett et al. [21, p. 5] find "even hours for which the two methods show significantly opposing results." They advice that the appropriateness of the different methods depends strongly on the applications and research question.

3. Methodology

The methodological approach consists of three sections, as shown in figure 1. The data preparation section matches two different databases to derive individual EFs per power plant for the CO_2-emissions. The next section calculates the four dynamic EFs to describe the hourly behaviour of the German electricity system. The final step is the ESM-model to determine an economic and environmental dispatch for an ESS in industry.

3.1. Data Preparation

To derive hourly emission profiles of the German energy system, we combined information of two databases: The ENTSO-E transparency platform (ENTSO-E)[22] and the EU Transaction Log (EUTL) [23]. The first offers data on hourly generation profiles"per generation unit" in MWh. EUTL contains data from the European emissions trading system (ETS). It lists the verified emissions per year for every installation in the ETS in tonnes of CO_2.

The data preparation is threefold. First step, we match the ENTSO-E-generation units to the EUTL-installation IDs. The matching table is shown in Braeuer et al. [24].

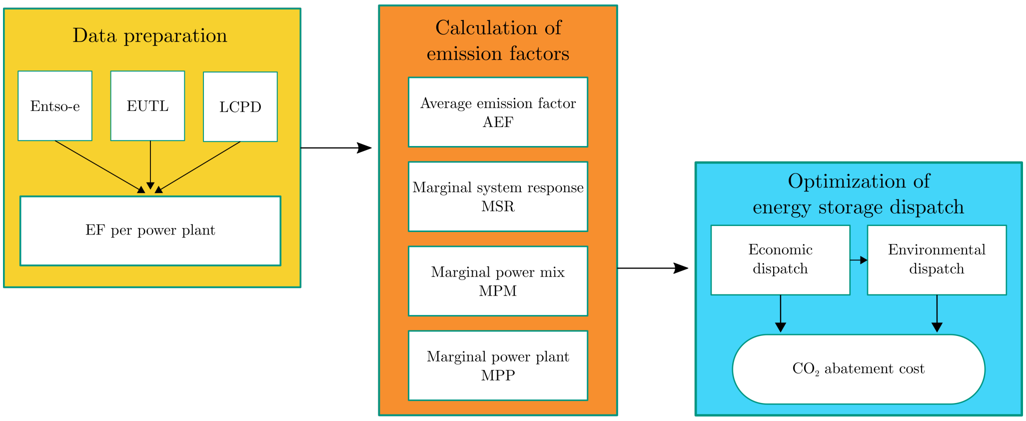

Figure 1: Illustration of the methodological approach

Second step, the total generation per year per power plant j is derived from the ENTSO-E-data and divided by the respective emissions per year per power plant derived from the EUTL-data. This results in the yearly average EF per power plant (EF_j), shown in equation 1. Last step, the EF_j is used to calculate the hourly emissions per power plant and eventually the hourly emissions of the German conventional energy mix ($m_{CO_2,t,j}$).

$$EF_j = \frac{m_{CO_2,j}}{E_{tot,j}} \tag{1}$$

$$L_{Res,t} = L_t - E_{RES,t} - E_{imp,t} + E_{exp,t} \tag{2}$$

Hourly load data is provided by ENTSO-E [22], as well as the generation of renewable energy sources (RES) and import/export balance. Equation 2 describes the resulting residual load without import and export ($L_{Res,t}$). Import and export is excluded due to a lack of data availability.

The matching of the two databases produce certain data inaccuracies. These are explained in the following paragraphs. First, it is not possible to match all generation units from ENTSO-E to an installation listed in EUTL. 6 out of 207 (2.9 %) of the generation units are not matched, which represents roughly 3 % of the total conventional energy generation in 2017. Furthermore, multiple generation units in ENTSO-E are listed under one single installation name in EUTL. In these cases, we estimate the theoretical share one generation unit has of the total CO_2-emissions of the entire power plant listed in EUTL. SI B further illustrates this approach. It concerns almost half of the generation units representing up to 60 % of the total conventional energy generation.

Additionally, there is a divergence between the hourly profiles listed in ENTSO-E [22] and the monthly domestic values for the generation per fuel type[22]. For fuel types with a high number of smaller generation units like waste and run-of-river plants, it can be explained by the fact that the hourly profiles list only large generation units. Nonetheless, the values for electricity generation from lignite and nuclear power plants differ in average over the year between 2% and 4% and for fossil hard coal with 13%.

Finally, missing values for verified emissions as well as unreasonable high EFs per power plant greater than 2 t/MWh diminish the data quality further[1]. For compensation, these values are manually adapted, see SI B.

3.2. Calculation of EFs

For the analysis in this study, we apply four different emissions factors.

1. Average EF (AEF)
2. Marginal system response (MSR)
3. Marginal power mix after [16] (MPM)
4. Marginal power plant (MPP)

The AEF is described in equation 3 [20, equation 2] as the sum of the CO_2-emissions of all power plants j over the total energy production of all power plants in period t. Therefore, AEF_t represents the average emissions in period t.

$$AEF_t = \frac{\sum_j m_{CO_2,t,j}}{\sum_j E_{t,j}}, \forall j \in J, t \in T \tag{3}$$

$$MSR_t = \frac{\sum_j m_{CO_2,t+1,j} - \sum_j m_{CO_2,t,j}}{L_{Res,t+1} - L_{Res,t}}, \forall j \in J, t \in T \tag{4}$$

The second factor is the *MSR*. It describes the reaction of the energy system in CO_2-emissions as the sum of emissions of all power plants ($m_{CO_2,j,t}$) to a change in the residual load (L_{Res}) from hour t to hour t+1, see equation 4. The *MPM* is derived from the work of Hawkes [16]. Over the course of one year, he assumes that the energy system reacts similar in every hour of the day. Analogous to Hawkes [16] for every hour of the day h, we build a linear regression model consisting of 365 samples. The slope of the hourly regression line is defined as the *MPM*[2]. Finally, the *MPP* results from a European electricity market model [25] and resembles the EF of the last accepted power plant on the wholesale market. To replicate the historic dispatch, generation availability and load levels have been scaled to match the values reported by ENTSO-E monthly domestic values. Additionally, outages for generation units and transmission elements have been implemented as reported by the e-transparency platform. Efficiencies are derived by age and technology of the power plants and for EF calculation we distinguish between full-load and part load operation. For part-load operation, efficiencies are reduced according to the regression formula reported in Brouwer et al. [26]. Thus, we obtain an effective EF depending on the ratio of power output and installed capacity for each marginal power plant in every hour.

