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Indispensable in the Decarbonized Energy Chain

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Abstract

Electricity will become the main energy supplier to deliver energy services to the end consumer, being it residential, commercial or industrial. However, as part of the road to a fully carbon neutral energy system by 2050, molecules as energy carriers will play a key role. The paper describes the challenges for decarbonizing the different energy vectors and how choices are impacting energy efficiency.

Two main routes exist to produce carbon-free hydrogen: classic approaches from carbon-based fuels equipped with Carbon Capture and Storage/incorporated in Carbon Capture and Use strategies, blue hydrogen or via electrolysis powered by renewable electric energy, green hydrogen.

The direct use of hydrogen as a supplier of energy services to the end user is limited. Due to the specific characteristics of the hydrogen molecule (very light, very low boiling temperature, very low energy density), mobile applications are doubtful. For stationary applications, the need for storage of energy is clearly present, but the required volume and the resulting pressure/temperature needs make hydrogen a poor choice. The same holds for strategic energy storage.

Hydrogen-based molecules, can be produced by combining CO2 captured from the air or industrial processes, making hydrogen an essential part of the carbon neutral post 2050 energy system, as an intermediate product. Molecules such as ammonia (NH3) may be used to transport hydrogen over long distances.

The analysis leads to conclusions on the need for a clear taxonomy of hydrogen. The basis has to be the carbon content in order to ensure carbon neutrality in the most effective way.

Keywords

Hydrogen; Energy transition; Renewable energy; Decarbonisation

1. Why do fossil fuels dominate the current energy system?

Much attention has been paid to the decarbonization of the electricity supply as the key element in the energy transition process - primarily by introducing massive amounts of intermittent renewables, which would result in an electricity system with a far more distributed nature. However, the energy requirements cannot be satisfied with electricity generation alone, and include transport, heating/cooling, and industrial processes.

Hydrogen is prominently mentioned in the media nowadays, as a great promise for all kinds of applications, such as heating, transport and electricity generation.

In this publication we more closely examine the priorities for sustainable synthetic molecules and the specific role of hydrogen, concluding that while there is a huge need for hydrogen in the future, the recent attention of media, investors and policy makers often targets its less desirable applications. Below we illustrate the overall challenges and the share of electricity versus molecules (gas or liquid) in our current energy system. In subsequent chapters, we detail how to source hydrogen and where it will play a role in the decarbonization of our society.

In the future, more energy services will be delivered to the final customer by electricity as the key energy vector, and the introduction of ICT and data management will enable a stable and reliable operation. Demand will be increasingly flexible and controlled and storage in batteries will offer the short-term balancing factor. Though there are concerns and questions concerning this scenario, it is clear that it will be the kernel of the future energy system.

When comparing the use of energy to the supply of electricity, electricity presents only one limited, but very important factor, for the time being.

The electricity consumption is the electric energy consumed by the users (e.g. lighting, white good, electronics in a house), and is only a small part of the overall energy consumption (e.g. car and heating in a house). In 2017 in Belgium for instance, electricity represents only 16.6%: 81.4 TWh of electricity is supplied to final consumers (85.4 TWh being generated), while the final energy consumption in Belgium is 424 TWh (including electricity, gas, petroleum, coal, biomass, waste, ...)[1]. Instead, the primary energy use is 541 TWh, the gross available energy is 746 TWh and includes the energy employed as basis for non-energy purposes, e.g. chemical products, coal in steel, as well as nuclear fuel. It is obvious that electricity as an energy supplying vector is not dominant. When looking at the European scene, the same holds true: the gross generation of electric energy is 3,294 TWh, while 18,154 TWh (= 1561 Mtoe) of primary energy is used (out of which 17.8 % is electric energy).

Electricity currently makes up less than a fifth of the final energy demand, but its importance is increasing

In regard to energy demand, one should not start from energy consumption but from the energy services needed by society. Three main user groups can be distinguished:

1. The first is buildings: residential, commercial/offices and special purpose buildings such as schools and hospitals. In general, the energy supply currently consists of electricity and a heating source, mostly from natural gas but also from petroleum, coal, biomass and electricity. For hot water, solar thermal installations are commonly used, certainly in the south of Europe.
2. The second service is for transport: cars (most common), road freight, inland and seaborne shipping and airplanes. They form the major users of petroleum-based fuel. For public transport and freight trains, a mix of electricity and petroleum is provided.

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[1] Source: Eurostat

3. Large industrial consumers generally use electricity and natural gas. Petroleum and natural gas (chemicals), coal (steel) and biomass (paper and pulp) are sources of carbon-based feedstock. The data industry, especially large data centers, shows a growing demand for massive amounts of reliable electric energy.

The answer to the question 'how much energy will we need and which energy vector is the most appropriate to deliver them the final customer' must first consider the demand side for energy services, putting the citizen in the center.

2. How to get to Hydrogen?

Hydrogen is the lightest element on earth, in its stable form consisting of just one proton and one electron. The hydrogen molecule H_2 as such, is not available freely in nature. There are excellent reports describing in detail how hydrogen can be produced[2]. Four main technologies are:

- So-called grey hydrogen is produced through steam reforming of natural gas, which results in the release of CO_2 into the atmosphere. This is currently the dominant and most cost-effective production method.
- When the process of grey hydrogen is extended through a capturing system for CO_2 where 80 to 90 % of the CO_2 emissions are captured, so-called blue hydrogen is produced. The CO_2 is compressed and may be liquefied, then transported and stored (CCS Carbon Capture and Storage) or supplied to a process, which reuses the CO_2 in new products (CCU Carbon Capture and Use). An interesting technology to reduce the emissions of hydrogen production is the pyrolysis of methane, producing solid carbon instead of CO_2, which then may be used for industrial applications[3].
- Coal gasification leads to black hydrogen, which is far less popular in modern installations in North America and Europe. However, it is the main source of hydrogen in Australia and Asia.
- Green hydrogen is most commonly produced by electrolysis using power from renewable electric energy. The electric energy powers water electrolysis, which splits H_2O into hydrogen and oxygen. The idea is to produce H_2 from demineralized water by adding electrons that receive electric energy from renewable power produced by wind or solar energy:

$$2H_2O + \text{Electric energy} \quad \Rightarrow \quad 2H_2 + O_2 + \text{heat}$$

  - There is a fifth way to get to hydrogen. In many industrial processes, hydrogen is a by-product, for instance in chlorine production, oil refining or steel production. The potential of collecting excess sources of hydrogen, instead of flaring it, is unknown, as data sources are scarce.

