Power-to-X: Between Electricity Storage, e-Production, and Demand Side Management

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Abstract - The common understanding of Power-to-X is exclusively the use of renewable electricity to manufacture products currently based on fossil sources. We argue that beyond such "e-Production", many of these technologies also include aspects related to demand side management and temporal storage of electricity. We therefore suggest a definition of Power-to-X that encompasses all three aspects. We discuss which of these are relevant under which conditions and highlight illustrative examples that show how process systems engineering can help address common challenges for Power-to-X technologies.

Keywords - demand side management, e-Production, electricity storage, Power-to-X

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1. Introduction

On a global scale, the share of renewable energy sources (RES) in electricity production is small but is growing continuously. In order to prevent economic losses and idle green resources caused by energy curtailments, corrective actions need to be taken. Moreover, RES must become accessible for sectors that still heavily rely on fossil resources, i.e., chemical industry, heating, and transportation [1], if global climate targets are to be met.

In this context, technologies termed "Power-to-[…]" (such as Power-to-Gas, Power-to-Chemicals, or Power-to-Fuels) have attracted increasing interest in recent years (cf. Sect. 2). The terminology has been used for an ever-increasing number of applications, and the large diversity of applications associated with this terminology has resulted in the term "Power-to-*X*". However, we are not aware of an established definition about what the "*X*" may or may not include. Looking at most instances of Power-to-X concepts, these aim at converting electricity into gases, liquids, heat, fuels, or even back from those into electricity (e.g., [2–7]). We believe that in addition to the new aspect of bringing renewable electricity into production processes to replace fossil-based products, many recently proposed technologies under the term "Power-to-X" are closely related to the much older concepts of electricity storage and demand side management (DSM).

We therefore propose a broad definition of Power-to-X as *processes with the goal to exploit the environmental and economic potential of renewable electricity.* This explicitly encompasses electricity storage and DSM, as well as the newer aspect that we call "e-Production". In the following, we first give a brief overview of the literature (Sect. 2). We then provide details on our definition and classification of Power-to-X, before discussing key challenges and benefits for given external conditions (Sect. 3). We also give illustrative examples that demonstrate how process systems engineering (PSE) methods support overcoming these challenges (Sect. 4). Finally, we summarize the most important findings and still open questions (Sect. 5).

2. The increasing awareness of Power-to-X

With the project "Strategieplattform Power-to-Gas" [8], which was initiated in 2011 with the objective to improve and promote Power-to-Gas technologies, the terminology "Power-to-[…]" has been used increasingly in the scientific community during the last years (Fig. 1). The extensive presence of this terminology indicates an increasing interest in related technologies, such that the terminology was also included in the German energy strategy (e.g., [9]), which highlights its relevance. The more general term "Power-to-X" was introduced later on, in order to combine all related "Power-to-[…]" technologies under one common terminology. This terminology is often used in the context of sector coupling, where Power-to-X technologies are considered a key element.

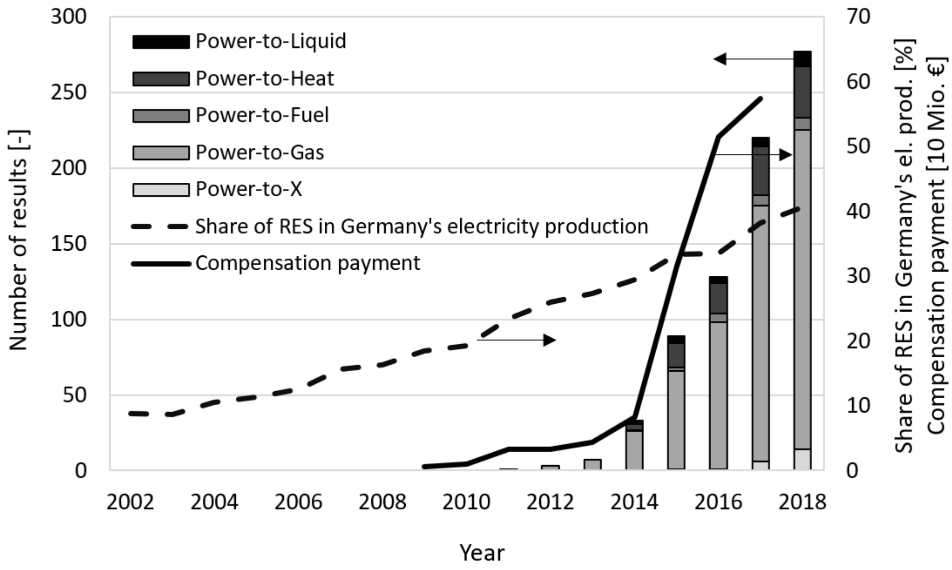

Figure 1: Share of RES in total electricity production in Germany (data from [10]*), number of publications with the terms "Power-to-[…]" stated in the legend (constituted on 14.06.2019 using the search engine "Web of Science"* [11] *with the basic search by topic, demand side management is not included), and compensation payments for electricity curtailments in Germany (data from* [12]*). The data for the number of publications exclude such related to relevant technologies but without the wording "Power-to-[…]".*

Interestingly, there is a correlation between the number of publications on "Power-to-[...]" technologies and the amount of compensation payments for curtailed energy in Germany, which have both increased seemingly exponentially in the last decade (Fig. 1). Taking the number of publications as an indicator for public investments into R&D, the correlation may indicate the high effort in avoiding electricity curtailments by investing in Power-to-X technologies. This gets even more plausible by interpreting the much steeper increase of compensation payments for curtailed electricity compared to the linear increase in share of RES in total electricity produced: The potentially usable energy from RES seems to be higher than what the current (grid) technology can handle without curtailment. In order to identify the key interests in Power-to-X technologies, we categorize recent studies into their main object of investigation and give examples for each field in the following.