For this study and the case of Germany, we only consider dispatchable production units as part of the power mix that actively react to changes in energy demand. Based on Graf and Marcantonini [27], Spork et al. [20], we describe these units in table 1. Thus, we exclude the output of the majority of RES. The German energy system prioritizes

[1]The issue might partly result from the fact that, for combined heat and power (CHP) units, all emissions for heat and power generation are accounted to the electricity sector as well as possible start-up procedures, where the power plant is not yet connected to the grid.

[2]Further elaboration see SI F.

the dispatch of renewable energy sources. The only reason to curtail renewable energies is due to grid congestion. Therefore, RES are (in the given system) rarely the marginal production unit.

3.3. Energy storage model

The ESM is based on Braeuer et al. [15]. The model identifies the optimal investment in an ESS for an industrial company to minimize cost for electricity. In line with the key findings of Braeuer et al. [15], this study only considers peak shaving as the most profitable business case for industry. Additionally, this study extends the model to minimize the CO_2-emissions.

The optimization is divided into two steps. The first step identifies the economic optimum for the ESS capacity and dispatch. The objective function f in equation 5 [15] minimizes the grid charges, the product of the yearly peak load (P_{peak}) and the price for the peak power (p_{peak}), along with annuity payment for the ESS (A_{ES}). For further explanation see SI C.

The second step of the optimization identifies the optimal environmental dispatch. A few equations from the economic optimization in Braeuer et al. [15] need to be altered. The objective g in equation 6 minimizes the total CO_2-emissions for one year in hourly resolution due to the resolution of the emissions data basis. The total CO_2-emissions are the sum of the product of the electricity from the grid ($x_{el,t}$) and the respective EF (EF_t). We fix the capacity of the ESS to the size in the economic optimization, equation 7 to allow for a direct comparison of the ESS's utilization between the economic and environmental dispatch. Moreover, the yearly peak load in the environmental dispatch cannot be greater than in the economic dispatch, equation 8. This constraint is needed to answer the question if idle capacity of the ESS could be utilized to lower the CO_2-emissions without infringing the economic goals of the peak shaving business case.

$$minf, f = P_{peak} \cdot p_{peak} + A_{ESS} \tag{5}$$

$$ming, g = \sum_{t=1}^{8760} (x_{el,t} \cdot EF_t) \tag{6}$$

$$cap_{ESS,econ} = cap_{ESS,envir} \tag{7}$$

$$P_{peak,econ} \geq P_{peak,envir} \geq x_{el,t} \tag{8}$$

3.4. Performance indicators for the environmental dispatch

For the evaluation of the environmental dispatch, we consider a variety of indicators. Equation 9 defines the amount of avoided CO_2-emissions between the economic and environmental dispatch ($\Delta CO_{2,i,k}$). It is the sum of the consumed electricity (x_{el}) for an economic dispatch (*econ*) minus the electricity for an environmental dispatch (*envir*) multiplied by the respective EF_k over all time steps t. It is calculated for all companies i and all EFs k. Equation 10 describes the utilization factor u_{cap}, which is a measure for how much CO_2-emissions can be avoided by a storage system with a capacity of $1\ kWh$. Equation 11 describes the CO_2-abatement cost as the fraction of additional costs for electricity consumption compared to the economic dispatch and the avoided CO_2-emissions. Finally, equation 12 describes the number of full cycles per day.

$$\Delta CO_{2,i,k} = \sum_{t=1}^{T} \Big((x_{el,i,t,econ} - x_{el,i,t,envir}) \cdot EF_{t,k} \Big), \forall i \in I, k \in K, t \in T \tag{9}$$

$$u_{cap,i,k} = \frac{\Delta CO_{2,i,k}}{cap_{stg,i,k}} \tag{10}$$

$$C_{abat,i,k} = \frac{C_{el,i,envir} - C_{el,i,econ}}{\Delta CO_{2,i,k}} \tag{11}$$

$$cycle_{day,i,k} = \frac{charg_{stg,i,k}}{cap_{stg,i,k}} \cdot \frac{1}{LT \cdot 365} \tag{12}$$

4. Application of the method

The evaluation is divided into 3 analytical steps. First, we compare the four different EFs. Second, we evaluate the dispatch of a generic storage system (GSS). The GSS is used to investigate the CO_2-reduction potential of a storage system without restricting cycle life conditions and a high efficiency of 98%. Third, we analyze the optimal dispatch of a battery storage system (BSS) with constraining cycling conditions, 4000 cycles and 90% efficiency.

4.1. Emission factors

As discussed in previous works, the four EFs differ significantly in both magnitude and volatility and thus produce different at times contrasting signals about the CO_2-intensity of the energy mix. Fig 2 shows the EFs for the week from July 10 to July 16, 2017, in the German electricity mix. Also shown is the electricity generated per timestep and fuel type. AEF, MSR and MPM are derived using empirical data from ENTSO-E [22], while the MPP is the result of the EEMM.