Blue hydrogen production faces two primary challenges. The first concerns technical hurdles in order to achieve both high CO_2 capture rates and low per-ton storage costs. Addressing these issues will require tapping into different parts of the steam reforming process and accessing long-term storage sites, for instance in depleted offshore gas fields. The second challenge is public acceptance of the development of storage facilities, a subject of heavy debate in most European countries.

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[2] See for instance

IEA, The future of hydrogen, IEA 2019 https://www.iea.org/hydrogen2019/

CEPS, The future of gas in Europe https://www.ceps.eu/ceps-publications/the-future-of-gas-in-europe/

[3] Keipi, T., Tolvanen, H., & Konttinen, J. (2018). Economic analysis of hydrogen production by methane thermal decomposition, 159, 264–273. doi:10.1016/j.enconman.2017.12.063

Semi-green hydrogen can be produced using power from the regular grid. In this way the operation time of the system can be increased to lower the CAPEX (CAPital Expenditure) cost of the investment. The hydrogen produced in that way generates CO_2, depending on the energy mix used in the power generation at a given instant in time. An extended analysis is needed, depending on the country/interconnected electricity system from which the installation is supplied.

'Semi-Green' hydrogen production today registers double the emissions of 'grey' hydrogen production, when taking into account the energy source used in the electricity generation.

The reaction, industrially performed in existing electrolyzers, would split , say, 18 kg of demineralized water into 2 kg of hydrogen gas and 16 kg of oxygen.

As such, green hydrogen can be produced at zero emissions if electricity is fully supplied from a renewable electricity source. Otherwise, one needs to take into account the electricity mix used to produce semi-green hydrogen.

If the electrolysis is supplied from the grid delivering semi-green hydrogen taking into account the current emissions associated with electricity generation in Europe of 296 g/kWh[4], around 16 kg CO_2 per kg hydrogen would be emitted[5].

The emissions of the so-called grey hydrogen production using steam methane reforming are in the order of 7 $kgCO_2/kg\ H_2$ [6] being substantially less than the semi-green hydrogen.

At present, switching from grey to semi-green hydrogen would double the volume of emissions, whereas by 2050, the hydrogen used in industry should be produced without emitting CO_2.

Hydrogen production process today is not cost efficient as equipment is subscale and operating costs are high for most configurations. Cost-efficient operations depend on two developments:

- Electrolyzer technology is mature on a rather small scale, being 5 to 10 MW units as deployed today. To reach an industrial level that would impact the carbon balance at a substantial level, current plans to scale up the technology should further increase the unit size output to 100 - 300 MW[7]. It would reduce costs by 50 % to below 500 €/kWel and increase efficiency by more than 5% to over 70 %[8].
- Hydrogen production units should operate with a renewable power configuration that allows high electrolyzer utilization, roughly 5000 hours per year or more. Such high operating hours are most probably achievable only by a combination of well-situated wind and solar energy systems or through the use of inherent storage capability (thermal solar)

This delicate relation between hydrogen production and the electricity sector highlights the importance of how the energy system as a whole, functions. It is not acceptable to consider one technology or sector and ignore the impact of this on other technologies employed in the energy system. Assume that 100 MW of green power from an offshore wind park is used to produce hydrogen and the wind park is

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[4] Source: European Environment Agency:

https://www.eea.europa.eu/data-and-maps/daviz/co2-emission-intensity-5#tab-googlechartid_chart_11_filters=%7B%22rowFilters%22%3A%7B%7D%3B%22columnFilters%22%3A%7B%22pre_config_ugeo%22%3A%5B%22European%20Union%20(current%20composition)%22%5D%7D%7D

[5] Assuming an electrolysis efficiency of 75%, using the specific energy of 40kWh/kg H_2

[6] Soltani, Reza & Rosen, Marc & Dincer, Ibrahim. (2014). Assessment of CO2 capture options from various points in steam methane reforming for hydrogen production. International Journal of Hydrogen Energy. 39. 10.1016/j.ijhydene.2014.09.161.

[7] For instance https://www.hydrogenics.com/2019/02/25/hydrogenics-to-deliver-worlds-largest-hydrogen-electrolysis-plant/ or https://www.hannovermesse.de/en/news/news-articles/hamburg-to-build-worlds-largest-hydrogen-electrolysis-plant

[8] https://www.bcg.com/publications/2019/real-promise-of-hydrogen.aspx

coupled to the grid. As long as there is no congestion in the grid, this electricity can also be used to cover demand in the remainder of the system. If that power is used to produce hydrogen, extra “grey” electricity is dispatched to cover the demand not served by the green electricity. This electricity will be produced by a power plant with a relatively high marginal cost, using inefficient natural gas (older unit) or coal (due to the high CO_2 price). Overall the CO_2 output will increase. Therefore, on a system level, semi-green hydrogen increases the CO_2 production of the energy supply; green hydrogen would be produced only if the electricity demand in the system (say, for instance, continental Europe) at a given moment could be covered by zero-carbon electricity generation.

