DECHEMA

ROADMAP

Water-for-X

Water for sustainable hydrogen production and follow-up PtX processes

WATERforX

by DECHEMA

Imprint

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Summary

Green hydrogen and follow-up PtX solutions are promising routes towards a climate-neutral economy. Water is a key for these routes. The Water-for-X management framework is connecting an integrated water management with the implementation of PtX processes to foster an economically, ecologically and socially strong transition to a climate-neutral economy. The framework builds up on a production-, industrial water- and integrated water-management shell.

With this roadmap we formalise the "Water-for-X" approach, provide the basis for its broad implementation, further development and highlight its necessity for a sustainable application of PtX technologies.

1. Motivation

Climate change with its new weather extremes highlights the fragility of the earth's atmosphere. Impacts to the supply chain, food and industrial production and even our daily lives are becoming noticeable. To solve these threatening problems, countries have agreed on strategies to achieve net zero emissions of greenhouse gases via the Paris Agreement (2015). To achieve this ambitious goal, society must move away from fossil carbon sources.

Secure and affordable energy is needed to achieve the European Commission's Green Deal[1] vision of a climate-neutral economy. Energy resilience is another global driver in the context of political and economic stability. The energy transition will involve new process designs, such as replacing fossil fuels with renewable electricity. On the other hand, there will be a high demand for converted and stored energy carriers based on (renewable) power, such as hydrogen, gas, kerosene etc., which are also known as Power-to-X (PtX) products. A key contribution for the defossilization of our energy consumption will come from green PtX technologies[1]. The first step within this value-chain is the generation of hydrogen. Hydrogen is then used directly or is utilized to produce other carbon- or nitrogen-based PtX products.

PtX processes depend on the availability of highly purified water – not only for hydrogen production, but also for process water and steam, cooling water and cleaning during the subsequent production of chemicals (kerosine, methanol, methane, etc.). To date, the interdependence of water and PtX process management is noted but not specifically addressed. On the one hand, the global green energy transition can put an extra demand on global freshwater sources, which are already at risk. On the other hand, connecting an integrated water management strategy with the implementation of PtX processes fosters an economically, ecologically and socially strong transition to a climate-neutral economy.

Focusing on this connection, this roadmap introduces the Water-for-X Management Framework, designed to:

a) Reveal the importance of water as a unique resource in sustainable PtX processes
b) Create synergies between the water and PtX sectors
c) Guide decision makers on the responsible use of water by highlighting local and regional social, economic, and environmental aspects
d) Altogether foster the vital contribution of PtX technologies for reaching net-zero goals

The Water-for-X concept is essential for a sustainable and secure energy transition, promoting an integrated and sustainable water management approach that is indispensable for successful PtX solutions.

[1]https://ec.europa.eu/info/strategy/priorities-2019-2024/european-green-deal_en, accessed 19.08.2022

For over a decade, DECHEMA has provided expertise on PtX processes in interaction with water management. Thus, this roadmap formalises the "Water-for-X" approach, provides the basis for its broad implementation and highlights its necessity for a sustainable application of PtX technologies.

2. Hydrogen production and follow-up PtX processes

In general, PtX processes use (renewable) electricity to produce gaseous (PtG) or liquid products (PtL) or heat (PtH). The best known PtX process is the generation of hydrogen. Here, (renewable) electricity is used to produce hydrogen via electrolysis. Afterwards, the hydrogen is separated, purified, and transferred for direct application or used as basic feedstock for further synthesis processes.

These further processes include the production of methane, methanol, ammonia, or Fischer-Tropsch (FT) hydrocarbons, for example. Therefore, most PtX products need a source of carbon or nitrogen in addition to hydrogen. Carbon sources include carbon from biogenous sources, industrial point sources of hard-to-abate sectors (e.g. cement production), or carbon taken from the atmosphere via direct air capture (DAC).

> Electrolytic hydrogen production is the first step in PtX processes. Increased application of hydrogen or follow-up PtX products will lead to higher hydrogen demands (in 2050 approximately 5 times higher than 2020).