The depicted week is a good example to illustrate the qualitative differences between the considered factors. The AEF ranges between 0.46 kg_{CO_2}/kWh and 0.86 kg_{CO_2}/kWh, being the lowest when the share of technologies with low emissions is the highest. For the German power system, this is the case when a large amount of generators are dispatched and the cheap lignite power plants are complemented by relatively low emission technologies like hard coal and gas. The AEF gets larger when the share of technologies with high emissions increases. This is the case when either the amount of lignite increases in almost-all-renewable hours or when the residual load decreases and gas and hard coal fired power plants cease operation. It can be observed in Figure 2 that the AEF is the lowest when total generation reaches its peak illustrating the described connection. With respect to a signaling effect for CO_2-reduction, the AEF provides a clear signal for hours of a high EF and hours of a low EF. However, as discussed in the literature review, it is questionable if the AEF is suited to indicate the additional emissions caused by an incremental increase in the electricity demand. Naturally, such an increase will not be answered by the power plant mixture but by an individual plant or a small group of plants.

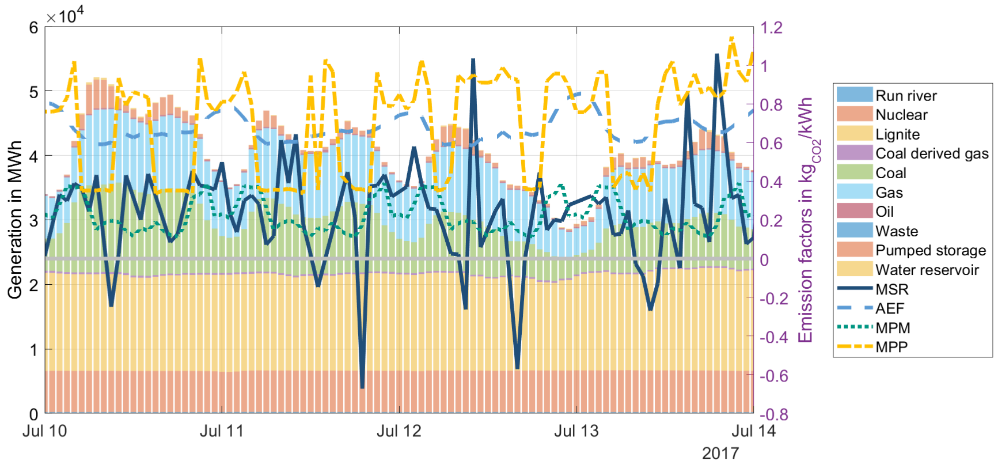

Figure 2: Hourly generation and EFs in week 28, 2017

The MPM shows by definition a periodical behaviour. It is notably lower than the AEF at all times. The MPM is based on a linear regression of the system response to shifts in generation and load and thus it represents a typical response. Therefore, this factor is most appropriate in hours which are least impacted by volatile renewable in-feed. This becomes more clear when looking at the value of the measure of determination (R^2) for the different hours of the day. Here, the MPM performs best in the night hours, when generation is at minimum load of many power plants and each shift in load is matched by a classic reaction of the power system. Nonetheless in hours where more flexible power plants are utilized, only the residual load has to be matched. Thus, the reaction of the power system is highly dependant on renewable in-feed. This results in very low R^2-values in the middle of the day (see Figure F.3). Moreover, the MPM reaches a local minimum when the AEF is at a local maximum. This can be observed regularly at the change of day. Due to its periodic behaviour it offers a well foreseeable potential for the use of flexibility, because the CO_2-EF for each time step is known in advance.

Similarly, the profile of the MPP implies a periodical behaviour. The MPP is not derived from empirical data since the data are insufficient to determine which power plant is marginal in each time step. Therefore, the EEMM determines the MPP, which represents the CO_2-EF of the marginal generation unit. The individual CO_2-EF of the marginal generation unit depends on the commissioning year and the technology. In many hours of high loads, the MPP is low as the marginal generation units are gas-fired power plants. In these hours, power plants with higher CO_2-emissions like lignite and coal are fully dispatched. These hours of low MPP-values coincide in many cases with low AEF-values. Simultaneously, hours of high MPP-values indicate low load in the system or a high share of renewable generators. The incremental energy demand increase is answered by a lignite-driven or coal-driven power plant. Again in many cases, hours of a high MPP coincide with hours of a high AEF. Exemptions can be observed in hours of relatively high renewable in-feed and relatively low loads. In these hours, most generators reduce their electricity output to their minimum must-run condition. In these cases, the MPP jumps between very high values, when lignite is the marginal fuel type, and values equals to zero when nuclear power plants or run-of-river plants answer the incremental increase in energy demand.

The MSR on the other hand is the most extreme factor by all means. With a standard deviation of 304.1 kg_{CO_2}/MWh it is by far the most volatile EF also reaching the global maximum and global minimum of all factors. Most striking are the negative values, which are not trivial to explain. Taking a closer look at the formulation, this can only occur when either the residual load is reduced but system emissions increase or vice versa, which seems not intuitive. We attribute this to the effect of ramping constraints, when slower power plants power up or down for the next/last hour without necessarily being directly connected to the change in residual load. However, the MSR offers the largest potential for CO_2-reduction due to the number and magnitude of peaks and valleys, which allow many adjustments within on day. The Table 2 shows the mean, minimum, maximum and standard deviation of the four EFs considered for the whole year.