From this overview, the need for a clear taxonomy of hydrogen as an energy carrier becomes evident. The basis has to be the carbon content. In this way ‘greening’ of hydrogen is avoided.

3. Is hydrogen a suitable energy carrier?

Harvesting solar and wind energy is a key factor in paving the way to a sustainable energy supply. PV panels and wind turbines are producing electric power that may be used directly for most of the energy services discussed above. When introducing hydrogen in the chain, there are two extra conversion steps needed. In the first one, electric energy from wind or sun is used to produce hydrogen molecules. The chemical energy in these molecules is, at the second conversion step, transformed back into electric energy and waste heat, if it is not used as feedstock. In a circular, sustainable economy, the second law of thermodynamics is important rather than the first (conservation of energy):

- Not all energy conversion steps function at a 100 % efficiency. Heat energy for instance can never be converted fully into mechanical energy;
- All energy conversion processes are irreversible. Heat energy cannot be totally converted due to the losses during the conversion process.

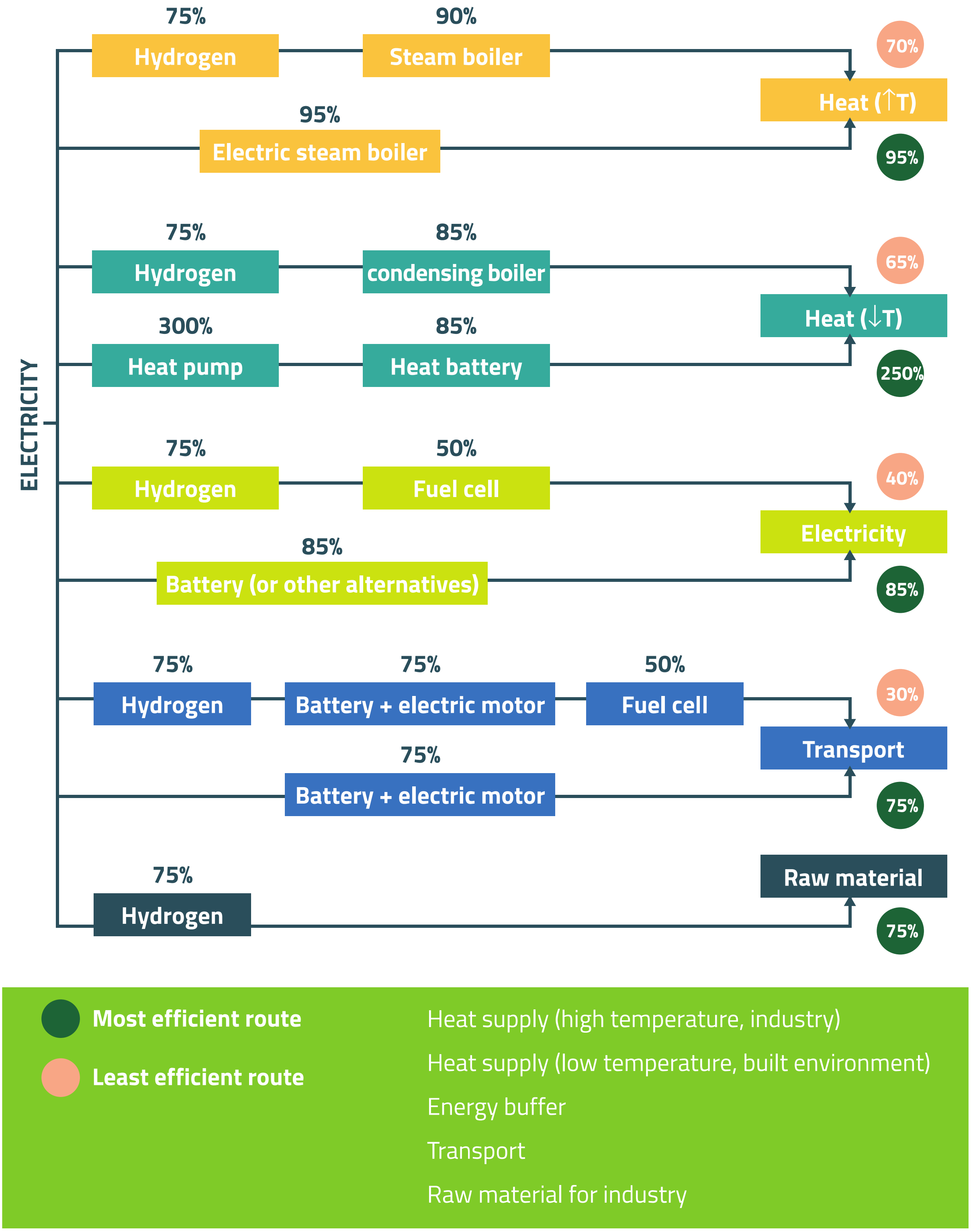
In a closed, sustainable, circular system, energy as such is never lost. Yet, due to the second law of thermodynamics, the quality of energy deteriorates: less and less mechanical energy or electrical energy, the most useful energy resources for applications, is available. This phenomenon is called the loss of ‘exergy’. Exergy cannot be recuperated. Therefore, this type of energy is a scarce resource. Generated electric energy should be used directly whenever possible. We will now illustrate this point specifically for hydrogen.

The fundamental question is how to provide the electric energy needed for splitting demineralized water as described above. We will investigate three basic scenarios to be distinguished in the long term for the production of green hydrogen:

- Long distance solar and wind energy harvesting
- Offshore energy harvesting in nearby sea
- Excess renewable electric energy in the grid

We will discuss the three energy flows from harvesting to use.

