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Editorial

Progress in Power-to-Gas Energy Systems

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1. Introduction

Hydrogen is expected to become a key component in the decarbonized energy systems of the future. Its unique chemical characteristics make hydrogen a carbon-free fuel that is suitable to be used as broadly as fossil fuels are used today. Since hydrogen can be produced by splitting water molecules using electricity as the only energy input needed, hydrogen offers the opportunity to produce a fully renewable fuel if the electricity input also only stems from renewable sources. Once renewable electricity is converted into hydrogen, it can be stored over long periods of time and transported over long, even intercontinental, distances. Underground hydrogen storage, pipelines, compressors, liquefaction-units, and transportation ships are infrastructures and suitable technologies to establish a global hydrogen energy system. Several chemical synthesis routes exist to produce more complex products from green hydrogen to fulfil the demands of various end-users and industries. One exemplary power-to-gas product is methane, which can be used as a natural gas substitute. Furthermore, ammonia, alcohols, kerosene, and all other important products from hydrocarbon chemistry can be synthesized using green hydrogen.

In the light of the continuously exacerbating crisis of global warming, the urgency of deploying green technologies could not be more pressing. Researchers and industry innovators worldwide study and develop all aspects of power-to-gas technologies, ranging from hydrogen production, conversion, transport, handling, etc., to the broad variety of end-use options. In the meanwhile, it remains an open research question to what extent the portfolio of power-to-gas technologies and products will enter the markets. For the various end-use sectors, the future defossilized energy mix will develop into different optima depending on the availability, flexibility, and cost of energy, as well as technical implications for the end users and the specific legal and regulatory framework. As a result, we will see different local or regional energy mixes and fuel compositions around the globe.

A major unknown variable is the depths in which direct electrification of processes will be implemented. Direct electrification—in cases where it leads to similar product qualities in industry or comfort in the mobility or household sectors—promises higher efficiencies and makes the more complex synthesis routes of power-to-gas technologies obsolete. However, a fully electrified energy system will lack the large scale and long-lasting storage option, not cover the fuel demands by high-temperature industrial processes, and lack back-up power plants needed for weather-conditions with insufficient renewable electricity supply. Thus, the role of molecules as energy carriers is very crucial, but at the same time is challenged by the competing direct electrification in some market segments.

A recent Special Issue of the open access journal *Energies* published ten research articles from the field of hydrogen and power-to-gas energy. The Special Issue entitled 'Progress in Power-to-Gas Energy Systems' covers several aspects of hydrogen energy systems, including hydrogen production, transport/distribution, storage, end use, as well as legal and regulatory aspects. This editorial summarizes the key findings. Finally, a brief discussion will pick up the main ideas of the introduction and place the research results of the Special Issue in the wider context of the defossilization of energy sectors and the competition of electrons vs. molecules.

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2. Special Issue Articles

The ten articles published in the Special Issue 'Progress in Power-to-Gas Energy Systems' are presented in Table 1, where an overview of the authors, research fields, titles and methodologies is given.

Table 1. Summary of the research fields, titles, and methodologies of the Special Issue articles.