4.2. Generic storage system

Table 3 shows the statistical values of the performance indicators. These are the statistical results of the optimization runs for the 50 companies. One can observe significant differences between the possible CO_2-reductions (ΔCO_2) of the four EFs. Hence, the mean values for ΔCO_2 range between 6.81 t for the AEF and 86.25 t for the MSR, which is 12 times as much. One explanation for different mean values, is the number of daily cycles. The number of daily cycles is very different for the considered EF and the respective company. In average, the AEF allows for 2 full cycles per day with only minor variation between the companies, the coefficient of variation is 7 %. The values for MSR, MPM and MPP are considerably higher with a mean value for the number of daily cycles of up to 5.41 and the coefficient of variation ranging between roughly 19 % and 21 %. This indicates that the MSR, the MPM and the MPP have a higher frequency of peaks and valleys compared to the AEF. Simultaneously, the companies have deviating potentials to exploit these spreads in the hourly EF. The coefficient of variation of ΔCO_2 is similar for all applied EFs. Therefore, the deviation in reduced CO_2-emissions for the different companies is similar for all EFs. To get a better understanding how the different EFs influence the environmental dispatch of the individual companies, we consider the utilization factor of the installed storage capacity (u_{cap}). In line with ΔCO_2, it shows that the level of possible CO_2-reductions per installed capacity vary widely. Nonetheless, the coefficient of variation presents different values for the respective EF. The coefficient of variation is the lowest for the AEF and the highest for the MSR. This shows that the dependency of the utilization factor on the individual load profile is low for the AEF, coefficient of variation is 10 %, higher for the MPP, MPM and MSR, 15 % to 22 %.

Considering the CO_2-abatement costs (C_{abat}), the MPP shows mean values in the range of current ETS prices of around 25 €$/t_{CO_2}$ (September 2019) and the MSR shows considerably lower mean values. With values around 62 €$/t_{CO_2}$, the AEF and MPM present notably higher results. With fixed electricity prices, the additional costs for CO_2-abatement are a result of efficiency losses during charging and discharging processes.

Concerning the coefficient of variation with values around 4 %, C_{abat} of the sample companies are fairly concentrated for the AEF and the MSR compared to the other EFs. This implies a weaker dependency of C_{abat} on individual load profiles. For the AEF, this can be explained by the low frequency of peaks in the EF and the resulting low number of cycles. In addition to a comparably small spread between the minimum and maximum value of the AEF, this does not allow for a high divergence among the companies. The low coefficient of variation for the MSR is somehow surprising as one can observe high variation among the companies considering the other three indicators. This might be a result of the extreme outliers of the MSR. The values of the C_{abat} following the MPP deviate the most, which implies a stronger dependency on the individual load profiles.

To further illustrate the above mentioned effects, Figure 3 compares the company 45 and company 46 showing the storage dispatch for the MSR. The figures show the load profile, the charging and discharging profile as well as the SoC on the left axis. The right axis indicates the respective EF. The horizontal dashed-dot lines indicate the maximum peak load that has to be achieved through peak shaving. All for two consecutive sample days, February 15th (Wednesday) till 17th (Friday) 2017.

While the two sample companies have a similar peak load level (translated into maximum energy per 15-minute interval, company 45 with 327 kWh and company 46 with 370 kWh) as well as comparable optimized storage capacities (company 45 with 219 kWh and company 46 with 319 kWh), the load profiles are fairly different. Company 45, an iron casting company, shows very high singular peaks of more than 300 kWh followed by periods of low energy demand, not more than 20 kWh. Sample company 46, a manufacturer of mixed spices, shows five peaks per day of up to 400 kWh. The lowest load during these sample days is around 80 kWh. Thus, the load profile of company 46 allows for discharge of the storage system in low load periods. Compared to company 45, this leads to CO_2-shifting during these periods. Thus, company 46 has a higher utilization factor than 45. This has no strong effect in case of the AEF, see Figure D.2, where the low frequency of the EF peaks results in two daily cycles. In Figure 3, one can observe a high correlation between the MSR and the load profile of company 46, which allows for a high utilization of the storage system. Still, for example between 6 am and noon on the 15th, the full CO_2-reduction potential cannot be reached as hours of a low MSR and a high load overlap. During these hours, charging is restricted due to peak shaving. Considering MSR, MPM and MPP, the GSS of company 46 is charged two times more than the GSS of company 45.

For further illustration of the environmental dispatch for all four EFs, we refer to Figures D.1 and D.2 in SI D.

4.3. Battery storage system

In this subsection, the model constraints were adapted to fit the real life setting of a BSS. The BSS cycle life is restricted to 4000 cycles over 11 years, which is equivalent to one cycle per day. Additionally, the charging and discharging efficiency is reduced to 90 %. This affects the environmental dispatch substantially compared to the GSS. Table 3 shows in the two BSS-columns on the right the statistical evaluation of the optimization results for an environmental dispatch following the MSR and the MPP. The table indicates that the possible ΔCO_2 is much lower for a BSS than for a GSS. The mean value of all 50 companies for a BSS is around 38 % of the mean value for the GSS following the MSR. Following the MPP, it is around 48 % of the GSS value. Partly, this great reduction is the result of the restricted cycle life. For both EFs, all 50 companies fully exploit the cycle life and reach 1 cycle per day. Next to the reduced cycle life, the lower efficiency of the charging process lowers the utilization factor of the BSS. A round-trip efficiency of 81 % results in a spread in an EF of more than 29 % that is needed for