Many early publications on Power-to-X evaluate to which extent the integration of a distinct technology into the energy system (e.g., [13–15]) and process industry (e.g., [1,16,17]) is beneficial, and how they influence one another. Typically, future energy scenarios are developed and the technology is assessed based on performance, economic, and environmental indicators. Independent of the sector the technology is applied in, the authors highlight the need for a consistent and predictable energy policy for a successful integration. Coupled with technological progress, such technologies may even become economically attractive. Concerning the environmental impacts of Power-to-X technologies, Koj et al. [18] give a review of life-cycle assessment (LCA) studies based on their understanding of Power-to-X.

The question about the integration of Power-to-X into an existing energy system or industry intrinsically includes the question which Power-to-X technology is suited best for which energy scenario. Most publications consider Power-to-Gas (e.g., [19–23]), Power-to-Liquid, often also referred to as Power-to-Fuel (e.g., [24–27]), Power-to-Heat (e.g., [28]), and Power-to-Chemicals (e.g., [7]) individually, some of them also collectively (e.g., [6,29]). The publications typically consider different performance indicators (i.e., economics, sustainability, efficiency, infrastructure, technology readiness level, etc.) as well as a variety of boundary conditions in order to provide a holistic assessment of the technology. The diversity in boundary conditions and assumptions makes the comparison between the publications difficult.

Going through the broad range of different literature on Power-to-X technologies, it is noticeable that their applications in most cases aim at the conversion of predominantly electric power into products that are currently based on fossil energy sources. Therein, the scientific community distinguishes between the product's state (i.e., Power-to-Gas or Power-to-Liquid), and the product's intended purpose (i.e., Power-to-Fuel or Power-to-Heat). This product-oriented classification has two shortcomings: First, the notations are ambiguous. Either of the terms “Power-to-Liquid” and “Power-to-Fuel” are used for the same notion. Additionally, “Liquid” may refer to fuels, a chemical feedstock, or both, and “Fuel” may refer to a liquid, a gas, or both. However, the intended purpose of the product or - even more precisely - of the Power-to-X application is very important for its environmental assessment (cf. [6,29]). Second, the broad usage of the terminology “Power-to-[…]” and the missing definition lead to the question which technologies to include and which not. For instance, there are DSM endeavors in which some electricity-intensive industrial processes are explicitly operated flexibly to make them utilize renewable electricity effectively (cf. Sect. 3.1). Such approaches are commonly not considered Power-to-X technologies, although flexible operation is a key aspect in many Power-to-[…] processes, and they pursue the same goal of improving the utilization of renewable electricity. This indicates a connection to more established process concepts that we excluded in the keyword search illustrated in Fig. 1. In order to indicate the increasing interest also in those, Fig. 2 exemplarily shows the number of publications related to some of them using a selection of keywords.

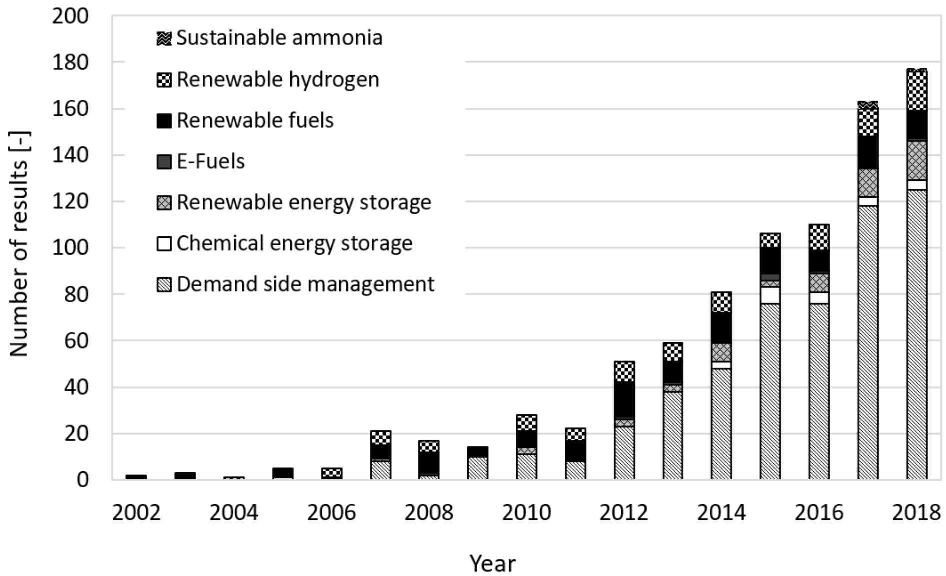

Figure 2: Number of publications related to the keywords stated in the legend (constituted on 18.09.2019 using the search engine “Web of Science” [11] *with the basic search by topic). We used the additional keywords “renewable” and “electricity” in order to narrow down the results for demand side management to relevant publications.*

In addition to the increasing general interest in these established technologies, the high amount of literature on demand side management with regard to renewable electricity utilization highlights its relevance for Power-to-X processes. We therefore propose a broader definition of Power-to-X and a classification based on the way Power-to-X pursues the common goal of a beneficial utilization of renewable electricity.