Article	Authors	Research Field	Title	Methodology
[1]	Yan Zhao, Vince McDonell, Scott Samuelsen	Combustion Science	Residential Fuel Transition and Fuel Interchangeability in Current Self-Aspirating Combustion Applications: Historical Development and Future Expectations	Review Article
[2]	Jörg Leicher, Johannes Schaffert, Hristina Cigarida, Eren Tali, Frank Burmeister, Anne Giese, Rolf Albus, Klaus Görner, Stéphane Carpentier, Patrick Milin, Jean Schweitzer	Combustion Science	The Impact of Hydrogen Admixture into Natural Gas on Residential and Commercial Gas Appliances	Combustion Theory, Calculations, Experimental Investigations
[3]	Paul Glanville, Alex Fridlyand, Brian Sutherland, Miroslaw Liszka, Yan Zhao, Luke Bingham, Kris Jorgensen	Combustion Science	Impact of Hydrogen/Natural Gas Blends on Partially Premixed Combustion Equipment: NOx Emission and Operational Performance	Experimental Research
[4]	David Tetzlaff, Vasanth Alagarasan, Christopher Simon, Daniel Siegmund, Kai junge Puring, Roland Marschall, Ulf-Peter Apfel	Electro Catalysis	[NiFe]-(Oxy)Sulfides Derived from $NiFe_2O_4$ for the Alkaline Hydrogen Evolution Reaction	Experimental Research
[5]	Andreas Zauner, Karin Fazeni-Fraisl, Philipp Wolf-Zoellner, Argjenta Veseli, Marie-Theres Holzleitner, Markus Lehner, Stephan Bauer, Markus Pichler	Energy Economy, Energy Storage	Multidisciplinary Assessment of a Novel Carbon Capture and Utilization Concept including Underground Sun Conversion	Techno-economic assessment Life cycle assessment Legal assessment
[6]	Janos Lucian Breuer, Juri Scholten, Jan Christian Koj, Felix Schorn, Marc Fiebrandt, Remzi Can Samsun, Rolf Albus, Klaus Görner, Detlef Stolten, Ralf Peters	Mobility	An Overview of Promising Alternative Fuels for Road, Rail, Air, and Inland Waterway Transport in Germany	Mobility Sector Modeling
[7]	Hannu Karjunen, Eero Inkeri, Tero Tynjälä	Energy System Analysis	Mapping Bio-CO_2 and Wind Resources for Decarbonized Steel, E-Methanol and District Heat Production in the Bothnian Bay	Potential Analysis
[8]	Johannes Schaffert, Hans Christian Gils, Max Fette, Hedda Gardian, Christine Brandstätt, Thomas Pregger, Nils Brücken, Eren Tali, Marc Fiebrandt, Rolf Albus, Frank Burmeister	Energy System Analysis	Integrating System and Operator Perspectives for the Evaluation of Power-to-Gas Plants in the Future German Energy System	Energy System Modeling, Energy Economics, Assessment of Regulatory Framework
[9]	Yifei Lu, Thiemo Pesch, Andrea Benigni	Energy System Analysis	Simulation of Coupled Power and Gas Systems with Hydrogen-Enriched Natural Gas	Energy Grid Modeling
[10]	Lena Maria Ringsgwandl, Johannes Schaffert, Nils Brücken, Rolf Albus, Klaus Görner	Energy Law and Regulation	Current Legislative Framework for Green Hydrogen Production by Electrolysis Plants in Germany	Legal and Regulatory Assessment

The contributions bring together various research fields. The first item in Table 1 contains a comprehensive review paper on the historic development of residential combustion technologies and fuel transitions that have been realized in the past [1]. The following two articles [2,3] stem from the field of combustion science and analyze in detail the impact of hydrogen admixture in natural gas (or methane). Both pieces of research include theoretical and experimental approaches. In [3], the focus is on partially premixed combustion, which plays a dominating role in the US-American natural gas appliances. One contribution from the field of catalysis describes a production method for facilitating the Alkaline Hydrogen Evolution Reaction [4]. In [5], the role of underground gas storage as a potential large-scale methanation reactors is addressed. Hydrogen and hydrogen-derived fuels in various mobility sectors are studied in [6]. Three articles were published from the field of energy system analysis. In [7], a detailed case study of a region in Finland is modeled, while in [8], the German energy system was modeled and assessed from system and operator points of view. Gas and electricity energy networks were modeled in [9] with a focus on co-simulation and hydrogen/natural gas blends. Finally, an assessment of the current legal framework for green hydrogen production in Germany was published in [10].

In the following, brief summaries of the ten research papers are given.

The work by Zhao et al. [1] provides a comprehensive literature review of the historic development of residential fuel transition and fuel interchangeability in self-aspirating combustion applications. The researchers from University of California, Irvine, CA, USA, go back in time and reflect on the fuel transitions in the domestic heating sector in the past centuries in great detail. The paper includes the history of coal substituting fuelwood in England starting in the 1500s, and the introduction of manufactured gases (amongst others the so-called town gas) starting in the early 19th century, followed by the town-gas-to-natural-gas transition in the second half of the 20th century. In England, this fuel switch led to 35 million appliances with 200 million burners being converted. The authors also address safety issues related to carbon monoxide poisoning and the development of gas quality standards. The emergence of renewable gases since the 1980s is summarized for the case of biogas and renewable hydrogen, including an outlook on future developments. The competing options of electrifying homes versus adopting renewable gases is discussed as well. A separate chapter of this work discusses technical considerations of adopting renewable fuels in residential burners in detail, explaining relevant combustion characteristics and formulae. Subsequently, the burner performance indicators efficiency, emissions, flame characteristics, and ignition are discussed.

