Dynamisation of Life Cycle Assessment Through the Integration of Energy System Modelling to Assess Alternative Fuels

Simon Pichlmaier, Anika Regett and Stephan Kigle

Abstract As greenhouse gas (GHG) emissions need to be reduced in order to limit the effects of climate change, Life Cycle Assessment (LCA) provides an internationally recognized framework to evaluate the environmental impact of energy supply and application technologies. However, standard LCA approaches are unable to depict the high dynamics of the future energy system. High shares of renewable energies and more variable loads intensify these dynamics according to a wide range of energy system scenarios. Therefore, a dynamisation and modularisation of the classic LCA approach is proposed in order to easily integrate the simulated electricity generation from energy system models on an hourly basis as well as future energy technologies. A special focus is put on Power-to-X (PtX) technologies in the transport sector due to its potential in deep decarbonisation scenarios.

Keywords Energy system modelling · Life cycle assessment (LCA) · Dynamic LCA · Power-to-X · Alternative fuels

1 Motivation and Problem Scope

The pathway to reach a sustainable supply of energy in the future is challenging. Nevertheless, a reduction of greenhouse gas (GHG) emissions is a pressing issue that needs to be addressed as soon as possible in order to stay below the limit of 1.5 °C of global warming [1]. The current primary energy supply is mainly based on fossil fuels. In 2016 fossil fuels accounted for 81.1% of the world's primary energy supply [2]. This applies globally as well as in Germany where in 2017 80.3% of the primary energy consumption was based on fossil fuels (hard coal, lignite, gas, oil) [3]. In order to fulfill the political agenda for decarbonisation a lot of research is conducted to illuminate the different routes towards sustainable energy supply.

S. Pichlmaier (✉) · A. Regett · S. Kigle
Forschungsstelle Für Energiewirtschaft e.V. (FfE), Am Blütenanger 71, 80995 Munich, Germany
e-mail: spichlmaier@ffe.de

F. Teuteberg et al. (eds.), *Progress in Life Cycle Assessment 2018*,
Sustainable Production, Life Cycle Engineering and Management,
https://doi.org/10.1007/978-3-030-12266-9_6

One main approach to model future energy supply are energy scenarios that are integrated in energy system models [4, 5]. A methodical framework is needed to assess the sustainability of these pathways. Life Cycle Assessment (LCA) provides such a framework and evolved to an accepted tool with international standards and norms [6], to evaluate the life cycle impact of different energy technologies [7, 8] and systems [9–11]. This article contains a detailed discussion of the requirements and limitations of the current state-of-the art of LCA of energy scenarios. It also makes a proposal to extend the current methodology to a dynamic and modulised LCA using the example of Power-to-X (PtX).

1.1 Deep Decarbonisation Energy Scenarios and the Relevance of Power-to-X Technologies

Most energy scenarios that are based on the political will to cut GHG emissions yield results that point into two slightly different directions—an electrification of energy applications or an electrification in combination with the production of synthetic fuels respectively PtX fuels [12, 13]. The main difference in whether the first or second alternative dominates, depends upon the level of decarbonisation. Especially ambitious levels of decarbonisation of up to 95% GHG emission reduction in 2050 compared to 1990, as for example aspired by the German government [14], favor a development of the energy sector towards an integration of PtX technologies [13].

The term PtX is not yet used uniformly in the literature and often causes confusion due to the variety of synonyms. Synthetic fuels, green fuels, renewable fuels, alternative fuels or electrofuels are just some of the many terms referring to fuels provided by similar technologies. In the present case PtX describes any technology that produces liquid or gaseous fuels which are produced from electricity. The key technology is the electrolysis for the separation of water into hydrogen and oxygen [15], which can be subdivided into alkaline electrolysers (AEL), proton exchange membrane (PEM) electrolysers and solid oxide electrolysers (SOEC). They differ mainly with regard to their efficiency, charge carriers and operating temperatures [16].