3. How can Power-to-X utilize electricity in a beneficial way?

We define Power-to-X processes as *processes with the goal to exploit the environmental and economic potential of renewable electricity*. This comprises the production of gases and liquids from renewable electricity, as well as the provision of heat with the intention to replace fossil-based products, which we call "e-Production". Additionally, our definition encompasses the older fields of electricity storage and DSM. With this definition, we do not restrict Power-to-X to technologies for the conversion of predominantly electric power into products that are currently based on fossil sources. With DSM, it also incorporates approaches that enable the utilization of renewable electricity for industrial processes that have not been able to utilize such in an effective way until now. We believe that such a broad definition is useful to highlight the relationship and overlap of these fields that becomes particularly apparent in many Power-to-X technologies falling into more than one of these three categories (grey areas in Fig. 3). We explicitly confine our definition to processes that aim at utilizing renewable electricity and exclude, e.g., general energy management technologies from our definition of Power-to-X. However, contrary to their intended purpose, associated technologies could in principle also utilize other types of energy sources, e.g., for producing synthetic fuels from nuclear power in one country and transport it to another one. In the following, we briefly introduce these three main approaches for a beneficial utilization of renewable electricity, identify their relations, and state their opportunities and common challenges.

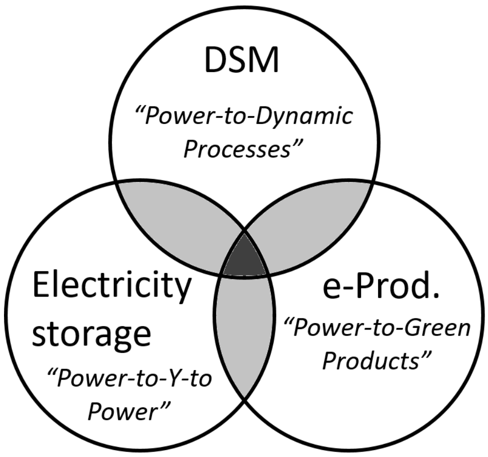

Figure 3: Power-to-X main approaches for an economically and environmentally beneficial renewable electricity utilization: demand side management (DSM), e-Production, and electricity storage. The white areas represent their individual application, whereas the shaded areas represent their combined application.

3.1. Demand side management

The fluctuating nature of renewable electricity, e.g., from solar and wind power, motivates adjusting the operation of existing (electricity-intensive) production processes to their electrical energy supply [30]. A dynamic (or flexible) operation of such processes by varying the production level [31] or changing the operational mode [32] helps to stabilize the electricity grid, as well as reduces electricity costs. With such a dynamic operation, these processes become able to benefit from renewable electricity in an economic and environmental way. This operation strategy is commonly called DSM and an integral part of many Power-to-X applications due to the fluctuating nature of the availability of RES.

Classification of DSM is twofold: dispatchable demand responses and non-dispatchable demand responses [33]. The former responses are requested by transmission system operators (TSO) in ancillary markets for balancing a power grid in exchange for monetary incentives. The latter responses consider electricity spot prices to reduce electrical energy costs. In addition to the economic benefits, environmental impacts, especially carbon footprint, can be mitigated by exploiting electricity with a high share of RES [34,35].

Especially for electricity-intensive industrial processes such as air separation units (ASU) [36–39], chlor-alkali (CA) electrolysis [32,40], seawater reverse osmosis [41], and aluminum production processes [42], DSM is particularly worthwhile.

3.2. e-Production

By e-Production we denote non-conventional processes that utilize renewable electricity predominantly, including the production of commodities for industry, the provision of heat, or the production of fuels for transportation. Electricity-intensive processes have existed already for a long time (e.g., air separation units, aluminum production) but are mainly based on fossil sources. With e-Production we explicitly refer to processes that are developed with the intention of using RES instead. This way, the resulting product has potentially a low carbon footprint and can directly replace its fossil-based alternative, which makes e-Production a key element for sector coupling [43,44]. For such sector coupling purposes, e-Production may be operated at steady-state. While this may seem counter-intuitive when considering fluctuating renewable power, *steady-state* e-Production has the advantage of better utilization of plant equipment (and hence capital investment) compared to a dynamically operated plant and avoids the difficulties related to dynamic operation. However, combinations of e-Production with dynamic operation in the sense of DSM exist (cf. grey areas in Fig. 3).

3.3. Electricity storage

Any process that can operate in different modes that encompass both net electricity consumption ("charging") and production ("discharging") can be used for temporal storage of electrical energy. In contrast to DSM, a pure electricity storage system is not intended to sell any material product and its sole purpose is to generate revenue by exploiting fluctuations in electricity prices or participating in ancillary markets, or to support the integration of renewable sources into the electricity grid.

