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POLYTECHNIQUE MONTRÉAL

affiliée à l'Université de Montréal

Use of the Life Cycle Approach for the Evaluation of Industrial Water Management Alternatives

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Mémoire présenté en vue de l'obtention du diplôme de *Maîtrise ès sciences appliquées*

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Ce mémoire intitulé :

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présenté par **Janaina SANTOS BOEIRA**

en vue de l'obtention du diplôme de *Maîtrise ès sciences appliquées*

a été dûment accepté par le jury d'examen constitué de :

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DEDICATION

When education is not liberating, the dream of the oppressed is to become the oppressor.

Paulo Freire

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RÉSUMÉ

La combinaison de l'augmentation de la demande et de la compétition pour l'eau a entraîné la nécessité de mettre en place des réglementations plus restrictives pour l'utilisation de l'eau afin de prévenir la rareté. De nombreuses industries ont opté pour la réutilisation de l'eau comme solution viable. Cependant, les technologies utilisées pour la réutilisation de l'eau nécessitent souvent des quantités importantes d'énergie. Si les combustibles fossiles constituent la principale source d'énergie, le surplus d'électricité généré contribue à augmenter les émissions de CO2 équivalent. Le changement climatique, provoqué par les émissions de gaz à effet de serre, se manifeste par des événements tels que des inondations et des sécheresses. Ainsi, si le recyclage de l'eau vise à protéger cette ressource vitale, il est essentiel d'évaluer ses impacts environnementaux associés pour ne pas les déplacer, voire les accroître.

Le choix d'une approche de gestion de l'eau doit concilier les exigences légales locales avec la performance environnementale pour garantir que l'une ne compromet pas l'autre. Une question fondamentale se pose donc : quels sont les impacts environnementaux associés aux options de gestion des eaux industrielles? Pour répondre à cette question, cette recherche mène une étude de cas, analysant différentes options de gestion de l'eau à partir d’une approche d'analyse du cycle de vie.

Une centrale électrique à cycle combiné a été choisie pour représenter le secteur industriel en raison de sa simplicité et de son importance en matière d'utilisation de l'eau. Trois options de récupération d’eau ont été analysées et ensuite combinées avec différentes sources de qualité de l'eau et options de rejet. De plus, tous les scénarios ont été virtuellement réaffectés à un autre contexte de pénurie d’eau pour une analyse de sensibilité géographique plus complète.

Les scénarios d'utilisation de l'eau ont été classés en fonction de la récupération. Pour zéro récupération, l’eau suit un flux de processus linéaire, représentant la configuration présente du scénario de base. La récupération partielle est obtenue par osmose inverse, tandis que la récupération totale, également connue sous le nom de Zero Liquid Discharge, utilise la distillation pour récupérer davantage l'eau provenant de l'osmose inverse.

Le recyclage de l’eau cause un impact sur l’ensemble du système d’eau. Lorsque l’eau est recyclée et réintroduite dans le système pour sa réutilisation, une réduction se produit pour les demandes de volume d’eau pour pré- et post-traitement. Au but de considérer la fonction du système d'eau dans

le processus de production, le choix de la production d'énergie a servi de scénario de base pour la comparaison au lieu des volumes d'eau. La fonction du système est de gérer l'eau pour produire 1 MWh d'électricité, où seules la structure et l'énergie liées à l'eau ont été prises en compte. De plus, un deuxième système a également été envisagé, dont la fonction est de produire 1 MWh d'électricité, où tous les impacts du site ont été pris en compte.

Les informations locales du site de 2021 ont été utilisées comme données de source principale. La littérature et des spécialistes ont été consultés pour obtenir les données supplémentaires requises. La centrale électrique a été modélisée dans OpenLCA en utilisant la base de données Ecoinvent pour les processus en amont. Les impacts ont été calculés à l'aide de la méthodologie IMPACTWorld+. Les résultats sont d'abord présentés en émissions d'équivalent de CO2 et en profil AWARE en tant qu'indicateurs mid-point. Des indicateurs de santé humaine et de qualité des écosystèmes sont également fournis pour évaluer la contribution relative du potentiel de réchauffement climatique et de la rareté de l'eau aux impacts globaux.

La consommation est définie comme le volume de prélèvement d'eau en soustrayant le volume de rejet, représentant la quantité d'eau incorporée dans un produit ou évaporée dans l'atmosphère. Dans le cadre de cette étude, le principal contributeur à la consommation d'eau sur site est la vapeur d'eau générée dans la tour de refroidissement. Cet équipement est indispensable pour dissiper la chaleur des cycles thermodynamiques impliqués dans la production d'électricité. Le recyclage n'ayant pas d'impact direct sur le processus de production d'électricité, la consommation d'eau sur site due à l'évaporation reste essentiellement égale. Néanmoins, les volumes d'eau prélevés et rejetés peuvent diminuer avec des taux de récupération plus élevés.

L'empreinte de la rareté d'eau est principalement influencée par l'utilisation d'eau douce sur site quand la fonction de gestion de l'eau est en évidence. Cependant, pour la production de 1 MWh d'électricité, le processus amont du gaz naturel est aussi important comme l'utilisation directe sur site. Les coefficients AWARE sont basés sur la consommation d'eau douce ; par conséquent, le recyclage n'entraîne pas nécessairement une diminution de la rareté d'eau lorsqu'il est considéré le prélèvement et le rejet d'eau douce. L'eau des océans n'étant pas considérée comme de l'eau douce, alors dans le cas du dessalement, aucune eau douce directe n'est consommée et seul le processus en amont présente des impacts. En outre, des crédits de rareté de l'eau peuvent être générés en libérant de l'eau dans un corps d'eau douce. Si l'eau est extraite de sources d'eau douce et rejetée dans l'océan, tout le volume extrait est considéré comme consommé. Dans ce cas, le recyclage a pour effet de réduire les impacts de rareté d'eau.

Les émissions de CO2 équivalent sont principalement causées par la combustion du gaz naturel pour produire de l'électricité. Les systèmes de recyclage consomment moins de 1 % de l'électricité produite. Par conséquent, les variations des émissions d'équivalent CO2 ne peuvent être détectables que si l'unité fonctionnelle de gestion de l'eau pour produire 1 MWh d'électricité est utilisée. Une récupération partielle de 50 % de l'osmose inverse par rapport au scénario de base présente des impacts similaires, voire inférieurs, selon que l'adoucissement ou le dessalement est utilisé comme prétraitement. Le dessalement consomme beaucoup plus d'énergie que l'adoucissement fait par le décarbonisateur et, par conséquent, des exigences de prétraitement moindres dues à la réutilisation de l'eau sont favorables si l'eau de mer est utilisée. Des récupérations plus élevées nécessitent plus d'énergie et peuvent ne pas être compensées par le prétraitement pour éviter les impacts. C'est particulièrement le cas du scénario ZLD, qui entraîne dans tous les cas des émissions d'équivalent CO2 plus élevées si aucune optimisation ne peut être appliquée. L'augmentation des récupérations par osmose inverse avant les systèmes d'évaporation est bénéfique pour minimiser les impacts ; cependant, elle présente des limites quant à la qualité de l'eau à traiter.

Les compromis analysés dans les paramètres montrent que le contexte de l'eau est crucial pour tirer des conclusions. Les impacts sur la santé humaine sont principalement dominés par le potentiel de réchauffement climatique dans les pays sans rareté en eau ou hautement développés. Cependant, les impacts d'eau peuvent être plus importants pour les pays où il y a la rareté et sont moins développés. La qualité des écosystèmes présente moins des variations que la santé humaine, mais les différences entre les scénarios sont aussi dominées par la variation du potentiel de réchauffement climatique. Lorsque l'on compare les extrêmes de coefficients de rareté d'eau pour la qualité des écosystèmes, les conclusions qualitatives comparant les scénarios restent les mêmes.

Le recyclage ne réduit pas nécessairement l'empreinte de rareté d'eau et peut entraîner une augmentation des émissions de gaz à effet de serre. Il est crucial de prendre en compte le contexte de pénurie d'eau et les compromis possibles avant de prendre des décisions concernant la gestion de l'eau. Une législation basée uniquement sur les volumes d'eau prélevés et rejetés peut résulter en impacts environnementaux indésirables, au-delà du fait de ne pas garantir les économies d'eau.

Cependant, lors des options de gestion de l'eau en discussion, le présent travail vise à faciliter une prise de décision éclairée concernant les impacts environnementaux potentiels.

ABSTRACT

The rising demand for water, coupled with intense competition among water users, has led to the implementation of more stringent regulations on water usage to protect from high scarcity. Many industries are turning to water recycling as a viable solution. However, it's important to note that the technologies employed for water reuse often require substantial amounts of energy. In cases where fossil fuel combustion is the primary energy source, the surplus electricity generated contributes to increased CO2-equivalent emissions. Climate change, caused by greenhouse gas emissions, manifests in events like floods and droughts. Therefore, while recycling water has the objective of protecting this vital resource, it's essential to assess its associated environmental impacts to not displace or even increase them.

The selection of a water-management approach must reconcile local legal requirements with environmental performance to ensure that one does not compromise the other. Therefore, a fundamental question arises: What are the environmental impacts associated with industrial water management options? To address this inquiry, this research conducts a case study, analyzing different water management options using a Life Cycle Analysis approach.

A Combined Cycle Power Plant was chosen to represent the industrial sector due to its simplicity and significance in terms of water use. Initially, three distinct recovery practices were analyzed and subsequently combined with different water quality sources and release options. Furthermore, all scenarios were virtually reassigned to another water-scarce context for a more comprehensive geographical sensitivity analysis.

The water use scenarios were categorized according to recovery. For zero-recovery scenario, water follows a linear process flow, representing the current base case configuration. Partial recovery is achieved through reverse osmosis, while total recovery, also known as Zero Liquid Discharge, utilizes thermo-distillation to further recover water from reverse osmosis.

Water recycling has a significant impact on the overall water system. When water is recycled and reintroduced into the process system, a reduction occurs in both pre- and post-treatment water volume demands. To considers the water system's function in the production process, the selection of energy production served as the base scenario for comparison instead of water volumes. The system's function is to manage water to produce 1 MWh of electricity, where only water-related

structure and energy were considered. Additionally, a second system was also considered, which its function is to produce 1 MWh of electricity, where all site impacts were considered.

The 2021 local site information was used as primary source data. Literature and specialists were consulted to additional required data. The power plant was modeled in OpenLCA using Ecoinvent database for upstream process. Impacts were calculated using IMPACTWorld+ methodology. Results are first presented in CO2-eq emissions and AWARE profile as mid-point indicators. Human Health and Ecosystem quality endpoint indicators are also given to evaluate the global warming potential and water scarcity relative contribution in the overall impacts.

Consumption is defined as water withdrawal minus release, representing the amount of water incorporated into a product or evaporated into the atmosphere. In the context of this study, the primary contributor to on-site water consumption is the water vapor generated in the cooling tower. This equipment is essential for dissipating heat from thermodynamic cycles involved in electricity production. As recycling does not directly impact the electricity production process, on-site water consumption due to evaporation remains essentially unchanged. Nevertheless, withdrawn and released water volumes may decrease with higher recovery rates.

The water scarcity footprint is primarily influenced by on-site freshwater use if the water management function is considered. However, for the production of 1 MWh of electricity, the natural gas upstream process shares importance with on-site direct use. AWARE coefficients are based on freshwater consumption; therefore, recycling does not necessarily result in lower water scarcity when considering freshwater withdrawal and release. As ocean water is not considered freshwater, in the case of desalinization, no direct freshwater is consumed, and only the upstream process presents impacts. Also, water scarcity credits can be generated by releasing water into a freshwater body. If water is withdrawn from freshwater sources and release in the ocean, all withdrawn volume is considered consumed, in this case, recycling impacts in lower water scarcity.

CO2-equivalent emissions are caused mainly due to natural gas burned to produce electricity. Recycling systems consumes less than 1% of the generated electricity, consequently, variances in CO2-eq emission can only be detectable if water management to produce 1 MWh electricity function unit is used. Fifty percent partial RO recovery compared to the base case scenario presents similar to lower impacts depending on whether softening or desalinization is used as pretreatment. Desalination consumes substantially higher energy than softening and therefore *lower pretreatment demands due to water reuse from recycling is favorable if ocean water is used. Higher recoveries demand more energy and may not be compensated by the pretreatment avoid impacts. This is especially the case for ZLD scenario, which has higher CO2-equivalent emissions in all cases if no optimization can be applied. Optimizing reverse osmosis recoveries before evaporation systems is beneficial to minimize impacts; however, it has limitations on the water quality to be treated.*

Trade-offs analyzed in endpoints show that the water context is crucial for drawing conclusions. Human health impacts are primarily dominated by global warming potential in non-water-scarce or highly developed countries. However, the water scarcity footprint impacts can be more significant for scarce and less developed countries. Ecosystem quality exhibits lower variation than human health, but the differences between scenarios are also dominated by global warming potential variation. When comparing the extremes in terms of water scarcity coefficients for ecosystem quality, qualitative conclusions comparing scenarios remain the same.

Recycling does not necessarily lead to lower water scarcity footprints and can result in higher greenhouse gas emissions. It is crucial to consider the water scarcity context and trade-offs before making decisions about water management. Legislation based solely on water withdrawal and release volumes may lead to undesirable environmental impacts, beyond not ensuring water savings. Nevertheless, when debating water management options, the present work aims to facilitate informed decision-making regarding potential environmental impacts.