The implementation of PtX processes is estimated to increase the demand for hydrogen by up to a factor of five by 2050. To put this into perspective, the global hydrogen demand in 2020 was around 90 megatons (Mt) [2]. The current demand mainly arises from refining processes as well as the production of ammonia and methanol. All these processes are mainly based on fossil resources such as natural gas, coal or oil. Forecasting future hydrogen demands, the International Energy Agency (IEA) estimates a demand of 530 Mt hydrogen in 2050 to fulfill their 'net-zero-emissions' scenario. Within this scenario, approximately 1/3 of the hydrogen demand will be utilized for the production of hydrogen-based fuels, e.g. ammonia, synthetic kerosene or methane [2]. Enhancing the current electrolysis capacities for green hydrogen production with renewable energy is the first step needed to reach this goal.

3. Water demand for selected PtX processes

Water is a key resource for the various PtX processes. Their stochiometric water consumption based on simplified water balances is listed in Table 1. Reading the table, the production of 1 kg of hydrogen by electrolysis leads to a stochiometric water consumption of 9.0 $kg_{H2O}/kg_{product}$. Utilizing green hydrogen for the production of follow-up products such as methanol, ammonia, methane or kerosene leads to a stochiometric water consumption between 1.7 – 4.5 $kg_{H2O}/kg_{product}$. This represents the theoretical minimum consumption of ultra-pure water (UPW). The required water qualities vary from UPW for electrolysis to lower qualities for cleaning. Since processes never achieve 100% efficiency, losses must be accounted, resulting in the real water demand. The wastewater generated in some PtX processes is contaminated and needs to be additionally treated. Thus, the real water demand is much higher than the stochiometric consumption.

> A growing demand for hydrogen and other PtX products will result in an water consumption of 9.0 – 13.5 $kg_{H2O}/kg_{product}$, on top of that, efficiency losses and demands for cooling, steam and cleaning.

Based on an estimated hydrogen demand of 530 Mt in the year 2050, this would add up to 4770 Mt of UPW, needed exclusively to produce green hydrogen via electrolysis. Putting this into perspective, this

[2] IEA Global hydrogen review 2021

amount equates to 0.1% of the global yearly water consumption, which is around 4250 km^3. In addition to these quantities, water demands for cooling, steam production, cleaning, and other processes in the range of ~5-20% (238.5 – 954 Mt), along with the requirements concerning the water source (groundwater, seawater, wastewater, etc.) of 20-60% (954 – 2862 Mt), are not considered in this equation [3].

Table 1: Water consumption to produce 1 kg of hydrogen, methanol, ammonia, methane or FT-kerosene/diesel.

(PtX) product	Reaction	Stochiometric water consumption [L_{H2O}/$kg_{product}$]
Hydrogen (H_2)	$H_2O \rightarrow H_2 + ½ O_2$	9.0
Methanol (CH_3OH)	$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$	1.7
Ammonia (NH_3)	$N_2 + 3H_2 \rightarrow 2NH_3$	1.8
FT-Kerosene/Diesel	$CO_2 + 3H_2 \rightarrow [-CH_2]- + 2H_2O$	3.0
Methane (CH_4)	$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$	4.5

Although the percentage of 0.1% seems rather small, regions with high potential for hydrogen production often lack the required freshwater resources. This demand will place additional water stress. The Netherlands, for example, estimate their extra water demand for hydrogen production in 2050 to be 4.6% (0.062 km^3/year) of the total drinking water consumption [4].

4. Global water availability and use

Earth retains natural water in different forms over its various parts: salt water in the oceans (97%), freshwater as ice, surface and groundwater (3%). About 1% of freshwater resources are accessible via rivers, lakes, wetlands, and aquifers [5]. This 1% is, however, unevenly distributed. Some resources are difficult to access or non-renewing (fossil). Thus, water availability is a regional/local issue with individual characteristics, requiring individual solutions for a sustainable use.

Water availability is limited in many countries based on regional specialties. This result in regional different levels of water risks. The level of water risk is expected to increase in the future. Thus, to cope with these developments, alternative water resources as seawater desalination or water reuse will become even more important.

