Ideal-Typical Utility Infrastructure at Chemical Sites – Definition, Operation and Defossilization

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The defossilization of the electricity and heat supply in the chemical industry poses a significant challenge. In particular, the intended feed-in of volatile renewable electricity into the chemical processes may conflict with the need for a constant, secure and affordable electricity and heat supply for chemical plants. Adapted concepts for the operation of the cogeneration plant, which is located at the chemical site, play a central role. The present work defines a so-called ideal-typical utility infrastructure (iUI). The iUI is a means to exemplarily investigate the operational behavior of utility infrastructures and furthermore to identify defossilization options for process steam and electricity supply at chemical sites.

Keywords: Chemical industry, Combined heat and power, Power-to-heat, Thermal energy storage

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1 Introduction and Overview of Flexibility Option Technologies

In the past, the focus in the chemical industry was mainly on efficiency improvements, whereas today's ambitious CO_2 reduction targets require changes beyond efficiency measures, e.g., use of "CO_2-free" gases. At the time of writing, typical chemical sites utilize mainly fossil sources. Hence, the reduction of CO_2 emissions is a fundamental challenge for the chemical industry. For example, Germany's greenhouse gas (GHG) targets for the chemical industry mandate GHG neutrality by 2045 [1]. The use of a significant amount of new renewable electricity via power-to-heat (PtH) in the processes is assumed as a key GHG mitigation measure. At the same time, the electricity demand for the chemical industry would increase by a factor of approx. 13 compared to the current value with extensive PtH use [2].

Fig. 1 shows a simplified scheme of a typical modern chemical site with the connection to the natural gas and electricity grid (left), the highly integrated end-use processes (right) and the on-site utility infrastructure including typically a combined heat and power unit (CHP, middle). The operation of the on-site utility infrastructure is typically adapted to process steam and electricity end-use demand. CHP, also called cogeneration, has a long tradition in the chemical and petrochemical sector because of numerous processes that require a large quantity of heat (mainly in the form of steam) and power that is efficiently provided by on-site CHP plants. A worldwide energy saving potential for efficient CHP in the chemical and petrochemical sector of 2 Exajoule was estimated. Therefore, along with other efficiency measures, an efficient CHP configuration is an important option for energy savings and CO_2 reductions in the chemical sector [3].

Most chemical processes in the production chain offer limited flexibility options. In order to operate the highly integrated processes efficiently, a continuous and secure supply of steam and electricity over the entire year is required. The identified flexibility options are limited in their potential. For example, the flexible operation of chlor-alkali electrolysis systems has been identified. However, there are disadvantages such as loss of production, additional investments in production capacity, lower thermodynamic efficiencies, and demanding storage solutions for chlorine products [4, 5].

Today, chemical sites are typically supplied by natural gas and electricity from transmission and local grids. Both

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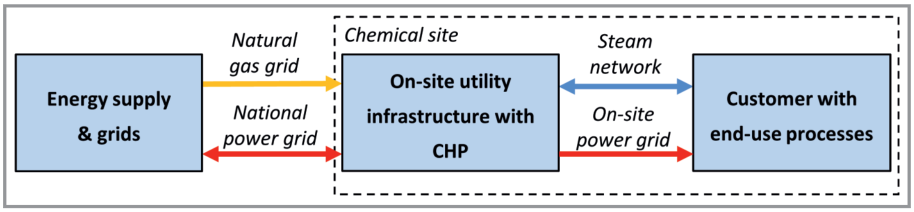

Figure 1. Simplified scheme of the supply structure of a typical modern chemical site.

sources have their own challenges. "CO_2-free" gas to replace natural gas is currently not available and is estimated to be more expensive (e.g., green hydrogen with 5.3 € kg^{-1} or 159 € MWh_{H2}^{-1} [6]). In addition, the chemical site faces potentially higher overall gas prices due to rising costs for CO_2 emission allowances. On the other hand, the CO_2 footprint of electricity is steadily decreasing with the expansion of renewable energies. For the chemical site, however, there are restrictions with regard to increasing electricity price fluctuations and the low availability of PV and wind power. On the demand side there is a remaining need of end-use processes to maintain a steady, secure, and affordable supply of steam and electricity (Fig. 1, right). This puts the utility infrastructure into focus. Ausfelder defines the boundary conditions and key figures of an ideal-typical utility infrastructure in the chemical sector and discusses the possibilities of using storage and renewable energy [4]. However, no previously published work could be identified that defines in detail an ideal-typical utility infrastructure (iUI) with all its components.

The main objective of this paper is to define an iUI with all components as well as to propose a methodology for studying the performance of this structure itself. Subsequently, the results of an optimized operation are presented to better understand and verify the operational behavior of the iUI. Finally, CO_2 reduction options within the utility infrastructure are qualitatively identified from literature sources and the acquired operational results.

2 Applied Methods

2.1 Definition of an Ideal-Typical Utility Infrastructure for Chemical Sites in Germany

The utility infrastructure of a chemical site consists mainly of an electricity distribution and a steam network at different pressure levels. Usually, a utility infrastructure has a connection to the public electricity grid as well as its own electricity production in form of on-site generators driven by gas and steam turbines. For the provision of steam at one or more pressure levels, a utility infrastructure typically contains heat recovery steam generators and natural gas fired boilers.

To make the results of this work and future studies applicable to many chemical sites, an ideal-typical utility infrastructure is defined. A proposal for such an iUI is outlined as a simplified block diagram in Fig. 2. The iUI was designed in close cooperation with Currenta and Covestro. Both companies operate chemical site supply infrastructures in Germany.