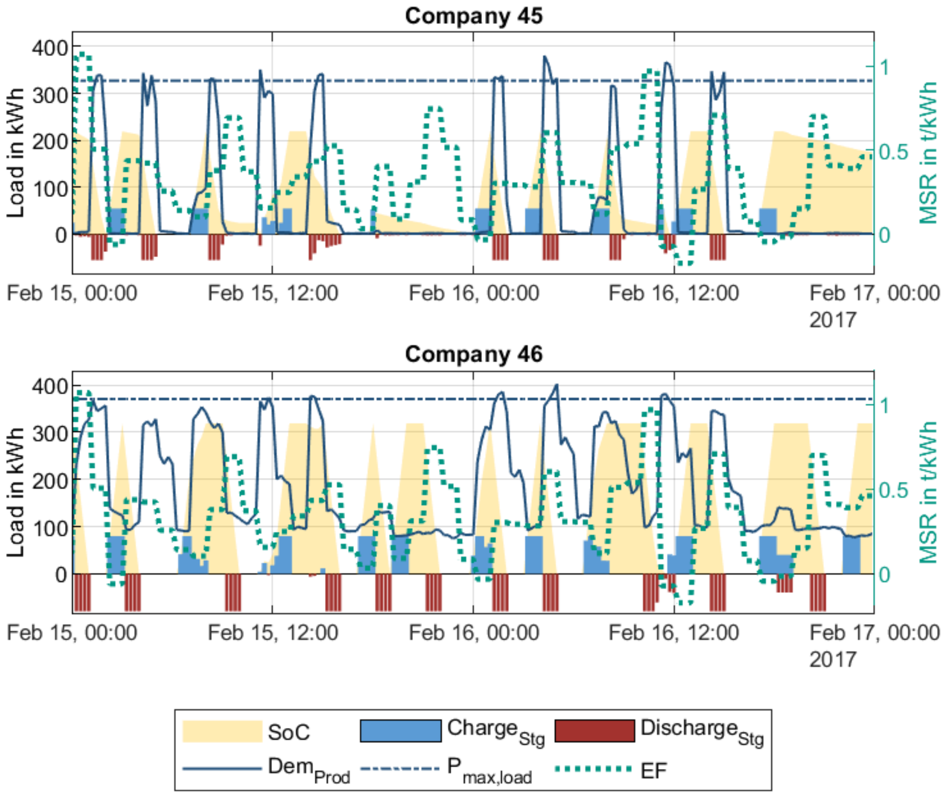

Figure 3: Comparing load and charging profile of company 45 and company 46 for 2 days, showing the MSR

the model to choose a CO_2-shifting dispatch. Figure 4 further illustrates these effects. The figure shows the environmental dispatch of a BSS for the MSR and the MPP for company 46. Compared to the GSS, the optimal peak load increases by roughly 6 % and the optimal BSS capacity is with 205 kWh around 21 % smaller than the GSS capacity. Considering Figure 4, only the highest spreads are utilized for CO_2-shifting due to the restricted life time. In the MSR-graph, the BSS is charged during a period of a negative MSR value and discharged during hours of an MSR around 1 t_{CO_2}/kWh. During the next charging phase, noon of February the 16th, the spread between the low MSR and the high MSR is not large enough for the BSS to be charged. For the MPP, the BSS is charged while a nuclear power plant is the marginal generation unit with a MPP-value of 0 t_{CO_2}/kWh and discharged while a lignite driven power plant is marginal. As such occurrences of spreads larger than 1 t_{CO_2}/kWh are fairly rare, the model chooses to charge the BSS in hours of a coal-driven marginal power plant, around 0.7 t_{CO_2}/kWh.

In case of the environmental dispatch no additional degradation effects are considered. Nonetheless, results show that CO_2-shifting coincides with very high c-rates. Additionally, to fully exploit the CO_2-reduction potential, the results indicate very high depths

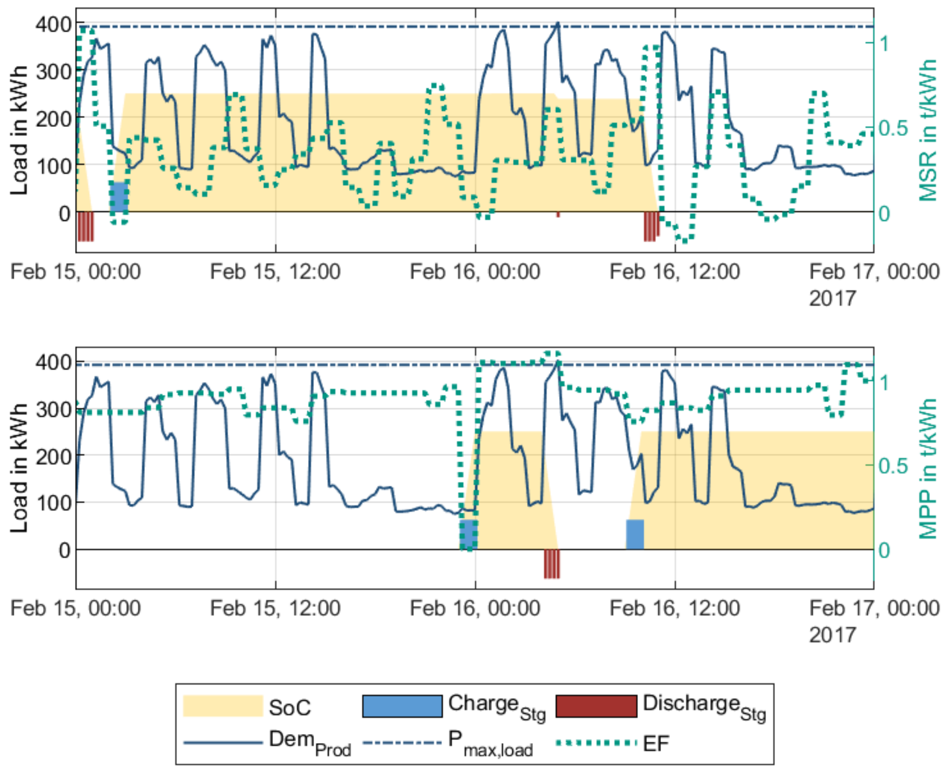

Figure 4: Load and charging profile of a BSS for company 46 for 2 days

of discharge for a CO_2-reducing dispatch. Both effects have a strong influence on the premature aging of a BSS resulting in premature capacity losses.