Leicher et al. [2] address the impact of hydrogen admixture into natural gas on residential and commercial gas appliances. Hydrogen admixture into existing natural gas grids is being discussed as a way for the gas industry to contribute to decarbonization efforts in the short-term. The work was carried out as part of the European Commission-funded research project THyGA, which currently investigates up to 100 appliances in laboratory tests with hydrogen blending levels up to 60% by volume [11–13].

The main findings of these theoretical considerations and the accompanying first measurements are that hydrogen admixture into natural gas can in many ways be treated as a conventional natural gas quality issue. Many effects of the changing fuel characteristics induced by hydrogen, e.g., in terms of laminar combustion velocities, combustion temperatures, or the formation of nitrogen oxides (NO_X), are largely compensated by shifts towards higher air excess ratios in uncontrolled residential appliances. In appliances with combustion control, the control systems were found to be unable to maintain a constant air excess ratio with increasing levels of H_2 admixture, at least at full load. This is, however, not a safety-relevant concern since air excess ratios increase with higher levels of hydrogen, making the formation of toxic carbon monoxide less likely. These findings are, to some extent, specific to certain technologies: fully premixed gas appliances, which are common in heating systems in the EU, are less sensitive to issues such as flame flash backs than partially premixed devices, which can be found in cooking applications and in American residential heating appliances.

The theoretical and experimental investigations in THyGA so far indicate that a hydrogen admixture of about 20 vol% into natural gas, as it is currently proposed, does not pose any safety-related challenges, e.g., in the form of flame flash backs, overheating, or increased pollutant emissions, to the appliance types found in the field today. There are additional aspects to consider, e.g., in the context of appliance adjustment in the field, which is a topic ongoing research within the THyGA project.

In Glanville et al. [3], six North American hydrogen/natural gas blending demonstrations were selected for a literature review that set the basis for the subsequent experimental approach. Through laboratory testing using purpose-built "simulators" and in situ tests and field sampling in a simulated operating environment, a series of short-term tests were performed on components and equipment. Performance, efficiency, emissions, and other factors were characterized as a function of hydrogen blending up to 30% by volume. In general, all appliances and their burners were able to tolerate this shift in fuel composition, without notable excursions in process temperatures or emissions, and anticipated trends were confirmed and further quantified for these appliances, ranging from the de-rating of heat input, to the increase in excess aeration, and to the NOx and CO emissions. For these partially premixed types of combustion appliances, the dominant impact of hydrogen blending without extra adjustments is the increase in excess air, often resulting in lower NOx emissions, surface temperatures, and other parameters. The most sensitive burners to hydrogen blending were of the "in-shot" variety, used by warm-air furnaces, tested in the laboratory. The flash back events observed were inconsistent and likely caused by either test procedures or sensitivities of the specific test stands used. Further investigation into these burners is recommended [3].

Tetzlaff et al. [4] focus on hydrogen production, more specifically, on precious-metal-free electrocatalysis, which is a key factor for industrial-scale hydrogen production. Using controlled (partial) sulfidation of Fe/Ni oxide nanoparticles, the authors describe a novel synthesis procedure for mixed Fe/Ni (oxy)sulfide materials. As a result, high overall activities of the synthesized electrocatalysts were reported for the electrochemical hydrogen evolution reaction and interpreted as a step forward towards designing transition metal chalcogenide catalyst materials for the hydrogen evolution reaction and efficient stoichiometric formulations of NiFe (oxy)sulfide-based catalysts. [4]