The main process unit is a gas turbine (GT) with a subsequent heat recovery steam generator (HRSG). The electrical output of the GT is equal to half of the average electricity demand of the end-use processes, depicted in the upper right corner of Fig. 2. In this way, the GT is able to achieve a high utilization. The HRSG comprises three steam generating stages: high-pressure (HP, 110 bar and 530 °C), medium-pressure (MP, 31 bar, 370 °C), and low-pressure (LP, 6 bar, 210 °C) steam. Steam temperatures within the iUI are higher than required for the end-use processes to improve the steam turbine (ST) efficiency. Thus, before steam is

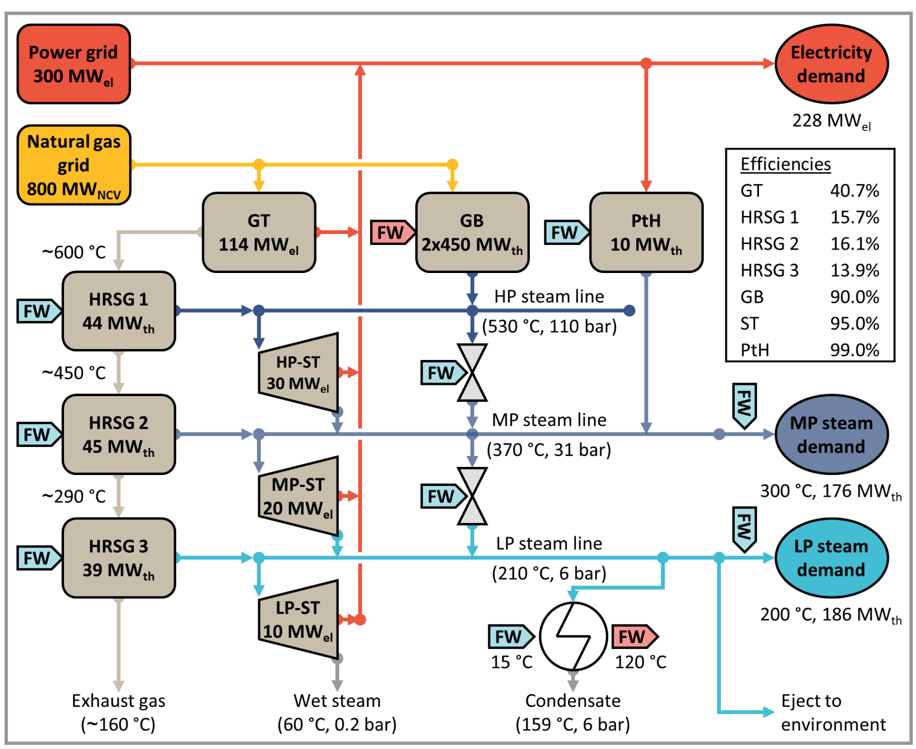

Figure 2. Simplified block scheme of an iUI for chemical sites.

delivered to the customers, pressurized water (feedwater, FW) is injected to reduce the temperature. The end-use processes require LP and MP steam. The average steam demands and temperature specifications are shown on the right side in Fig. 2 (for further details see Sect. 2.2). The HP steam line gives the iUI more potential for on-site power generation. The selected high-pressure steam specifications of 110 bar and 530 °C are within the typical parameter range of power plant-scale steam generators [7]. The performance of a process component is determined by the relation between efficiency, useful output and input. As long as two of these properties are defined, the third one is also fixed. In the following, the efficiency is always given as the ratio of the useful output to the input for better comprehensibility. The efficiencies of the GT and a single HRSG stage are defined as follows:

$$\eta_{\mathrm{GT}} = \frac{P_{\mathrm{el,GT}}}{\dot{m}_{\mathrm{NG,GT}} NCV} \tag{1}$$

$$\eta_{\mathrm{HRSG}} = \frac{\dot{m}_{\mathrm{FW,HRSG}} \left(h_{\mathrm{St}} - h_{\mathrm{FW,15\,^\circ C}} \right)}{\dot{m}_{\mathrm{NG,GT}} NCV} \tag{2}$$

$P_{\mathrm{el,GT}}$ refers to the electrical output of the GT. $\dot{m}_{\mathrm{NG,GT}}$ is the mass flow rate of natural gas combusted for the GT process of which the net calorific value is *NCV*. The mass flow rate of feedwater passing through one of the HRSG stages is denoted by $\dot{m}_{\mathrm{FW,HRSG}}$. h_{St} and h_{FW} are the specific enthalpies of steam at the considered steam line and feedwater at 15 °C, respectively. Note that the total efficiency of the CHP unit, consisting of the GT and HRSG, equals the sum of the component efficiencies (86.4 %).

Two identical gas boilers (GB1 and GB2) can produce additional HP steam. A single GB together with the HRSG is able to cover the complete steam demand including a reserve, even at times of high steam demand. The efficiency of the two identical gas boilers can be calculated from

$$\eta_{\mathrm{GB}} = \frac{\dot{m}_{\mathrm{FW,GB}} \left(h_{\mathrm{HP}} - h_{\mathrm{FW,120\,^\circ C}} \right)}{\dot{m}_{\mathrm{NG,GB}} NCV} \tag{3}$$

where $\dot{m}_{\mathrm{FW,GB}}$ denotes the feedwater mass flow rate through the GB, h_{HP} and $h_{\mathrm{FW,120^\circ C}}$ are the specific enthalpies of high-pressure steam and feedwater at 120 °C, respectively, and $\dot{m}_{\mathrm{NG,GB}}$ represents the natural gas combusted for the GB process. LP steam is used to preheat the GB feedwater to the desired temperature (see bottom of Fig. 2).

PtH units with thermal outputs in the small double-digit MW range are increasingly being implemented in chemical site utility infrastructures [8, 9]. Hence, the iUI also includes a relatively small 10 $\mathrm{MW_{th}}$ PtH unit that produces MP steam. The conversion efficiency from electricity to heat of the PtH unit is defined by

$$\eta_{\mathrm{PtH}} = \frac{\dot{m}_{\mathrm{FW,PtH}} \left(h_{\mathrm{MP}} - h_{\mathrm{FW,15\,^\circ C}} \right)}{P_{\mathrm{el,PtH}}} \tag{4}$$

with the mass flow rate of feedwater processed through the PtH unit $\dot{m}_{\mathrm{FW,PtH}}$, the specific enthalpy of the medium pressure steam line h_{MP} and the power consumption of the PtH unit $P_{\mathrm{el,PtH}}$. Transformer losses are not included in the stated efficiency value of 99%.

The three steam lines are connected by steam turbines and steam pressure and temperature reducing stations. During periods of high electricity prices, the high-pressure (HP-ST), medium-pressure (MP-ST) and low-pressure steam turbine (LP-ST) are ramped up to reduce the amount of electricity required from the grid. The steam turbine conversion efficiency can be determined from

$$\eta_{\mathrm{ST}} = \frac{P_{\mathrm{el,ST}}}{\dot{m}_{\mathrm{St,ST}} \left(h_{\mathrm{St,in}} - h_{\mathrm{St,out}} \right)} \tag{5}$$

$P_{\mathrm{el,ST}}$ refers to the electrical output of the ST. $\dot{m}_{\mathrm{St,ST}}$ is the steam mass flow rate flowing through the ST with the specific enthalpies at the inlet $h_{\mathrm{St,in}}$ and outlet $h_{\mathrm{St,out}}$. At low electricity prices, the steam turbines are bypassed, and steam is simply processed over the reducing stations.