5. Discussion and outlook

5.1. General methodology

This contribution employs two energy system models based on linear programming, one taking a micro-economic perspective for an individual company (ESM) and one taking a macro-economic perspective for Germany and surrounding countries (EEMM). Both of these models suffer from common limitations of linear optimization models, which for these particular instances are discussed elsewhere [15] and [25]. The remainder of this subsection therefore concentrates on the methodological focus of this paper, namely on the definition and analysis of different emissions factors for integrated electricity systems.

Data input. As described in the section Data Preparation, this study introduces a novel data basis to allocate CO_2-emissions to the respective hourly energy generation of power plants. We provide a solution to overcome the missing matches between EUTL account holders and generation units in the ENTSO-E database. Yet, the deduction of hourly CO_2-emissions factors from the yearly verified CO_2-emissions remains a source of inaccuracies. To increase the robustness of the data, a larger number of years could be used. Additionally, with information about the individual part-load behavior of the generation units, it would be possible to estimate a part-load dependent EF. Without detailed knowledge about CHP units and their respective dispatch logic, how much heat is generated and sold, the data accuracy remains weakened.

General EF-approach. The results indicate that the four different EFs considered have different signaling effects for an environmentally-oriented dispatch.

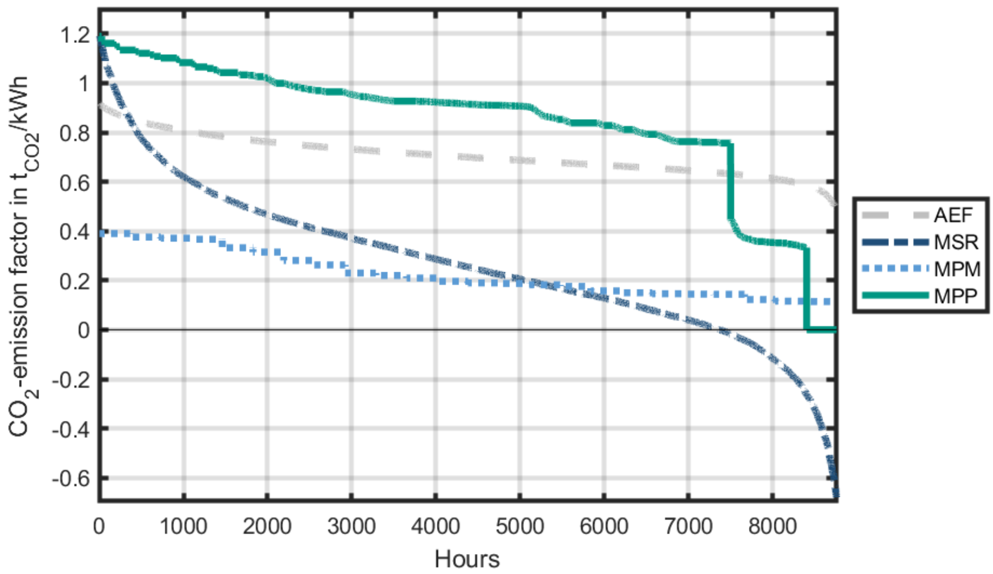

Figure 5: Annual sorted duration curve of the EFs

In addition to Table 2, based on the annual sorted duration curve for the four EF approaches in Figure 5, it is possible to reach some general insights. Firstly, the overall range of the factors is comparable for all methods, with the exception of the MPM, which is much lower than the others. This is due to the fact, that the hourly linear-regression model insufficiently approximates hourly CO_2-emissions changes. In addition, the differences in the extrema of the different factors are clearly visible.

AEF and MPM show an averaging effect, the AEF due to the large number of different technologies, the MPM due to the large number of hours per time-step. Both duration curves show a smaller range between the extrema then the MSR and MPP, which aim to describe the marginal reaction of the system and are more responsive to the CO_2-intensity of single technologies.

Furthermore, the number of hours with high and low CO_2-intensity are clearly visible in contrast to the weekly graph in Figure 3 and Figure 4 where the focus lies on volatility. The MSR and the MPP present a relative high number of extreme hours compared to the other two EFs. This high number together with high volatility strongly impacts storage dispatch decisions. Finally, the "drops" between marginal technologies are only visible in the MPP as this EF is technology specific. In contrast, the other EFs resemble the system's reaction.

Concerning the four different EF, we follow a production-based approach. For an energy system the size of Germany's, we assume a negligible influence of imported and exported energy flows. This is in line with the findings of Pareschi et al. [28], but this simplification can still be challenged. An exception is the MPP, where market coupling is explicitly included in the model and the selection of the MPP thus also depends on the level of exchange with neighbouring countries.

Related to the above point, the marginal approach adopted for all of the EFs is only valid for small samples at the margin. In the case that a large number of consumers adopt electrical storages and implement the business models analyzed here, they will cease to be marginal. In other words, they will cease to be price takers and will become price setters, in this context affecting the marginal emissions factors that they are employing. This therefore needs to be borne in mind when analysing these dynamic emissions factors for a large number of distributed consumers. If all 50 companies would apply the optimized environmental dispatch the maximum load change would range around 5 MW.

AEF. This study analyzes the dynamic change in load and the energy system's reaction based on four EF approaches, which only consider the dispatchable generation units. In other words, the non-dispatchable generation is exogeneously fixed and defined by historical generation and feed-in profiles for renewables. This leads to an AEF that deviates from existing studies, whereby the AEF shows two peaks per day. However, the exclusion of RES as non-dispatchable units results in high values for the AEF in hours with a large share of RES in the system and vice versa. This is contrary to existing studies, which include RES into the AEF and indicate low values during periods of high RES share.

MSR. To identify the system's reaction, we postulate the EF MSR, which is oriented towards Hawkes [16]. This approach has obvious shortcomings, as it yields negative values in some hours, which is due to changes of load and emissions in opposite directions. This is counter-intuitive for the energy system in the year 2017 and as long as renewable energy sources are considered as non-dispatchable. An explanation could be a high share of CHP-units with uncertain heat production and ramp-up processes in hard-coal and lignite power plants. Additionally, a reaction of the generation units too small to be listed in the ENTSO-E data base is not accounted for by the MSR.