Zauner et al. [5] approach the Power-to-Gas topic and more specifically, the underground storage of renewable methane synthesized from hydrogen and carbon dioxide from economic, technical simulation, greenhouse gas emissions, and legal points of view. The so-called Underground Sun Conversion or geo-methanation process uses green hydrogen and carbon dioxide captured from industrial emitters. The gases are injected into depleted underground hydrocarbon reservoirs, where the methane synthesis is realized by biochemical processes. The resulting gas is cleaned to achieve natural gas grid compliant feed-in quality before it is used in industry, closing a carbon cycle. Results show, that the novel synthesis route for methane production may be at comparable or lower cost compared to conventional above-ground methane synthesis. However, it must be taken into account that in order to produce geomethane with an underground sun conversion plant, according to current knowledge, large quantities of carrier gas are required by the process and must be stored simultaneously with the hydrogen and carbon dioxide used for underground methanation. Therefore, the underground sun conversion technology is particularly suitable when large quantities of gas have to be stored already. This commonly occurs for reasons of system relevance or supply security. As an additional benefit of this storage process, geomethane can be produced from renewable hydrogen and carbon dioxide, thus contributing to the achievement of climate targets. However, a list of legal or regulatory barriers or gaps, along with technical uncertainties, preventing project realization on an industrial scale is reported [5].

Karjunen, Inkeri, and Tynjälä [7] performed a regional resource analysis for a potential hydrogen valley (i.e., a promising early adoption site for hydrogen). Open data sources were used to identify the existing local industrial facilities from the northern region of

Sweden and Finland. The steel industry alone could require 55 TWh of additional renewable electricity by 2045 for producing the required hydrogen for carbon-neutral steel production. The production of renewable methanol from electricity and CO_2 could also require up to 85 TWh of electricity annually if all of the available biogenic CO_2 resources in the area were to be utilized. To put these numbers in perspective, the current annual electricity consumption of Sweden and Finland is 127 and 81 TWh, respectively. The study also evaluated the role of wind power production as a source of additional renewable power generation in the region. Existing projects in the area already amounts to 16 TWh of annual electricity production, but even 100 TWh could be exceeded in the following decades. The study also performed an analysis of the utilization of residual electrolyzer heat in the district heat supply when primed with heat pumps. The required industrial volumes of hydrogen are so vast that eventually a significant oversupply of low-grade heat is to be expected, but first demonstrations still show great integration benefits. Future studies are recommended to assess the dynamic performance of the system, leading to a more concise implementation plan for the region.

Breuer et al. [6] review alternative fuels based on Power-to-Gas and Power-to-Liquid processes, as well as corresponding propulsions systems, to solve challenges of decarbonizing the road, rail, air, and inland waterway transport sectors. On the production side, the criteria of technical maturity, costs, as well as environmental impacts were evaluated. On the utilization side, possible blending with existing fossil fuels and the satisfaction of the required distances are composed. From today's perspective, the electrification of most long-distance, heavy-duty road, shipping, and aircraft transportation is highly unlikely. In conclusion, Methanol-to-Gasoline, Fischer–Tropsch diesel and kerosene, hydrogen, battery-electric propulsion, HVO, DME, and natural gas were identified as promising future fueling options. All the above-named alternative fuels can reach near-zero greenhouse gas emissions bounded to preconditions. The results of the cost value review highlight the insecurities around the regarded cost levels, production costs, cross-border prices, and end-user prices. The extracted interval sizes of cross-border prices for 2020 are 7 EURct/kWh_LHV for H_2, 10 EURct/kWh_LHV for SNG, and 8 EURct/kWh_LHV for unspecified PtL fuels. Cost insecurity increases for 2030 and 2050, as does the length of the value chains. At present, cost comparisons indicate that lower production costs of H_2 are almost compensated by higher transport costs in comparison to fuels that offer existing infrastructural compatibility.

In their energy system analysis, Schaffert et al. [8] study in what way, and in which sectors, renewable energy will be integrated in the German Energy System by 2030, 2040, and 2050 and what role hydrogen and methane from power-to-gas processes will play in this integration.