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LISTE OF SYMBOLS AND ABBREVIATIONS

AWARE	Available remaining water
CC	Combined cycle Unit
CF	Coefficient Factor
CR	Crystallizer Unit
CT	Cooling tower Unit
DALY	Disability-adjusted life year
DM	Demineralization Unit
DZ	Algeria
EQ	Ecosystem Quality
EV	Evaporator Unit
FR	France
g	Grams
GWP	Global Warming Potential
HH	Human Health
LCA	Life cycle analysis
m^3	Cubic meter
MD	Membrane distillation
MJ	Megajoules
MLD	Minimal Liquid Discharge
MSF	Multistage Flash
MVC	Mechanical Vapour Compressor
MW	Megawatt
MWh	Megawatt-hour

NGCC	Natural Gas Combined Cycle
NF	Nanofiltration
PDF.m2.yr	Potentially Disappeared Fraction of species per square meter per year
ppm	One part per million
RO	Reverse osmosis Unit
ST	Softening Unit
TW	Tap water production per Desalination Unit
UF	Functional Unit
US	United States of America
WW	Biological-Wastewater treatment Unit
ZLD	Zero Liquid Discharge
μS	Micro Siemens

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CHAPTER 1 INTRODUCTION AND LITERATURE REVIEW

1.1 Context

Climate change is an ongoing process caused by greenhouse gas emissions, particularly CO2. Its consequences vary globally, leading to floods in some places and droughts in others. Europe has been experiencing water shortages since 2018 [1] and this issue is expected to intensify, affecting up to 17% of the European population by 2050 [2]. Despite a decrease in water abstraction in Europe, the areas impacted by drought remain constant, indicating the need for additional efforts to mitigate water scarcity [3].

Off-stream water use, defined as removed water from its natural water body [4] can be categorized into industrial, domestic, agricultural, fisheries, hydropower, transport, and recreation [5]. Water quality standards are specific for the desired application. Domestic water use standards aims to prevent human health risks whereas for industrial standards vary according to the process production. Domestic standards may be suitable for some industry uses; however, process water is not considerable potable.

Industries and the energy sector account for 19% of the world's total freshwater withdrawals [6], with higher contributions in Europe and the United States. In the U.S., thermoelectric power generation alone is responsible for 41% of total withdrawals [7]. Cooling purposes represent a significant portion of water usage [8].

Industries are also pointed as an important source of contaminants to groundwater. Oil and gas extraction can contaminate waters with aromatic hydrocarbons, whereas coal mining with acids and heavy metals [6].

To safeguard water resources, stringent regulations are now in place, restricting withdrawal and release volumes. Withdrawal regulations aim to prevent scarcity, while release regulations address the risk of water unavailability due to contamination. The Indian government, recognizing the need for environmental protection, has mandated Zero Liquid Discharge (ZLD) water management for its high-pollution industries [9]. Similarly, the U.S. government's effluent guidelines express a preference for zero discharge [10]. In France, water use limitations are decreed during drought periods [11], but this can compromise electricity production, compelling alternative measures [12, 13]. The adoption of ZLD technology is increasing globally, notably in the USA, China, and India, driven by its environmental benefits, including protection for human uses [14]. Notably, the power plant sector stands out, with approximately 70% of ZLD plants falling within this industry [15].

In this context, industrial water recycling and reuse emerges as promising alternatives, facilitated by a range of established technologies. Options such as reverse osmosis, evaporators, and crystallizers have been widely used. Despite their effectiveness, the high-energy requirements for water recovery have led to the emergence of new technologies, including membrane distillation, forward osmosis, and electrodialysis. However, these later technologies still need to assess their performance on a industrial application.

1.1.1 TotalEnergies Power Plant

The 440 MW Combined Cycle Power Plant located in France, owned by TotalEnergies, serves as an example of the water challenges faced by industries. The current site water management is characterized as linear, with water flowing from pretreatment to the use phase process and then sent to post-treatment for discharge. In 2021, the plant withdrew 1.2 Mm^3 of water from groundwater, released 0.28 Mm^3 into the river, and produced 1543000 MWh of electricity over 4197 hours of production. Necessary to release heat from electricity generation fluids, the cooling tower system accounts for the largest water use, evaporating approximately 75% of the total water withdrawn. Water is constantly fed and purged from the tower to maintain the required water quality, making the cooling tower a focal point in terms of water flows.

The unit needs to reduce its water withdrawals volumes by 10 to 20% during water scarcity periods to meet local regulations. Impossible to meet the stricter decree while in normal operation, energy production needs to be shut down. There are also regulations in terms of release water. Maximum water discharge is 70 m^3/h in summer while 55 m^3/h in other seasons. The presence of pollutants in release water is limited in terms of concentrations. Currently, some chemical species such as chlorine and phosphate are already at their maximum allowed concentration, restricting further concentrations with the aim of lowering water volume release.

Other water management options include recycling water at different rates, ranging from partial recovery to total recovery, also known as Zero Liquid Discharge. This involves applying additional technologies to effectively remove wastewater pollutants, meeting the necessary water quality requirements. Recycling water for reuse enables reduced water withdrawals and releases. However, it's important to note that the potential surplus energy required for this process may lead to higher environmental impacts, particularly if derived from a fossil energy base.

Looking for solutions to maintain normal operations, TotalEnergies is interested to understand trade-offs between water use and other environmental impacts to guide decision-making in terms of water management practices.

For a comprehensive perspective, various water sources and discharges were considered. The required pre- and post-treatment differs due to water quality, leading to distinct impacts. Although the power plant unit is located in France, this study aims to understand how water scarcity scenarios in other regions can influence trade-offs. To assess regional variability, the unit was virtually relocated to other countries to capture extremes in terms of water availability.

1.2 Literature review

1.2.1 Methodological basis

Life cycle analysis involves considering the impacts of the entire production chain of a product or service. This approach helps avoid the transfer of impacts from one process to another. The results are presented in the form of various indicators to prevent the consideration of different emissions of different compounds, avoiding the loss of information when substituting one category of impact for another.

Life cycle analysis divides the world into two spheres, as represented in Figure 1.1. The Technosphere is where the production of goods and services occurs, considering a network of internal flows. On the other hand, the Ecosphere encompasses everything in nature outside the Technosphere. The exchanges between the Technosphere and the Ecosphere involve flows of materials extracted and sent to nature as a consequence of Technosphere processes, also known as elementary flows. These flows are quantified and translated into impact indicators using established impact models.

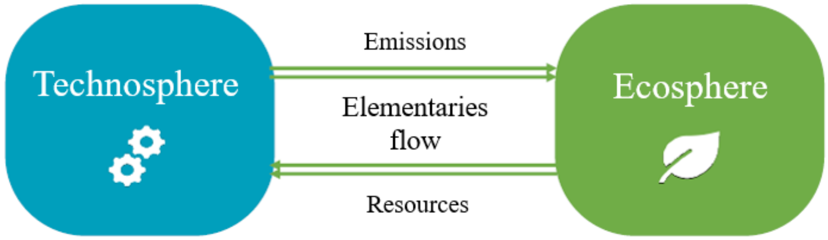


Figure 1.1 LCA Techno and Ecosphere and elementary flows. Adapted from [16].

The Technosphere is often represented by a system product, as illustrated in Figure 1.2. It comprises a group of elementary processes with specific inputs and outputs, representing the production chain for a particular function. The internal changing flows within this system are referred to as technological flows.

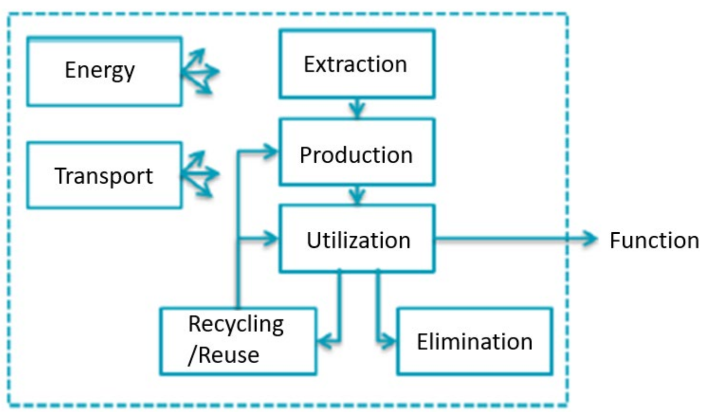


Figure 1.2 Product system representation. Adapted from [16].

This methodology is supported by the ISO 14040:2006 [17] and ISO 14044:2006 [18] standards, consisting of four interconnected main steps. Figure 1.3 illustrates the iterative nature between each step, essential for constant refinement if necessary. The framework includes the definition of objectives, determine inventory, assessment of impacts, and subsequent interpretation of results. Each step's development is detailed in the following subsections. It is crucial for the ACV steps to be aligned with the desired analysis application. Examples of possible Life Cycle Assessment (LCA) applications include product development and improvement, strategic planning, public policy, and marketing. The application of this study is to support decision-making regarding water management for power plant units.

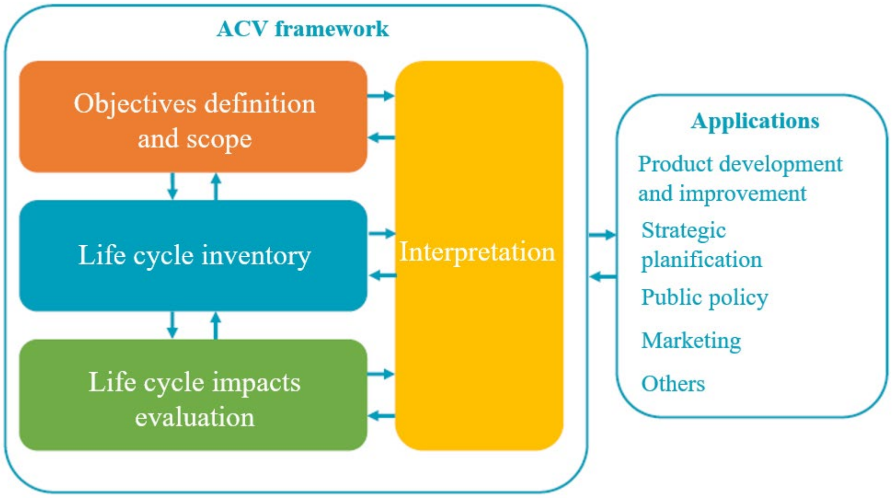


Figure 1.3 LCA framework and applications. Adapted from [16].

1.2.2 Water treatment technologies and impacts

An overview of the technologies in focus in presented in the Table 1. Specific functioning details are presented in section 2.2. Water treatment is a sum of various unit operations combined that are dependent on the input water characteristics and product water quality requirements. It can be divided in pre- and post-treatment technologies, even though some are present in both stages. Desalination is applied to ocean withdrawals and its technologies are mainly based on reverse osmosis, and/ or evaporator and or not followed by a crystallizer in different configurations. Reverse osmosis, evaporator and crystallizer are also present in post-treatment stages because allows the possibility to recycle wastewater.

With a focus on different water treatment technologies, in terms of impacts is important mention water footprint. The consensus base water footprint is the AWARE (Available Water REmainig) methodology which is based on the volume of consumed (withdrawal minus release) freshwater in relation of the available water minus the human and ecosystem needs in perspective of the world average [19]. More details in section 2.3.1. Another important indicator is the carbon footprint. Considering water treatment technologies, the energy source is the main responsible for CO2-eq emissions [20].

Table 1 Water treatment technologies explored in this work.

Treatment stage	Technology	Principle
Pre-treatment	Softening	Precipitation to remove hardness specially from groundwater. Produce softened water and sludge
Pre-(desalination) and post treatment (water recovery)	Reverse Osmosis	Pression to filtrate water against reverse osmosis membrane. Produce high quality water in terms of dissolved salts and a concentrate.
	Evaporator	Evaporates water using heat. Produce and high-quality water in terms of dissolved salts and a concentrate.
	Crystallizer	Evaporates water using heat. Produce salts high quality water in terms of dissolved salts and salts.
Post-treatment	Biological treatment	Uses bacteria to degradation and filtrate wastewater. Produce water with low DBO and sludge.

Analyzing pre-treatment for different sources of water, due to energy consumption, those required for surface and groundwater present from one third to half less global warming potential impacts compared to desalination, used for ocean water; on the other hand, desalination has lower freshwater consumption [20]. Additionally, groundwater is a preferred source of water for industries due to its clean characteristics, requiring fewer treatment stages [6].

As presented in Table 1, recycling water technologies are similar to the ones used in desalinization. Reverse osmosis and evaporation technologies are also applied to recover wastewater. The most established route for water recovery involves first membrane separation followed by thermo-technologies as needed to achieve high recovery rates. Due to high energy requirements, thermo-distillation has 2 to 19 times higher impact relative to the RO system, depending on the impact method [20].

The RO system has shown potential in reducing water streams (in and out) in cooling tower systems; however, the recovery rates are limited by high salinity, causing high osmotic pressure to be overcome, and scaling potential causing fouling [21]. RO membrane recoveries depend on salinity and applied pressure in general. Higher the salinity, higher the pressure needed. Standard membrane recoveries can start at 35%, up to 80% [22, 23]. High-pressure membranes can achieve even higher recoveries, more than 90% [24] concentrating water up to 70 mg/l [14] or even 120 mg/l [25], but at the cost of increased energy consumption.

Thermo-desalinization consists of the evaporator and crystallizer. In the evaporator, separation occurs through a change in the water phase after receiving heat. Water vapor is recovered and can be reused, while the highly concentrated solution feeds into the crystallizer. Evaporators can concentrate up to 250 mg/l of salt concentration [26]. Further concentration is achieved in the crystallizer, where crystallization is performed by oversaturation of a brine by means of evaporation using thermal energy (heat).

Standard wastewater treatment requires a wide range of electricity, from 0.005 to 0.8 kWh/m^3 [27], while RO 1.5 – 6 kWh/m^3 of product water [28], 14 - 25 kWh/m^3 of product water for MVC evaporator [15, 26] and 50 - 59 kWh/m^3 of treated water for crystallizers [15, 26].

Despite the intention to save water, recovery does not necessarily imply a reduction in water consumption (withdrawal minus release). The associated increase or decrease in Global Warming Potential (GWP) impacts depends on the environmental effort ratio between standard treatment and recovery technologies [29]. NGCC plants, for instance, can reduce water withdrawals by 18%, consuming less than 0.8% of facility electricity production when applying zero liquid discharge technologies [30]. However, the additional energy requirement to recycle water can result in more water use due water consumption in energy production occurring in the upstream process. In the context of China, recycling 1 m^3 of water end up consuming more than 1.64 m^3 of freshwater [31].