From the viewpoint of operational need, it may be required that low-pressure steam is sometimes ejected to the environment. The iUI is connected to the natural gas and power grids and thus must consider the existing electricity and gas tariffs. These tariffs depend on the scenario considered and the simplifications made with respect to the political framework, taxes and other fees (see Sect. 2.3). The maximum electricity capacity of the power grid connection is 300 $\mathrm{MW_{el}}$. Thus, the maximum electricity demand of the end-use processes plus the maximum power consumption of the PtH unit, including a reserve, can be completely covered from the grid. The maximum gas consumption related to the net calorific value is set at 800 $\mathrm{MW_{NCV}}$. This is sufficient to operate a single GB and the GT simultaneously and at full load.

The selected maximum output power of each process unit (numerator in Eq. (1) through Eq. (5)) and its efficiency are included in the block scheme (Fig. 2). Any simplifications applied are listed in the following:

- Feedwater preheating for the HRSG is realized internally though a recirculation.
- The power consumption of water pumps is neglected. Preliminary evaluations have shown that it amounts to less than 1 % of the electricity demand of the end-use processes.
- Production of utilities like pressured air or cold is not considered.
- A constant efficiency of all components is assumed. There are no restrictions on the minimum part load, with the exception of the GT and HRSG (50 % minimum part load).
- Process units are free of heat losses and therefore must not be kept at temperature by an auxiliary heat supply during standstill periods.
- There are no delays during start-up and load change processes.

To conclude this description, the iUI is designed with a built-in backup capacity. Even if one of the components fails, the iUI still has enough steam generation capacity to meet the demand at any time. In further studies, efficient and cost-effective backup strategies can be investigated. However, the focus of this work is on the development and the optimized operation of the iUI.

2.2 Definition of Ideal-Typical Electricity and Process Steam Demands of the End-Use Processes

In reference to the technical connection and delivery conditions of Currenta, the process steam demand is divided into a medium-pressure (31 bar and 300 °C) and a low-pressure level (6 bar and 200 °C) [10]. The average electricity and total process steam loads were adopted from Ausfelder et al. [4] (a reference state of 1 bar and 25 °C is selected for this work). According to Ausfelder et al. the electricity demand has a daily variation due to batch processes and the steam demand shows a seasonal variation caused by higher heating loads in winter (this is included in the LP steam demand here). The basic progression of the load profiles was adopted from Ausfelder et al. However, the seasonal variation of the LP steam demand was adapted and additional random hourly fluctuations (electricity, MP and LP steam) were added to represent more realistic demand profiles. The magnitude of the seasonal variation and random hourly fluctuations was adjusted to approximate real data provided by Currenta. Fig. 3 shows the final demand profiles and Fig. 2 includes the average values.

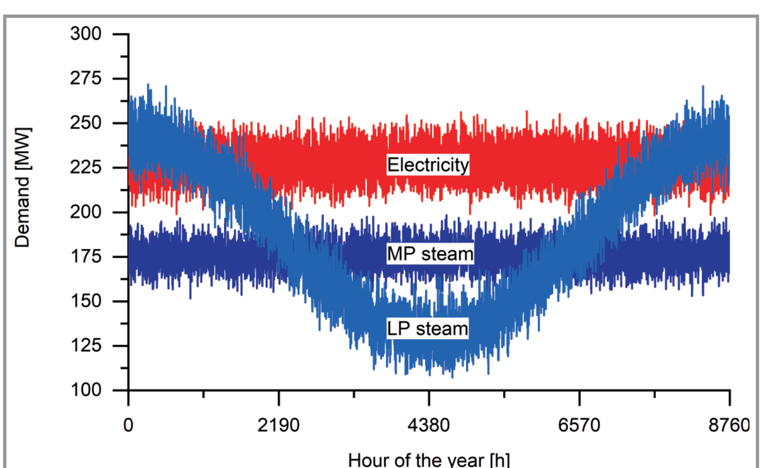

Figure 3. Electricity and process steam demand of the iUI end-use processes.

2.3 Input Parameters for the Operational Optimization of the iUI

The operation of the iUI can be optimized with respect to minimum operating costs (electricity, natural gas and European Emission Allowances) or minimum CO_2 emissions. The optimized operation depends, inter alia, on the selected input parameters. These input parameters are considered as hourly (electricity price, CO_2 emission factor of electricity, temperature) and quarterly (gas price) resolved time series or constant values (European Emission Allowances, emission factor of natural gas) and were determined for 2019. The required input parameters are collated in Tab. 1 together with their average and extreme values, the temporal resolution as well as corresponding reference. Taxes and other expenses for gas and electricity have an impact but are site dependent. Thus, they were not considered.

From the above input parameters, the electricity-to-clean-gas-price ratio can be derived, which is an important coefficient for the evaluation of the optimization results. The electricity-to-clean-gas-price ratio is defined as

$$R = \frac{c_{\mathrm{el}}}{c_{\mathrm{NG,clean}}} \tag{6}$$

c_{el} is the electricity price and $c_{\mathrm{NG,clean}}$ is the so-called clean gas price and consists of the gas price itself and the cost for European emission allowances (EUA):

$$c_{\mathrm{NG,clean}} = c_{\mathrm{NG}} + EF_{\mathrm{NG}} c_{\mathrm{EUA}} \tag{7}$$

c_{NG} is the gas price, EF_{NG} refers to the emission factor of the considered natural gas and c_{EUA} denotes the cost for a EUA that grants the right to emit one metric ton of CO_2 (see Tab. 1).

2.4 Implementation and Optimization of the iUI in TOP-Energy® Software

Chemical site models implemented in TOP-Energy® are currently used for the daily dispatch of energy plants. New operating schedules are generated each day based on the optimization results. Forecasts for gas and electricity prices are used as input data. Furthermore, models of real chemical sites in TOP-Energy® allow for optimal design of energy systems in brown and green field planning.

The iUI is implemented in the commercial software TOP-Energy® Version 2.11 as shown in Fig. 4 [16]. On the left-hand side, the primary energy suppliers are shown. Depicted below the suppliers is the GT with HRSG. Represented in the middle of the scheme are the STs, the PtH unit and the two GBs. Shown on the right-hand

Table 1. Input parameters for the optimization of the iUI operation for 2019.