The resulting hydrogen can then either be used directly as a final energy carrier [17] or, in a further step, be synthesised into a carbon-containing energy carrier [18] (see Fig. 1). Currently, in literature there are two main synthesis routes for liquid energy carriers, namely methanol and Fischer-Tropsch synthesis [19]. Methanol synthesis uses CO_2 in combination with hydrogen as process inputs [20]. In the case of Fischer-Tropsch synthesis, CO is required. Therefore, CO_2 has to be converted to CO in a preceding reverse water gas shift reaction [21]. For the production of gaseous carbon-containing fuels methanation is one possible synthesis process to convert hydrogen to methane [22].

In any case, a CO_2 source is necessary. For an ultimately CO_2-neutral energy carrier, the CO_2 must not be obtained from the combustion of fossil energy sources.

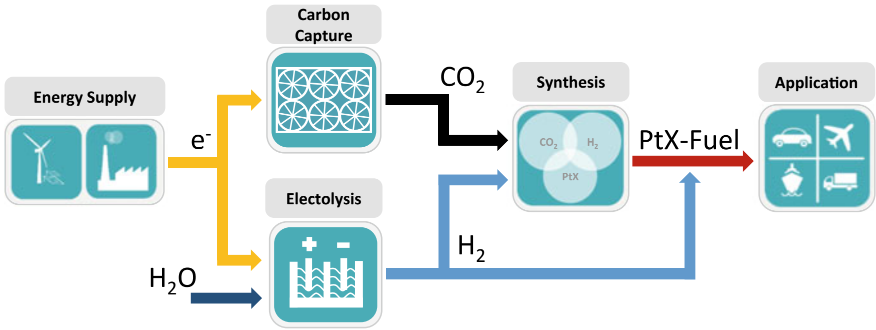

Fig. 1 Schematic representation of the production of PtX fuels

Direct air capture, the combustion of biomass or process emissions in the industry are suitable options [23].

For ambitious levels of decarbonisation these fuels are important as they possess two distinct advantages in contrast to the direct use of electrical energy:

1. PtX fuels have a high energy density. A high energy density is crucial in applications that are critical in respect to space or weight limitations such as e.g. the aviation sector.
2. PtX fuels offer the opportunity to store electricity surpluses from renewables over long periods of time.

Even though the energy efficiency is significantly lower than in case of a direct use of electrical energy [20–22], the advantages are taken to be crucial for an ambitious decarbonisation scenario.

Due to the fact that these technologies have not yet been assigned such a major role in the energy system transformation process, sustainability analyses are very rare in the literature. In addition, PtX is integrated into a highly dynamic energy system. A static assessment assuming a constant power supply is only valid to a certain degree. In the case of larger PtX plants, the repercussions on the energy system would also have to be considered. Furthermore, even with the integration of small plants and the associated marginal change in load without an effect on the energy system, it is not possible to depict the effects using a classical LCA.

1.2 *Limitations of Classic LCA Approaches and the Development Towards Dynamic LCA*

LCA methodology is commonly used to quantify the environmental impact of products or service systems [24]. For liquid and gaseous energy carriers a lot of research has been done on biofuels [25]. PtX fuels, however, only recently gained more attention. Additionally, only few research has been done on dynamic LCA such as e. g. the integration of LCA methodology into time-dependent energy system modelling.

A big hurdle to apply LCA to complete energy systems is missing data on future key technologies and production plants [10]. Furthermore, there are methodical limitations to standard LCA approaches such as double counting and shifting system boundaries in the analysis of the total energy system [11]. Another problem of LCAs of energy systems is more inherent to the energy system itself. In the context of a decarbonisation of the energy system a greater amount of renewable energies will be integrated into the power plant park. This integration will lead to higher dynamics in the provision of electricity as electricity from wind and photovoltaic plants is subject to volatile generation. However, not only the total amount of generated electricity and its provision is important, but also the flexibility of the demand-side technology and its ramp-up time to react to changes in the load. This may especially be important for the production of PtX fuels as their economic profitability strongly depends on the full load hours [26]. Therefore, the often used assumption of just deploying excess electricity from renewables is not strictly valid, but may possess potential for PtX fuels [27]. For it to be specified, a time-resolved consideration of renewable electricity generation and resulting operation strategies for PtX plants are required.

In the following a modular, dynamised LCA approach is proposed aiming at providing a more detailed assessment of future energy scenarios and the problem of volatility. The developed methodology is applied to the described case of PtX technologies.