Due to high energy requirements in ZLD systems, Minimal Liquid Discharge (MLD) is another recovery option. Lower recovery can significantly reduce energy consumption. MLD, with 84.6% recovery, consumes 5.4 kWh/m^3, while a ZLD system achieving 98.15% recovery consumes 10.43 kWh/m^3 [32]. On the other hand, more brine volume needs to be handled for final disposal. As brine becomes concentrated, it may reach hazardous specifications and therefore need to follow specific regulations regarding final disposal resulting in associated financial costs [15].

Water treatment options are often explored in LCA analysis [20] but are typically analyzed separately as pre- , as in Raluy et al, 2006 [33]or post-treatment as on Yang et al, 2020 [31]. Water reuse is also a frequent study subject; however, it usually focuses on water volumes and process optimization without the LCA analysis as example on the 2022 study from Plata et al [30]. The found exception was a 2023 paper from Markus Berger and Sebastian Thiede [29], however, it was not conducted considering site data, only sensitivity parameter in terms of environmental efforts using a standard municipal wastewater facility and suggest industrial related study cases to support results. With this, LCA studies integrating all water treatment phases for a real industry case water management system, considering water qualities and scarce locations, were not found.

1.3 Objectives

The idea of protecting water bodies through sea desalination and water recovery or recycling is well accepted socially. However, these practices also come with negative environmental aspects. The technologies involved in water recovery/recycling require large amounts of energy, which can be fossil-based and thus contribute to climate change. Therefore, it is necessary to understand the potential impacts of different practices regarding water management options. Thus, a question arises: *What are the environmental impacts associated with industrial water management options?*

Therefore, the objective of this work is to evaluate the environmental performance, using LCA approach, of the industrial wastewater management options to help decision-making. More specifically:

1. Quantify water management contributions to the total impacts of the power plant.
2. Evaluate trade-offs between water footprint and climate change indicator for different water recovery practices and water quality at mid and endpoint level.
3. Analyse the regional sensitivity of the results and conclusions in respect to different water scarcity context.

CHAPTER 2 METHODOLOGY

To evaluate the environmental performance of the different water management option, life cycle approach was applied aiming to guide TotalEnergies decision-making.

2.1 Scope

2.1.1 Case study

Aiming to analyze the environmental performance of water management options, a real industrial unit was selected. It is a Combined Cycle Power Plant 440 MW year capacity located in France, belonging to TotalEnergies.

The power plant employs a linear water use configuration without recycling. Figure 2.1 illustrates the simplified water flows in the studied system. Table 2 represents flows and compositions for the represented streams in ideal operational conditions, however not all the chemical composition was available for all streams and therefore was represented as n. d. (no data). Additionally, for vapor and demineralised water, the contaminants were considered to be zero (0*).

Groundwater, represented by stream number "1" serves as an intake flow to the softening unit where the hardness is removed using chemical promoting coagulation, flocculation, and decantation. Sludge is produced constantly and removed with frequency. The product softened water, represented by stream number "2" is majorly directed to the cooling tower basin as makeup flow and a small part to the demineralization system.

The demineralization unit supplies demineralised water, represented by the stream number "3" to the combined cycle. The softened water pass through a sequence of ion exchange units to remove the remaining contaminants to achieve the water quality required in the combined cycle boilers. The ion-exchangers resin needs to be clean after certain amount of operation time, this requires wash water flow and chemical additives. Therefore, wastewater is produced, represented by the stream number "4".

The combined cycle system is composed by boilers and turbines. Natural gas is burned following the Rankine cycle to produce energy. Energetic efficiency is achieved by a second thermodynamic cycle, called Brayton, to further use the potential energy source to produce electricity. The combination of Rankine and Brayton cycles gives the technology name as combined cycle. Heat release is necessary to maintain the cycles and it is achieved by the use of a cooled water passing into a heat exchanger where heat transferred is enough to increase around 10°C the cooled water. The cooled water is not represented on Figure 2.1 because there is no water transfer to the combined cycle unit, only heat. Some vapour is release in the atmosphere and represented by the stream number “5”. Due to the vapor release, some contaminants become concentrated and needs to be purged even though demineralized water is used. The purge, represented by the stream number “6” has enough quality to be used in the cooling tower. Chemicals containing ammonia, phosphate and sodium are used in this unit to maintain operational standards, however its concentration in the purge was not assessed, therefore, only represented as different from zero.

The cooling tower produce cooled water used to remove heat from the combined cycle. After having exchanged heat, water goes back to the cooling tower where it is distributed internally in the cooling tower to fall dawn against fan forced ambient air going upwards. The counter air flow partially evaporates, stream number “7”, thus, due to the vaporization heat, cools down the water falling stream. Once cooled, the water is retained in a basin and directed to the combined cycle heat exchanger. Chemicals additives are necessary to maintain the water quality, however, as contaminants concentration increase as the evaporation occurs. Similar to the combined cycle, a water purge, named blowdown is necessary to maintain the water quality and is represented by the stream number “8”. Also, as large volumes of water are evaporated and send to the atmosphere, constant softened water feed, make-up, is necessary to maintain the operations basin water level.

Cooling tower blowdown and water resin regeneration from demineralization system are combined and treated in the biological wastewater treatment unit. Using biofilters and chemical additives, chemicals compounds are degraded allowing water to meet local regulations for the final disposal into the river, represented by the stream number “9”.

The current water system was named the 'base case.' Other water management options were created using literature data, internal TotalEnergies projects, and specialist consultation. The alternatives first involve recycling wastewater partially and totally. Partial recovery was chosen to be achieved using reverse osmosis because it is a stablished technology and there was a previous internal project applied to this site. Full recovery under Zero Liquid Discharge most industrial stablished route is to use the RO concentrate to feed an evaporator to remove water followed by a crystallizer to recover the remaining water content. Other routes are exposed in the section 2.1.4.3.

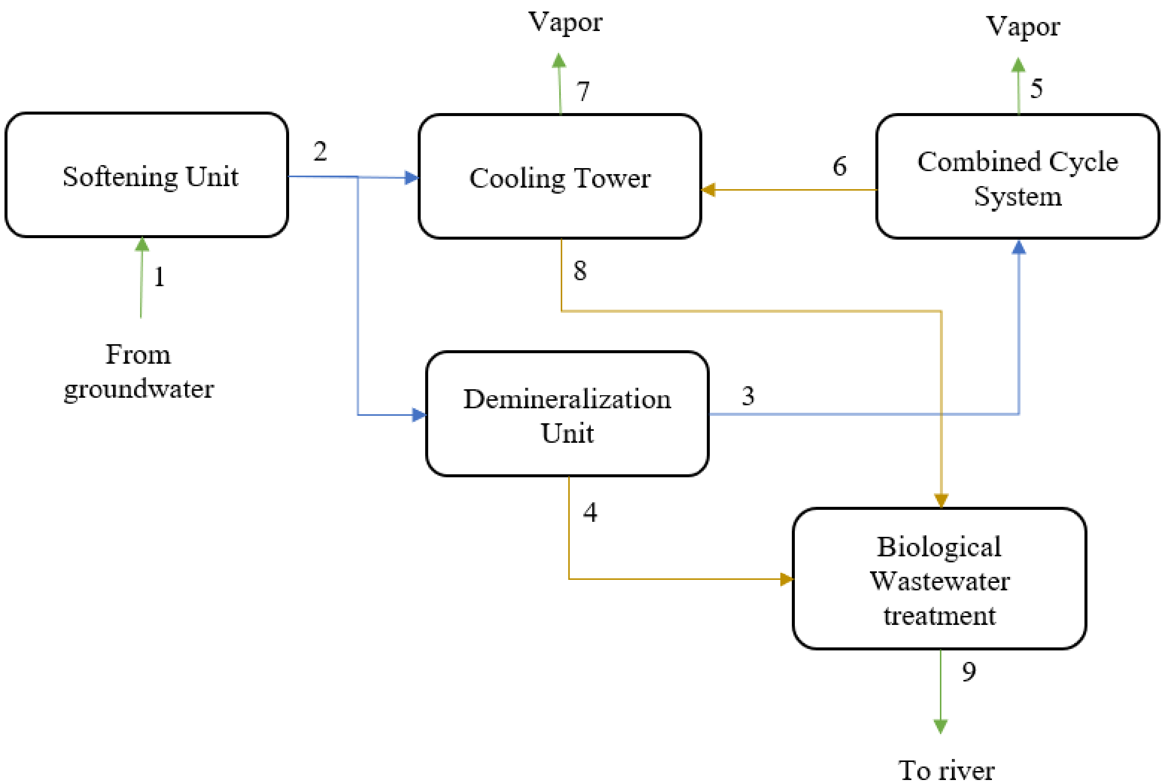


Figure 2.1 Simplified water flowsheet for TotalEnergies power plant.

For a broad perspective, both water source and discharge were considered. The required pre- and post-treatment differs, and consequently, have distinct impacts. Groundwater use requires softening, as presented in the site reality, while if ocean water source is used, desalination is necessary to meet process water quality standards. On the other side, river disposals are subject to stricter regulations in terms of Total Dissolved Solids compared to discharges into ocean bodies, therefore, more treatment is required for wastewater into freshwater bodies disposal.

Even though the case study unit is in France, this study aims to understand how other water-scarce scenarios can change trade-offs. To evaluate regional variability, the unit was virtually relocated to other countries to capture extremes in terms of water use impacts.

Table 2 Streams chemical composition represented in Figure 2.1.

Parameter	units	1	2	3	4	5	6	7	8	9
Flow	m3/h	261	261	9	0	6	3	210	42	45
Conductivity	us/cm	685	358	0.1	n. d.	0*	n. d.	0*	2289	n. d.
Total disolved solids	mg/l	469	n. d.	0*	n. d.	0*	n. d.	0*	2442	n. d.
Total alkalinity	mgCaCO3/L	292	58	0*	n. d.	0*	n. d.	0*	n. d.	n. d.
Carbonate alkalinity	mgCaCO3/L	2	31	0*	n. d.	0*	n. d.	0*	448	n. d.
Total hardness	mgCaCO3/L	437	163	0*	n. d.	0*	n. d.	0*	n. d.	n. d.
Suspention metter	mg/L	2	n. d.	0*	n. d.	0*	n. d.	0*	n. d.	2
Turbidity	NTU	2	3	0*	n. d.	0*	n. d.	0*	n. d.	n. d.
Chemical oxygen demand	mg/l	20	n. d.	0*	n. d.	0*	n. d.	0*	n. d.	8
Biological oxygen demand	mg/l	4	n. d.	0*	n. d.	0*	n. d.	0*	n. d.	4
Nitrate	mg/l	20	20	0*	n. d.	0*	n. d.	0*	n. d.	9
Ammonia	mg/l	0	n. d.	0*	n. d.	0*	≠ 0	0*	n. d.	n. d.
Ortho-phosphate	mg/l	0	n. d.	0*	n. d.	0*	≠ 0	0*	n. d.	8
Sulfate	mg/l	59	87	0*	14483	0*	n. d.	0*	954	445
Calcium	mg/l	111	25	0*	n. d.	0*	n. d.	0*	330	n. d.
Chloride	mg/l	24	24	0*	n. d.	0*	n. d.	0*	324	112
Magnesium	mg/l	32	24	0*	n. d.	0*	n. d.	0*	186	n. d.
Silicon	mg/l	15	10	0*	n. d.	0*	n. d.	0*	n. d.	n. d.
Sodium	mg/l	7	13	0*	3813	0*	≠ 0	0*	152	n. d.

2.1.2 Function and functional unit

The water treatment system serves the function of guaranteeing water flows necessary to produce energy. Considering that water volumes may change due to recycling practices; a production base unit was chosen. The main functional unit is *water management for 1 MWh of electricity production*. For this, only impacts associated with water management were considered.

As the energy required in the water treatment unit comes from the studied power plant, a second function was created, which is *1 MWh of electricity production*. The system burdens include infrastructure, energy consumption, and natural gas use for process units other than those solely for water management. This is also useful for comparing the relative contribution of the water management into the entire energy production.

2.1.3 Product system

To address the objectives of this case study, two product systems were created to represent each one of the two functional units.

The product system for all scenarios is represented in Figure 2.2. Specific product system for each scenario is also available in the following sections and in the annex. Although all elementary processes are depicted, the frontier limits differ for each scenario and functional unit. The dashed blue line represents the base case limits, the dashed orange line represents the partial recovery, and the dashed pink lines represent the zero liquid discharge scenario. The blue, dark-yellow, orange, pink, light-yellow, and red continuous line arrows represent internal water flows from various providers. The green continuous line arrow is used for elementary water flows, and gray continuous line arrows represent upstream processes. The gray dashed line arrows and rectangles represent additional processes considered for electricity production. The purple continuous line arrow represents the cooling function delivered by the cooling tower, but it also signifies the delivered function if only the water systems part of the cooling tower is considered.

For the first function unit, *water management for 1 MWh of electricity production*, elementary flows are represented by continuous black lines on a white background. The base case scenario consists of process water production (softening process for freshwater and desalination for ocean water use), demineralize unit, water management for the cooling tower, water management for the combined cycle, biological wastewater treatment, and its respective upstream processes. Chemicals production, sludge final disposal, infrastructure, and energy production are considered as upstream processes. In the partial recovery scenario, the base case is augmented by adding the reverse osmosis unit. It is important to note that this implies changes in requirements for other elementary units. Pretreatment provides less water if the system is partially fed with recovered wastewater. Similarly, bio-wastewater treatment treats a smaller water volume. Additionally, the chemicals required for bio-treatment change according to the water quality to be treated. The Zero Liquid

Discharge scenario has additional evaporator and crystallizer units while excluding bio-wastewater treatment.