Freshwater use has increased by a factor of six to seven over the last 100 years, reaching an amount of more than 4000 km^3/a in 2010. The latest predictions show a similar increase for the decade 2010-2020. Agriculture consumes the largest share of water, totalling almost 70% globally, followed by industries. The steady increase in water usage of all sectors, combined with lower rainfalls and a slower groundwater recharge, exacerbated by climate change, increases the pressure on the available resources and leads to so-called water stress [6]. The overall ”water risk“ as a qualitative indicator summarizes all water-related risks (including water stress), by aggregating all selected indicators from the physical quantity, quality and regulatory & reputational risk categories [7] (see Figure 2).

[3] Catarino, J., Picado, A., & Lopes, T. (2021). Assessing water availability and use for electrolysis in hydrogen production. March. https://doi.org/10.13140/RG.2.2.18531.27685
[4] Oesterholt, F. et. al. (2016). The role of water in a future hydrogen economy.
[5] The United Nations World Water Development Report 2022
[6] When a territory withdraws 25 % or more of its renewable freshwater resources, https://www.unwater.org/publications/summary-progress-update-2021-sdg-6-water-and-sanitation-for-all/ accessed 19.08.2022
[7] https://www.wri.org/applications/aqueduct/water-risk-atlas accessed 02.08.2022

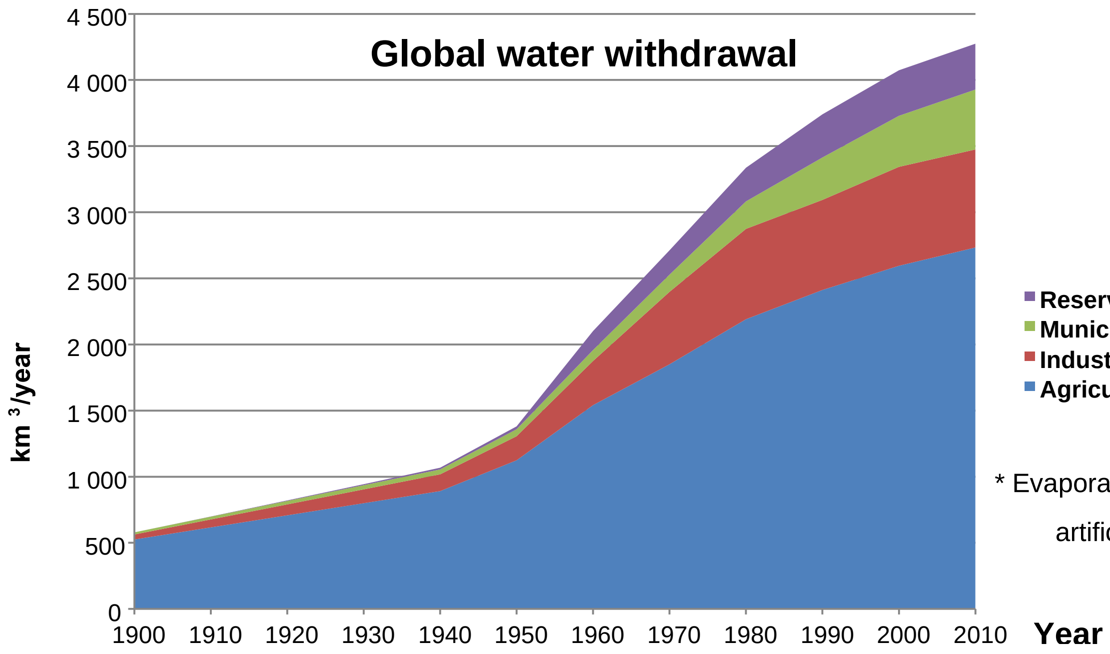

Figure 1: Global water withdrawals, 1900-2010[8]

Considering climate change perspectives, water risks will increase, forcing the need for sustainable water use. Strategies for a sustainable water use include introducing alternative resources, such as water reuse both from municipal and industrial sources, rainwater harvesting, in addition to increasing efficiency in water use.