MPM. The evaluation of the MPM, the approach by Hawkes [16], might not be fit to describe the German energy system in 2017. Hawkes [16] focuses on the British energy system until 2009. With a higher share of volatile RESs, it seems no longer suitable to assume a reoccurring behavior of the electricity mix for one representative day over one year. In Figure F.8, this study does not show sufficient values for the coefficient of determination for the hourly resolution. Thus except for three hours in the morning, the load change in one hour of the day (independent variable) is not sufficient to approximate the change in CO_2-emissions (dependent variable).

MPP. The model-based EF MPP appears to be most suitable to evaluate the effect of an increase in electricity demand. Nonetheless, because of the conformity issues of model results it lacks comparability to other energy models and possibly to reality. In reality, there might be additional operational constraints not fully implemented in the EEMM. Moreover, the dispatch of power plants might be subject to portfolio optimization of the owner's fleet with different or even changing objectives. In return, this makes it very hard to identify an individual power plants, which would react market-wise to the change in demand implied by the flexibility provider.

5.2. Comparison with other studies

In this section, we briefly compare our results with the literature. Near-real time and historic EFs for Germany are available from Agora Energiewende [29]. The data on power generation is also based on ENTSO-E publications, while EFs are fuel specific based on Icha [30]. Emissions are only accounted for the generated power in Germany ignoring imports but also accounting for exported energy. This assumption is in line with our presented approach. However, Agora Energiewende [29] include renewable energy sources in the calculation. Nonetheless, our presented approach is more detailed as we provide a mapping table for actual emissions reported to EUTL and power generation reported by ENTSO-E.

In contrast to our approach, Wörner et al. [31] consider the life cycle emissions of each technology and Tranberg et al. [32] include CO_2-emissions of the complete fuel chain. The former base the technology specific emissions on the ProBas database, the later base the fuel specific emissions on ecoinvent database; calculations outside the scope of our article, as we consider generation-based EFs. However, the results in [31] show that the inclusion of life cycle aspects only produce an offset in the CO_2-factor and have little qualitative impact on the dynamic EFs.

Furthermore, Wörner et al. [31] present a representative winter and summer week for which the EFs of our current article compare as follows: in the characterized winter week our methodology leads to more volatile factors following more closely the load patterns of the day and also quantitatively higher than described by Wörner et al. [31]. We find the same effect of the summer week having significantly lower EFs than the winter weeks. We attribute this to the lower amount of residual load because of higher solar intensity. Apart from the two weeks a comparison is unfortunately not possible.

Tranberg et al. [32] present a real-time carbon accounting method for the European electricity markets. The average CO_2-intensities are specific for each generation technology, thus neglecting the merit order within fuel types as well as must-run or part-load operation. The analysis is based on commercial data from electricitymap [33], so we were not able to compare the results.

Deetjen and Azevedo [34] chose a different approach, by developing a simplified merit order model. The data sources are specific to some US power markets. They address ramping constraints by explicitly modelling constraints in the dispatch model. While their definition of dynamic emissions is similar to our MEF, their proposed moving average approach is a deviation to our methodology. A comparison to our results is not possible due to the different geographic scope of the articles.

5.3. Outlook

The results of the study implicate that rewarding environmental dispatch could incentivize industrial companies to exploit their load flexibility options. At the same time, the utilization of a BSS for the reduction of CO_2-emissions does not seem practicable. However, there might exist other technologies and measures for industrial companies that offer flexible electricity demand with higher efficiencies and longer lifetime than a BSS.

While the time series of the estimated EFs for the current energy system can be intuitively explained, the results of this study indicate the challenges for future studies. As the AEF presents a more inert behaviour than the MPP, one can still identify a correlation between the value of the EF and the share of RES in the system. However, for a few hours in 2017 the share of RES was so high that nuclear power plants became the marginal generation unit. While this does not influence the AEF, it results in a jump of the MPP from the minimum value in case of a nuclear driven power plant to the maximum value for lignite. In future cases with increasing shares of RES and dispatchable RES, such situations might occur more regularly. Operating hours of formally base-load generation units such as lignite power plants are decreasing. To apply the proposed methodology in such a case, we need to obtain a more detailed knowledge about the must-run conditions and other operational constraints of conventional generators as well as dispatchable RES. This becomes increasingly important, since they may determine the plants dispatch. Furthermore, the coal-phase-out potentially changes the merit order on the energy market and leads to an almost binary EF (zero for RES and positive for the remaining conventional power plants, mainly gas). Increasing prices for CO_2-certificates may lead to a fuel switch, which would result in an alignment of production cost and CO_2-intensity in the merit order, making a signalling function of EFs redundant.

In addition, the regional aggregation level influences the conceptual approach. Considering smaller regions such as autonomous municipalities or congested electricity grid nodes, introduction of sophisticated regional electricity prices could help to reduce regional emissions. Such prices should orient on dynamic EFs. In these cases, the effect on the non-CO_2-emissions, which mostly have a local effect, should be considered. SI E expands the methodology to estimate the EFs for other emissions SO_2, NO_x and Dust.

Based on the foregoing discussion, the following recommendations for further work can be given:

- improve method for calculating hourly values based on European Pollutant Release and Transfer Register (E-PRTR) [35] and EUTL data
- improve modelling of part load and must-run capacities etc.
- extend the validation of the method based on measured/empirical data for power generation and CO2 emissions
- further assess the CO_2-reduction potential of BSSs, combining the economic and environmental objectives
- further develop such an approach to a more local/regional context, which may operate in partially off-grid mode with regional markets and prices
- extend the consideration of micro-economic and macro-economic aspects in more integrated framework to overcome the lavine/snowball effects that might be encountered.