	Average	Maximum	Minimum	Resolution	Ref.
Ambient temperature of Leverkusen [°C]	11.1	29.2	–7.3	Hourly	[11]
Electricity price c_{el} [€ MWh_{el}^{-1}]	37.7	121.5	–90.0	Hourly	[12]
Emission factor of electricity [t-CO_2 MWh_{el}^{-1}]	0.397	0.637	0.141	Hourly	[13]
Gas price c_{NG} [€ MWh_{NCV}^{-1}]	Q1: 21.3	–	–	Quarterly	[14]
	Q2: 15.1				
	Q3: 11.6				
	Q4: 12.9				
EUA price c_{EUA} [€ t-CO_2^{-1}]	24.9	–	–	Constant	[14]
Emission factor of natural gas EF_{NG} [t-CO_2 MWh_{NCV}^{-1}]	0.202	–	–	Constant	[15]

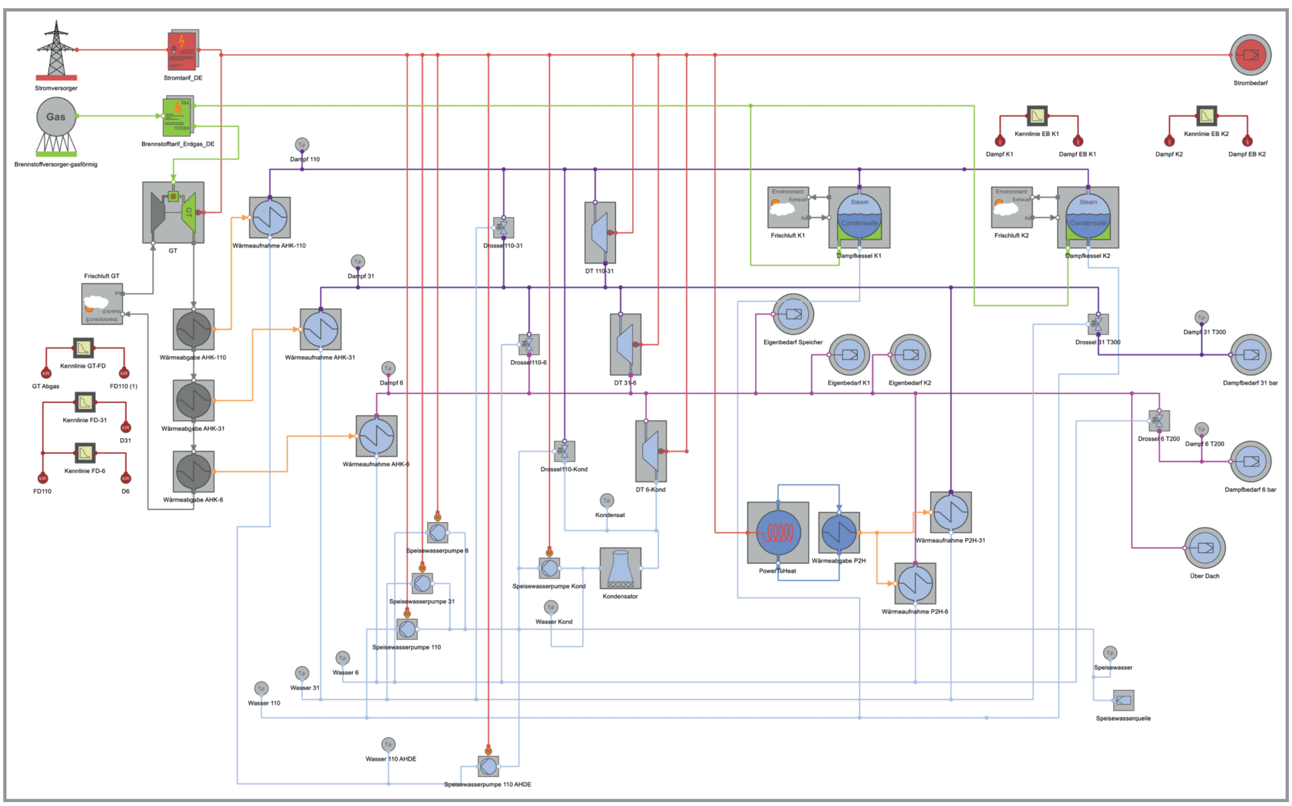

Figure 4. Screenshot of the iUI implemented in the software TOP-Energy®.

side are the electricity and steam demands of the end-use processes.

The operation of a process equipment can be assessed by its utilization expressed in full load hours per year *FLH*, where $P_{t(i)}$ is the actual power within one time step and P_{peak} is the installed power of the component:

$$FLH = \frac{\sum_{i=1}^{8760} P_{t(i)} \cdot 1\mathrm{h}}{P_{peak}} \tag{9}$$

In contrast, the operating hour value is defined as the time the component was switched on in partial or full load. Hence, the operating hours are equal to or larger than the *FLH*.

In the following, the method is presented to optimize and thus investigate the operating behavior of the iUI depending on the different fixed input variables (mainly electricity price) and fixed output variables (steam and electricity demand of the end-use processes). The operating behavior is controlled by an optimization algorithm on an hourly basis with either minimum operating costs or minimum CO_2 emissions as optimization target. When minimizing one of the targets, the algorithm solves an optimization problem formulated as MILP (mixed integer linear programming). The objective function for cost minimization is the minimum sum of operating costs for all energy system components (j) ($C_{OP,j}$) and energy costs for all forms of energy (l) (price multiplied by primary energy supply from the grids ($c_l\dot{Q}_l$), calculated over all time steps (t):

$$\min\left\{\sum c_{l,t}\dot{Q}_{l,t} + \sum C_{OP,j,t}\right\} \qquad (10)$$

For CO_2 emission optimization, the specific emission factors of every energy form (l) are multiplied by the corresponding primary energy supply, summarized and minimized over all time steps (t). Typical constraints and conditions for energy system optimization are energy demands, which need to be satisfied in every time step, or efficiency factors, which define the energy conversion in system components.

3 Operational Optimization and Performance of the iUI

To obtain a better understanding of the behavior of the iUI, a TOP-Energy® optimization with a 1-hour resolution was conducted for the year 2019. Operating costs were chosen as the optimization target. The behavior of the iUI is best characterized by the on-site electricity generation. The on-site electricity generation is plotted against the electricity-to-clean-gas-price ratio R in Fig. 5. Each data point is the optimization result from one of the 8760 considered time intervals. Negative R values correspond to a limited number of operating hours with negative electricity prices. According to Fig. 5, the iUI is operated in two different ways.