Water management for the cooling tower and for the combined cycle only considers chemicals and water consumption. Electricity requirements and infrastructure construction were challenging to dissociate from the main equipment function. For the cooling tower, the primary function is cooling, and for the combined cycle, it is to produce 1 MWh of electricity. However, water consumption was considered part of water management even if it was not directly caused by water treatment. This choice was made due to the interest of this work in assessing the site's water footprint.

For the second functional unit represented in Figure 2.2, *1 MWh of electricity production*, the system is similar to the previous one. However, for the cooling tower and combined cycle, infrastructure, energy consumption, and natural gas use are in this case also counted.

All the required energy for each elementary unit system uses electricity from the process tree whose function is '1 MWh of electricity production.' This means that a feedback effect also contributes to variations in environmental impacts.

Water quality changes were not represented in Figure 2.2. Only a generic pretreatment named 'process water production' was used. This is better explained in subsequent sections. It should be noted that if groundwater is withdrawn, softening is required. On the other hand, if the ocean is used as feed water, desalination is necessary. The pollutants concentration for river bodies discharges is conditioned by local regulation, restricting partial recovery to 50%. However, in ocean discharges higher pollutant concentrations are allowed, therefore, higher recovery is possible.

Wastewater management is represented as an input flow because it signifies the necessity for treatment, not the water flows themselves, as in a process flow diagram. A similar approach was conducted for recovery systems, reverse osmosis, evaporator, and crystallizers, which were also represented as input service necessities. Additionally, the recovery and post-treatment services were modeled in separate blocks directly linked with the consumer processes, the cooling tower and demineralization unit. Therefore, they do not aim to represent process relationships in a realistic perspective, only for LCA purposes.

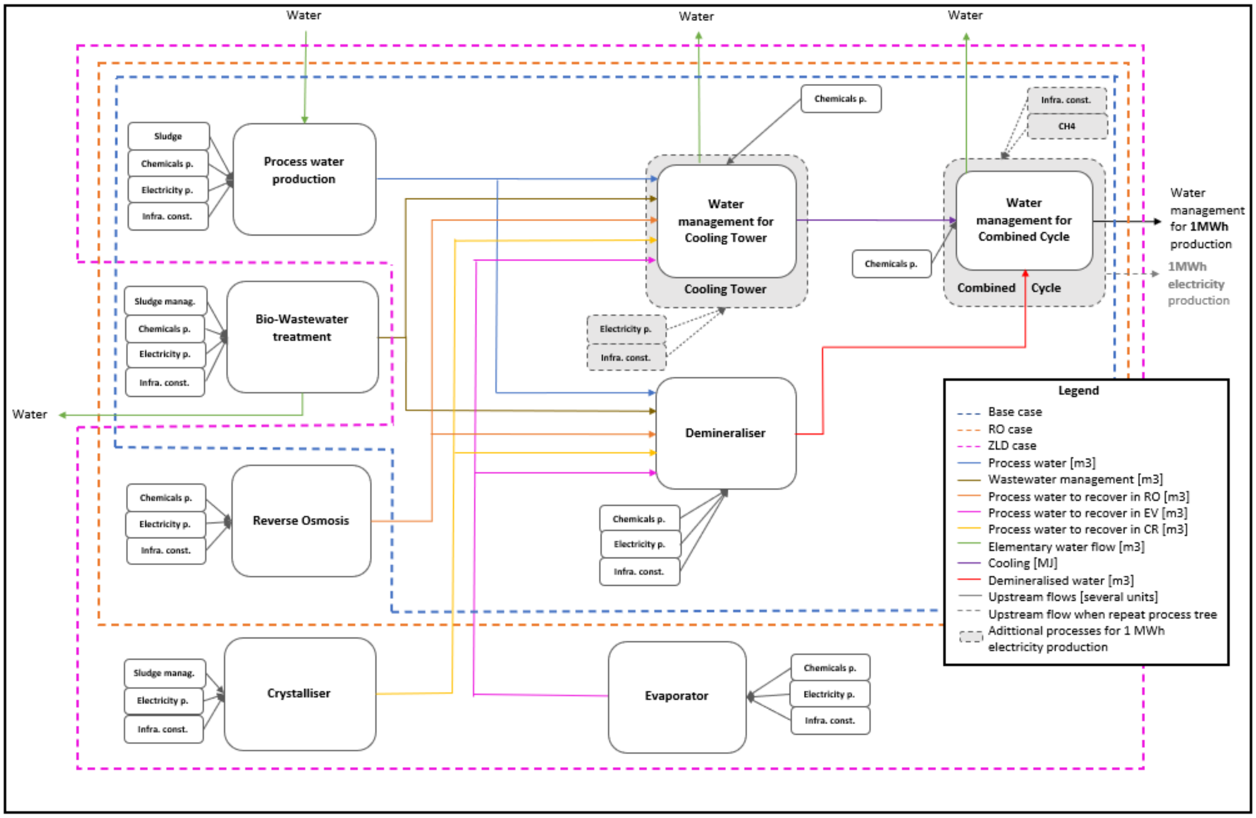


Figure 2.2 Product system for two different functional units: Water management for the production of 1 MWh electricity and 1 MWh electricity production, respectively.

2.1.4 Scenarios and system boundaries

The following water management scenarios were assessed: Base case for no water recycling, partial recovery and zero liquid discharge for total recycling. The recycling rates can be combined with water source and release options (freshwater or ocean). Figure 2.3 represents schematically the studied scenarios.

The base case represents the actual water treatment practice used in the power plant, where no water is recovered. Freshwater from groundwater sources is used, and wastewater is treated to be released into the local freshwater body. Partial recovery is achieved through reverse osmosis, and for the freshwater receiving body, only 50% recovery is considered due to pollutants final concentration in the release stream. Total recovery recycles 99% of the wastewater. The released salts contain around 50% water. Total recovery was studied in two different configurations, named Option 1 and Option 2. The options differ in exploring membrane recovery before distillation, ranging from 50% to 97%. In all scenarios, recovered water returns into the system as process water. Therefore, the higher the recovery rate, the lower the amount of withdrawal water necessary.

Water sources can be either freshwater or ocean origin. Freshwater requires softening pretreatment, whereas ocean water use needs desalination. Release water into freshwater bodies such as rivers has stricter regulations for discharged chemical species, therefore limiting reverse osmosis (RO) recovery. The power plant has already investigated RO unit to recover 50% of the wastewater, so this previous project served as partial recovery scenario. In this case, the pollutants concentration in release water is twice higher than the present situation, however maintaining the same total mass. Discharges into ocean water allow up to 70,000 ppm salts concentration. Thus, partial recovery can be increased to higher rates if nanofiltration and high-recovery membranes are added.

The use phase is similar for all scenarios, consisting of the demineralization system, cooling tower, and combined cycle. Vapor comes mainly from the cooling tower unit; however, a small amount is also generated in the combined cycle. As all the required energy is provided by the system itself, higher energy-intensive scenarios cause more pronounced feedback effect. To produce the surplus energy, additional water management system is required; thus, a looping is presently adding consistently smaller sums of required flows. All the impacts associated with the surplus energy were classified as energy-related impacts. Additionally, as the recovery water has higher water quality, it affects the demineralization system.

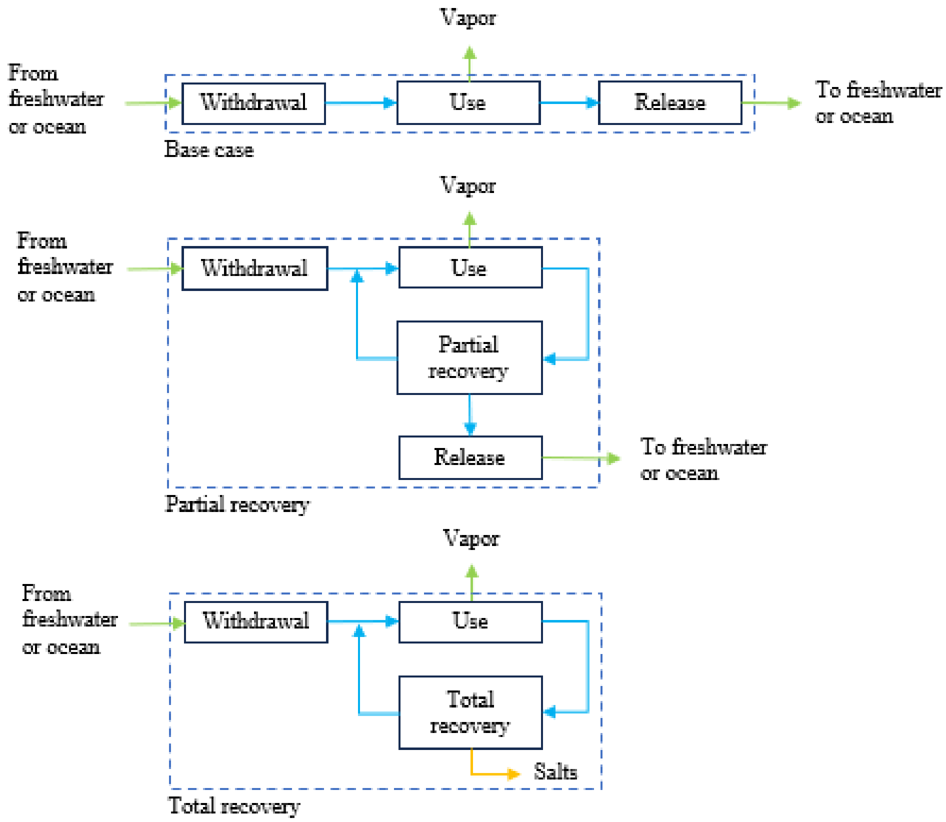


Figure 2.3 The three water management scenarios that have been defined for the water management for the production of 1MWh of electricity

Changing the power plant unit's location does not alter the site technologies or the required upstream providers. Consequently, only on-site water value changes will be captured.

An attributive analysis was considered, meaning that migrating from the base case to other scenarios' impacts were not taken into account. It was assumed that all scenarios were already constructed in the final format.

Table 1 provides an overview of all studied scenarios and its particularities. More detailed scenarios regarding water flows are presented in the following subsections. Evaporated water flows are represented in m^3. This is equivalent as liquid water at ambient temperature and not real vapor state volume. TW: Tap water production from desalination; ST: Softening; CT: Cooling Tower; DM: Demineraliser; RO: Reverse Osmosis; NF: Nanofiltration; CC: Combined Cycle; WW: Wastewater biological treatment; EV: evaporator; CR: Crystallizer.

Table 3 Unit operations presence for each water management scenario.

Process unit	Scenarios										
	Freshwater withdrawal and release				Ocean withdrawal, freshwater release				Ocean withdrawal and release		Freshwater withdrawal and ocean release
	Case base	Partial rec.	ZLD, option 1	ZLD, option 2	Case base	Partial rec.	ZLD, option 1	ZLD, option 2	Partial rec.	Base case	Partial rec.
TW	-	-	-	-	x	x	x	x	x	-	-
ST	x	x	x	x	-	-	-	-	-	x	x
CT	x	x	x	x	x	x	x	x	x	x	x
DM	x	x	x	x	x	x	x	x	x	x	x
RO*	-	50.0%	50.0%	97.6%	-	50.0%	50.0%	97.6%	96.5%	50.0%	96.5%
NF	-	-	-	x	-	-	-	x	x	-	x
CC	x	x	x	x	x	x	x	x	x	x	x
WW*	x	x	-	-	x	x	-	-	x	x	x
EV*	-	-	98.1%	61.6%	-	-	98.1%	61.6%	-	-	-
CR	-	-	x	x	-	-	x	x	-	-	-

* Processes have some differences between scenarios, such as recovery, energy consumption and chemical additives.

2.1.4.1 Base Case

Figure 2.4 show water flows when freshwater is used and released for the base case. 0.7917 m^3 of water is withdrawn and treated in the softening unit. 4.28x10^{-4} m^3 is discharged in the sludge generation and 0.7912 m^3 of softened water is produced. From this, 0.7703 m^3 feeds cooling tower system and 0.0209 m^3, the demineralization unit. The Cooling tower also receives 0.0059 m^3 wastewater from combined cycle through a virtual process named “CC valorized water for CT”. Cooling system evaporates 0.5935 m^3 of water and generates 0.1828 m^3 of blowdown wastewater. The demineralization unit produces 0.0195 m^3 demineralized water to be sent to the Combined Cycle while 0.0014 m^3 of wastewater is sent to bio-wastewater treatment. The Combined Cycle consumes demineralized water, generates 0.0136 m^3 vapor and its wastewater have enough quality to be used in the cooling tower. Bio-wastewater treatment receives 0.018 m^3 of wastewater. Biotreatment consumes 0.0012 m^3 water due to natural evaporation and 6.75x10^{-6} m^3 due to sludge generation. Thus, 0.1829 m^3 of water is released back into the water basin. Water flows for a process perspective are available in Appendix E.

Approximately 0.79 m^3 of water is withdrawn for each 1 MWh of electricity produced. Within those, approximately 0.61 m^3 is evaporated: 0.5935 m^3 from the cooling tower, 0.0136 m^3 from the combined cycle system, and 0.0012 m^3 from wastewater treatment. Then, 0.1829 m^3 will be returned to the water body. Thus, around 0.61 m^3 of water is consumed. The biggest water consumer is the cooling tower unit, followed by the combined cycle. However, some water is also consumed in the softening and in the bio-wastewater treatment.

The flows described in Figure 2.4 are specific for freshwater use and bio-wastewater treatment. Some powerplants use freshwater and discharge into saline water without recovery. This scenario is explored as the base case – freshwater withdrawal, ocean release. For scenarios with seawater use, the softening unit is replaced by a desalination system.