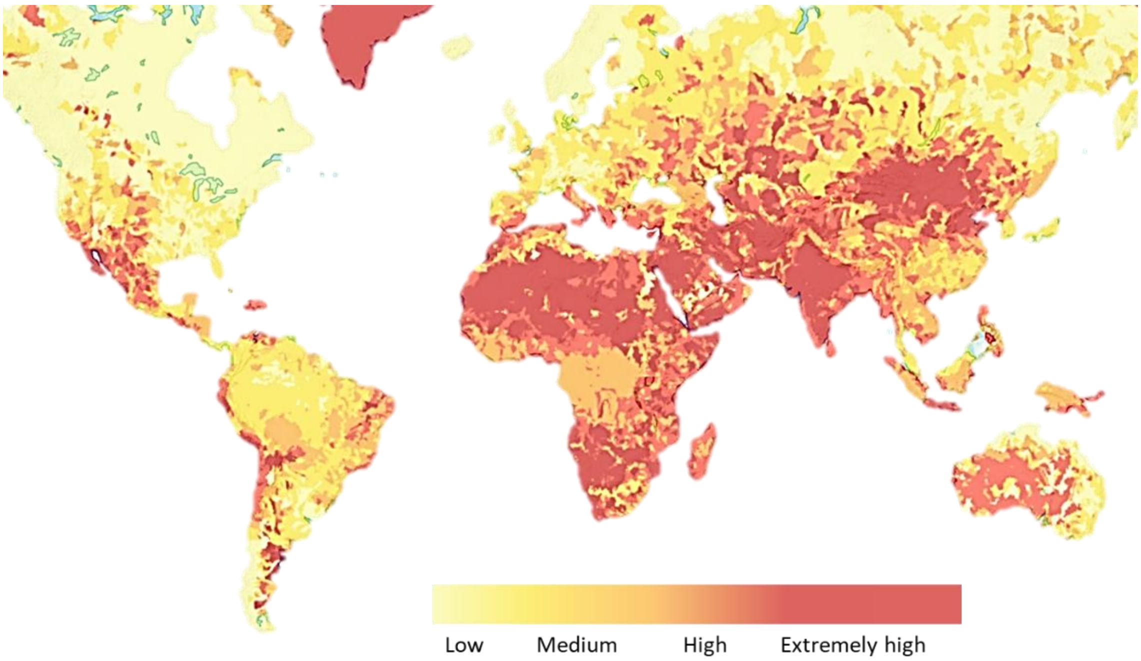

Figure 2: Overall Water Risk [9]

Another way to reduce pressure on freshwater resources is the use of seawater desalination. Today, more than 174 countries use desalination to meet sector water demand, supplying over 300 million

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[8] FAO-AQUASTAT: 2010; I.A. Shiklomanov: 1900- 2000, https://www.fao.org/aquastat/en/overview/methodology/water-use/, accessed 24.01.2024

[9] https://www.wri.org/applications/aqueduct/water-risk-atlas, accessed 02.08.2022, adapted

people with potable water [10]. Despite declining costs, most desalination facilities are in high-income countries (67%), accounting for 71% of the global desalination capacity. Conversely, less than 0.1% of the capacity occurs in low-income countries [11].

5. Resources nexus: water - renewable energy

Like water resources, the potential for renewable energy production is unevenly distributed around the globe, as shown with the photovoltaic power potential and wind speed potential in Figures 3 and 4, respectively.