ELECTRICITY ROUTES WITH AND WITHOUT HYDROGEN



Source: Tomas Mathijsen, Ingrid Giebels and Peter-Paul Smoor in 'Over Morgen': 'De positie van waterstof in de energietransitie – een nuancering van de belofte', November 2018

3.1 Long distance solar and wind energy harvesting

Many reports discuss the possibility of generating electric power in deserts where there is a lot of sunshine, the temperature is high and space is available. The Sahara, the Middle East and Australia are cited in literature as potential areas. To bring the energy to Europe from the Sahara, two possibilities exist in principle: HVDC (high voltage direct current) electrical transport or chemical energy, i.e. the transport of molecules.

The electricity would probably be generated using solar thermal systems, rather than photovoltaic panels. Such a solar thermal unit produces heat, part of which is used immediately to produce steam, which is delivered via a classical Rankine cycle electric energy (CSP Concentrated Solar Power). Another part is used to heat a thermal buffer (High Temperature Phase Change Material), which provides the energy to the steam cycle during the night. In this way the solar thermal system can generate continuous electric power (constant or dispatched, due to demand). If we assume an electric output power of 1000 MW, the energy produced is 8,76 TWh/year. The continuous electric energy supply reduces the power rating of the electrolyzer. The cost of this approach is still very difficult to estimate, as no real industrial systems are readily available. The combination CSP/smaller electrolyzer has to be compared to that of the combination of photovoltaic/larger electrolyzer. For electricity production the difference that CSP is as a ‘dispatchable’ power source leading to a smaller rating of the electricity system, while PV requires a higher rating of the power system.

If we assume the electrical route to transport the energy, the power is converted into HVDC via transformers and power electronic converters. We assume an efficiency of 95 %. The long-distance power transfer is executed at a very high voltage, say 800 kV dc. This leads to a highly efficient transport, assume again 95 %. In Belgium or elsewhere in Europe, the power is injected into a high voltage ac grid via transformers and power electronic converters, again assuming an efficiency of 95 %. Finally, the ac power is delivered to the consumer, assuming a minimum efficiency of 92 %, when the final consumption is at the low voltage distribution grid; if the consumption is at a higher voltage, the efficiency is higher. The overall efficiency is the multiplication of all percentage values, leading to 79 %, or, in the case considered here, 789 MW is delivered to final consumer.

It is always more efficient to make use of electricity directly compared to conversion to hydrogen and re-electrification.

When the hydrogen route to provide energy is used, an electrolyzer is the first step, to produce H_2 out of H_2O. While availability of water in the Sahara or any desert environment may be a major challenge, this factor is not considered here. The efficiency of the hydrogen production is assumed to be 70%. Cryogenic transport with ships is the most efficient way to bring the hydrogen to Europe. Due to the extremely low boiling point of hydrogen (-255°C), liquefaction is an intensely energy demanding process. Different values are found in literature. Here a value of 70 % is assumed for this step[9]. The energy use for transport is estimated at 10 %; this is assigned an efficiency of 90 %. This efficiency includes the energy needed to bring the hydrogen by pipeline to the coast where liquefaction takes place. The evaporation requires another 5 % of energy, leading to an overall efficiency of around 40 %. Approximately 397 MW of hydrogen energy arrives at the final destination. It may be injected in the natural gas grid and delivered to the final consumer as such. If it is further converted to electricity, and assigning a fuel cell an efficiency of 60 % at the premises of the end user, the final electric power available is 251 MW. In the latter case pure hydrogen is required, and a separate hydrogen grid is needed if methane is also distributed along the same pipeline. The electricity generation is performed close to the final consumer, so no electric grid losses are taken into account.

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[9] The future of hydrogen, IEA 2019 https://www.iea.org/hydrogen2019/

An alternative route is to convert the hydrogen using CO_2, captured from the air or brought in by pipeline, into methane. The efficiency of the process (producing hydrogen and methanization) is estimated to be 60 %. Methane liquefaction is far more efficient, i.e. 95 %, and methane transport is more efficient than the liquefaction and transport of hydrogen. Methane energy losses are recorded at around 0,1 % per day (assume 2 weeks per journey, i.e. one month, being 3 %), while the evaporation efficiency is set at 99 %. This leads to an overall system efficiency of 53,1 %. For producing electricity, a regular high efficiency power plant (65 %) can be used. The electricity generation is performed centrally and the losses in the grid have to be taken into account (efficiency 92 %), giving an overall efficiency of 31,7 %, or 317 MW delivered to the final consumer.

3.2 Offshore wind energy harvesting in nearby sea

For offshore wind energy harvesting, a rated power of 1000 MW is assumed. The production of hydrogen and the generation of power depends on the availability of wind.

The electrical approach for such energy is almost identical to the one found for the Sahara approach. The voltage used in the HVDC system may be somewhat lower as the distance is shorter. The efficiency, while somewhat lower for the HVDC, partly due to the lower voltage, is actually higher in the end, due to the shorter distance.

The hydrogen route is easier. After production (efficiency 70 %), hydrogen can be injected into a nearby natural gas pipeline after compression (efficiency 90 %), thus transported efficiently. It is unclear whether or not the existing pipelines can carry this mixture and what the maximum percentage of hydrogen may be, but we assume this to be not a problem for the time being. The system efficiency is 63 %. If the energy is returned into electric energy, a regular power plant is used with an efficiency of 65 %, leading to an overall efficiency of 41 %.

The disadvantage of an approach where a methane route or a mixture of hydrogen and methane is used, is that the hydrogen is available in a mixture of methane (or natural gas) and hydrogen, making it far less useful as feedstock for chemistry or other industrial processes like steel making, and thus far less economically valuable. If pure hydrogen is used instead, the Sahara approach with hydrogen liquefaction, is the only valid one, or a full-blown separate pipeline system for hydrogen has to be foreseen.