6. Summary and conclusions

As one possibility to increase flexibility, battery storage systems will play a key role in the transition of the energy system. From an economic point of view, BSSs have been studied and proven in a variety of business cases. How storage system can help to reduce the CO_2-emission of an energy system by flexibly shifting the load is still an open question. In this paper, we introduce a novel data basis for the determination of the energy system's emissions. This is a match between the ENTSO-E database and the EUTL database. Furthermore, we postulate four different dynamic EFs to determine the hourly emissions caused through a change in electricity demand. This is the average EF, the marginal power mix, the marginal system response and the marginal power plant. The signaling effect of these EFs are tested for a storage system combined with an industrial load. We differentiate between a generic storage system, which might be applicable to a variety of technologies offering flexibility, and a specific battery storage system. The linear optimization is divided into two levels. On the first level, the optimization determines the size and economic dispatch of the storage system considering peak-shaving. The second level finds the environmental optimum by minimizing the emissions of the electricity drawn from the grid for the respective EF. The results of the four EFs are statistically evaluated for a set of 50 small and medium sized companies in Germany.

The four different EFs have different signaling effects for an environmental storage dispatch. The AEF and the MPP lead to a similar CO_2-reduction and allow for roughly two cycles per day for the generic storage system. The MSR and MPM show a higher volatility, which leads to a higher utilization of the storage system. For the single companies, peak shaving is prioritized over CO_2-shifting. Therefore, if a high portion of the storage system is used for peak shaving the CO_2-reduction potential is low. Furthermore, a high correlation of the load profile and the profile of the hourly EF supports high CO_2-reduction. Similar to an arbitrage trading dispatch, the charging behavior of an environmental results in high levels of additional degradation of the BSS.

To further assess the CO_2-reduction potential of BSSs, future research needs to focus on combining the economic and environmental objectives as well as assessing local/regional energy systems. In addition, future research needs to increase the robustness of the marginal EFs. For this, supplementary information about the behavior of CHP-plants and ramp-up process of hard-coal and lignite plants should be included in the data basis.

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8. Conflict of interest

The authors declare no competing interests.

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Nomenclature

Acronyms		*Symbol*	
AEF	average emission factor	ΔCO_2	avoided CO_2-emissions
BSS	battery storage systems	C_{abat}	CO_2-abatement cost
CHP	combined heat and power	C_{el}	cost for electricity
EEMM	European electricity market model	cap_{stg}	capacity of storage
EF	emission factor	$charg_{stg}$	energy charged in storage per year
entso	ENTSO-E database	$cycle_{day}$	full daily cycles
ESM	energy storage model	E	energy
ESS	energy storage system	EF	emission factor
ETS	emission trading system	L	load
EUTL	European Union Transaction Log	LT	life time
GHG	greenhouse gas	m_{CO_2}	mass of CO_2
LCPD	Large Combustion Plants Directive	u_{cap}	utilization factor
MEF	marginal emission factor		
MPM	marginal power mix	*Index*	
MPP	marginal power plant	exp	export
MSR	marginal system response	h	hour of a day
RES	renewable energy sources	i	company
SME	small and medium sized enterprises	imp	import
		j	power Plant
Variables and parameters		k	emission factor
A_{ESS}	annuity for ESS [€]	Res	residual
$cap_{ESS,econ}$	capacity of ESS of economic dispatch [kWh]	RES	renewable energy sources
$cap_{ESS,envir}$	capacity of ESS of environmental dispatch	t	hour of the year
P_{peak}	peak power from grid per year [MW]	tot	total amount per year
p_{peak}	peak price [€$/kWa$]		
$x_{el,t}$	electrical energy flow [kWh]		

Table 1: Dispatchable production units by fuel type

Fuel type
Nuclear
Fossil Brown coal/Lignite
Biomass
Other
Waste
Fossil Hard coal
Fossil Oil
Fossil Coal-derived gas
Fossil Gas

Table 2: Characteristics of the EFs

	CO_2 *in* kg_{CO_2}/MWh			
	AEF	MSR	MPM	MPP
Min	486.5	-679.1	114.2	0.0
Max	915.6	1190.3	390.1	1189.8
Mean	707.5	268.1	224.1	840.2
Std	76.1	304.1	90.4	267.0
Varcoef	0.1	1.1	0.4	0.3

Table 3: Statistical overview of results

			GSS				BSS	
		Unit	AEF	MSR	MPM	MPP	MSR	MPP
ΔCO_2	Min	t	0.29	4.33	0.76	1.43	1.88	0.82
	Max	t	82.75	1038.37	201.72	371.68	344.98	153.49
	Mean	t	6.81	86.25	16.58	30.99	32.92	14.78
	Varcoef	%	187	188	189	186	2	2
u_{cap}	Min	kg/kWh	45.54	372.58	86.51	182.26	341.91	154.99
	Max	kg/kWh	74.99	1109.66	194.47	366.27	443.01	194.32
	Mean	kg/kWh	68.08	861.89	165.39	310.76	411.65	185.61
	Varcoef	%	10	22	16	15	0	0
C_{abat}	Min	€/t_{CO_2}	53.33	11.86	46.61	16.73	26.38	58.48
	Max	€/t_{CO_2}	65.05	14.60	72.33	27.23	34.20	75.44
	Mean	€/t_{CO_2}	61.77	14.13	63.55	24.26	28.26	62.63
	Varcoef	%	4	4	10	11	0	0
$cycle_{day}$	Min	#	1.59	2.57	2.32	1.88	1.00	1.00
	Max	#	2.23	6.80	5.99	4.25	1.00	1.00
	Mean	#	2.00	5.41	4.73	3.46	1.00	1.00
	Varcoef	%	7	21	20	19	0	0

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