Electricity storage technologies can be interpreted as *Power-to-Y-to-Power* processes. Existing approaches use a wide range of energy forms *Y* for storage between charging and discharging periods [45]. In the context of Power-to-X, gaseous or liquid energy carriers, i.e., chemicals, are of particular interest since they constitute an intermediate *Y* that could also be sold instead of re-conversion (cf. Sect. 3.4). Such systems are attractive for large-scale stationary storage because of their very low self-discharge and the possibility to independently design achievable charge/discharge rates and storage capacity (in contrast to batteries) [45]. The latter enables favorable scaling of cost with storage capacity because the tank required to store most gases or liquids typically is not the main cost driver [46].

3.4. Combined approaches

The shaded regions in Fig. 3 denote approaches that lie in between the three extremes of *steady-state* e-Production, pure DSM, and pure electricity storage described above. The area between e-Production and DSM contains approaches that aim both at enabling the use of renewable electricity for other sectors, and at providing a flexible load that can operate according to the availability of renewable electricity. The area between electricity storage and DSM encompasses systems that utilize storage technologies (e.g., batteries) to improve the dynamic response of DSM approaches. The area between e-Production and electricity storage represents approaches where a product from *steady-state* e-Production can be re-converted to electricity, e.g., depending on current market conditions. Finally, the dark gray area where all three approaches overlap denotes systems that produce a new product flexibly according to electricity availability and that dynamically either sell this product or re-convert it to electricity. One example for this case is flexible Power-to-Methane with re-conversion in gas power plants [47].

3.5. When is their application beneficial?

Given that Power-to-X technologies aim at achieving economic and/or environmental benefits by utilizing renewable electricity, the question arises which approach is favorable under which conditions. In Fig. 4, we give general trends where the decisive factors that affect the economic viability are twofold: the average electricity price and its fluctuations. Herein, the fluctuations indicate the absolute changes in price with time. From the environmental point of view, particularly for mitigating greenhouse gas (GHG) emissions, the Power-to-X applications are evaluated according to the average electricity carbon footprint and its absolute fluctuations over time.

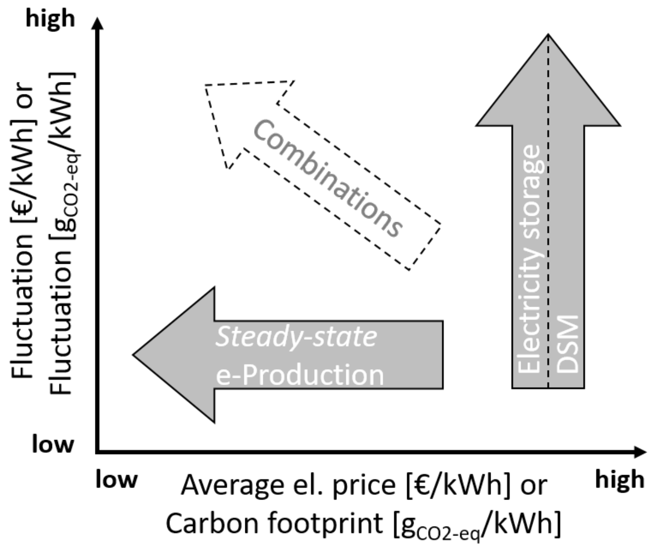

Figure 4: Preferred direction of operation of different Power-to-X approaches for utilizing renewable electricity within the electricity market.

E-Production in steady-state operation becomes more viable with decreasing average electricity price as this is its major operating cost factor. This way, e-Products can become cost-competitive with fossil-based products only if the average electricity price is low. Similarly, e-Production must consume electricity with a low carbon footprint to result in low GHG emissions. Utilizing electricity with a high carbon footprint GHG emissions might even exceed those of fossil-based products [48]. For steady-state operation, the fluctuations in both factors have no influence on process economics and environmental impact, because the plant does not adapt to those fluctuations.

Power-to-X applications for DSM and electricity storage are economically beneficial if the fluctuations in electricity prices are high. In such a case, the capacity of processes operated under DSM and processes for electricity storage can be increased when electricity is available at low costs and the load can be reduced or the energy can be re-converted at high electricity prices, respectively. The benefit needs to recoup the capital investment for gaining operational flexibility. The achievable cost savings do not depend on the average price, because the (absolute) revenue of both buying and re-selling electricity and of shifting periods of electricity consumption only depends on the magnitude of fluctuation. Electricity storage facilities and DSM favor a high fluctuation in carbon footprint of the electricity mix in order to exploit the environmental potential. Electricity is used/stored when the share of RES in the electricity grid is high, and re-converted when the share is low [35].

As already stated in Sect. 3.4, combinations of these applications can outperform individual applications. One combination could be DSM for e-Production with an increased production rate when electricity prices are low. Then, equipment oversizing that enables flexible operation should be addressed in process design.

The considered fluctuations occur on very different time scales: hourly, daily, or even seasonal. Depending on the dynamics of the processes and their ability to adapt their operation to the fluctuating electricity, all types of fluctuations can be beneficial for both electricity storage and DSM. Faster process dynamics allow faster changes of the operating point and thus a faster reaction to changed electricity prices, i.e., greater profits can be achieved. The fluctuations in electricity prices may occur due to volatile availability of RES or due to the participation in different electricity markets, e.g., the spot market or futures trading.