To address their research questions, techno-economic energy system modeling was performed. Evaluation of the resulting operation of energy technologies was carried out from system and business points of view. Special consideration of gas technologies, such as hydrogen production, transport, and storage, was taken as a large-scale and long-term energy storage option and a key enabler for the decarbonization of the non-electric sectors. The broad set of results gives insight into the entangled interactions of the future energy technology portfolio and its operation within a coupled energy system. Amongst other energy demands, CO_2 emissions, hydrogen production, and future power plant capacities are presented. One main conclusion is that integrating the first elements of a large-scale hydrogen infrastructure into the German energy system by 2030 is necessary for ensuring the supply of upscaling demands across all sectors. Within the regulatory regime of 2020, authors suggest that investment decisions for large scale hydrogen infrastructures may come too late and might jeopardize the chances of achieving transition targets within the 2050 horizon [8].

In a second contribution from the field of energy system analysis, Yifei et al. [9] simulate coupled power and gas energy systems, including the option of hydrogen-enriched natural gas. Their methodological approach can handle different gas compositions and is thus able to accurately analyze the impact of hydrogen injections into natural gas pipelines. An exemplary co-simulation of coupled power and gas networks proves the capabilities of the new model. The authors implemented a detailed description of the physical properties of the gas mixtures, which allows tackling co-simulation research questions in the future. The importance of detailed technical simulation is highlighted for a number of examples including the necessity of considering different and—importantly—varying gas compositions in simulations. [9]

The work by Ringsgwandl et al. [10] contributed to this Special Issue's topic from a complementary point of view by addressing the current legislative framework for implementing green hydrogen production plants. For the case of Germany, the authors analyze laws and ordinances to identify potential obstacles to the rollout of green hydrogen. Especially the implications on potential hydrogen production plant operators are focused on. Due to unbundling-related constraints, potential operators from the group of electricity transport system and distribution system operators lacking permission to operate hydrogen production plants. Moreover, ownership remains forbidden for them. The same applies to natural gas transport system operators. The case is less clear for natural gas distribution system operators, where explicit regulation is missing. It is finally analyzed if the production of green hydrogen production, in its competition with fossil hydrogen production, is currently supported, not only by the legal framework but also by the National Hydrogen Strategy and the Amendment of the Renewable Energies Act. It can be concluded that in recent amendments of German energy legislation, regulatory support for green hydrogen in Germany was found. The latest legislation has clarified crucial points concerning the ownership and operation of electrolyzers and the treatment of green hydrogen as a renewable energy carrier. This can be seen as a step forward towards a green hydrogen rollout; nevertheless, a number of clarifications are still needed to allow a swift, large-scale implementation of green hydrogen in a deeply decarbonized energy system. As an outlook, the already proposed amendment for the Renewable Energy Directive by the European Commission is expected to bring quotas for renewable hydrogen used in industry. This might become a game-changer and lead to a drastic acceleration of hydrogen deployment in European member states.

3. The Current Status of Research in the Field of Power-to-Gas Energy Systems

Power-to-Gas energy systems is a research field within Energy Science, that requires interdisciplinary approaches. This is especially due to the coupling functions that Power-to-Gas technologies perform, e.g., between the electricity and gas energy sectors. Technical development alone does not suffice to enable a mass roll-out of Power-to-Gas plants and Power-to-Gas products. Rather, complementary research fields need to work coherently to assess the strengths, weaknesses, chances, and risks of implementing Power-to-Gas technologies in today's energy systems.

The broad portfolio of research fields in energy science that intensely study the future prospects of hydrogen and related energy carriers is also reflected in the recent Special Issue of *Energies* [14], which is summarized in this editorial. We received contributions from combustion science [1–3], which is a field currently studying the hydrogen tolerability of today's gas applications. We also received a manuscript from the field of catalysis [4], a research field that focuses on the development of energy- and cost-effective materials for hydrogen production. Furthermore, one contribution deals with large-scale energy storage and hydrogen-to-methane conversion [5]. In addition, one paper that assesses various renewable fuel options for the mobility sector [6] has been included. Energy System Analysis is a broad topic itself, with three papers being published in this Special Issue. One of them modeled a region in Finland [7] as a case study for large-scale industrial energy applications. A second paper modeled the future German Energy System and assessed the results from techno-economic as well as operator perspective [8]. The third contribution focused on the technical modeling of power and gas networks including the option of hydrogen/natural gas blends [9]. Finally, one article is dedicated to the legal framework for implementing green hydrogen for the case of Germany [10].