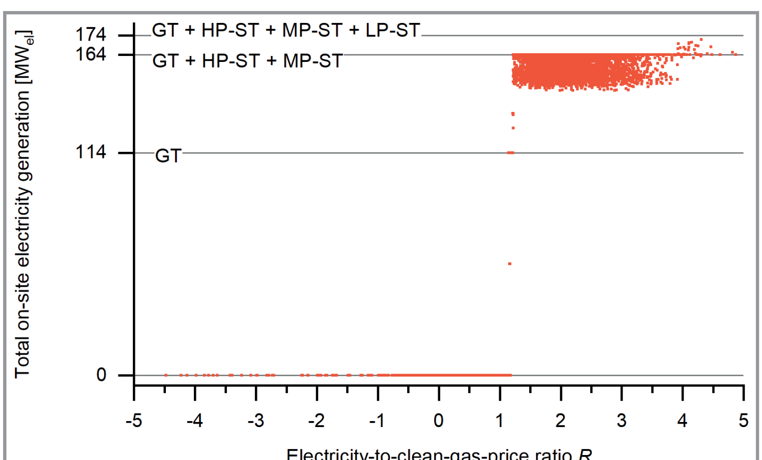

Figure 5. Total on-site electricity generation of the iUI in dependence of the electricity-to-clean-gas-price ratio R for the year 2019.

1. Power grid mode: Whenever the price of electricity is low compared to the clean gas price, the iUI shuts down all on-site electricity generation (gas and steam turbines) and the entire electricity demand of the end-use processes is covered through the power grid. The threshold is at an electricity-to-clean-gas-price ratio of approximately R = 1.2. Due to the efficiencies of the various process units, the threshold is not exactly 1.0, as might be expected. The required steam is produced primarily by GB1 and to a small extent by the PtH unit. In times of high steam demand, GB2 may also have to be switched on. Steam is distributed between the different pressure levels via the available reducing stations.

2. Electricity generation mode: When R exceeds a value of 1.2, on-site electricity generation is ramped up. The gas turbine generates 114 MW_{el}. The HP-ST and the MP-ST are capable of producing another 50 MW_{el}. However, as can be observed in Fig. 5, the two steam turbines cannot always be operated at full load. During periods of low steam demand, the disponible process steam is not sufficient to operate the HP-ST and MP-ST at full capacity. Moreover, a pure power plant operation mode of the iUI, i.e., steam generation for the sole purpose of producing electricity by steam condensing, appears to be uneconomical. Only at R values of about 4 and above, as well as high steam demand the LP-ST is switched on. Even when the iUI is in electricity generation mode, part of the electricity demand must still be covered by the grid. The required steam is produced by the HRSG and GB1.

The average power output of the GT, HP-ST and MP-ST, as well as the electricity procurement from the grid are shown in Fig. 6a. The LP-ST is not considered due to its low operating hours and contribution. More than one third of the 228.9 MW_{el} total power output is covered through the power grid. The total average power output is slightly higher than the average electricity demand of 228.0 MW_{el}, since the PtH unit must also be supplied with electricity. The average electricity demand of the PtH unit is just 0.9 MW_{el} because it is only operated at $R < 1.2$ and thus achieves limited full load hours.

Fig. 6b illustrates the average thermal output of the steam generation units. GB1 and the HRSG are the main steam generators. The contributions of GB2 and the PtH unit account for only a small fraction of steam production. The total thermal output exceeds the steam demand of the end-use processes, because steam is also needed for feedwater preheating and the enthalpy drop over the steam turbines must also be accounted for.

To conclude this section, Tab. 2 lists the full load and operating hours of the process units. By setting the GT power output to half of the average electricity demand of the end-use processes, the GT and HRSG achieve a high number of operating hours. In fact, full load and

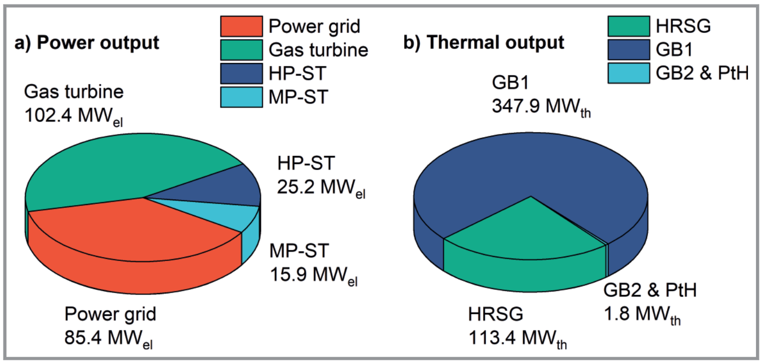

Figure 6. Distribution of the average a) power output and b) thermal output among the various process components of the iUI for the year 2019.

operating hours are almost identical. Only in a single instance, at an electricity-to-clean-gas-price ratio of around 1.2, the GT is operated at half load (see also Fig. 5). GB1 must run 8760 h per year to produce a sufficient amount of steam. If the HRSG is running, GB1 does not have to be operated at full load, which explains why the full load hours are less than the operating hours. Operation of the HP-ST and LP-ST is economical with an electricity-to-clean-gas-price ratio above 1.2. Operating hours and full load hours differ because the steam demand of the end-use processes can limit the power output. As discussed, operation of the LP-ST is profitable only in a few cases. The PtH unit achieves only limited operating and full load hours. This illustrates that a larger PtH unit is not useful in 2019.

Table 2. Full load and operating hours of the process units for the year 2019.

	Full load hours [h]	Operating hours [h]
Gas turbine and HRSG	7870	7871
Gas boiler 1	5957	8760
Gas boiler 2	13	306
High-pressure steam turbine	7359	7808
Medium-pressure steam turbine	6970	7814
Low-pressure steam turbine	9	23
PtH unit	872	872

4 Options for CO_2 Reduction within the iUI

Tab. 3 lists different options identified in this work to reduce CO_2 emissions of the energy supply by the on-site utility infrastructure. Only options that include proven components with a high technology readiness level were considered. The term "secure supply" is defined. It is assumed that the continuous operation of iUI with high power levels requires hybrid heat generation based on electricity and gas for an affordable heat supply. Thus, electricity as a sole source is assumed to provide "no secure supply". The term "CO_2-free" is used for energy sources and carriers that, strictly speaking, have a low CO_2 emission factor (e.g., wind and photovoltaics as renewable electricity sources, green hydrogen).

