DECHEMA

WHITE PAPER

Water-for-X
Water for sustainable hydrogen and follow-up PtX processes

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.

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 white paper 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.

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[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 white paper 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.

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).

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).

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 megatonnes (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 demand 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 demand of 9.0 $kg_{H2O}/kg_{product}$. Utilizing this kind of hydrogen for the production of follow-up products such as methanol, ammonia, methane or kerosene leads to additional stochiometric water demands between 1.7 – 4.5 $kg_{H2O}/kg_{product}$. These stochiometric water demands represent the theoretical minimum water demand. As processes never meet efficiencies of 100%, losses must also be added to the estimation. Thus, the estimated real water demand is even higher, as outlined in the far-right column in Table 1.

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[2] IEA Global hydrogen review 2021

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

(PtX) product	**Reaction**	**Stochiometric water demand [$L_{H2O}/kg_{product}$]**	**Additional water demand in practice [$L_{H2O}/kg_{product}$]**
Hydrogen (H_2)	$H_2O \rightarrow H_2 + \frac{1}{2} O_2$	9.0	1-2 [3]
Methanol (H_3COH)	$CO_2 + 3H_2$ --> $H_3COH + H_2O$	1.7	0.5 (No clear range reported) [4]
Ammonia (NH_3)	$N_2 + 3H_2 \rightarrow 2NH_3$	1.8	0.6 (No clear range reported)[4]
FT-Kerosene/Diesel	$CO_2 + 3H_2 \rightarrow$ $[-CH_2]- + 2H_2O$	3.0	1.4 (No clear range reported)[4]
Methane (CH_4)	$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$	4.5	1.1-1.4 (No clear range reported)[4]

Based on an estimated hydrogen demand of 530 Mt in the year 2050, this would add up to 4770 Mt of water needed exclusively to produce hydrogen via electrolysis. Considering water losses of ~5-20%[5] based on water treatment processes during the production of hydrogen, an additional 238.5 – 954 Mt of water would be needed. Putting this into perspective, this amount equates to approximately 0.23% of the global yearly water consumption, which is around 4250 km^3. On top of these amounts, water demands for cooling, steam production, cleaning and other processes need to be considered. The required water qualities vary from ultrapure water for electrolysis to lower qualities for basic cleaning processes.

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

Although the percentage of 0.23% seems rather small, regions with high potential for hydrogen production often lack the required freshwater resources and this demand can place additional stress on the countries' water consumptions. 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[6]. In all these estimations, follow-up PtX processes, which require an additional water demand (see Table 1), are not considered.

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[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] Deutsche Energie-Agentur (dena), Factsheets: Power Fuels, 2018

[5] https://www.digitaleschweiz.ch/wp-content/uploads/2021/06/25-VBI_LF_EE_2015_Print_final.pdf

[6] Oesterholt, F. I. H. M., Koeman-Stein, N. E., Oldenbroek, V. D. W. M., Boere1, J. A., Van, A. J. M., & Wijk1. (2016). The role of water in a future hydrogen economy. October 2016, 9.

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[7]. 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.

Independent from its source, 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.