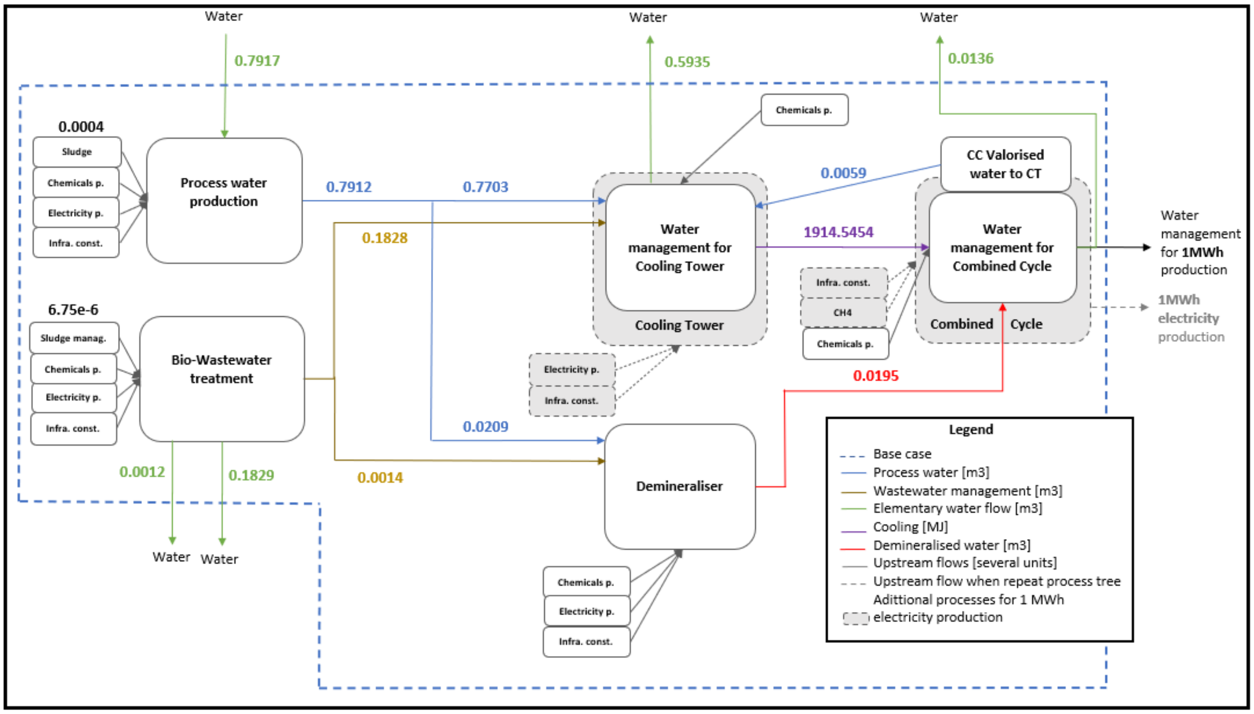


Figure 2.4 Product system with main flows values for base case scenario using freshwater source.

2.1.4.2 Partial Recovery

Partial recovery is present in four distinct scenarios. Process configurations for the same recovery rates have differences only in terms of pre-treatment technology. Softening for freshwater use and desalination for seawater use, as a consequence of elementary water flow for the pre-treatment unit, may change. As all other flow values remain the same, only freshwater use is represented. Recovery rates of 50% and 96.5% are represented in Figure 2.5 and Figure 2.6 respectively.

A higher recovery is possible when releasing in saline water. Legislation allows up to 70,000 ppm dissolved salts. This concentration is achieved when RO recovers 96.5% of the wastewater. This is only possible if an additional nanofiltration stage is applied upfront and high-pressure RO downstream. It's important to notice that this is only possible if low TDS wastewater is treated, characterizing brackish water.

When partial recovery is applied, water still needs to be treated in bio-wastewater treatment to remove organic compounds. In this case, bio-treatment was considered capable of treating concentrated water, only requiring chemical adjustments, which may not reflect the reality since microbiota needs special conditions to be capable of digesting organic compounds.

The water use phase remains similar to the one in the base-case scenario. The feedback effect is only captured when modeling is run in the software. The difference is in the demineralization unit. It won't receive water from the pre-treatment system. It is fed directly from recovery water due to its higher water quality. Thus, less resin recovery is necessary, generating less wastewater to be sent to bio-treatment.

Due to the increase in water quality when it comes from the RO system compared to pre-treatment technologies, it is prioritized to use recycling water in the demineralization system instead of equally distributing the recycled flows.

Figure 2.5 represents water flows for a partial recovery of 50%. Only freshwater is used and released. 0.6990 m^3 of water is withdrawn by the softening system. 3.7810^{-4} m^3 is discharged as part of the generated sludge. 0.6986 m^3 of softened water is generated and sent to the cooling tower. The cooling tower also receives 0.0059 m^3 from the combined cycle using the virtual process named 'CC valorizes water to CT'. 0.5935 m^3 is evaporated in the cooling system, and blowdown water needs to be treated in the wastewater system and reverse osmosis. The demineralization unit receives only recycled water: 0.0198 m^3 recycled water, being 0.0197 m^3 from CT blowdown through a virtual process named 'RO recovered water from CT', is used to produce 0.0195 m^3 of demineralized water and $2.48\text{x}10^{-4}$ m^3 as wastewater, being $1.24\text{x}10^{-4}$ m^3 recovered in the reverse osmose unit. The combined cycle unit consumes demineralized water and produce 0.0136 m^3 vapor water. From the bio-wastewater treatment, 0.0909 m^3 of water is released back after $6.92\text{x}10^{-6}$ m^3 and $6.4\text{x}10^{-4}$ m^3 water are consumed, respectively, in the sludge and vapor generation in the bio-wastewater treatment.

Figure 2.6 represents water flows for a partial recovery of 96.5%. In this configuration 0.6139 m^3 of water is withdrawn by the softening system. 0.003 m^3 is discharged as part of the generated sludge. 0.6135 m^3 of softened water is generated and sent to the cooling tower. Water use phase flows are similar to those with 50% and the differences are in RO and wastewater processes. 0.0064 m^3 of water is released in the ocean body.

Water flows in process perspective is shown in annex E.

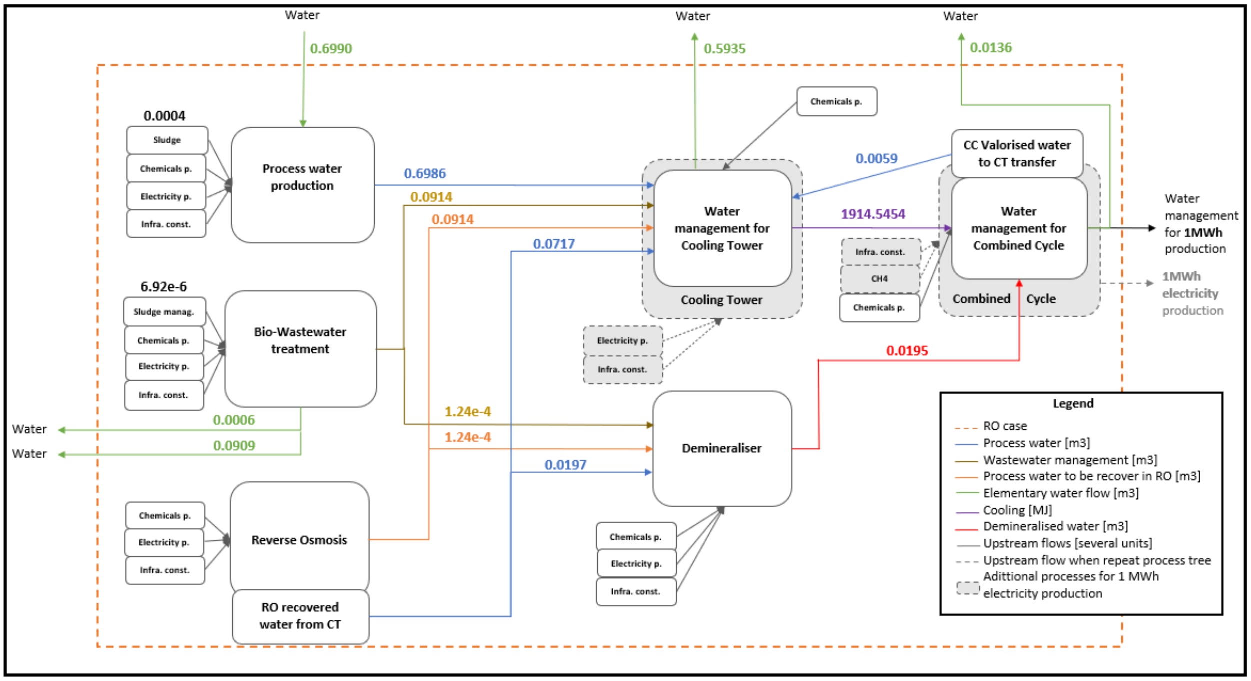


Figure 2.5 Product system with main water flows for 50% recovery scenario

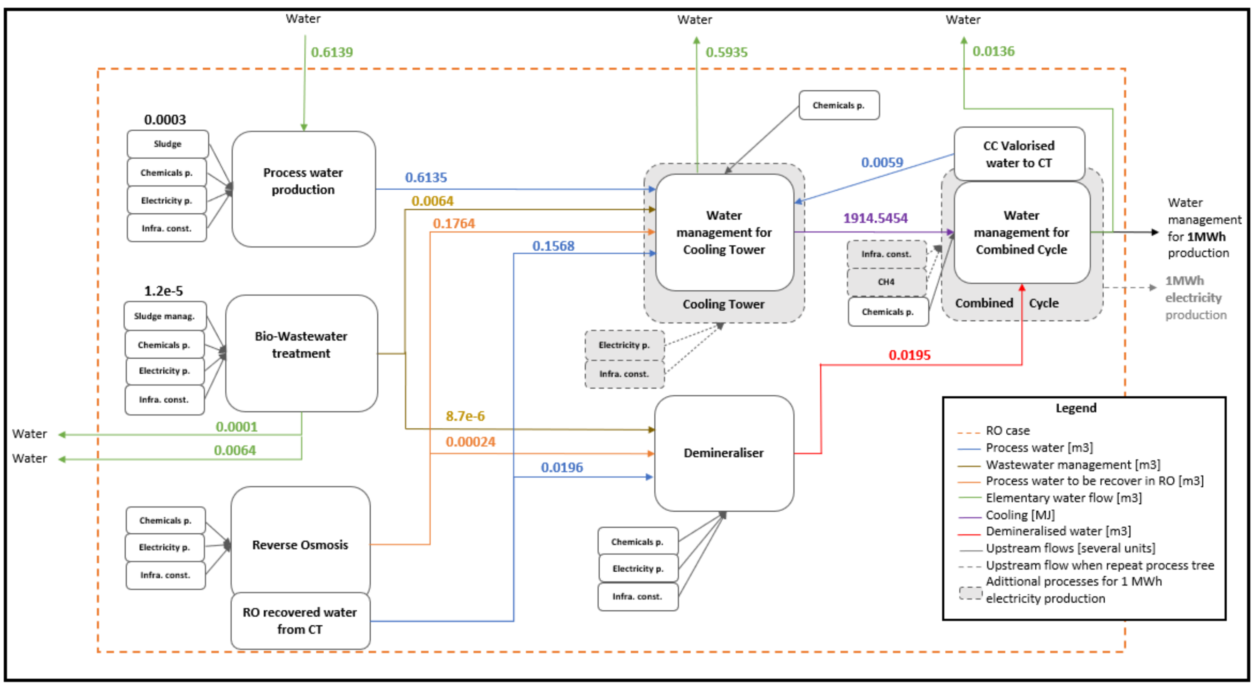


Figure 2.6 Product system with main water flows for 96.5% recovery scenario

2.1.4.3 Zero Liquid Discharge

Zero liquid discharge is not confined to a singular technology, but rather the integration of technologies and process units to avoid liquid sewage to be discharged. Various are the technologies to be used and define the best route to achieve no liquid discharge. The most established technology is evaporator and crystallizer. But due to its high energy requirements, new routes have been developed. Elevates recovery in reverse osmosis' system helps to energy savings. Emergent technologies, such as membrane distillation promises further energy savings if low-waste heat can be used.

Five different options for zero liquid discharge were evaluated and are presented in Figure 2.7. The first option, the most established route, involves applying 50% reverse osmosis, followed by 98.12% recovery in an evaporator and crystallizer. The second option includes a two-stage reverse osmosis process, with high-pressure reverse osmosis in the second stage allowing for 97.55% recovery. The concentrate is then 61.6% recovered in the evaporator and subsequently in a crystallizer. The third option involves replacing the evaporator with membrane distillation to allow for low heat waste utilization. The fourth option substitutes the second stage high-pressure membrane for membrane distillation to enable greater heat integration. Finally, the fifth option involves substituting both reverse osmosis stages with membrane distillation.

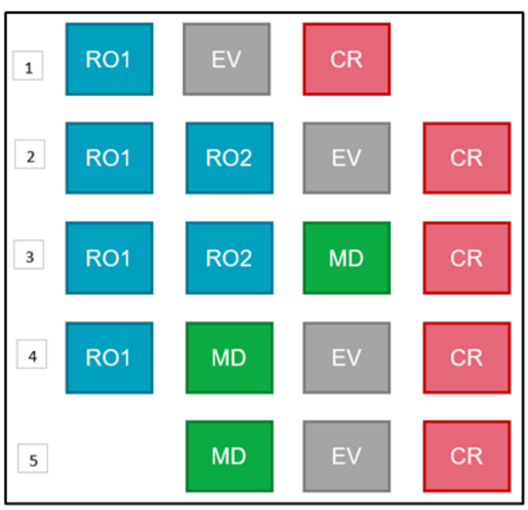


Figure 2.7 technologies routes for ZLD water management under study

Low waste heat is available in the unit, generated through saturated low-pressure vapor in the combined cycle. Additionally, the combined cycle demands high cooling capacity, leading to the substantial evaporation of water into the atmosphere caused by the cooling tower. If this low-grade heat can be addressed into water recovery technologies, it reduces the need for the cooling, consequently decreasing water consumption.