Existing literature on optimal operation of electricity storage facilities and DSM focuses predominantly on economic metrics, i.e., the electricity price and its fluctuations, rather than environmental impacts. However, markets will change, possibly assigning an economic value to the environmental impact (e.g., imposing carbon taxes), which leads to an increased impact of carbon footprint on decision-making.

3.6. Challenges for successful implementation of Power-to-X technologies

Power-to-X technologies face a number of challenges for successful implementation, some of which differ from those of classical process systems. We discuss technical challenges and exclude political boundary conditions (e.g., carbon tax or climate targets [49]), social acceptance (e.g., preferences for potential Power-to-X products [50]), and similar issues.

3.6.1. Process: Efficient flexible operation

Power-to-X processes are energy-intensive by definition, and therefore energy efficiency is of prime importance both for economic and environmental reasons [6,48,51]. Beyond high efficiency at a single design point, Power-to-X processes aiming at DSM or electricity storage need to retain high efficiency over a wide range of operating conditions in order be able to operate according to electricity price or some other signal for availability of electricity [33] instead of operating at steady-state like today's process systems. Such changes in operating conditions also need to occur sufficiently fast to follow the changes in electricity supply in the desired time scale. Processes with inherently fast dynamic response can thus easily be used for DSM by appropriate scheduling, e.g., seawater reverse osmosis [41]. Other processes exhibiting slower dynamic response, such as ASU [36], demand advanced control strategies to enable flexible operation for DSM. Additional challenges are associated with the implications of flexible operation on the performance and lifetime of plant equipment and in particular catalysts, that are only beginning to be understood [52].

3.6.2. Supply chain: From new raw materials to new products

Beyond the change to renewable electricity as main energy source, many Power-to-X technologies also require new types of raw materials, particularly CO_2 and/or biomass [53]. Therefore, sizing and location of Power-to-X plants are not only impacted by the temporal and spatial availability of suitable renewable power sources considered (e.g., in [54,55]), but also of raw materials [56,57]. Additional challenges arise regarding the quality of raw materials (e.g., CO_2 purity [58] or exact composition of biomass).

As Power-to-X is in principle indifferent to type of product, both product and process design are needed, ideally combined. This applies both at a high-level view point when looking for Power-to-X technologies in general [6], but also when targeting specific applications, e.g. Power-to-Fuel for light-duty vehicle applications [59]. This freedom in designing both process and product obviously holds significant promise for achieving solutions that have favorable properties on both sides. On the downside, it entails complexity in decision-making, and so far only few truly integrated approaches for combined process and product design have been developed [60].

3.6.3. Uncertainties

Finally, Power-to-X technologies are subject to various types of uncertainties. Beyond the inherent uncertainty associated with any new technology, there is the uncertainty regarding temporal profiles of electricity price or availability. This type of uncertainty will remain even after a plant is built and running since it is inherent when relying on volatile renewable electricity supply. A plant relying on such electricity supply will not only experience different price profiles throughout its life time, these price profiles are also unknown in advance. They thus need to be approximated with an (imperfect) prediction [61]. This will require increasing use of methods for optimization under uncertainty to enable good decision making [33].

4. The role of PSE in Power-to-X – Illustrative examples

In the following, we discuss examples for DSM, e-Production, and electricity storage, as well as examples in between these extremes. In particular, we demonstrate how PSE methods can help to address some of the challenges highlighted above.

4.1. Chlor-alkali electrolysis – DSM by oversizing and operational mode switching

CA electrolysis is an electricity-intensive technology, e.g., amounting for 4.25% of the total German industrial electricity consumption in 2017 [62]. Half of the total production costs are due to electricity consumption [63]. Therefore, DSM of CA processes seems promising and desirable.

CA electrolyzers are technologically well fit for variable operation (i.e., varying the production level) because of their fast dynamics [64]. However, industrial CA electrolyzers are mostly operated at over 95% capacity utilization [65]. Thus, further investment costs for oversizing the process are incurred for providing operational flexibility. Additionally, Cl_2 is utilized downstream thus either necessitating to operate also these downstream processes dynamically or to temporarily store Cl_2. Increasing the storage capacity is very costly or even prohibited due to the strict regulations for ensuring safety [66].