2 Developed Methodology and Exemplary Application

According to DIN 14040/14044 an LCA can be structured in four phases: the definition of goal and scope, the life cycle inventory (LCI), the life cycle impact assessment (LCIA) and the interpretation. In Sect. 2.2 a method is explained to modularization and dynamics the determination of the LCI in order to assess the production and application of a PtX fuel in transport. The modularization allows different system boundaries and therefore different scopes of the LCA. This topic is discussed in Sect. 2.1. As an exemplary application of the methodology, in Sect. 2.3, the production of a PtX fuel with a dynamic energy system providing the electrical energy input is discussed.

2.1 Discussion of Goal and Scope for the Proposed Methodology

The proposed methodology does not imply one particular goal. Moreover, the goal has to be defined as soon as the level of modularisation is set. If the environmental

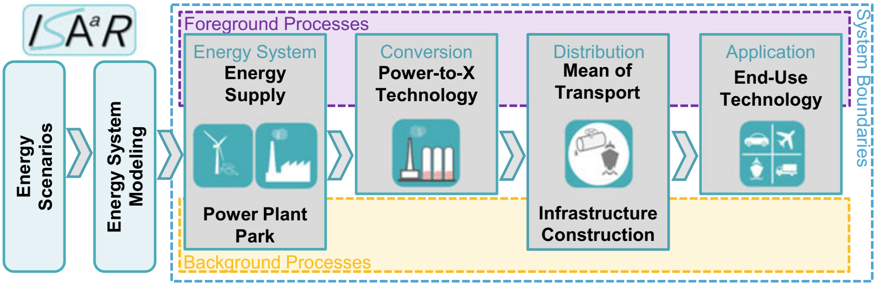

Fig. 2 Modularisation for the LCA of PtX fuels for transport applications with integration of the energy system model ISAaR

impact of the provision of 1 passenger-km (pkm) wants to be assessed, the scope and therefore the level of modularisation has to be set accordingly. But also parts of the life cycle, such as the provision of 1 kWh PtX fuel, can be assessed as explained in the following chapters. The scopes in these two cases are different and hence the system boundaries are different. Consequently, the modularisation adds flexibility to the choice of system boundaries.

In the following, first, Sect. 2.2 explains the method for the system boundaries according to a Well-to-Wheel analysis. Consequently, in addition to the operational considerations, the upstream chains of the individual life cycle stages are also considered. However, in Sect. 2.3 the focus is set on the fuel supply and the assessment method is shown for a functional unit of 1 kWh PtX fuel.

2.2 *Modularisation and Dynamisation of LCA*

Looking at the whole life cycle of a PtX fuel, it can be divided into energy supply, conversion, distribution and end use. Figure 2 illustrates these four steps within the system boundaries. It also shows which parts of the fuel life cycle are regarded as foreground and background processes. The foreground processes are part of detailed considerations, while the background processes are assessed using the database ecoinvent 3.5.

The energy system model ISAaR, developed at the Research Center for Energy Economics (FfE), provides the hourly German energy supply embedded in a European energy system. Among others, the energy sources considered include electrical energy, district heating and gas. By setting the boundary conditions, including the energy consumption by energy carriers, the dispatch of the supply systems for scenarios up to 2050 can be simulated [28] (see also Fig. 4). Additionally, the results contain economic as well as ecological indicators such as electricity prices and GHG emissions. The output of ISAaR in hourly resolution serves as an input for the LCA. Hence, the use of fuels for power supply can be considered a foreground process. This

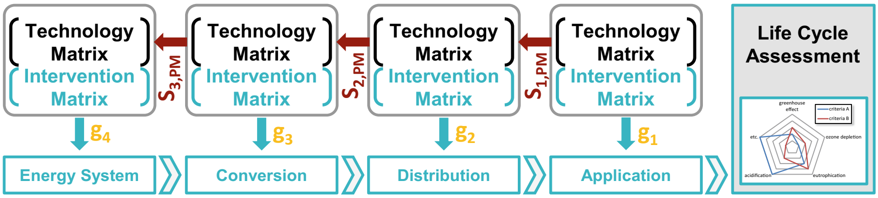

Fig. 3 Matrix interpretation of the modules to carry out the LCA. The part of the scaling vector described as $s_{i,PM}$ is the one to be handed over to the preceding system [see also Eqs. (4) and (5)]. The inventory vector g_i can be derived for each module

enables the time-dependent assessment of the environmental impact of the further PtX fuel production in the foreground and thus the inclusion of possible peaks in the power supply of volatile renewable energies. In addition, the applications such as cars and other means of transport are also considered in the foreground. This allows the comparison with transport applications using other energy sources with less favorable storage properties, such as electricity. In addition to the modeled foreground processes, the background processes are assessed with the help of the ecoinvent 3.5 database. Examples of background processes are the construction of required plants and means of transport as well as the provision of raw materials for power generation.