3.3 Renewable electric energy in the grid

Renewable electric energy in the grid is comparable to the offshore wind energy situation when hydrogen is being transported. Compared to pure wind, more production hours may be available for renewable electric energy, as a surplus of power may be due to both wind and sun. The efficiency numbers are comparable.

The main use of hydrogen is not to valorize excess renewable energy. Electrolyzers are capital intensive, requiring a high number of operating hours.

An important note in all these examples is that the total cost will be the main driver for the system, in terms of new investments and operating hours. For instance, for this last example, the electrolyzer will run for more hours to harness offshore wind energy than when operating only in times of excess renewable energy: electrolyzers are capital intensive investments. As noted before, the concept of ‘green’ hydrogen is heavily dependent on the electricity mix.

4. The place of hydrogen in the energy system

As illustrated above, direct use of electricity is more efficient and cost effective than conversion to molecules and re-electrification (hydrogen process). This has profound implications on the overall energy system.

First of all, flexibility on the demand side will increase, driven by the more frequent periods of low marginal cost of renewable electricity, and, consequently, higher variability of the electricity price. Industrial processes will maximize their profit margins, and the residential consumer will be able to save a considerable amount on the energy bill, for instance, by charging electric vehicles during periods with abundant renewable energy available.

Even then, it is not always possible or preferable to supply the present energy demand by electricity coming from renewables for all energy services needed now and in the future. Molecules will be needed for different parts of the value chain. By ‘molecules’ we mean energy carried by gaseous or liquid fuels, as opposed to carriage via electrons (electricity). Clearly, these molecules will have to come from a carbon neutral source; otherwise the energy transition towards a carbon neutral system will not be attained. As an alternative or an intermediate solution, carbon capturing with storage or use may be envisaged. First, we will provide an overview of the molecules available, not only hydrogen, but also in fuels containing hydrogen.

4.1 Different molecules for different applications

In addition to hydrogen and natural gas, there are other liquid or gaseous energy carriers, for instance, methanol, ethanol, ammonia and biofuels. In general, such a molecule is denoted by X.

The choice of the appropriate molecule for a specific application is closely linked to the physical parameters. For transport applications, the energy density per unit weight and/or per unit volume are very important. With respect to the pressure needed to increase those values to acceptable levels, the weight of the containment is a critical element. When deep cooling is needed to liquify the fuel, the energy needed for this cooling process has to be considered, as we noted above, with hydrogen.

The table below provides key advantages of some important fuels, both classical carbon-based and potential candidates for Power-to-X applications. We do not aim to provide a full overview of the possible molecules in this text. A further table in the annex contains an overview of the relevant physical parameters of some molecules.

The basis for comparison is energy density, measured as a per unit weight or per unit volume. The higher the value, the more useful a carrier becomes as an energy service supplier. Higher valued energy means that which is easier to store and more convenient to include in mobile applications.

Table 1: Overview of some synthetic molecules/energy carriers and their main advantages and disadvantages

	Production cost	**Storage**	**Transport across long-distances**	**Distribution**
Green Hydrogen	building block for other synthetic fuels	Needs large volumes (salt caverns, huge tanks)	Liquefaction for shipping is energy intensive	To a certain extent possible with existing gas grid, safety issues
Methane	Needs CO_2 source	existing infrastructure	existing infrastructure	Transportable
Methanol	Needs CO_2 source	Easily storable	existing infrastructure	Transportable
FT Diesel	Needs CO_2 source, more costly	Easily storable	existing infrastructure	Transportable
Ammonia	Extra step wrt H_2	Storable but toxic	Possible	Serious safety issues, best for industrial use only

Green hydrogen is the simplest of the molecules and can be produced in a carbon-free way using electrolysis. However, international transport, in a liquid phase, poses serious challenges. The energy density of liquid methane is double the value of liquid hydrogen. As a consequence, for a given shipment volume, double the energy can be transported. Furthermore, the low boiling temperature of hydrogen (-255°C) compared to methane (-160°C) sets high challenges for the materials used in containments, pumps and compressors. If the hydrogen itself were to be used to provide the energy for liquefaction, between around 25% and 35% of the initial quantity of hydrogen would be required[10]. This is significantly more than the energy required to liquefy natural gas, which consumes around 5 % of the initial energy quantity of gas.

The transport of hydrogen by pipeline also poses challenges. It is possible to build a dedicated transmission infrastructure (in Belgium there is, in fact, a hydrogen network commercially operated by Air Liquide); a new infrastructure would need to be built across Europe. Hydrogen can only be mixed to a certain extent into the gas grid (which may even be undesirable - see next chapter). The existing distribution grid may be suitable to transport hydrogen from a technical perspective, but the challenge lies at the consumer end where simultaneous retrofits of boilers, meters and new safety procedures would be required.

> *There are different molecules to transport energy over long distances or use in mobile applications -for all of which hydrogen is a key ingredient.*

By contrast, synthetic methane is much more appropriate for the end consumer applications, where the existing infrastructure can simply be reused. In addition, there is a well-established infrastructure for transport over long distances, either by shipping or pipelines.

The trade-off here lies in the production of synthetic methane[11], a process that involves a reaction between H_2 and CO_2 to create CH_4. in a strongly decarbonized society, a highly concentrated and pure source of

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[10] Ohlig, K. and L. Decker (2014), "The latest developments and outlook for hydrogen liquefaction technology", *AIP Conference Proceedings*, Vol. 1573, Issue 1 , https://doi.org/10.1063/1.4860858.

[11] For instance https://www.sciencedirect.com/science/article/pii/S0306261919312681

CO_2 might not be available. And while it can be captured directly from the air, this will incur additional energy demand and costs.