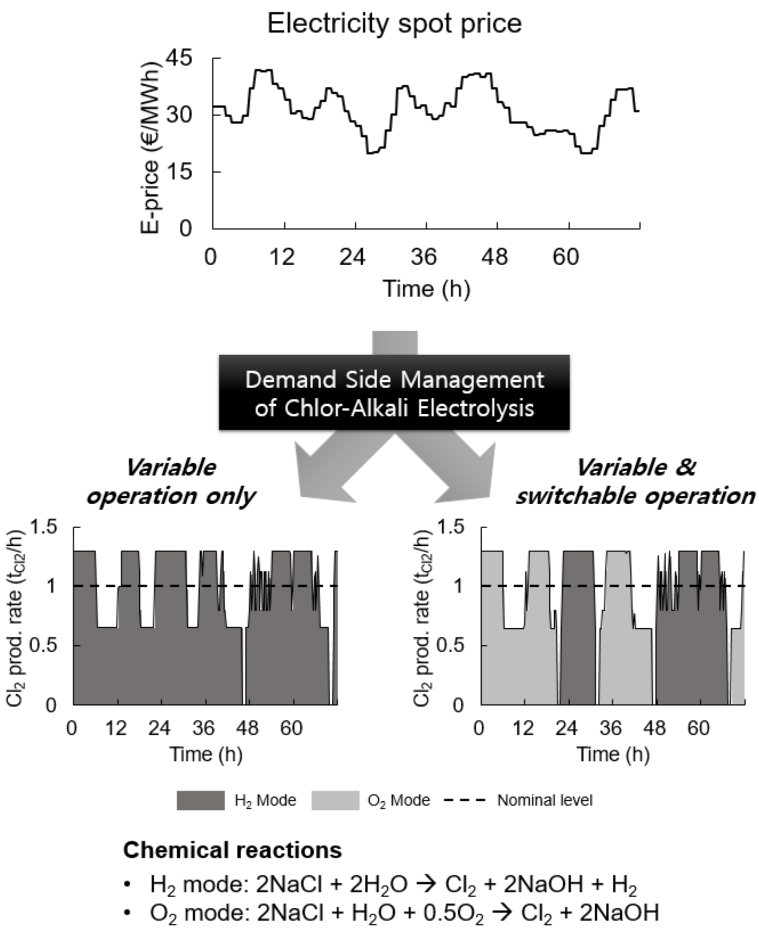

Figure 5: Illustration of two strategies for demand side management in CA electrolysis.

These challenges concerning the limited Cl_2 tank size as well as production capacity can be overcome by utilization of a bi-functional cathode [67] allowing for operational mode switching between the so-called hydrogen (H_2) mode and oxygen (O_2) mode. Both modes are characterized by the same process conditions (e.g., ramping constraints). They guarantee the same production rates of Cl_2 and sodium hydroxide (NaOH) but the O_2 mode demands 30% less electricity than the H_2 mode due to a change in side reactions. As shown in the chemical reactions in Fig. 5, the H_2 mode produces additional H_2, whereas the other consumes O_2. If electricity prices are low, it is beneficial to produce additional H_2 by consuming more electricity (i.e., H_2 mode). If electricity prices are high, consuming O_2 and less electricity (i.e., O_2 mode) is advantageous. Thus, switching the operational mode allows providing flexibility for a long duration even under limited Cl_2 storage capacity. A challenge to overcome is the electrolyzer cleaning when it is switched between the modes in order to suppress the explosive reaction of H_2 and O_2 [32]. Thus, a certain downtime of the plant has to be accepted for removing the respective gases by a purge with nitrogen. The technology can be used in new plants or by retrofit of conventional CA electrolyzers [32].

Brée et al. [32] and Roh et al. [68] analyzed the economic potential of switchable operation (in combination with variable operation) of the bi-functional CA electrolyzers in comparison with variable operation of the conventional CA electrolyzers. Solving mixed-integer linear programs (MILP) to minimize the total production costs, they determined the optimal oversizing and operation schedule of the electrolyzers. In the bottom plots in Fig. 5, the overall profiles of the optimal Cl_2 production rate of the two cases are similar. However, in the case of switchable operation, the O_2 mode is preferred when the electricity price is high while the H_2 mode becomes active when the electricity is cheap. When the electricity price fluctuates strongly, the switchable operation promises savings of 14% and 1.5% in electricity and operating costs, respectively, compared to its sole variable operation [68]. Considering the investment costs, the sole variable operation in one mode is likely to have a shorter pay-out time (POT) than the novel operation due to the absence of the capital investment for retrofitting conventional CA electrolyzers (e.g., 2.5 years for the sole variable operation, and 7.0 years for the switchable CA electrolysis [68]). However, the switchable operation has a higher capacity for DSM and thus allows for higher benefit once the POT is reached.

4.2. Process and product analysis for e-Production

The variety of applications for commodities from e-Production (e.g., transportation, chemical industry) coupled with many uncertain parameters regarding technology, policy, and society (cf. Sect. 3.6) result in a high complexity for the selection of the most beneficial product and corresponding production process. For a fair comparison, two aspects are essential for decision-making:

- Consideration of the entire life cycle and interest groups
- Consistent boundary conditions and assumptions

Regarding e-Production for transportation, Bongartz et al. [59] compared different e-Fuels (H_2, CH_4, dimethyl ether (DME), and methanol) using diverse performance indicators: overall efficiency, energy/power density, infrastructure, pollutant formation, environmental impact, and handling/safety. The analyses were entirely based on the same boundary conditions (i.e., equal sources for H_2, CO_2, and electricity, steady-state operation), as well as methods (i.e., detailed simulations, equal cost models [69], DIN norms for LCA [70] and engine measurements). The respective experts evaluated each performance indicator in an interdisciplinary setting, before the indicators were weighted for a holistic comparison. The analyses showed that a steady-state operation of the e-Production processes with renewable H_2 enables significant reduction of GHG emissions (up to 90% [59]) and pollutant formation for all e-Fuels (e.g., 95% in particulate matter emissions for DME [59]) compared to fossil fuels. However, cheap H_2 (e.g., below 5 €/kg_{H2} for DME production), and thus, a cheap average electricity price for cost competitiveness with fossil fuels need to be available. Apart from these clear results, most performance indicators turned out to be reverse for different fuels: In contrast to CH_4, DME, and methanol, H_2 is advantageous regarding fuel cost, emissions, and overall electricity consumption. The H_2 infrastructure, however, is not given and its technology less advanced, which makes its fast implementation challenging.