The two major approaches to defossilize the on-site utility infrastructure include the switch to chemical fuels with a lower CO_2 footprint synthesized via electrolysis (e.g., green hydrogen) and extended renewable electricity utilization via PtH technology to produce steam. To a lesser extent, alternative solution options such as CHP with carbon capture and storage (CCS), high-temperature heat pumps, and biomass fuels are also mentioned in the technical literature (Tab. 3) [4, 5, 17–20].

To date, the integration of thermal energy storage (TES) into on-site cogeneration for process steam has been identified as an option in the literature but has not been realized and has only been investigated to a small extent [4, 17, 21]. Ausfelder suggested that the TES is charged with excess flue gas heat of the gas turbine. This option could be attractive in the summer half of the year with a lower steam demand [8].

Both the PtH and fuel switch route have their own challenges. Fig. 7 compares the Sankey diagrams of PtH (left) and Power-to-Gas-to-Combined-Heat-and-Power (PtGtCHP, right). It can be seen that the PtH technology has a high overall efficiency but no storage option. The PtGtCHP concept has a low overall efficiency compared to PtH and Power-to-Heat-to-Combined-Heat-and-Power (PtHtCHP, middle) + TES. The latter is a rather unknown option for combined heat and power supply. The PtGtCHP overall efficiency value is only 37 %, while PtHtCHP has a high overall efficiency of 87.4 %. Further details and a discussion about hybrid configurations of PtHtCHP and PtGtCHP can be found in literature [4, 22].

The previous discussion did not focus on the fact that renewable PV- and wind electricity sources are volatile and have limited annual operation hours. For example, photovoltaics has about 1000 full load hours and on- and offshore wind from 1500 to 4500 full load hours in Germany. On the other hand, larger chemical sites require a continuous steam and electricity supply over the entire year (8760 h). With the extension of volatile renewable sources, the mismatch between renewable supply and demand grows and requires flexibility solutions [4]. Energy storage is therefore an important aspect for a comprehensive renewable energy supply for the chemical industry.

Fig. 8 shows the indicative total as-spent capital (TASC) at the time of writing, based on the discharge power C_p for large-scale grid-connected electric storage technologies (CHP operation is not included for simplicity here). The value C_p is the sum of the capacity unit cost c_c multiplied with the storage duration $t(h)$ plus the power unit cost c_p

Table 3. Options to reduce CO_2 emissions caused by the operation of the on-site utility infrastructure. The table is divided into three sections: options with adapted gas supply (''molecule options'', top), options with adapted electricity supply (''electron options'', middle), and options including TES (bottom).

Option	Description	Pros	Cons
Electricity islanding capability	Larger gas and steam turbines are implemented to cover the entire electricity demand of processes	– high CHP efficiency of gas use – iUI has larger flexibility to support the power grid – allows "secure supply"	– on-site investment with space requirement – requires affordable "CO_2-free" gas
CCS	Further use of natural gas with carbon capture on-site, transport and subsequent CO_2 storage	– high CHP efficiency of gas use – natural gas grid available, no additional grid investment – allows "secure supply"	– on-site investment with space requirement – efficiency loss due to CCS – CO_2 transport – CO_2 storage is currently not pursued in Germany
Biogas	Natural gas is gradually replaced by biogas	– high CHP efficiency of gas use – no on-site investment with space requirement – natural gas grid available, no additional grid investment – available biogas storage – allows "secure supply"	– limited availability of biogas in Germany compared to total demand of chemical industry – limited resource potential for biogas extension in Germany – competing other biogas use cases
Power to Hydrogen	Natural gas is gradually replaced by hydrogen	– high CHP efficiency of gas use – no additional methanization with costs and efficiency losses – allows "secure supply"	– H_2 adaption/investment in iUI – H_2 grid extension required – demanding/costly storage of H_2 – limited efficiency of H_2 production from renewable electricity – limited resource potential of green H_2 in Germany may require H_2 transport/import – oversizing and limited operating hours of the relatively expensive electrolysis units could lead to costly "CO_2-free" H_2
Power to Methane	Natural gas is gradually replaced by "CO_2-free" methane	– high CHP efficiency of gas use – natural gas grid available – no adaption of iUI required – available methane storage – allows "secure supply"	– low conversion efficiency of methane production (additional methanization step compared to H_2) – limited renewable resource potential may require "CO_2-free" methane transport/import – emission free CO_2-source required – oversizing and limited operating hours of relatively expensive electrolysis and methanization units could lead to costly methane
Battery	The on-site batteries are charged with surplus electricity and discharged when there is a power shortage	– temporal shift of electricity use to times with low CO_2 emissions – fast response, e.g., for short-term electricity markets	– electricity grid extension required – limited annual operation hours with renewable electricity – on-site investment with space requirement – allows "no secure supply" – limited to shorter storage periods due to high capital costs – relatively low lifetime
PtH-steam	Electrode boilers and continuous flow heaters generate steam directly with electricity	– increased use of electricity with low CO_2 emission factor – high conversion efficiency for electricity to heat – low capital cost – switchable load for power grid	– electricity grid extension required – limited annual renewable operation – on-site investment with space requirement – demanding/costly storage of steam – allows "no secure supply"
High temperature heat pump	Environmental or waste heat is upgraded to process steam via a high-temperature heat pump	– increased use of electricity with low CO_2 emission factor – one unit of electricity generates more than one unit of heat – integration of waste heat flows feasible to improve performance	– electricity grid extension required – limited annual renewable operation – on-site investment with space requirement – allows "no secure supply" – low coefficient of performance – limited market maturity

Table 3. Continued.