Methanol, the simplest type of alcohol, can be produced as well, based on CO_2 and hydrogen. Having half of the energy density of heating oil, this molecule would be suitable for mobile applications like transport.

Producing electricity will never be the main application of hydrogen.

Worldwide, there is already a lot of experience with internal combustion engines using alcohol molecules. Furthermore, there are other energy carriers, such as Fischer-Tropsch diesel fuel, that offer high quality but also, higher production costs, or organic carriers of hydrogen. The latter are still in a pre-industrialization phase.

Another option to transport hydrogen over long distances more efficiently is to convert it to a more compressible molecule, for instance, ammonia. (NH_3). This has a much higher energy density (see table in annex). Ammonia is easier to transport but poses safety problems. It can be used as direct feedstock for fertilizers.

The capture of nitrogen, needed for producing ammonia, may be less costly. However, ammonia's toxic nature makes it unsuitable for decentral applications. Its more efficient transport, compared to hydrogen, must be weighed against costs for conversion and reconversion.

In addition to the synthetic fuels discussed above, biofuels are also an option for supplying part of the carbon neutral molecules. Obviously, it is essential that biofuels should only be an option when produced sustainably.

In summary, every molecule based on hydrogen has its own advantages and limitations/drawbacks, in terms of production cost, transport, storage and handling. The final choice between energy carriers must compare operational and capital costs for the overall system. Safety costs and putting to good use available experience, including the use of existing infrastructure, will need to be considered.

Another consideration, with respect to decarbonization, is the production of such molecules, which will enormously increase the need for renewable electricity. As an example, around 1000 TWh and 700 TWh of electricity would be needed as input for synthetic fuels to replace 1% of current global oil and gas production respectively, representing around 4% and 3% of global electricity generation[12].

Concluding this paper, we now review in detail the energy services in society where one or more of these molecules will find their use.

4.2 Electricity storage

Hydrogen – or synthetic fuels based on hydrogen – which gets the most attention in the media - can be used in electricity storage. When there are periods with excessive solar and wind energy, hydrogen is produced and can then be reconverted to electricity in periods with low solar and wind power.

However, the applicability of hydrogen for electricity storage is largely overestimated for the following reasons:

First of all, as we have seen in chapter 1, the round trip efficiency of 'electricity – hydrogen – electricity' is only 35-41%.

Secondly, a 'Dunkelflaute', an extended period of time with low wind and sun, is a relatively infrequent phenomenon. There is more production of offshore wind in winter than in summer, and transmission grids connect the countries in Europe quite effectively. While it is important to have a

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[12] The future of hydrogen, IEA 2019 https://www.iea.org/hydrogen2019/

backup source of energy during a ‘Dunkelflaute’, and hydrogen could play a role providing electricity during these times, the total percentage of generated electricity will be limited.

Finally, while studies using energy system models like TIMES[13] and PRIMES [14] take into account all relations within the energy system including industry, transport, heating and electricity, it remains very hard to incorporate ‘disruptive technologies’ i.e. technologies that can have rapid cost reductions but are not yet commercially viable today. An example seen during the last decade is the extremely fast price reduction of batteries that has surprised are modelers of energy systems.

For electricity storage, competing technologies are being developed, such as liquefaction of air[15] or heating of stones[16]. Their ultimate potential for commercialization has yet to be seen. The key factors will be based on investment/operational costs, storage time and volume, power during charging and discharging, geographical limitations and roundtrip efficiencies.

We conclude that green hydrogen may play a role in providing electricity in a future decarbonized energy system, however this will never be its main application.

As an off-topic note, the strategic storage of energy has to be mentioned. At this moment, countries have a strategic reserve of 90 days of liquid fuels (for Belgium www.apetra.be). Whether such reserve volumes are still needed when more and more energy is harvested within Europe is an open question. New volumes and new energy carriers can be agreed upon for storage and strategic reserves. Given the limited volume, liquid fuels will be the best choice. This strategic reserve can be linked with the storage needed for the ‘Dunkelflaute’.

4.3 The future energy supply of buildings

To follow we discuss different building categories.

Residential buildings will continue to require electricity connection, no matter what. Heating and cooling, including the heat needed for tap water may be electrified using heat pumps. A water tank may be used for storage and flexibility, in combination with a battery and PV panels. Depending on the availability of a local green thermal energy, a heat network may be used to supply the basic heat, and serve as input for the heat pump. Extra electricity demand may be seen due to the charging point for the private vehicle or other mobility assets (electric bikes for instance). Within a neighborhood, centralized storage of molecules may be installed (for instance using locally produced hydrogen or a tank of molecules produced centrally) to overcome ‘Dunkelflaute’ on a local basis in a grid-disconnected approach.

- For apartments, office and commercial buildings heat pumps both for cooling and heating will be the appropriate choice, for the most part. A low temperature heat network may be used to feed the basic heating/cooling energy to the heat pumps, certainly in cities where individual heat storage around the building may be difficult to achieve. In specific cases industrial excess heat sources or heat generated by large data hubs can be injected in the district heating grid. A roof as the site of solar panels, is normally far from sufficient to supply all necessary energy and a connection with the medium voltage grid has to be foreseen, potentially in parallel with the afore- mentioned heat network. Electric vehicles, too, may be a part of the challenge as charging points will be made available in parking lots. Molecules may not be needed in this system; due to investments in the building shell, the requirement for energy is reduced. The building mass may be used as heat

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[13] For instance https://op.europa.eu/en/publication-detail/-/publication/1c25c504-1878-11e9-8d04-01aa75ed71a1/language-en/format-PDF/source-94601869

[14] https://ec.europa.eu/clima/sites/clima/files/docs/pages/com_2018_733_analysis_in_support_en_0.pdf

[15] https://www.highviewpower.com/technology/

[16] https://www.siemensgamesa.com/products-and-services/hybrid-and-storage/thermal-energy-storage-with-etes

storage. Back up energy to address potential ‘Dunkelflaute’ would be stored at a distance, more centrally.