This example highlights the complexity in deciding how to utilize renewable electricity for e-Production in the most beneficial way: Even a systematic assessment by quantification and weighting of performance indicators does not provide clear answers. In this regard, optimization-based methods considering multiple objective functions represent a powerful tool for supporting the decision-making process. Such a method is the Reaction Network Flux Analysis (RNFA) [71] that finds the most promising reaction pathway towards a fuel candidate. While this method is based on reaction stoichiometry and yield only, Process Network Flux Analysis (PNFA) [53,72] also accounts for minimum energy demand for separation. Conflicting objectives (e.g., low cost and low global warming impact) are handled by a multi-objective optimization problem. The optimization results are Pareto fronts, where each point corresponds to a Pareto-optimal pathway. The Pareto fronts represent a rational basis for evaluating different e-Products and processes, and support decision-making for given circumstances. Recently, RNFA was coupled with computer-aided molecular design (CAMD) in order to realize an integrated product and pathway design [60].

Once a promising fuel candidate has been found, more detailed process models become necessary. They are used for obtaining more reliable estimates of the process' performance, such that bottlenecks can be identified. Model-based optimization is then performed in order to eliminate these bottlenecks reducing production cost and GHG emissions (cf. Sect. 3.6). For the industrial production of OME_1, which is a promising e-Fuel candidate with outstanding combustion properties [73], the formation of the intermediate formaldehyde was found to be responsible for the biggest exergy losses [74]. With a more direct synthesis route (i.e., the reduction of methanol to OME_1 [75]) a more efficient process could be developed and the efficiency of OME_1 production could be increased from 73% to 86%. Additionally, reasonable global warming potential (GWP) reductions were achieved [48]. Similar improvements can be expected for the production of $OME_{3\text{-}5}$, which offer a better compatibility with existing diesel engines while maintaining outstanding combustion properties [76]. Their production with established process concepts is limited to about 54% [77] starting from H_2 and CO_2, whereas novel process technologies reach an efficiency of up to 72% [78]. These examples show that system-level process analyses using detailed models enable significant improvements regarding production cost, efficiency, as well as GWP reductions of e-Production applications.

4.3. Efficient large-scale electricity storage based on ammonia

Ammonia (NH_3) is one of the most produced chemicals in the world [79] and synthesized almost exclusively via the Haber-Bosch process from nitrogen (N_2) and H_2 according to the reaction

$$\mathrm{N_2 + 3H_2 \leftrightarrow 2NH_3} \qquad R1$$

While N_2 is obtained from air separation, H_2 is predominantly obtained from steam reforming of natural gas. Since reaction R1 is reversible [79], NH_3 can act as an H_2 storage medium [80], and by combining NH_3 synthesis and decomposition with an electrolyzer and a fuel cell, one can devise an electricity storage process based on NH_3.

To this end, Wang et al. [46] proposed a process that uses a reversible solid-oxide fuel cell (RSOFC) integrated with ammonia synthesis and decomposition (Fig. 6). During charging, the RSOFC electrolyses steam to produce H_2 that is then converted to NH_3, while the heat of reaction of R1 is used to generate steam for the RSOFC. During discharging, the process is reversed and the hot product stream leaving the RSOFC in fuel cell mode provides heat for endothermic decomposition of NH_3. A steam power cycle is used to convert remaining thermal energy to electricity, and heat integration is performed between liquefaction and evaporation of O_2 and N_2 in both modes. Wang et al. conducted optimization-based process design considering steady-state operation in charging and discharging mode for equal times and demonstrated that the system can achieve round-trip efficiencies above 70% and similar storage costs as pumped hydroelectric and compressed air energy storage.

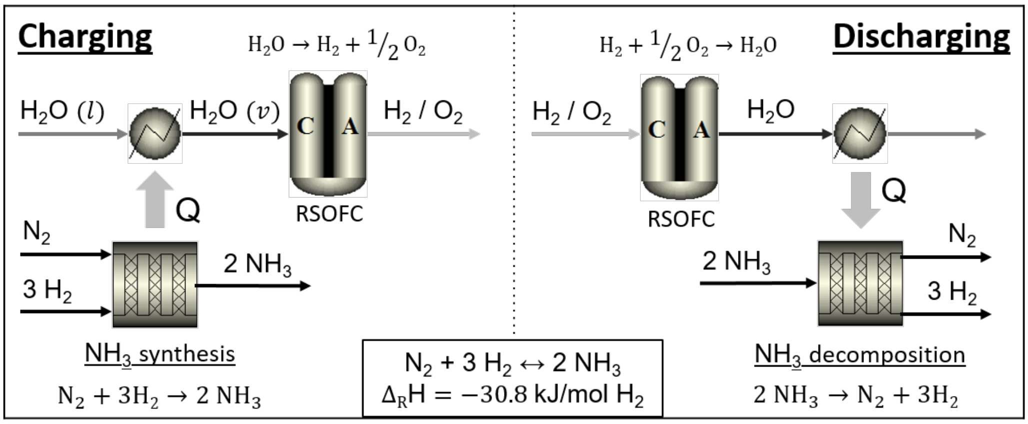

Figure 6: Heat integration between the two modes of the ammonia-based electricity storage system.