The modularisation of the LCA along life cycle phases is carried out to facilitate data integration and contribution analysis. It enables the smooth modification of known modules as well as the easy integration of new modules from e.g. PtX implementation projects. Furthermore, this approach allows individual sub-areas of the life cycle to be assessed in a transparent way, which simplifies the identification and communication of possible drivers of environmental impacts. As shown in Fig. 3 each module is represented by a separate technology matrix.

The matrix representation follows Heijungs et al. [29]. Therein the square technology matrix A is used to carry out the inventory analysis. A contains the input processes associated with a unit output process. For example, 1 m^3 hydrogen is assigned a certain amount of power generation. Given a final demand f the scaling vector s is to be carried out with Eq. (1):

$$s = A^{-1} f \tag{1}$$

The scaling vector serves to scale the unit processes of the technology matrix. With the use of s and the intervention matrix B, it is then possible to calculate the environmental flow vector g:

$$g = Bs \tag{2}$$

The emissions related to each unit output process are described in the intervention matrix B. It contains for example the CO_2 emissions of the combustion of coal to produce 1 kWh of electricity.

To connect the different modules, the elements in the scaling vector s of the processes to be considered in a preceding module are handed over as elements of a new final demand vector f. This concept is clarified in the following chapter using the example of a PtX fuel.

Eventually, all environmental flow vectors g_i are cumulated to derive the LCI. Ultimately, based on the LCI the LCIA can be conducted for each module separately or for all modules collectively.

2.3 Exemplary Application for the Production of PtX Fuel

The case of PtX fuel production is now considered more closely as an exemplary application of the methodological approach explained before. For this purpose, two systems of equations are set up. One represents the production of a PtX fuel and the other one describes the generation of electrical energy. The output of the whole system is a PtX fuel with the functional unit of 1 kWh referred to the lower heating value. According to Eq. (1) the first system of equations consequently results as follows:

$$\begin{pmatrix} a_{11,PtX} & a_{12,PtX} & \cdots & a_{1n,PtX} \\ a_{21,PtX} & a_{22,PtX} & \cdots & a_{2n,PtX} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1,PtX} & a_{m2,PtX} & \cdots & a_{mn,PtX} \end{pmatrix} \begin{pmatrix} s_{1,PtX} \\ s_{2,PtX} \\ \vdots \\ s_{n,PtX} \end{pmatrix} = \begin{pmatrix} f_{1,PtX} \\ f_{2,PtX} \\ \vdots \\ f_{n,PtX} \end{pmatrix} = \begin{pmatrix} 1\,\text{kWh} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (3)$$

Thereby the first row of A_{PtX}, s_{PtX} and f_{PtX} represent the PtX fuel production process. The final demand vector consists of the functional unit in the first row and zeros in every other row. Each column in the technology matrix A_{PtX} represents a unit output process. The rows contain the respective input processes. For the step of fuel conversion, the technology matrix contains, among others, the processes of operating materials such as water, CO_2 and electricity as well as the construction of the synthesis plant. Every entry a_{ij} of the matrix where $i = j$ is one. The system of equations is used to calculate the scaling vector as described above. The scaling vector contains entries of processes assessed in the PtX module and processes to be handed over to the previous module. The processes which are not handed over are used to determine the environmental flow of the PtX module g_{PtX}. For the other processes the resulting scaling vector elements are handed over as the final demand vector element of the preceding system of equations (see Fig. 3). Thus, if row α in Eq. (3) represents the provision of electrical energy, the scaling vector can be divided into one to be considered in the preceding module (PM) and one to be considered in the current module (CM):

$$s_{PtX} = s_{PtX,PM} + s_{PtX,CM} = \begin{pmatrix} 0 \\ \vdots \\ s_{\alpha,PtX,PM} = s_{\alpha,PtX} \\ \vdots \\ 0 \end{pmatrix} + \begin{pmatrix} s_{1,PtX,CM} \\ \vdots \\ s_{\alpha,PtX,CM} = 0 \\ \vdots \\ s_{n,PtX,CM} \end{pmatrix} \quad (4)$$