- Special buildings require specific answers. Schools, for instance, have a lot of rooftop space, but the use of energy during sunny periods is very low. They can, therefore, act as an energy supplier for their neighborhoods. In hospitals, for example, the availability of energy is critical. Mostly diesel generators are used. Here on-site stored molecules will be needed, either for diesel-type generators or fuel cells. Maybe the same will become important in other types of critical infrastructures: telecommunication systems, data centers, traffic control or in homes for the elderly, Reliable electricity is a life saver (for instance it is essential for assisted breathing equipment) requiring molecules (for instance, mobile small generator sets).

4.4 Molecules for transport

It is often said that the role of molecules in the future appears brighter when looking at the transport sector. Various traffic modi require different approaches.

The first modus is the “two-wheeled” one. Electric bikes are becoming very popular, including high speed, so-called speed pedelecs, being a substitute for the very popular mopeds (especially for delivery services in cities). The battery energy for such a speed pedelec is 500 to 600 Wh. On the downside, electric bikes have a somewhat lower speed capacity. Energy transport for two-wheeled modi will no longer need molecules in the future.

Motorbikes are finding their electric homologues, although more slowly than are electric cars. In the long run, no molecules will be needed for motorbikes.

The same holds for electric cars for personal mobility. When compared to hydrogen, battery-electric cars and bike-likes offer a cost advantage in individual mobility, one that fuel cell supplied vehicles are unlikely to achieve. This is thanks to the direct use of electric energy with its higher round-trip efficiency and the ability to leverage established infrastructure, As a result, using hydrogen in passenger cars is not very likely.

An energy refit for freight transport on the road is not clear yet. The first high electric power lorries have already been introduced and another approach is being considered by Siemens, in which highways are equipped with a catenary wire so that vehicles can tap into the grid. The battery will then only be used for the “first” and the “last” mile. The need for molecules may become low or even vanish.

Rail, buses and local transport will be increasingly electrified. For long distance buses and freight trains, molecules may still be the best energy source as with freight transport. For heavily used transport systems (such as forklifts or public transport buses for which there is almost continuous demand), molecules may be a viable alternative to batteries, which require charging time during the active operation.

Inland shipping might see electrification, too, however it is unclear yet if the batteries can provide sufficient energy density to cover long trips, while not adding too much weight or requiring too much space on the ship. This is true, to an even higher extent, for seaborne shipping: batteries can never meet the energy demands; molecules will remain key. Here molecules such as methanol, biofuels or liquid methane may play a key role.

The same holds for airplanes where molecules will be an essential element, though there are already first steps towards short haul small electric airplanes. Drones will have an important place in future mobility in delivery services, and maybe as taxis in cities); they are already electricity supplied. For long distance flights, the situation is clear: only liquid fuels at normal temperatures and pressures are feasible.

4.5 Molecules as industrial feedstock

When looking at large, energy intensive industry, the need for molecules is obvious - as an energy vector, but even more, as basic material/feedstock or as part of the process.

In many processes in the chemical industry, such as ammonia and methanol production, hydrogen is needed in a pure form. The processes and produced molecules in the chemical industry are very diverse and decarbonization possibilities need to be evaluated on a case-by-case basis.

Mixing pure hydrogen in the gas grid prevents its highest value use as a feedstock for industry.

In oil refineries, hydrogen is used for desulphurization of crude oil. In steel production, direct reduction (removal of oxygen in iron ore) in blast furnaces by hydrogen may be used to replace coal, and first demonstrations are ongoing[17]. It is not yet clear however if hydrogen will play a role there in the long term, as iron pellets cannot be produced without the use of fossil fuels. Electric-based technologies and CO_2 capturing in rather classic approaches may be options as well.

We conclude that for industrial applications, the value of hydrogen is the highest.

It is important to reiterate that for many industrial processes, a high purity of hydrogen is needed. A mixture of hydrogen stream in the gas grid is useless for numerous highly valued applications. Instead, the mix delivers lower-quality heating services for which a good number of alternatives exist. Therefore, mixing pure hydrogen in natural gas grids is not a good idea.

As a general conclusion of the overview of the energy services and their need for molecules, it is clear that “residential” application will be very low. The use of molecules for building heating and cooling is not to be envisaged and their use for individual transport (bike types and cars) is far less efficient, both technically and economically (new infrastructure) than the use of batteries and electric drives. Therefore, setting up a retail market for hydrogen and synthetic fuels is not required.

5. Conclusions

In a fully decarbonized society, the need for hydrogen produced from carbon free resources is going to be massive. It is a critical intermediate step towards a final fuel for specific energy services and an essential feedstock to industry.

Two main routes exist to produce carbon-free hydrogen:

- classic approaches from carbon-based fuels equipped with CCS (Carbon Capture and Storage) or incorporated in CCU ‘Carbon Capture and Use) strategies, blue hydrogen
- via electrolysis powered by renewable electric energy, green hydrogen

The choice will depend on the cost of both options, the availability of the required renewable energy resources for green hydrogen and the acceptability by society of CCS, more particularly, in the storage of carbon dioxide, for blue hydrogen.

Which of the two routes will be the winner, if either, is yet to be determined. The CCS route is better for large systems, integrated in the chemical and steel clusters and linked by a network of pipeline systems and the potential of Storage and/or Use. The renewable energy route is far more fragmented and can start with smaller investments. Both have a long learning curve ahead, though some of the elements, for instance the electrolyzers, are a fully mature technology.