Heat integration is key for the performance of the system and enables round-trip efficiencies that are much higher than those typically associated with chemicals-based storage [45]. In fact, through synergistic effects between plant components, the combined system is more efficient than storage based directly on H_2 [81] despite adding additional conversion steps, which is in contrast to intuitive expectations. Such synergies can only be fully exploited through optimization-based approaches.

5. Summary and outlook

We define Power-to-X technologies more generally than in conventional literature as *processes with the goal to exploit the environmental and economic potential of renewable electricity*. According to this definition, such technologies comprise DSM, e-Production, and electricity storage. These different approaches for the common goal of utilization of electricity with a high share of RES offer different economic and environmental benefits depending on average electricity prices and fluctuations, as well as depending on the electricity average carbon footprint and fluctuations, but share common challenges.

DSM is worthwhile especially for electricity-intensive processes: For CA electrolysis, electricity costs can be saved if variable operation is implemented and oversizing considered. However, the dynamic operation also brings challenges, e.g., limitations on Cl_2 storage. It is demonstrated how such a limitation can be overcome by a novel mode-switching operation. For e-Production, two main challenges are identified: technology selection and efficiency improvement. Optimization-based methods give insight into conflicting performance indicators of competing products and processes (e.g., production cost and GWP reduction for e-Fuel production), and support decision-making systematically. An additional system-level process analysis using detailed models reveals bottlenecks and can finally lead to significant efficiency improvements, as well as GWP and cost reductions. For the ammonia-based electricity storage, optimization-based process design enables a round-trip efficiency of the combined synthesis process that can even exceed the one of electricity storage based on H_2 directly.

Despite many challenges that have been addressed successfully by PSE methods, there are still open questions and challenges left. Particularly relevant for electrolysis, i.e., a key element of many Power-to-X technologies, the risk of deteriorating equipment lifetime due to flexible operation of Power-to-X processes needs to be investigated. Research regarding this via both experiments and simulations is ongoing; however, long-term compatibility of the material under highly dynamic operation has not been demonstrated conclusively yet. In addition, uncertainties due to external parameters influence decision-making regarding Power-to-X technologies significantly and must be addressed in process design and operation. Especially, uncertainties in future electricity price and carbon footprint in both short- and long-terms need to be accounted for via prediction methods. This will play a key role for a successful implementation of Power-to-X technologies. All these challenges need to be tackled by further research.

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CVs and pictures

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Abbreviations

ASU	air separation unit
CA	chlor-alkali
CAMD	computer-aided molecular design
DME	dimethyl ether
DSM	demand side management
GHG	greenhouse gas
GWP	global warming potential
LCA	life cycle assessment
MILP	mixed-integer linear program
PNFA	process network flux analysis
POT	pay-out time
PSE	process systems engineering
RES	renewable energy sources
RNFA	reaction network flux analysis
RSOFC	reversible solid-oxide fuel cell
TSO	transmission system operators

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List of Figures

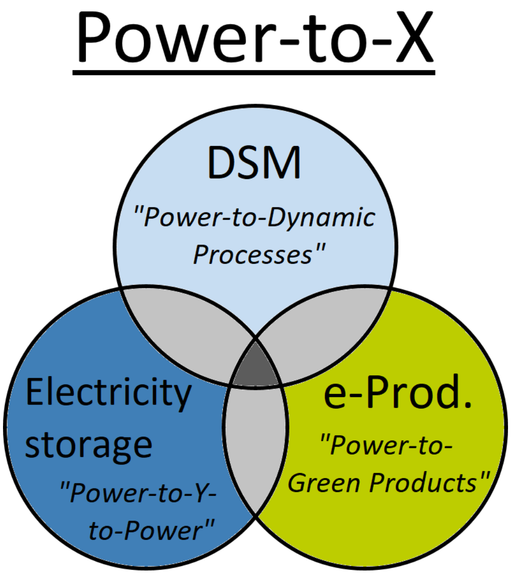
Table of Contents (TOC): Graphical Abstract

Power-to-X: Between Electricity Storage, e-Production, and Demand Side Management

J. Burre, D. Bongartz, L. Brée, K. Roh, A. Mitsos*

Review Article

A successful implementation of Power-to-X is difficult due to newly upcoming challenges. It is therefore essential to define Power-to-X and identify which technology is beneficial for which electricity scenario. We derive such trends and show how process systems engineering methods can maximize the benefits and finally support a successful implementation.


Power-to-X
DSM
"Power-to-Dynamic Processes"
Electricity storage
"Power-to-Y-to-Power"
e-Prod.
"Power-to-Green Products"