The feasibility of heat integration is assessed through pinch analysis, which involves defining the minimal temperature difference between the hot and cold streams to enable heat exchange. In a heat load and temperature diagram, curves representing the requirements for hot and cold streams are plotted. By always maintaining the minimal temperature difference, the point where the curves reach their closest proximity is termed the 'pinch point.' The analysis is then divided into above and below the pinch point. Following specific rules, heat can be transferred between different streams to minimize the need for cold and heat utilities.

The heat pump is a device that facilitates the utilization of waste heat when its temperature is below the required pinch. It operates by employing compression and expansion to extract heat from a lower-temperature stream and release it into another stream at a higher temperature. However, its energy requirements can be significant, depending on the specific demands and available heat streams.

Pinch analysis was performed using the ROSMOSE software[34] for the ZLD option 1 to assess the feasibility of heat integration. The analysis revealed that all energy requirements remain unchanged. This is due to the selected evaporator system being a mechanical vapor compressor. This type of evaporator solely relies on electrical energy. Its compressor system works by raising the vapor temperature to internally integrate its heat, effectively serving as a heat pump. The decision to opt for this electricity-intensive evaporator is since the required energy is sourced from the power plant under study. Consequently, from an industrial perspective, it is offset.

As for ZLD option 2 utilize the same thermos-distillation technology, there is no need for energy integration study. Its energy requirements were calculated bases on the equipment's energy consumptions only.

To calculate energy integrations gains for ZLD option 3, 4 and 5, the same pinch was used. However, the energy requirements to the heat pump and the energy savins from lower cooling demand were conducted manually in excel sheet. Used equations and considerations are disponible in Appendix B whereas water flows for all ZLD options.

Membrane distillation, used in ZLD options 3, 4 and 5, is an emerging technology, and as such, there is a wide range of reported heating and cooling requirements in the literature. The specific requirements chosen for this study were obtained from an internal TotalEnergies study and cannot be disclosed. The heat pump was necessary to utilize a heat stream from the combined cycle to achieve the required temperatures in the distillation system, thereby reducing the cooling needs for the combined cycle release heat. However, it's important to note that membrane distillation also requires cooling systems, and these must be taken into account.

To calculate energy integration gains for ZLD option 3, 4 and 5, the same pinch was used. However, the energy requirements to the heat pump and the energy savin from lower cooling demand were conducted manually in excel spreadsheets. Used equations and considerations are available in Appendix B.

Table 2 presents energy requirements results for the 5 different configurations options. It can be concluded that applying membrane distillation to utilize low-grade waste heat is not viable due to the high energy consumption of the heat pump systems. In Case 1, the energy consumption is 3.37 MW for the recovery system and cooling requirements. Case 2 requires 3.09 MW of electricity while maintaining the same cooling requirements. Case 3 yields similar results to Case 2, but with additional cooling needs and energy requirements for heat pumps. Case 4 consumes 4.19 MW, and Case 5 requires 5.47 MW.

Aiming to select established and energy optimized technology, options 1 and 2 were selected.

Table 4 Energy requirements for different ZLD routes

ZLD Options	1	2	3	4	5
CC heat used	0	0	70.9 kW	2300 kW	4600 kW
MD ad. cooling	0	0	79 kW	2570 kW	5130 kW
Delta	0	0	-8.11 kW	-266 kW	-536 kW
Energy consumption	3.37 MW	3.09 MW	3.11 MW	4.19 MW	5.47 MW

2.1.4.3.1 Option 1

The ZLD option 1 has the advantage of treat a large range of water salinities and being an established technology. Figure 2.8 presents the main flow values for zero liquid discharge option 1 scenario. 0.6076 m^3 of elementary water feeds the process water production, softening. 0.003 m^3 of water is discharged with softening sludge production. 0.6072 m^3 of process water is necessary in the cooling tower water management. 0.0914 m^3 needs to be regenerated in the reverse osmose system, while 0.0897 m^3 in the evaporator and 0.0016 m^3 in the crystallizer. Also 0.0059 m^3 of water from CC origin is used in the cooling system to generate 1914.5454 MJ of cooling to be used in the combined cycle to be able to produce 1 MWh of electricity. 0.5935 m^3 and 0.0136 m^3 of water is evaporated to the atmosphere from cooling tower and combined cycle respectively. Demineralizer consumes only recycled water in higher volume than it requires the recycling system, so to represent this difference, 0.0195 m^3 recycled water from CT free of associated impact is allocated into this unit. Due demineralization wastewater generation, recycling system is necessary, being divided as 0.0001 m^3, 8.05x10^{-5} m^3 and 1.44x10^{-6} m^3 of water to be recycled in the reverse osmosis, evaporator, and crystallizer respectively. Water management for the combined cycle requires 0.0195 m^3 of demineralized water. 0.0001 m^3 of water is discharged in the salts production from the crystallizer.

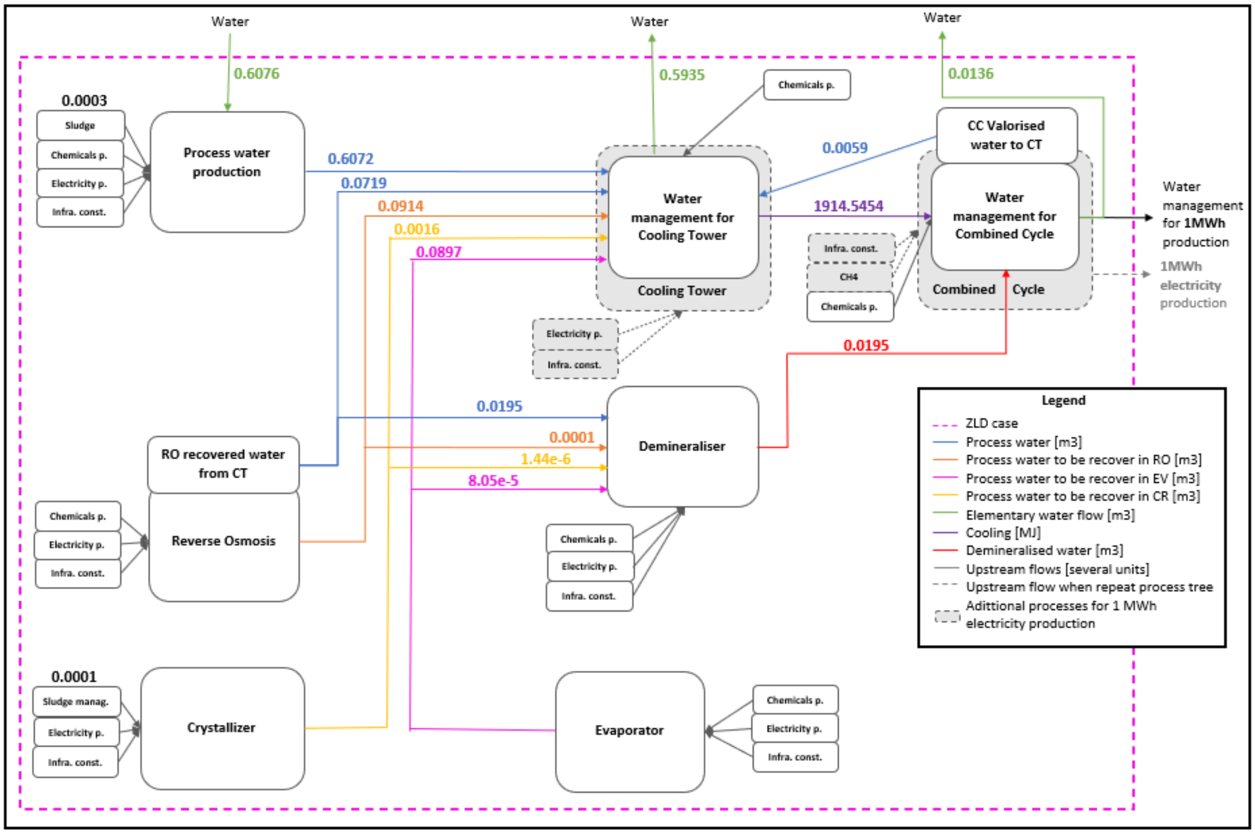


Figure 2.8 Product system with main water flows for zero liquid discharge, option 1 scenario

2.1.4.3.2 Option 2

Zero liquid discharge option 2 is only possible due to low salts concentration in the wastewater to be treated. It focuses on removing the maximum volume of water in the membrane reverse osmose before the use of thermo-separation to improve energy efficiency.

Figure 2.9 introduces the linkage flows between the main process units for the zero liquid discharge option 2 scenario. Water management for the cooling tower has the same output values for all scenarios, and water management for the combined cycle presents the same inputs and outputs across all scenarios. Additionally, the process water production maintains the same values as for ZLD option 1. The only variations occur in the recycling water-related flows of the evaporator and reverse osmosis. In this case, 0.1783 m^3 of water is needed to be recycled in the RO unit for the cooling tower water management, while only 0.0028 m^3 is required in the evaporator. The demineralizer also demands higher flows to be recycled in the RO unit and lower flows in the evaporator.

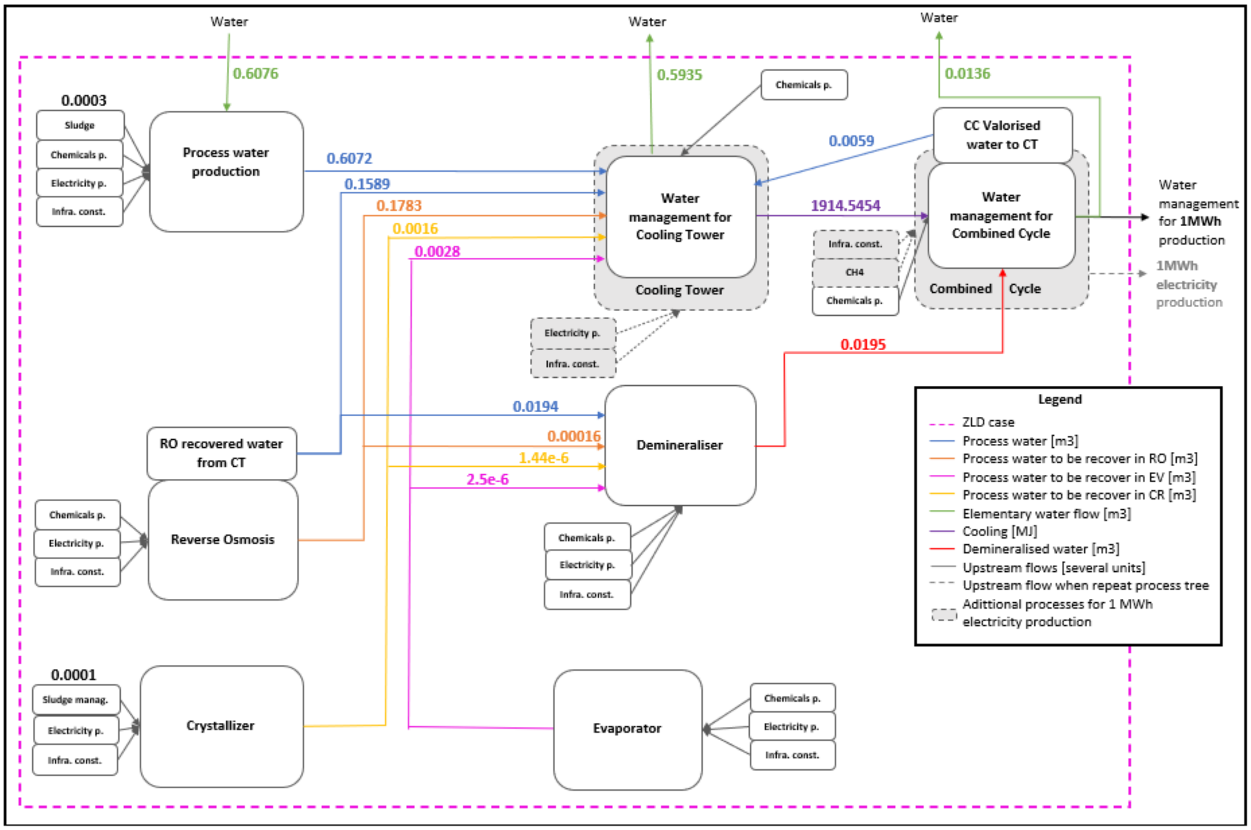


Figure 2.9 Product system with main water flows for zero liquid discharge, option 2 scenario.

2.1.5 Multifunctionality of internal processes

The recycling processes, such as reverse osmosis, evaporator, and crystallizer, can be comprehended as multifunctional processes. While providing wastewater treatment, clean water is simultaneously produced as the recycled water is fed back into the electricity production process. Consequently, recycling units serve as both pre- and post-treatment. However, since both recycling functions contribute to the water management burdens, no impact allocation was deemed necessary. For modeling simplicity, recycling process units were considered solely as wastewater treatment.

The consequence of the multifunctionality of the recycling process is a non-zero water balance because the respective pretreatment function is not explicitly accounted for. Therefore, for a correct water balance, flows from evaporator and crystalliser should be counted both as feed process water and wastewater. The process water from this process units have the same values as the wastewater flows and were not represented in the scenarios process flow to simplified lecture. Process water from reverse osmosis doesn't have the same values as the respective wastewater flows for demineralization and cooling tower units because its proportion were not maintained. As the recovered water exhibits better water quality compared to softened water, it is primarily directed towards the consumption of the demineralization unit. Consequently, the proportions of pre- and post-treatment functions are not the same for the Cooling Tower and Demineralization unit. The cooling tower necessitates a higher use of the wastewater function, while demineralization requires the pretreatment function, leading to an imbalance in water flows. To address this difference and better represent the process reality, the virtual process 'RO recovered water' was introduced. No impacts were attributed to this virtual process, and its purpose is solely to clarify water flows without affecting LCA results.