Option	Description	Pros	Cons
PtHtCHP + TES	Continuous flow heaters generate heat directly with electricity. Heat is transferred to a thermal energy storage system, which supplies high-temperature heat for power and heat supply on demand.	– shifting electricity use to times with low CO_2 emission factors by relatively inexpensive TES – decoupling of demand side and gas/electricity prices – high CHP efficiency – highly switchable grid load and secure HP steam from TES – extended PtH operating hours – combinable with GT-TES concept	– electricity grid extension required – limited annual renewable operation – on-site investment with space requirement – allows "no secure supply"
GT + TES	The gas turbine is sized larger to allow flexible power generation, and the excess heat in the flue gas is transferred to the TES for later power and heat supply in the chemical site.	– flexible operation of GT for peak power supply at low steam demand – shifting excess heat with relatively inexpensive TES – chemical site acts as heat sink; high CHP efficiency of gas use – allows "secure supply" – combinable with PtHtCHP+TES	– on-site investment with space requirement – GT operation hours can be limited if TES is fully charged – large GT oversizing can lead to condensing steam turbine operation (limited CHP efficiency)

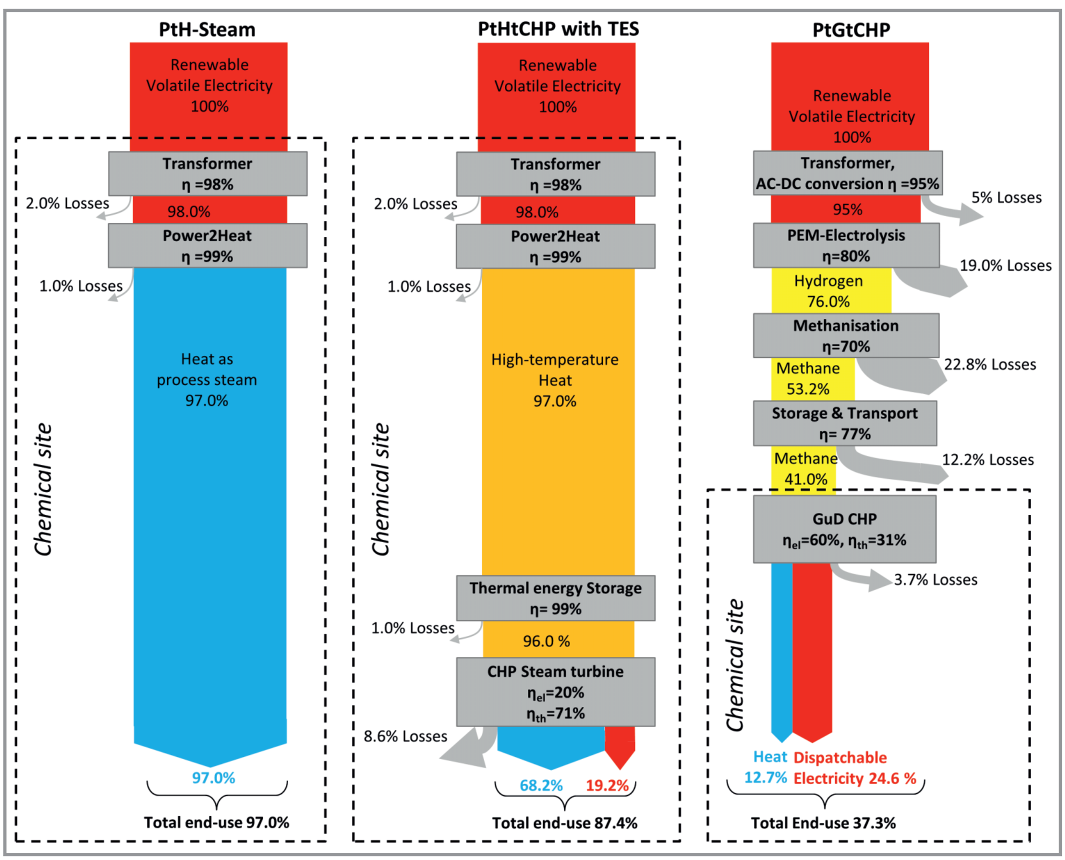

Figure 7. Energy Sankey diagrams of renewable electricity and process steam supply: Power-to-Heat (PtH) technology with direct steam generation and without storage (left), Power-to-Heat-to-Combined-Heat-and-Power (PtHtCHP) with thermal energy storage (middle), and Power-to-Gas-to-Combined-Heat-and-Power (PtGtCHP) with gas storage (right); partly redrawn from [4, 22].

(see equation in Fig. 8) [23–29]. Power-to-Gas-to-Power (PtGtP) requires electrolysis and methanization units for charging (included in c_p), a cavern for storage (included in c_c) and a gas turbine is assumed for discharging (included

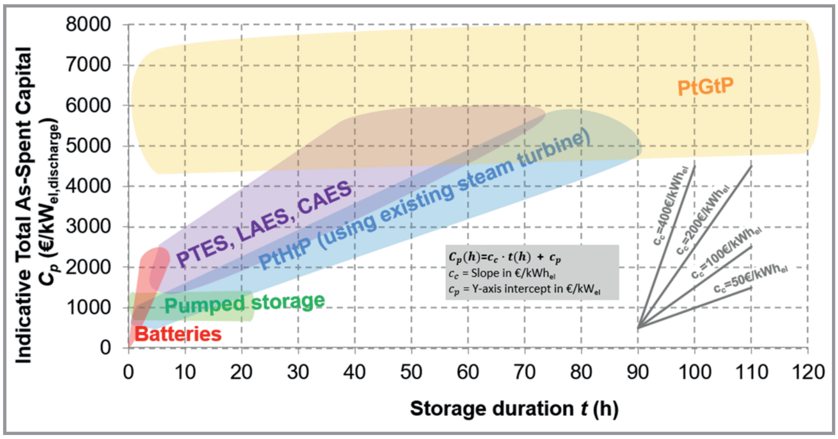

Figure 8. Indicative total as-spent capital at the time of writing, based on the discharge power C_p for large-scale grid-connected electric storage technologies.

in c_p). While the gas cavern and the gas turbine are relatively inexpensive, the electrolysis and methanization investment is significant. The low conversion efficiency leads to an oversizing and higher TASC of the electrolysis and methanization components of the PtGtP route (see Fig. 7). One main advantage of the PtGtP route is that large quantities of gas can be stored and discharged during the cold and dark season for a secure gas supply. Pumped thermal energy storage (PTES), liquid air energy storage (LAES) and compressed air energy storage (CAES) are predicted to have indicative power unit cost c_p values of about 1000–2000 € kW_{el}^{-1} and capacity unit cost c_c values of 50–100 € kWh_{el}^{-1}. Power-to-Heat-to-Power (PtHtP) systems can have relatively low power unit cost c_p values if electric heater, heat exchangers and existing steam turbines are utilized. The capacity unit cost c_c is based on high-temperature TES costs of several 10 € kWh_{el}^{-1}. Batteries based primarily on lithium-ion technology do not have separate capacity and power units. The values of the power unit cost c_p are approx. zero and the costs scale with the capacity unit cost c_c. With these technologies and cost assumptions, three classes of grid-connected electrical storage systems emerge: batteries as short-term storage (a few hours), medium type storage PTES, LAES, CAES and PtHtP (several hours to days) and long-term storage with PtGtP (days, weeks and season). It should be considered that the simplified diagram includes merely approximated capital costs including the conversion route and storage duration. Other important parameters for storage selection are not considered (e.g., availability of sites, lifetime, levelized cost of storage, CHP operation).