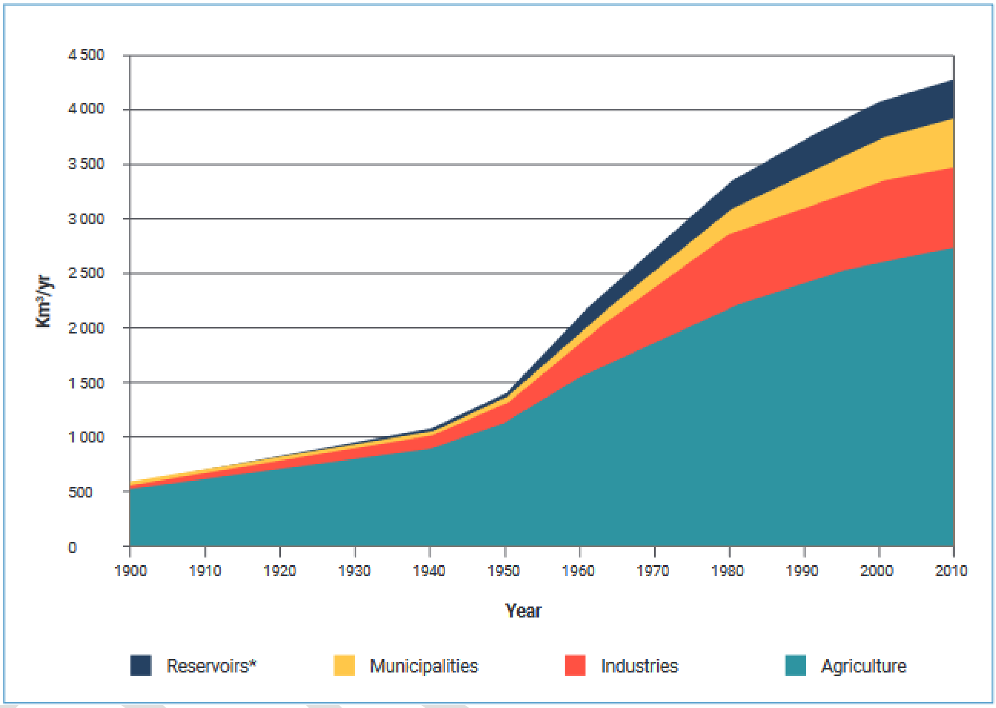

Figure 1: Global water withdrawals, 1900-2010[7]

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[8]. 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[9]. Figure 2 provides an overview of the global water risk distribution. Considering climate change perspectives, water risks will increase in the future, forcing the need for sustainable water use.

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[7] The United Nations World Water Development Report 2022

[8] When a territory withdraws 25 % or more of its renewable freshwater resources, https://www.un-water.org/publications/summary-progress-update-2021-sdg-6-water-and-sanitation-for-all/ accessed 19.08.2022

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

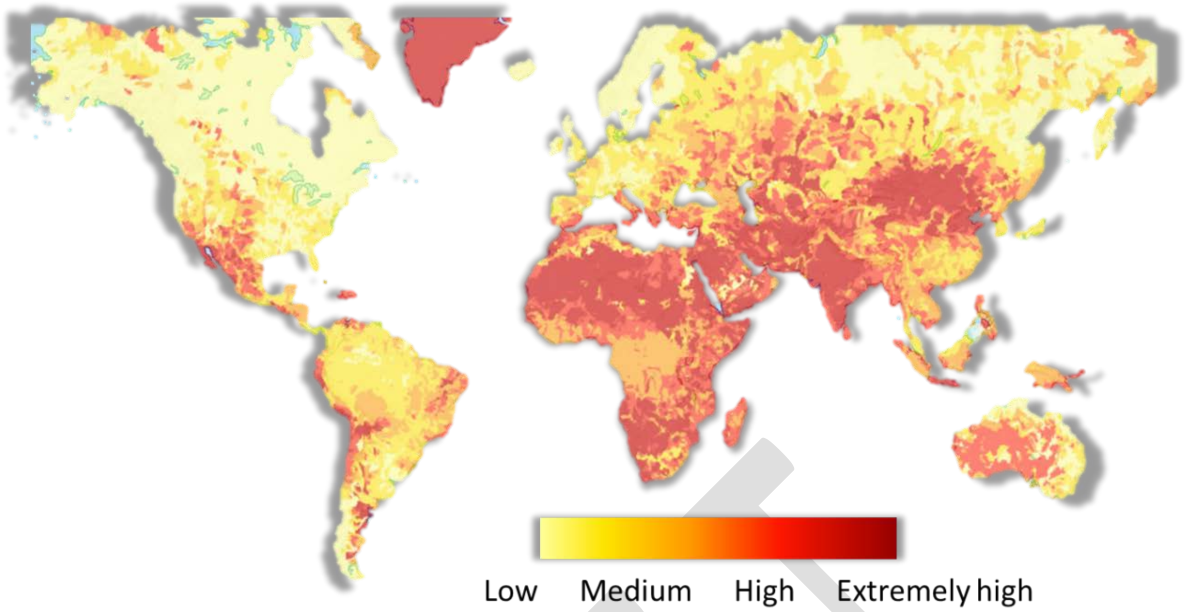

Figure 2: Overall Water Risk[10]

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.