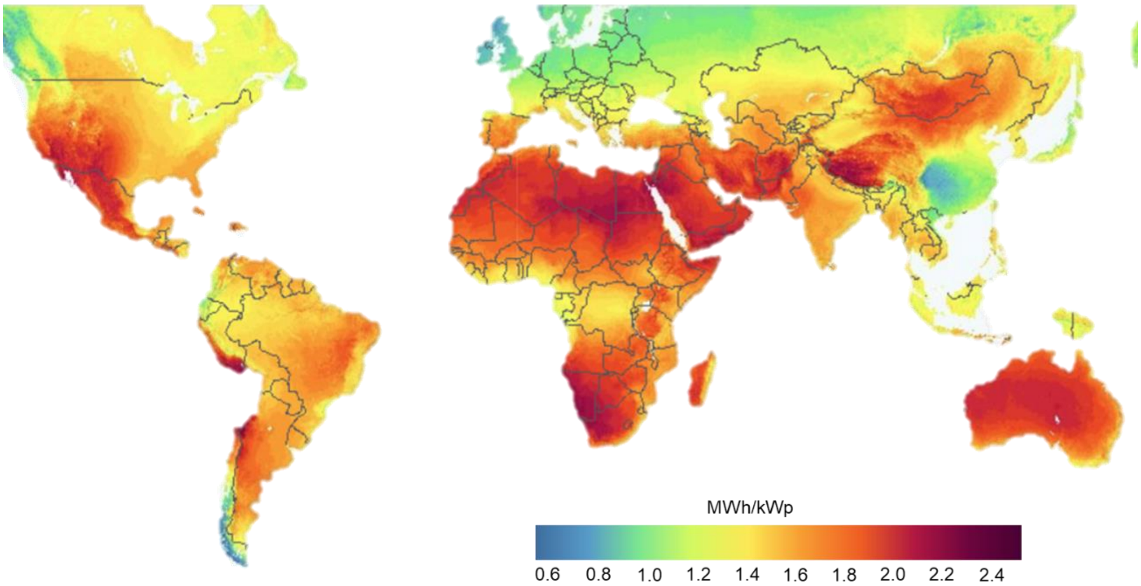

Figure 3: Long-term average of photovoltaic power (PVOUT) [12]

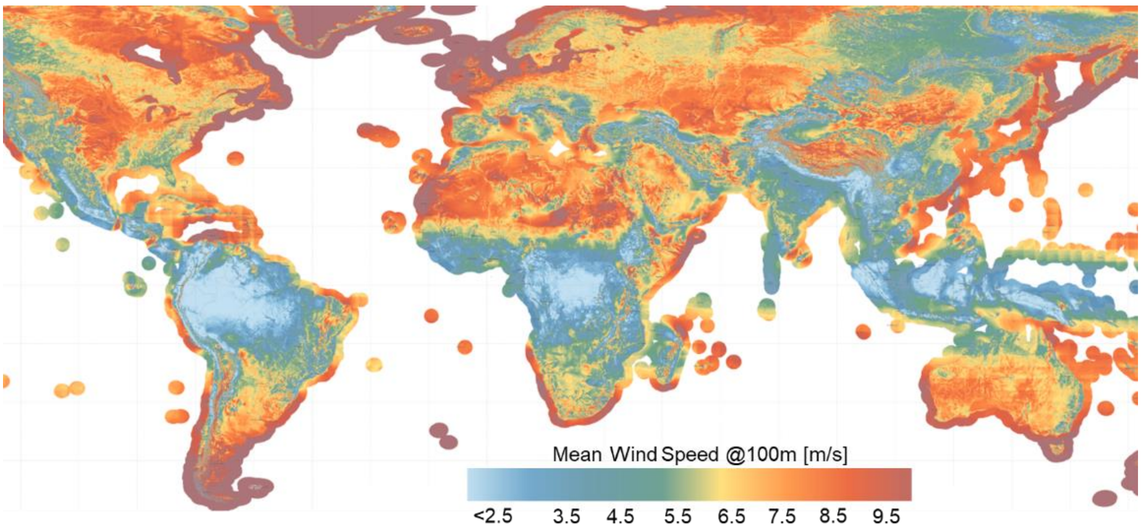

Figure 4: Mean wind speed potential [13]

[10] IDA (International Desalination Association). 2020. Desalination and Water Reuse by the Numbers. IDA website. https://idadesal.org

[11] Jones, E., Qadira, M., van Vliet, M.T.H., Smakhtina, V., Kangac, S. (2019). The state of desalination and brine production: A global outlook. https://doi.org/10.1016/j.scitotenv.2018.12.076

[12] 2019 World Bank, Global Solar Atlas 2.0, Solar resource data: Solargis, adapted

[13] https://globalwindatlas.info © 2019 World Bank, DTU Wind Energy, Vortex, OpenStreetMap.org, accessed 19.08.2022, adapted

Globally regions with severe water risks strongly conflict with high potential regions for Hydrogen production and PtX routes.