Only by reflecting the progress of Power-to-Gas-related research from all relevant disciplines can the current status and remaining challenges of this transition be understood. The Special Issue discussed here can only yield punctual insights into current research. Many more crucial research fields remain untouched. As an example, the important topic of social acceptance of technologies and policies shall be mentioned here.

The technologies needed to supply economies with clean energy, to convert it into the desired form, to store, to distribute and to utilize it, are available and are constantly being optimized. Research in this field must bridge the gap between academic understanding of clean energy technologies on the one hand side and a very constructive applied science approach on the other hand side. By this re-focussing on the implementation of the various energy applications, the remaining knowledge gaps must be identified and filled to facilitate the mass roll-out of clean energy technologies.

Let us have a more detailed look at the research topics mentioned above. The three publications from the field of **combustion science** describe in high technical detail the chances of blending hydrogen into existing natural gas distribution networks and using it with todays' end-use appliances. Highly depending on the exact design of appliances, i.e., geometrical, burners, fuel–air mixing, combustion controls, etc., some hydrogen admixture may be tolerable without changing the appliances in the field. Operation safety is the dominating concern when debating the use of existing appliances with new gas properties, while in general, the distribution of (defossilized) gaseous fuels distributed through existing grid infrastructure appears advantageous for quick decarbonization effects in the heating sector. For high hydrogen contents in distributed gas mixtures, e.g., above 20 vol-% or 30 vol-%, and especially for the case of a pure hydrogen distribution on the household level, new appliance types designed for this purpose will need to be installed. Fuel cells would be a high-efficiency option here. Also, a hydrogen combustion-based heat supply in households can be realised. The electric-driven heat pump is in the lead so far. For well-insulated buildings, it can be a very cost-effective option. In industry, however, especially in high-temperature processes, fuels will be needed, e.g., for energy-intensive melting, blast furnaces or direct reduction of iron, where electricity cannot supersede gases or fuels. Here, a strong demand for hydrogen can clearly be expected. **Underground gas storage** facilities such as the salt domes used today are available technology to store hydrogen in very large quantities and over seasonal time-scales. It is more complex for the case of pore storages, such as that studied in [5], where biological methanation reactions could be used to upgrade the heating value of a stored gas mixture. If this option is drawn in the future, regions that lack salt deposits suitable for hydrogen storage could benefit from pore storage potentials.

In the **mobility sector**, it appears obvious that small vehicles, especially those that make up the large fleets of private passenger cars, may be equipped with electric propulsion systems and batteries at lower cost and higher energy efficiency compared to hydrogen or other power-to-gas products. The case is different for heavy-duty transportation on the road, rail, waterways, and, obviously, aircrafts, where the high energy densities of (liquid) fuels or compressed/liquefied gases remain advantageous compared to battery energy storage.

The research field of **Energy System Analysis** delivers insights generated in the toolbox of energy system models. Researchers cope with the above-mentioned uncertainties concerning future energy mixes by parametrizing their energy system models with assumptions for the studied technologies and optimizing the energy systems within predefined boundary conditions. The latter are based on scenarios that contain economic and regulatory base assumptions, which are in turn based on scenarios. Scenario variations allow for identifying sensitivities and assess the robustness of results. While specific quantitative results are to be interpreted carefully and only against the background of all assumptions and boundary conditions, general trends that robustly emerge for various scenarios lead to resilient results.

As far as a green energy transition is a technical issue with available solutions at hand, decision makers do have the option to realize the transformation of fossil-dominated into renewable energy systems. Various disciplines of research, some of which have been mentioned here, support policy makers with technology developments and results from their simulation-based tool-boxes. The state of progress in power-to-gas energy research suggests that future research focus should be placed on technology implementation in energy systems. By addressing the details of real-world applications of power-to-gas technologies, the concepts have to prove themselves suitable for the manifold requirements and boundary conditions. By turning to applied research, future studies should follow the progressing technology readiness of power-to-gas technologies and prepare the next steps towards mass roll-out. Detailed technical studies of power-to-gas technologies in interaction and competition with existing technologies in the field are needed. In addition, technology acceptance research from the social science perspective, as well as the development of legal and regulatory frameworks and appropriate funding schemes, are needed to guide policy makers in creating investment security for decision makers in renewable energy markets worldwide.

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