> Water availability is limited in many countries based on regional specialties, which result in different levels of water risks that are 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.

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 people with potable water[11]. 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[12].

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

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

[12] 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

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.

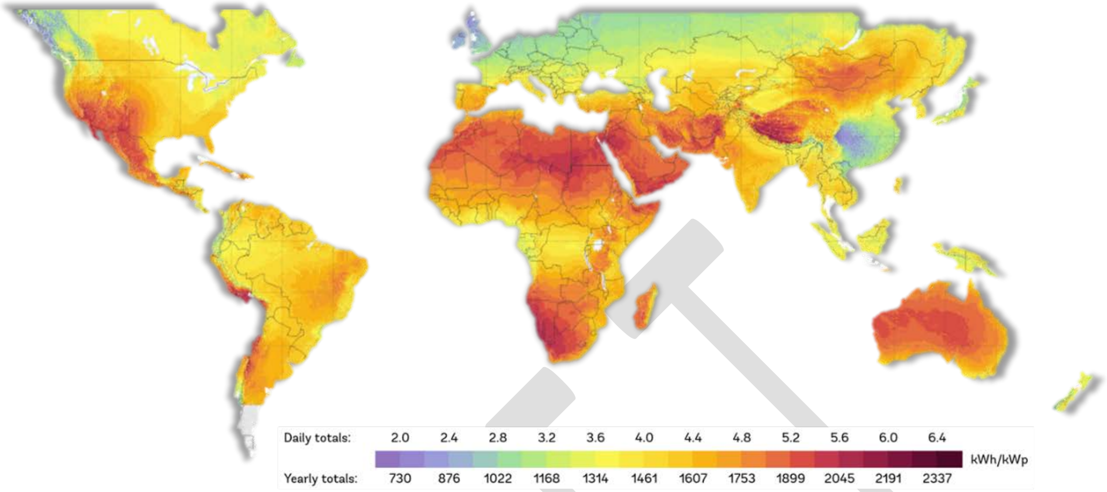

Figure 3: Long-term average of photovoltaic power (PVOUT)[13]

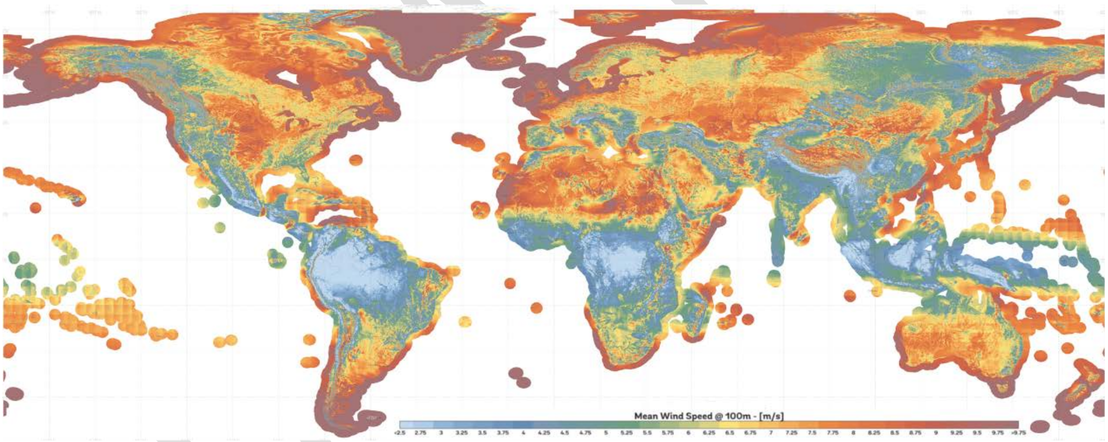

Figure 4: Mean wind speed potential[14]

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 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.