By comparing the availability of freshwater and renewable energy (see Figure 2-4), a clear conflict emerges: regions with a high renewable energy potential overlap with those regions facing water risk (e.g. MENA-region, Namibia, Australia). An integrated management framework combining hydrogen and follow-up PtX production with sustainable water management is essential.

6. Water-for-X the PtX Water Management Framework

Definition

Water-for-X by DECHEMA is a sketch for a sustainable water management framework for the hydrogen economy. It incorporates the water management and the interaction with hydrogen production and (follow-up) PtX processes as a holistic and integrated approach via three interconnected shells:

I. Production management shell
II. Industrial water management shell
III. Integrated water management shell

Water-for-X by DECHEMA combines the production management of PtX technologies with industrial and integrated water management to enable sustainable PtX solutions.

The three Water-for-X shells interact with and build upon each other, with an increasing scope size from production to industrial water to integrated water management. The role of water in each of the shells is as follows:

Integrated water management shell

a) Management of raw water resources required for operating hydrogen and PtX plants
b) Management of treated raw water streams not directly used in hydrogen or PtX processes
c) Management of treated product and waste water, e.g. off-site reuse or release to water bodies
d) Treatment and valorisation of residues from (waste) water

Industrial water management shell

a) Upgrading of raw water to process and cooling water for hydrogen and PtX processes
b) Treatment of all types of generated waste- or used water, as (I) residual streams from upgrading raw water, (II) used process water, (III) produced water and (IV) cooling water for reuse, alternative use or final release
c) Handling of residual streams generated during all (waste) water treatment processes (e.g. concentrate from membrane processes, sludge or valorisation or safe discharge)

Production management shell

a) Ultra-pure water and steam use in hydrogen and (follow-up) PtX processes
b) Hydrogen and PtX processes, incl. water from CCU/DAC, ASU etc.