The combined cycle also exhibits multifunctionality as it produces energy, and its blowdown water serves as process water for use in the cooling tower. However, this water flow represents less than 1% of all intake water. For modeling simplification, the Combined Cycle unit was considered monofunctional, only producing electricity. To account for the difference in water flows resulting from this modeling choice, the generated process water was reallocated to the virtual process named 'CC water valorization for CT,' with no associated impacts.

2.1.6 End of life

End of life impacts or credits were addresses in the cut-off approach for up and foreground processes. This modeling address waste management impacts to the waste producer. Also, potential credits due to waste valorization are not given to the primary producer. As a consequence, the use of recycled material if free of impacts, being only recycling process impacts counted.

Most infrastructure modeling considers market share for raw materials and end-of-life impacts. However, some process in Ecoinvent database does not count for end-of-life impacts due either to lack of data or because it is assumed that all materials are recycled.

Even though end-of-life material may present lower data quality, it was already demonstrated that its contribution to water management practices is negligible [35]. Additionally, a study review state that the infrastructure contribution is significantly lower than operations and maintenance associated impacts [20].

2.2 Inventory

The primary data source is the 2021 TotalEnergies power plant site data. However, due to its limitations for the base case system, internal TotalEnergies projects were also consulted, particularly for partial recovery and zero liquid discharge scenarios. Additionally, literature was used to fill data gaps. The last data source level used is the Ecoinvent 3.8 database, which has a significant contribution for upstream process and elementary flows quantification.

Each process unit represented in Figure 2.2 was modeled as a separate block, and its technological and elementary flows were scaled down to a specific delivered function. Detailed considerations and equations for all elementary units are displayed in the Appendix A. To expose the procedure, softening unit scaling example is presented in the following subsections and also the water flows subdivision for demineralisation unit.

OpenLCA was the chosen software due to its open access. It is developed by GreenDelta. The used version is 1.10.3.

2.2.1 Softening

This process treats well freshwater to remove hardness. Figure 2.10 represents the process tree for softening process. Its function is to produce process water. Internally coagulation, flocculation, and clarification occur. Then, chemicals, infrastructure, energy, and final sludge disposal are requirements to this service as represented.

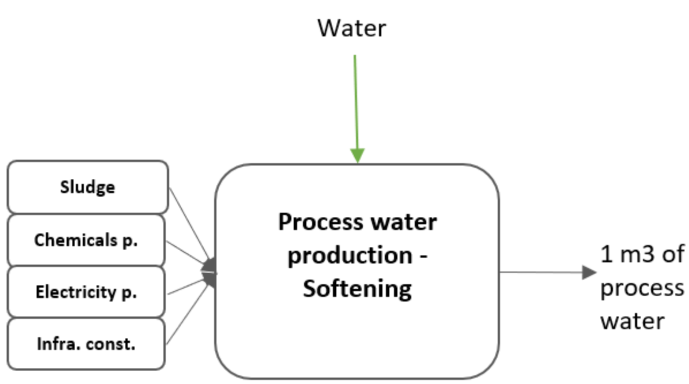


Figure 2.10 Softening elementary process tree.

Site data was used, and some assumptions were necessary. Table 3 presents data collected, sources and considerations. Scaling process is demonstrated in Table 4. Final input-out put elementary processes are evident in Table 5.

Providers in Table 5 represents process blocks and were either directly selected from Ecoinvent database or refers to a previously created elementary process. Lime production was already modeled in Ecoinvent; thus, no modifications were required. However, ‘drewfloc production’ is an example of created process because it was not available in the adopted database. Infrastructure and sludge management were modeled separately to better organize results and can be consulted in the Appendix A.

Table 5 Input data to softening unit.

Input parameters			
Name	Value	Description	Source
capacity	480	m^3/h	Site data / manufacturer
av_production	261	m^3/h	Site data
life_expectation	20	year	Assumption
Drewfloc_274	1	ton/year	Site data
Ferric sulfate_44%	108	ton/year	Site data
lime_hydrated	277	ton/year	Site data
In_water	1221195	m^3/year	Site data
water_sludge	50	% mass	Site data
total_sludge_production	1320	ton/year	Site data
Electricity_st_cons	44.8	kW	Site data

Table 6 Dependent parameters to Softening unit.

Dependent parameters			
Name	Formula	Value	unit
total_capacity	capacity*life_expectation*365*24	84096000	m^3
unit	1/total_capacity	1.189E-08	item
floculant_st_con	(Drewfloc_274/In_water)*E6	0.82	ppm
iron_sulfate_st_con	(Ferric sulfate_44%/In_water)*E6	89	ppm
cao_st_con	(lime_hydrated/In_water)*E6	227	ppm
water_sludge_m3	total_sludge_production*water_sludge	660	m^3
eff_st	(In_water-water_sludge_m3)/In_water	0.99946	dimentionles s
in_water_st	1/eff_st	1.000541	m^3
drewfloc_274_st	floculant_st_con/eff_st	0.825	g
ferric_sulfate_st	iron_sulfate_st_con/eff_st	89.248	g
lime_st	cao_st_con/eff_st	227.123	g
Electricity_st	(Electricity_st_cons/av_production)/10 00	1.72E-04	MWh

Table 7 Input and output flows description for Softening Unit.

Inputs				
Category	Flow	Amount	Unit	Provider
Chemicals prod.	Drewfloc 274	drewfloc_274_st	g	Drewfloc 274 production - created process - FR
	Ferric sulfate 44%	ferric_sulfate_st	gr	Ferric sulfate 44% production- created process - FR
	lime, hydrated, packed	lime_st	g	market for lime, hydrated, packed | lime, hydrated, packed | Cutoff, U - RER
Energy prod.	electricity, high voltage	Electricity_st	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	Decarbo	unit	Item(s)	Decarbo construction
Sludge manag.	sludge	1	Item(s)	Softened water production, internal unit, TotalEnergies - Sludge
Water	Water, well, FR	in_water_st	m^3	-
Output				
UF	water, softened	1	m^3	

2.2.2 Desalination

Desalination is used when salt water is fed into the system. This process is already modeled in Ecoinvent 3.8 by the name: 'seawater reverse osmosis module production, 8-inch spiral wound, enhanced | seawater reverse osmosis module | Cutoff, U'. However, to adapt the process into the study case, electricity requirements were provided by the power plant in study and water flows changed for the desired location.

2.2.3 Cooling Tower

The cooling tower is employed to cool water flows through fan-induced evaporation. Cold water flows from the cooling tower to the combined cycle. Once the heat is exchanged, water became approximately 10 degrees Celsius higher, flows back to the cooling tower basin.

Approximately its 77% of the inlet water volume is evaporated. Make-up water is necessary to maintain the operational cooling tower basin volume. Additionally, due to evaporation, the concentration of salts increases in the reservoir. To prevent salts from causing corrosion, a purge is necessary, referred to as blowdown. The ratio between make-up and blowdown flows is known as the Cycles of Concentration (COC). The present unit has an average COC of 4.2.

Some chemicals are necessary to maintain water quality. Biocide, anti-scaling agents, and sodium hypochlorite are consistently added to the water. Additionally, a small amount of ammonia is present due to the combined cycle blowdown flow entering the cooling tower.

2.2.4 Demineralization Unit

This unit process is essential for removing remaining salts from softened water. Ultra-pure water is required for combined cycle use. Anionic and cationic resins adsorb the present ions. After a specific running period, these resins become saturated and need to be regenerated. To do so, sodium hydroxide and sulfuric acid, along with backwash, are applied.

The regeneration frequency depends on the inflow water characteristics. The higher the dissolved solids, the more frequent the regeneration. Softened water has a conductivity of 358 μS, recovered water from reverse osmosis has 65 μS, and water from evaporation systems is considered to have a conductivity of 22 μS. Therefore, the demineralization system prioritizes the use of recovered water to reduce the regeneration frequency. When using reverse osmosis recovery water, the regeneration frequency diminishes by a factor of 5.5, and for zero liquid discharge, it diminishes by a factor of 8.3. It's important to note that even with ZLD, where the conductivity is low enough to be accepted by the combined cycle system, the demineralization system would still be necessary to ensure water quality.

As represented in Figure 2.11, the delivered function is 1 m^3 of demineralized water. This unit consumes chemicals, electricity, infrastructure, and water. All input and dependent parameters and process modeling are disponible in Appendix A. Fed water flow has different providers: Process water production (softening unit or desalination) or from recovery systems, reverse osmosis, evaporator, and crystallizers. Its produced wastewater also has options depending on the scenario. Bio-wastewater treatment only if the base case, additionally reverse osmosis if partial recovery and reverse osmosis, evaporator, and crystallizers if zero liquid discharge. Recovery system due to its nature, function as in and output water. However, in and out flows are not the same as already explain in the multifunctionality section.

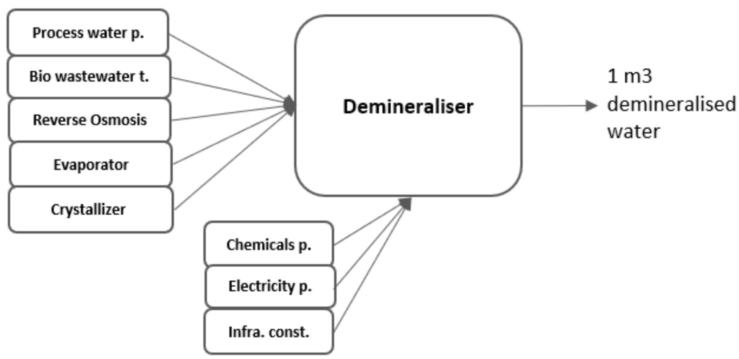
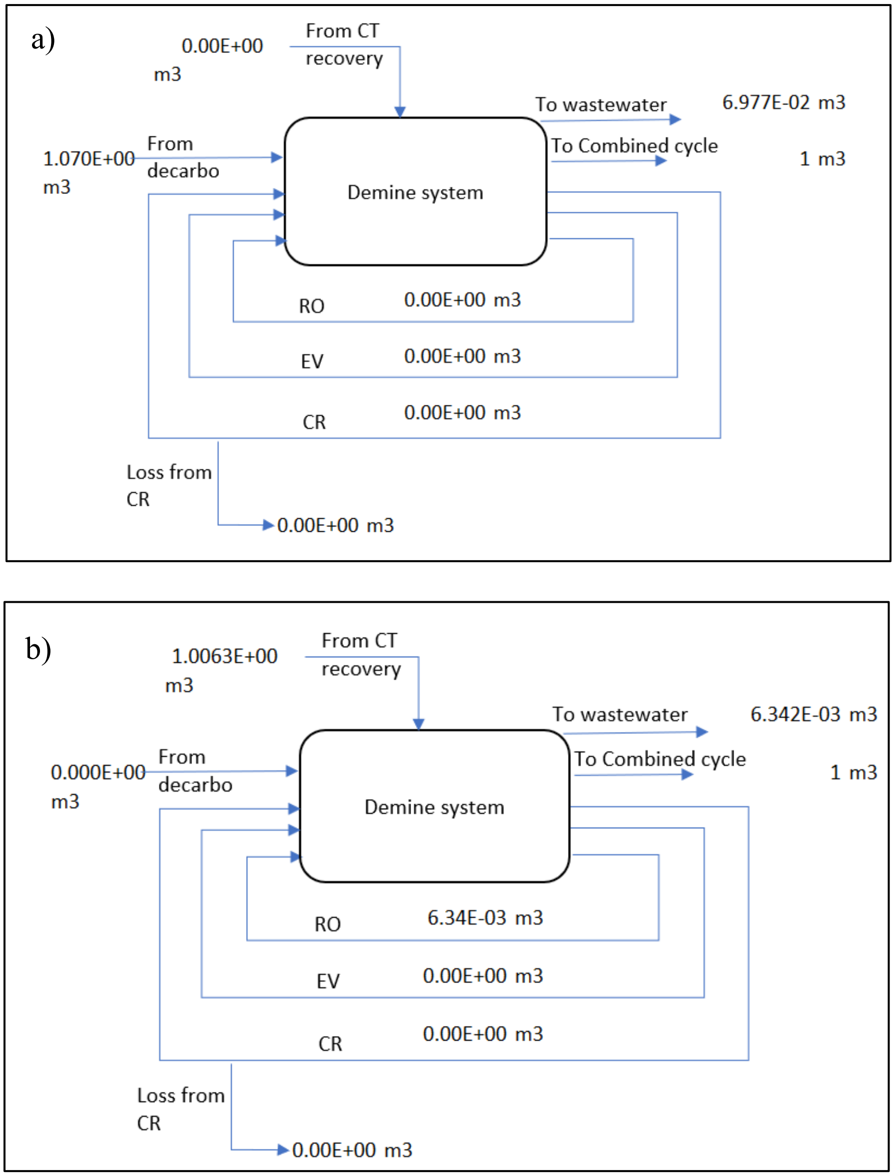


Figure 2.11 Demineralization unit process system.