Consequently, the final demand vector of the energy system (ES) results in:

$$f_{ES} = \begin{pmatrix} f_{1,ES} = s_{\alpha,PtX} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (5)$$

Thus, the first row in the system of equations of the energy system corresponds to electrical energy. All other elements of the final demand vector are zero. With the use of the technology matrix of the energy system A_{ES}, the underlying environmental flow for the supply of electrical energy can now be determined as explained in Eqs. (1) and (2).

However, the high dynamics of the energy system must be included. Figure 4 illustrates the time dependency of the technology matrix of the energy system. A simulated dispatch for the provision of electrical energy for the year 2030 using the energy system model ISAaR is depicted.

The electrical energy generation of power plants is shown divided by type, such as i.e. gas, lignite and hard coal. In addition, the load and the export of electrical energy are presented. It can be seen that the deployment of the different types of power plants is subject to great variability. As an example, the technology matrices of two hours $t = 2300$ and $t = 2700$ are set up.

As a consequence, the resulting environmental flow will also vary over time. Therefore, the described system of equations must be solved for each time step, in this case each hour of the year.

Since in this example the energy system is the last set of processes to be considered, the cumulative environmental flow of the overall system for each time step can finally be calculated as follows:

$$\boldsymbol{g} = \boldsymbol{g}_{PtX} + \boldsymbol{g}_{ES} = B_{PtX} \cdot s_{PtX,CM} + B_{ES} \cdot A_{ES}^{-1} \cdot f_{ES} \quad (6)$$

As the formation of the inverse of a large, sparsely occupied matrix is a complex arithmetic operation, it is important to keep the technology matrix A_{ES} and therefore also the intervention matrix B_{ES} and the final demand vector f_{ES} as small as possible. In contrast to the consideration of the whole system, the modularisation and the associated partitioning of the technology matrix already allows a significant reduction of complexity. Additionally, the second term can be cleared of unused processes.

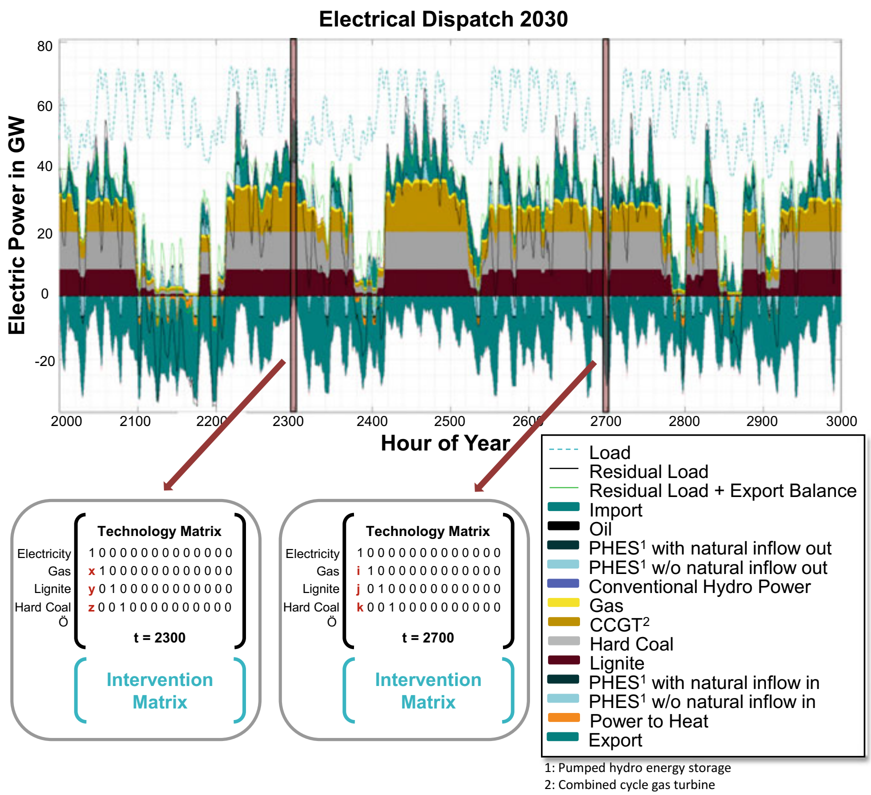

Fig. 4 Exemplary electrical dispatch for the hours 2000–3000 of the year 2030 and schematic representation of the technology matrices for two hours (t = 2300, t = 2700)