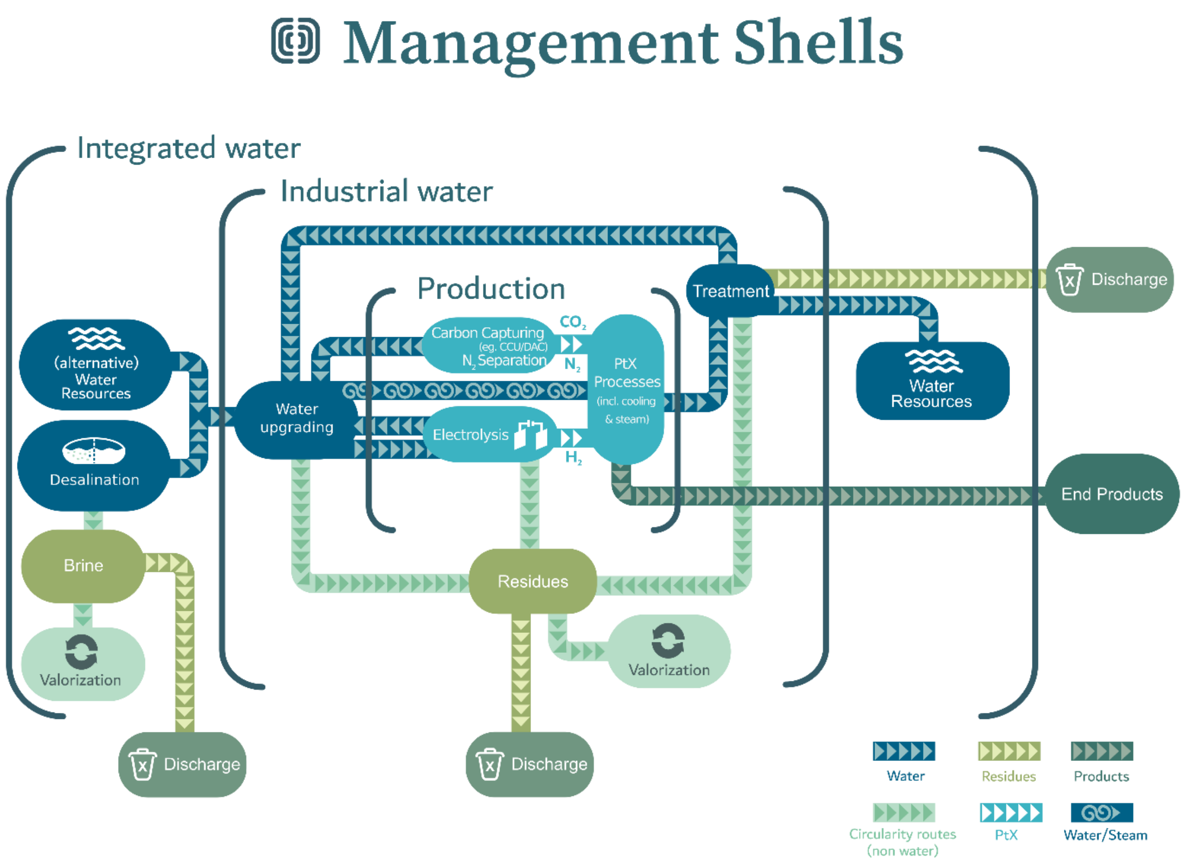

Figure 5: DECHEMA's Water-for-X Management Framework concept

The Water-for-X Management Framework needs to be integrated directly during the initial steps of planning and realizing hydrogen and follow-up PtX production sites.

Circularity and Sustainability

Additionally to the circularity aspects covered by Water-for-X (see Figure. 5), the approach with its identification and characterisation of water, energy, materials and residue streams provides direct interfaces to integrate further circularity routes, e.g. the valorisation of residue streams.

By following an integrated and holistic approach, Water-for-X enables the integration of socio-ecological and socio-economical aspects, like:

- valorisation of alternative water resources, e.g. municipal or industrial wastewater
- minimizing the impact on natural water ecosystems and other water users in a catchment, comparable to the water stewardship approach
- combining industrial and urban development, especially in arid and water stressed regions and in locations where new H_2 and/or PtX production sites are built

7. Application scenarios for the Water-for-X Management Framework

Based on the global distribution of regions with high potentials for photovoltaic power and wind speed (see Figures 3 and 4), three basic, water-related scenarios for hydrogen production as the initial step in the PtX value chain can be characterized (see Figure 6).

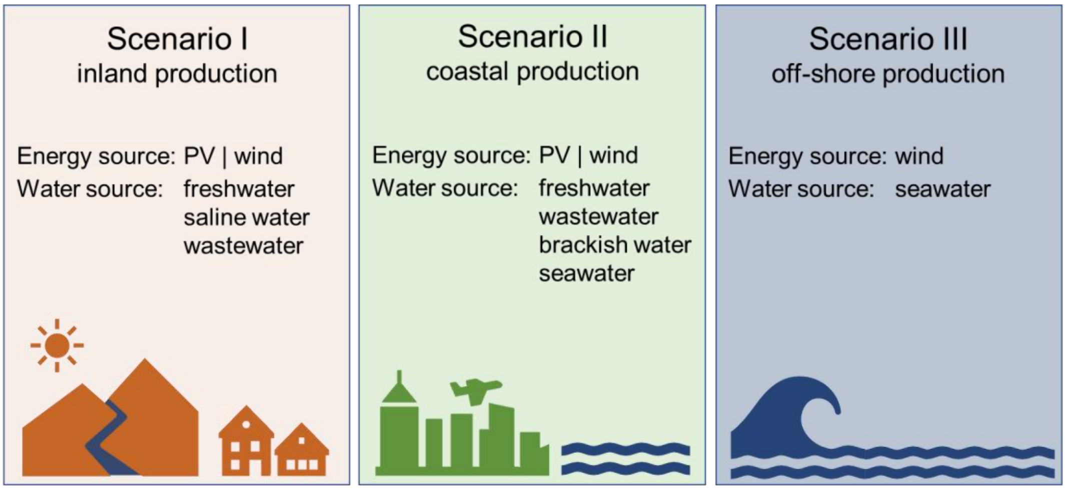

Figure 6: PtX production scenarios (PV = photovoltaic power) with potential energy and water resources