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[17] https://www.thyssenkrupp-steel.com/en/company/sustainability/climate-strategy/

There is a bright future for hydrogen, not in the frontline, but as an indispensable supplier of the backbone for the future energy and industrial feedstock system.

The direct use of hydrogen as a supplier of energy services to the end user is limited. Due to the specific characteristics of the hydrogen molecule (very light, very low boiling temperature, very low energy density), mobile applications are doubtful. For stationary applications, the need for storage of energy is clearly present, but again the required volume and the resulting pressure/temperature needs make hydrogen a poor choice. The same holds for strategic energy storage, which is now based on liquid petroleum products.

However, hydrogen-based molecules, such as methane CH_4, methanol CH_3OH, ethanol C_2H_5OH, can be produced by combining CO_2 captured from the air or directly from industrial processes, making hydrogen an essential part of the carbon neutral post 2050 energy system, as an intermediate product. Molecules such as ammonia (NH_3) may be used to transport hydrogen over long distances and directly used as feedstock, for instance, for fertilizers.

Which energy route will be taken depends on costs and efficiency. Choices are not easy and will require a great deal of engineering, design and economic studies. Again, public acceptability and safety will be part of the decision process, together with the possibility of reusing part of the existing infrastructure.

Hydrogen is key for the sustainability for many industrial processes. Here the existing demand for hydrogen feedstock, which currently comes from petroleum, coal or methane, (grey or black hydrogen) must be substituted. New demand will come from other feedstock molecules.

It is important to note that, especially for assessing the potential for hydrogen applications, an energy system view has to be considered at all times. There is not one ‘silver bullet’ technology: the decarbonized energy system will be a complex toolbox of many different technologies and processes. Especially for green hydrogen production, there is a very complicated relation with the electricity production sector.

Electricity will become the main energy supplier to deliver energy services to the end consumer, being it residential, commercial or industrial. However, as part of the road to a fully carbon neutral energy system by 2050, molecules as energy carriers will play a key role. Depending on the application, an appropriate molecule has to be chosen. As an intermediate between power, generated by wind, hydro or solar energy, hydrogen will be needed in massive amounts. Due to its physical characteristics, its use in the final application will be limited and other molecules will be used for transporting the energy and driving the application.

Overall, we conclude that there is a bright future for hydrogen, not in the frontline, but as an indispensable supplier of the backbone for the future energy and feedstock system.

6. Potential policy measures

The answer to the question “how much energy will we need and which energy vector is the most appropriate to deliver this the final customer” has to begin with the demand side for energy services, putting the citizen in the center.

From this overview, the need for a clear taxonomy of hydrogen becomes evident. The basis has to be the carbon content. In this way the ‘greening’ of hydrogen is avoided.

In a closed, sustainable, circular system, energy as such is never lost. But due to the second law of thermodynamics, the quality of energy deteriorates: less and less useful mechanical energy or electrical energy. These are most useful energy resources for applications available. Generated electric energy should be used directly whenever possible.

The long-distance transport of hydrogen using liquefaction for shipping is very energy demanding. When possible, electric transport is the better approach. When molecules have to be used due to the geography, a transformation to other molecules, e.g. methanol, methane or ammonia, will be the more efficient route.

However, in addition to hydrogen and natural gas there are other liquid or gaseous energy carriers, for instance methanol, ethanol, ammonia, biofuels etc. The choice of the appropriate molecule for a specific application is closely linked to the physical parameters.

Every molecule based on hydrogen has its own advantages and limitations/drawbacks in terms of production cost, transport, storage and handling. The final choice between energy carriers can be achieved by comparing operational and capital costs for the overall system.

There are many options for storing energy in different time horizons. The challenges of the “Dunkelflaute” are known; hydrogen is faced with its limitations and combining the strategic storage with the shorter horizon Dunkelflaute has to be considered.

The use of molecules for building heating and cooling is not to be envisaged and their use for individual transport (bike type and cars) is far less efficient, both technically and economically (new infrastructure) than is the use of batteries or electric drives. The direct involvement of the citizen with hydrogen will be very low, so setting up a retail market for hydrogen and synthetic fuels is not required.

Annex

Physical parameters of energy carriers:

	Specific energy	Energy density	Specific mass
	MJ/kg	MJ/l	kg/m^3
Residential heating oil	46,2	37,3	807,359
Natural gas	53,6	0,0364	0,679
Methanol	19,7	15,6	791,878
Methane (1,013 bar, 15°C)	55,6	0,0378	0,680
LPG propane	49,6	25,3	510,081
LPG butane	49,1	27,7	564,155
LNG (NG at -160°C)	53,6	22,2	414,179
Liquid ammonia (combusted to N_2+H_2O)	18,6	11,5	618,280
Jet Fuel	43	35	813,953
Hydrogen liquid (HHV)	141,86	10,044	70,802
Hydrogen liquid (LHV)	119,93	8,491	70,800
Hydrogen at 1 atm @ 15,5°C (HHV)	141,86	0,01188	0,084
Hydrogen at 1 atm @15,5°C (LHV)	119,93	0,01005	0,084
Hydrogen at 690 atm @ 15,5°C (HHV)	141,86	5,323	37,523
Hydrogen at 690 atm @15,5°C (LHV)	119,93	4,5	37,522
Gasoline (petrol)	46,4	34,2	737,069
Ethanol	30	24	800,000
Diesel fuel	45,6	38,6	846,491
Crude oil	41,868	37	883,730
CNG (250 bar)	53,6	9	167,910
Biodiesel oil	42,2	33	781,991

LPG Liquified Petroleum Gas
LNG Liquified Natural Gas
HHV Higher Heating Value
LHV Lower Heating Value
CNG Compressed Natural Gas

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