Then, in order to enable the addition with the vector g_{PtX}, the vector g_{ES} must again be extended by the corresponding zeros to match the length of the vector g_{PtX}.

In the present case, it is assumed that only the energy system varies over time. For example, in the event of a variable operation of an electrolyser, the system of equations for the conversion can also be time-dependent. In this case, the existing system can also be extended by a time dependency of the load. Therefore, e.g. partial load capable electrolysers can also be investigated.

3 Outlook and Future Projects

The methodology proposed above adds new aspects to classic LCA approaches. By being able to integrate distinct time series for the production of electricity and the related energy generation parks, a new level of dynamisation can be reached. The high temporal resolution adds to the accuracy of the LCA as the highly fluctuating composition of the electricity mix from different generation technologies can be taken into account. Additionally, the environmental impact of different electricity generation technologies can be compared according to different future energy scenarios.

The modularisation of the LCA adds the advantage to easily interchange, modify and add process data without the need to calculate the whole fuel life cycle all over again. Therefore, competing life cycles can easily be compared with regard to their environmental impact and new data of future technologies can be integrated to track environmental improvements. In addition, the computational complexity for the formation of matrix inversions can be reduced by the modularisation.

This newly developed methodology is implemented, in a first step, in a case study of different PtX production chains in the context of the project BEniVer. In a second step, a full integration into the energy system model ISaAR is aspired. By feeding the results of the LCA back into ISaAR it is possible to use them as an optimisation criteria in the plant expansion and deployment planning.

Acknowledgements This work was performed within the project BEniVer, which is funded by the Federal Ministry of Economic Affairs and Energy on the basis of a resolution of the German Bundestag under the funding reference 03EIV116C.

References

1. IPCC (2018) Global warming of 1.5 °C. An IPCC special report on the impacts of global warming of 1.5 °C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty. In: Masson-Delmotte V, Zhai P, Pörtner HO, Roberts D, Skea J, Shukla PR, Pirani A, Chen Y, Connors S, Gomis M, Lonnoy E, Matthews JBR, Moufouma-Okia W, Péan C, Pidcock R, Reay N, Tignor M, Waterfield T, Zhou X (eds). In Press
2. IEA (2018) Key World Energy Statistics 2018. IEA, Paris
3. BMWi (2018) Energiedaten: Gesamtausgabe. BMWi, Berlin
4. Wang, Z et al (2017) Outline of principles for building scenarios—transition toward more sustainable energy systems. In: Applied energy, vol 185 Part 2. Elsevier, Amsterdam
5. Lopion P et al (2018) A review of current challenges and trends in energy systems modeling. In: Renewable and sustainable energy reviews vol. 96. Elsevier, Amsterdam
6. Finkbeiner M et al (2006) The new international standards for life cycle assessment: ISO 14040 and ISO 14044. In: The international journal of life cycle assessment vol. 11, issue 2. Springer Nature Switzerland AG, Cham
7. Cherubini F et al (2009) Energy- and greenhouse gas-based LCA of biofuel and bioenergy systems: key issues, ranges and recommendations. In: Resources, conservation and recycling 53. Elsevier, Amsterdam
8. Turconi R Boldrin A Astrup T (2013) Life cycle assessment (lca) of electricity generation technologies: overview, comparability and limitations In: Renewable and sustainable energy reviews 28:565–565. Elsevier, Philadelphia