Scenario I represents production of hydrogen at an inland site, Scenario II at a coastal location, and Scenario III represents off-shore production. While the energy source can vary depending on location (photovoltaic power, wind), the scenarios mainly differ in their operational, environmental and water resources criteria. For example, when applying Scenario I or II, both green field (i.e. new plant development) and brown field (i.e. an existing plant) production sites can be considered. Further, all scenarios can vary in the targeted on-site PtX processes: hydrogen production, hydrogen and follow-up PtX production, follow-up PtX production (while hydrogen is produced off-site).

The Water-for-X Management Framework enables the evaluation of projects for hydrogen and PtX production for a most efficient and sustainable use of water, considering also the role and availability of renewable energy resources.

8. Water-for-X perspectives

Green hydrogen and follow-up PtX processes offer promising routes towards achieving a climate-neutral economy. Therefore, an increasing number of projects for the various PtX production scenarios can be expected in the near future. Water will be key for their successful realization. As individual projects will be locally / regionally based, the Water-for-X Management Framework provides sustainable water management solutions for regions with a high potential to realize the implementation of hydrogen and follow-up PtX processes.

In the nationally funded (BMBF) project H2Mare/TransferWind [14] the framework will be enhanced towards stand-alone solutions together with partners DVGW-EBI and KIT-IMVT [15]. Furthermore, the framework also finds use in international projects, such as GreeN-H2-Namibia and Nigeria4H2.

[14] https://www.wasserstoff-leitprojekte.de

[15] BMBF: Federal Ministry of Education and Research www.bmbf.de; DVGW-EBI (Research Center at Engler-Bunte-Institut of Karlsruhe Institute of Technology): https://www.dvgw-ebi.de; KIT-IMVT (Institute for Micro Process Engineering): https://www.imvt.kit.edu

The following aspects will be important for achieving sustainable PtX production and serve as the foundation for the Water-for-X Management Framework:

Achieving climate goals using PtX requires water

Hydrogen and follow-up PtX products will contribute to a fossil-free economy and to long-term energy security and resilience. An estimated hydrogen demand of 530 Mt in 2050 is required to realize a 'net-zero-emissions' scenario [16].

- As water is indispensable for PtX processes, this will lead to an increasing water demand.
- Based on the individual PtX production scenario, a production site could be a new additional water user in an existing local/regional water use context.

Sustainable water management is the route forward

By comparing the availability of both resources, freshwater and renewable energy (see Figures 2-4), a clear conflict emerges: regions with a high renewable energy potential strongly overlap with regions at water risk.

- Considering water stewardship is indispensable for long-term energy security.
- Many countries suffer from water stress already. Thus, alternative water resources will become even more important, e.g. seawater desalination and water reuse. New wastewater discharge challenges and valorisation opportunities (e.g. brines, concentrates) will occur.

The Water-for-X Framework provides PtX and water management solutions

- For sustainable PtX solutions, the conflict between the availability of (fresh) water and the availability of renewable energies has to be addressed.
- Integrated, sustainable water management is essential for successful PtX solutions.
- Water and wastewater treatment technologies and management concepts are available but need to be adapted to the Water-for-X application scenarios.
- Expertise and planning in water management and PtX technologies need to go hand in hand.

DECHEMA, with experts in both areas of water management and PtX processes, created this roadmap to establish a foundation for the "Water-for-X Management Framework" to support sustainable hydrogen and follow-up PtX processes. The Framework highlights the criteria that must be considered and provides a methodology to do so. As research and implementation in this field progress, the "Water-for-X Management Framework" will play a major role to realize both sustainable hydrogen and follow-up PtX production, together with integrated, sustainable water management.

[16] IEA Global Hydrogen review (2021) https://www.iea.org/reports/global-hydrogen-review-2021/executive-summary, accessed 19.08.2022

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