In general, there is very limited literature available on the TES benefits, TES operation modes, integration details and type of TES technology in industrial CHP sites. Available literature is summarized by Klasing [21]. A main approach to negative flexibility is the conversion of volatile renewable electricity via PtH, high temperature storage and the provision of high-temperature steam (e.g., for a back-pressure steam turbine operated in CHP mode). An approach to positive flexibility is to oversize the gas turbine so that it can generate additional electricity while temporarily storing the additional high-temperature waste heat until it can be used later in the processes. Further potential benefits of TES utilization can include reduction of price peaks, provision of backup power, improved energy efficiency, extension of turbine lifetime due to steadier operation, reduction of dumped energy and smaller sizing of power components (downsizing). It is important to mention that TES does not defossilize the CHP unit itself. Instead, TES temporally shifts energy and needs to be seen as enabler for flexibility and efficiency improvements, as well as extended operation hours and cost reduction of the previously mentioned PtH and fuel switch technologies.

5 Summary, Conclusion and Outlook

According to current knowledge, "CO_2-free" gas (e.g., green hydrogen) and the use of renewable electricity are the most suitable options for defossilization of heat and electricity supply in the chemical industry. The availability, necessary transport infrastructure and prices of these new energy sources are different from the existing supply (fossil heat and power generation). Therefore, the focus is on optimizing the utility infrastructure located between the electricity and gas networks and the chemical processes. The utility infrastructure must deal with significant challenges in the future. On the one hand, there is an increasingly fluctuating renewable power supply and rising gas prices. On the other hand, there is a need for a constant, secure, and affordable supply of steam and electricity to the processes.

In order to examine suitable adaptation options of the utility infrastructure for the future, this work defined an ideal-typical utility infrastructure (iUI) as a publicly accessible basis. The iUI was defined based on typical German chemical sites and includes a gas turbine with heat recovery steam generator, gas boilers, steam turbines and a small PtH unit. This supply structure can be operated flexibly to minimize either electricity and gas operating costs or CO_2 emissions. The iUI was implemented in the commercial software TOP-Energy® to optimize its operation.

To provide an understanding of the iUI behavior, an operating cost optimization was performed for 2019. Results showed that the main influencing factor on the operational behavior is the electricity-to-clean-gas-price ratio. At electricity-to-clean-gas-price ratios below 1.2 the iUI goes into power grid mode. The gas and steam turbines are shut down and the entire electricity demand of the end-use processes is covered from the grid. Steam is produced by the gas boilers and PtH unit. At electricity-to-clean-gas-price ratios above 1.2 the iUI runs in electricity generation mode. The gas and steam turbines are switched on and reduce the required power consumption from the electricity grid. The extent to which the steam turbines can be ramped up is determined by the current steam demand. According to the high full load and operating hours, the gas turbine, heat recovery steam generator, high-pressure and medium-pressure steam turbine are crucial components of the iUI. The low-pressure steam turbine and PtH unit are only used under very favorable boundary conditions and therefore currently achieve low full load and operating hours.

In this work, technology options for defossilization of the heat and electricity supply by the iUI were identified and qualitatively evaluated. Examples are the extension of existing components (e.g., gas turbine, heat recovery steam generator, steam turbines, power-to-heat unit) or the integration of additional components (e.g., high-temperature heat pump, thermal energy storage, battery). Currently, two main routes for a complete defossilization of the process steam and power supply are seen in the literature: 1) "CO_2 free" gas, and 2) the use of renewable electricity via PtH. In the case of "CO_2-free" gases, the gas costs in particular can be seen as critical. With PtH, on the other hand, renewable electricity is not always available, which leads to a limited number of operating hours. The integration of thermal energy storage has hardly been considered in this context so far and has not been analyzed in detail. The combination of PtH and TES shown in this article could enable a cost-effective steam supply with extended operation hours compared to PtH alone. The iUI defined in this work is a valuable resource for further investigations to examine such solutions for a safe, cost-effective, and CO_2-neutral operation of chemical sites in future years.

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Symbols used

C	[€ kW^{-1}, €]	Indicative total as-spent capital or operating cost
c	[€ kW^{-1}, € kWh^{-1}, € MWh^{-1}, € t-$CO_2$$^{-1}$]	Specific cost
EF	[t-CO_2 MWh^{-1}]	Emission factor
FLH	[h]	Full load hours
h	[J kg^{-1}]	Specific enthalpy
$\dot{m}$	[kg s^{-1}]	Mass flow rate
NCV	[J kg^{-1}]	Net calorific value
P	[W]	Power
$\dot{Q}$	[MW]	Primary energy supply
R	[–]	Electricity-to-clean-gas-price ratio
t	[h]	Storage duration
η	[–]	Efficiency

Subscripts

c	Based on storage capacity
clean	Including cost of European Emission Allowances
el	Electric
EUA	European Emission Allowance
FW	Feedwater
GB	Property of the gas boiler
GT	Property of the gas turbine
HP	High-pressure
HRSG	Property of the heat recovery steam generator
in	At inlet of a component
j	Running number for components
l	Running number for type of primary energy supply
MP	Medium-pressure
NG	Property of the natural gas
OP	Operational expenditure
out	At outlet of a component
p	Based on discharge power
peak	Installed capacity of the component
PtH	Property of the power to heat unit
ST	Property of a steam turbine
St	Property of the steam
t	Running number for time step

Abbreviations

CAES	Compressed air energy storage
CCS	Carbon capture and storage
CHP	Combined heat and power
FW	Feedwater
GB	Gas boiler
GHG	Greenhouse gas
GT	Gas turbine
HRSG	Heat recovery steam generator
HP	High-pressure
iUI	Ideal-typical utility infrastructure
LAES	Liquid air energy storage
LP	Low-pressure
MP	Medium-pressure
PTES	Pumped thermal energy storage
PtH	Power-to-Heat
PtHtP	Power-to-Heat-to-Power
PtHtCHP	Power-to-Heat-to-Combined-Heat-and-Power
PtGtP	Power-to-Gas-to-Power
PtGtCHP	Power-to-Gas-to-Combined-Heat-and-Power
ST	Steam turbine

TASC Total as-spent capital
TES Thermal energy storage

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