9. Rauner S et al (2017) Holistic energy system modeling combining multi-objective optimization and life cycle assessment. In: Environmental research letters 12. IOP Publishing, Bristol
10. Volkart K et al (2018) Integrating life cycle assessment and energy system modelling: methodology and application to the world energy scenarios. In: Sustainable production and consumption 16. Elsevier, Amsterdam
11. Vandepaer L et al (2018) The integration of energy scenarios into LCA: LCM2017 conference workshop. In: The international journal of life cycle assessment 01/2018. Springer-Verlag GmbH Germany, Berlin
12. Gebert P et al (2018) Klimapfade für Deutschland. München: The Boston Consulting Group (BCG), Prognos
13. Bründlinger T et al (2018) dena-Leitstudie Integrierte Energiewende—Impulse für die Gestaltung des Energiesystems bis 2050—Teil A: Ergebnisbericht und Handlungsempfehlungen (dena)—Teil B: Gutachterbericht (ewi Energy Research & Scenarios gGmbH). Deutsche Energie-Agentur GmbH, Berlin
14. Klimaschutzplan 2050—Klimaschutzpolitische Grundsätze und Ziele der Bundesregierung. Berlin: Bundesministerium für Umwelt, Naturschutz, Bau und Reaktorsicherheit (BMU), 2016
15. Foit SR et al (2017) Power-to-syngas: an enabling technology for the transition of the energy system? In: Angewandte Chemie—International Edition vol. 56, issue 20. Wiley-VCH Verlag GmbH, Weinheim
16. Ursúa A et al (2012) Hydrogen production from water electrolysis: current status and future trends. In: Proceedings of the IEEE vo1. 100, issue 2. Piscataway: IEEE—Institute of Electrical and Electronics Engineers Inc
17. Gamba M et al (2016) Power-to-gas hydrogen: techno-economic assessment of processes towards a multi-purpose energy carrier. Politecnico di Torino, Torino, Italy
18. Tremel A (2017) Green hydrogen and downstream products—electricity-based fuels for the transportation sector. In: Internationaler Motorenkongress 2017, Proceedings. Springer Fachmedien, Wiesbaden
19. Dayton DC, Spath PL (2003) Preliminary screening—technical and economic assessment of synthesis gas to fuels and chemicals with emphasis on the potential for biomass-derived syngas. National Renewable Energy Laboratory, Golden, Colorado
20. Fasihi M et al (2017) Synthetic methanol and dimethyl ether production based on hybrid PV-wind power plants. Lappeenranta University of Technology, Lappeenranta (Finland)
21. Fasihi M et al (2016) Techno-economic assessment of power-to-liquids (PtL) fuels production and global trading based on hybrid PV-wind power plants. Lappeenranta University of Technology, Lappeenranta (Finland)
22. Götz M, Lefebvre J, Mörs F, Koch AM, Graf F, Bajohr S, Reimert R, Kolb T (2016) Renewable power-to-gas: a technological and economic review. Karlsruhe Karlsruhe Instituts für Technologie 85:1371–1390
23. Purr K et al (2016) Integration of power to gas/ power to liquids into the ongoing transformation process. German Environment Agency, Dessau-Roßlau
24. Finkbeiner Ms (2014) The international standards as the constitution of life cycle assessment. In: Klöpffer Walter (ed) Background and future prospects in life cycle assessment. Springer, Netherlands
25. Menten F et al (2013) A review of LCA greenhouse gas emissions results for advanced biofuels: the use of meta-regression analysis. In: Renewable and sustainable energy reviews, vol. 26. Elsevier, Amsterdam
26. Regett A, Pellinger C, Eller S (2014) Power2Gas—Hype oder Schlüssel zur Energiewende in: Energiewirtschaftliche Tagesfragen—64. Jg. (2014) Heft 10. etv Energieverlag GmbH, Essen
27. Uusitalo V et al (2017) Potential for greenhouse gas emission reductions using surplus electricity in hydrogen, methane and methanol production via electrolysis. In: Energy conversion and management, vol 134. Elsevier, Amsterdam

28. Pellinger C (2016) Mehrwert Funktionaler Energiespeicher aus System- und Akteurssicht—Dissertation an der Fakultät für Elektrotechnik und Informationstechnik an der TU München, durchgeführt an der Forschungsstelle für Energiewirtschaft e.V., München
29. Heijungs R et al (2002) The computational structure of life cycle assessment. Centre of Environmental Science Leiden University, Leiden