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

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[13] 2019 World Bank, Global Solar Atlas 2.0, Solar resource data: Solargis

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

6. Water-for-X Management Framework

Definition

Water-for-X by DECHEMA incorporates the entire water management framework 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

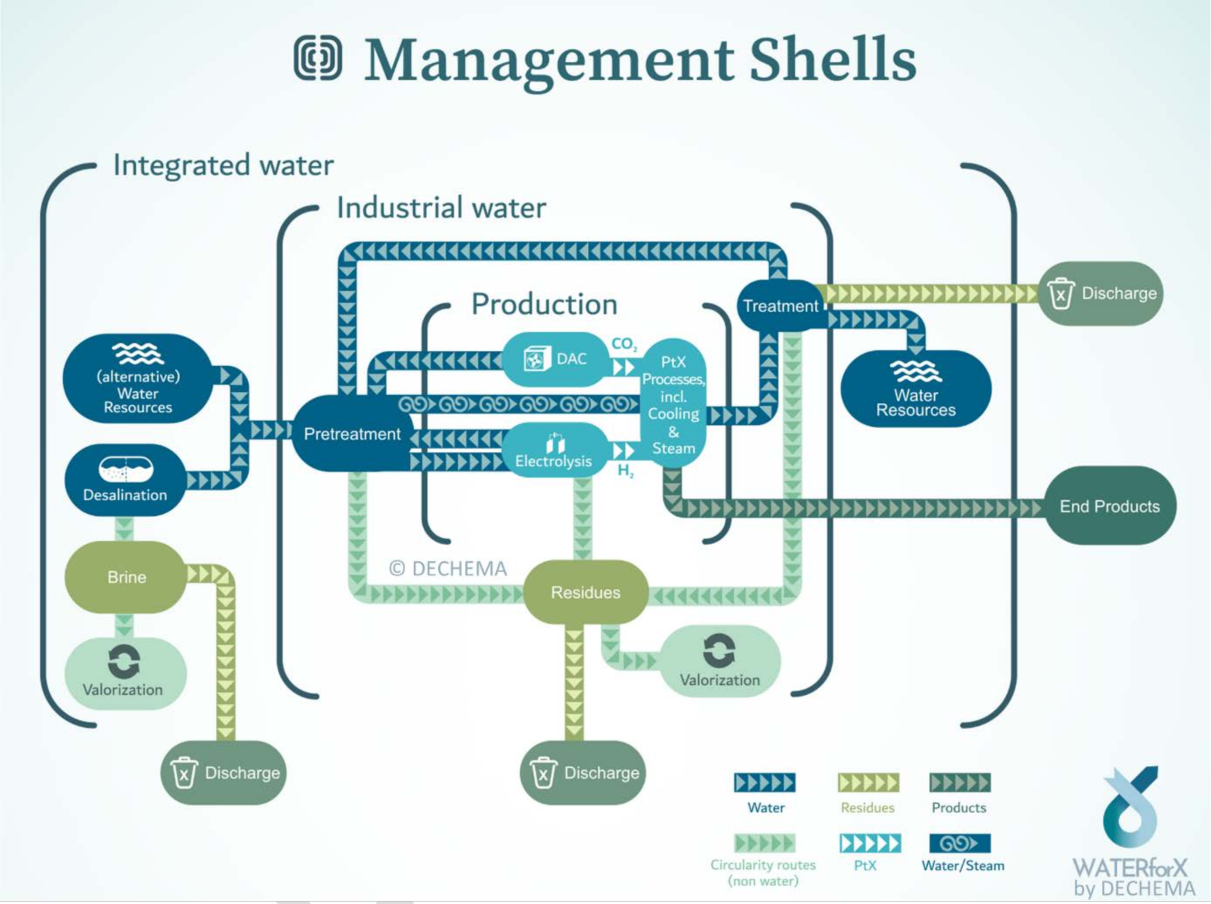

Figure 5: DECHEMA's Water-for-X Management Framework concept

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:

1. **Production management shell**

a) Direct water and steam use in hydrogen production and (follow-up) PtX processes
b) Hydrogen production and (follow-up) PtX processes, including produced water during DAC and PtX processes (e.g. Fischer-Tropsch Synthesis)

2. **Industrial water management shell:**
   a) Upgrading of raw water to process and cooling water and for steam production required for H_2 production and/or in 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. concentrates from membrane processes, sludge, or valorisation or safe discharge

3. **Integrated water management shell:**
   a) Management of raw water resources required for operating H_2 and PtX plants (seawater, brackish water, freshwater, alternative water resources)
   b) Management of treated raw water streams not directly used in H_2 production and/or PtX processes
   c) Management of treated industrial wastewater, e.g. for off-site reuse or release to water bodies
   d) Treatment and valorisation of residues from (waste)water treatment

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

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

In addition to the circularity aspects directly covered by Water-for-X (see Figure 5), the approach with its clear 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).

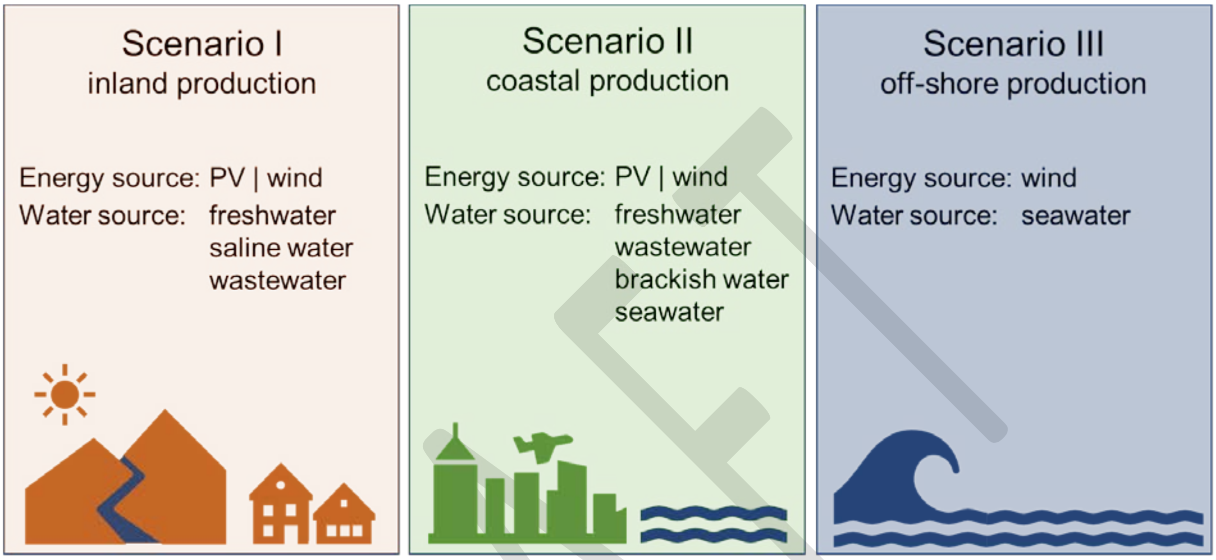

Figure 6: PtX production scenarios (PV = photovoltaic power) with potential energy and water resources

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.

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).

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.

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 strongly 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[15].
- 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 valorization opportunities (e.g. brines, concentrates) will occur.

The Water-for-X Management 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 white paper 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.

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