In Figure 2.12 a), all in water flows come from softening system. Nothing is recycled. All wastewater is sent to wastewater treatment. In b), partial recovery occurs. Half of the wastewater generated is recovered in the reverse osmosis and the remaining is treated in the bio-wastewater unit. Feed water comes from recycling originated from cooling tower blowdown water, and it is represented as ‘recycling from CT’. No softening water is necessary. Recycling system provides the required water volume. C) represents ZLD configuration. All wastewater generated is sent to recovery system. Even though it is named total recovery, a small amount of water is a loss in the final crystals generated at the crystallizer unit. Similar to partial recovery, all required in water is provided by the recovery system from RO and from CT.


a)
0.00E+00
m3
From CT
recovery
To wastewater
6.977E-02 m3
1.070E+00
m3
From
decarbo
To Combined cycle
1 m3
Demine system
RO
0.00E+00 m3
EV
0.00E+00 m3
CR
0.00E+00 m3
Loss from
CR
0.00E+00 m3
b)
1.0063E+00
m3
From CT
recovery
To wastewater
6.342E-03 m3
0.000E+00
m3
From
decarbo
To Combined cycle
1 m3
Demine system
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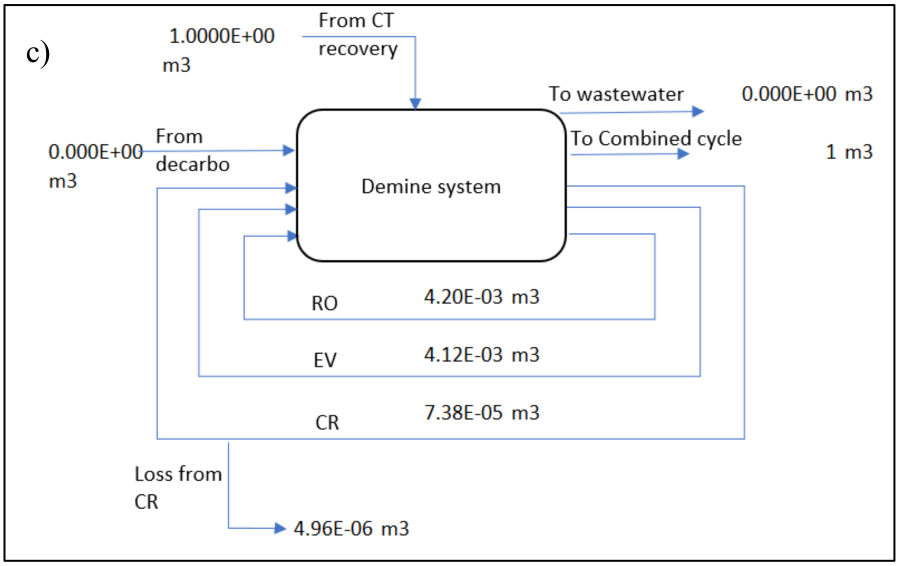

Figure 2.12 Water flows for demineralisation unit for different base scenarios using freshwater. a) base case; b) partial recovery; c) zero liquid discharge.

2.2.5 Combined Cycle

Electricity is generated in the combined cycle, named for the combination of the Rankine and Brayton cycles. Natural gas is burned and serves as a heat source in the Rankine cycle. The remaining heat is collected and used as a heat source in the Brayton cycle.

Similarly, to the cooling tower, this unit also generates vapor, and, therefore, needs constantly make-up water and blowdown flows. Make-up flows comes from the demineralization unit and blowdown flows goes directly to cooling tower basin.

Some chemicals are necessary to guarantee water quality. Carbohydrazide and different concentrations of ammonium are required. Carbohydrazide is used to avoid corrosion caused by oxygen, while ammonium is used as anti scaling due to its evaporation capacity, being able to follow water vapors cycles.

2.2.6 Biological Wastewater unit

The biological wastewater unit uses biofilters to decompose organic matter and remove solids. Bacterial growth is a result of organic decomposition, generating sludge. Acetic acid, phosphoric acid, and flocculants are necessary. The first two chemicals are used for biological growth, and the last one is used to separate the generated sludge more easily.

Biological sludge in this unit contains around 5% mass of water. Its final disposal is similar to the softening unit, manure.

The chemical usage is proportional to the organic concentration in the feed water. As such, chemical concentrations for the base case are lower than those in partial recovery. Partial recovery concentrates organic compounds to be treated in this unit.

2.2.7 Reverse Osmosis

Physically absent in the power plant, the reverse osmosis unit was modeled based on internal projects, TotalEnergies specialists, and research papers. The primary goal of this unit is to eliminate salts by subjecting the water to pressure higher than the osmotic pressure. The filtered water is reintroduced into the production process, serving as an inlet to the demineralization and cooling tower units. The concentrated stream undergoes further treatment, either biological treatment or the evaporator, depending on the scenario. To prevent membrane fouling, upstream nanofiltration and the use of chemicals such as sulfuric acid, sodium hydrogen sulfite, and commercial antiscalants are applied across all scenarios.

Recovery coefficients vary among different scenarios. For freshwater disposal and ZLD option 1, partial recovery is set at 50%, consuming 1.5 kWh/m^3 of treated water and involving only RO modules. Partial recovery for ocean discharge includes nanofiltration and additional high-pressure RO membrane, resulting in a 96.5% recovery and 3.1 kWh/m^3 of treated water. In ZLD option 2, the configuration is similar to ocean discharge, but with a 97.55% recovery and the same energy consumption.

In its modeling, the reverse osmosis unit is classified as multifunctional, serving as both pre- and post-treatment. However, for simplicity, all impacts were attributed as wastewater treatment. Its functional unit is the recovered water process.

2.2.8 Evaporator

The evaporator is a device used for producing distilled water while concentrating salts. The distilled water is reintroduced into the system, while the concentrate is directed to the crystallizer.

In this study, the choice was made to use a mechanical vapor compressor evaporator (MVC) due to its low total energy consumption (electric and thermal energy), even though its electric energy usage is high. This decision is justified by the fact that the required electricity is supplied by its own power plant.

The recovery rate for the evaporator is set at 98.12% for ZLD option 1 and 61.6% for ZLD option 2. This is due to the difficulty in achieving further concentrations beyond these rates, primarily because of the rising boiling point. The salt concentration limit is 250 ppm [26].

To maintain the process, certain chemicals are necessary. Antifoam, hydrochloric acid, and anti-scaling agents were considered based on TotalEnergies' internal project for another industrial unit.

2.2.9 Crystallizer

The crystallizer operates on a principle similar to that of the evaporator, but it can achieve higher temperatures, allowing for the recovery of the remaining water. However, its energy consumption is higher, amounting to 60 kWh/m^3 of treated water. Although it involves both thermal and electric energy, for the purposes of this study, only electric energy is considered.

In this process, the distilled water is reintroduced into the system. The sludge produced contains 25% mass of water and is directed to landfill for final disposal. No chemicals were considered for this process unit.

2.3 Evaluation

Potential impacts were evaluated using IMPACTWorld+. This impact assessment methodology consists of various impact categories for a broad range of indicators. Figure 2.13 shows all categories impacts included in the methodology.

Potential impacts can be presented in midpoint and endpoint level indicators. Mid point refers to problems while endpoint, to consequences. Midpoint units are variable and are dependent on the associated problems. Endpoint units are DALY for Human Health area and PDF.m2.year for Ecosystem Quality. Endpoint indicators are useful to aggregate various impact categories and then, measure the total impact for each area of impact. However, the pathway from mid to endpoint ads uncertainties.

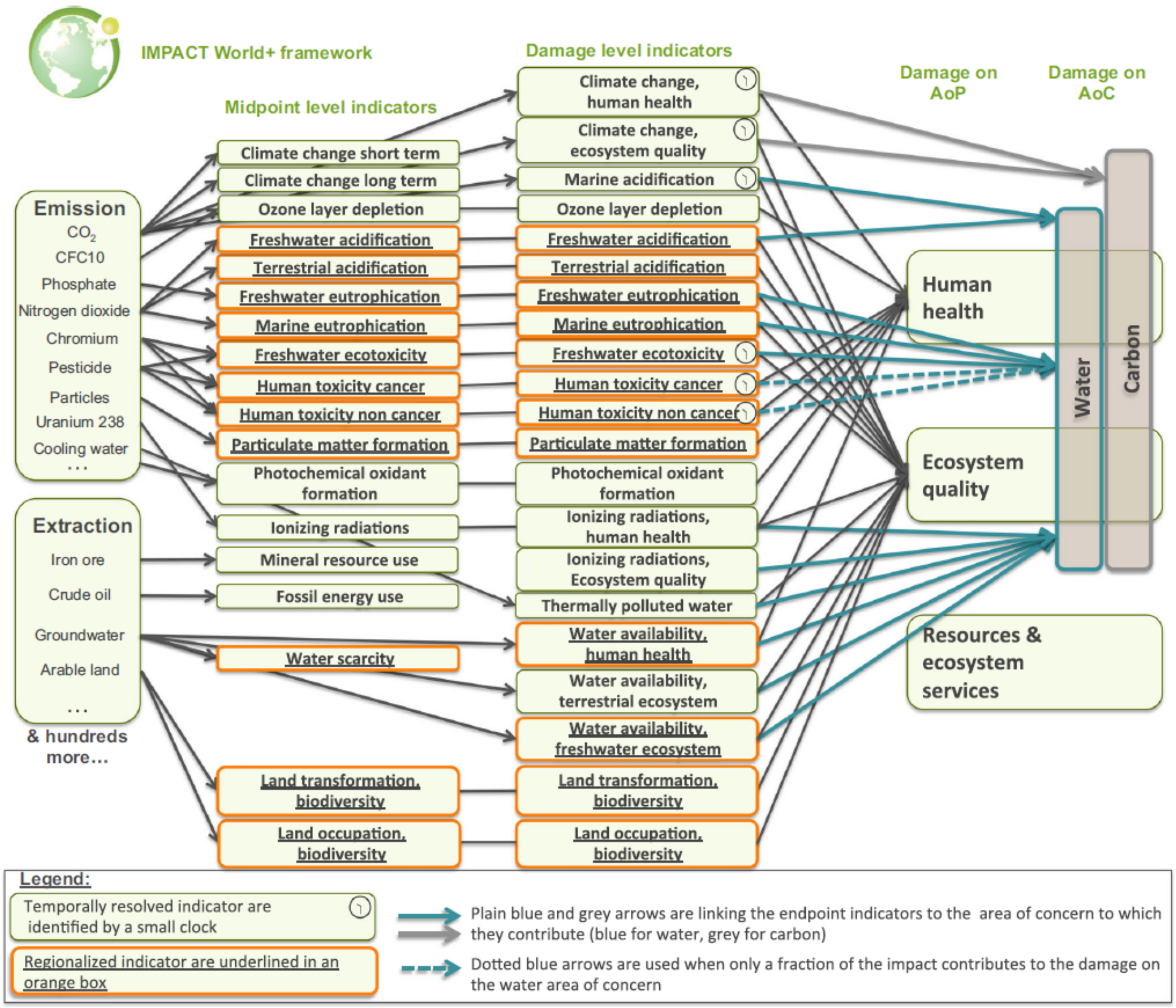

Figure 2.13 IMPACTWorld+ framework indicators [36].

2.3.1 AWARE

AWARE [19] is a proxy midpoint indicator for water scarcity. As illustrated in Figure 2.13, water scarcity doesn't lead to endpoint indicator. However, it already considers human end ecosystem needs into water demands. It is a regionalized indicator and proportional to the world average water scarcity.

AWARE indicators are regionalized, meaning that consuming 1m^3 of water in the Amazonia Basin has lower impacts compared to North Africa basins. Coefficients such as 0.1 signify that water is 10 times less scarce than the world average, while a coefficient value of 100 corresponds to water being 100 times scarcer than the world average. Figure 2.14 represents the geographic variation for water scarcity indicator.

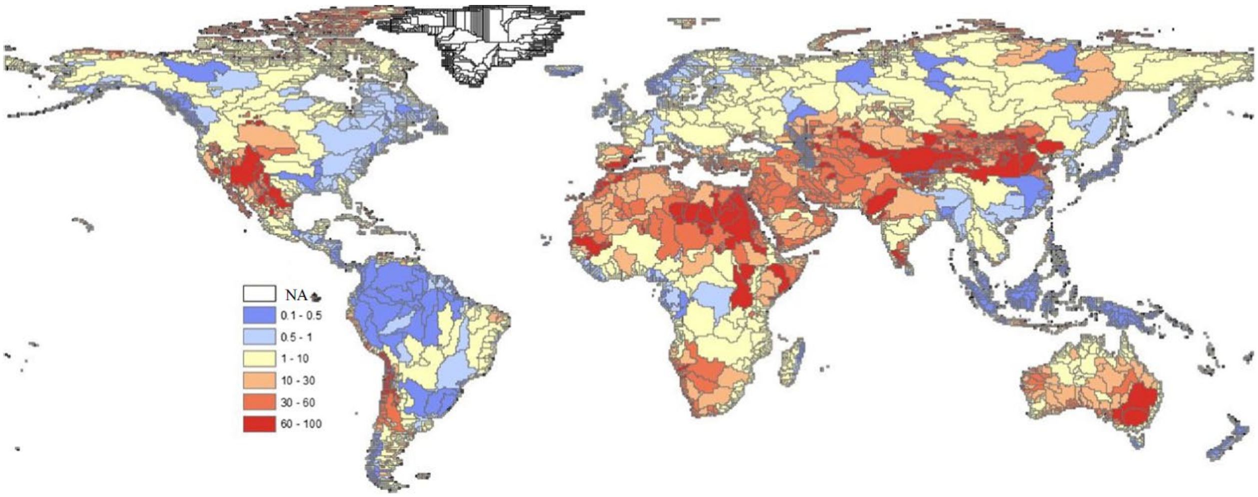

Figure 2.14 AWARE indicator for basin water consumption [19]

2.3.2 Climate change (CO2-eq)

This mid-point indicator aggregates all greenhouse gas by converting in CO2 radiative forcing potential. It is not a regionalize indicator due to non-limit effect for climate change.

2.3.3 HH – water related impacts

The consequences of water use for human health are captured in the water availability indicator developed by Boulay [37]. This indicator takes into account local scarcity and the potential for compensation measures, with these measures being based on Gross National Income. As a result, countries facing water scarcity can compensate for water deprivation, leading to no water use impacts on human health. This is particularly evident in countries such as the United States and Europe.

To assess the local sensitivity to water use, the power plant case study was reallocated from its original location in France, a country with no direct human health-related water use impacts, to Algeria, a country characterized by high water scarcity and no compensatory measures.

2.3.4 EQ – water related impacts

Similar to Human Health, Ecosystem water impacts are a consequence of various impact categories. Marine acidification, freshwater acidification, marine eutrophication, freshwater eutrophication, freshwater toxicity, ionizing radiation, thermally polluted water, water availability on terrestrial ecosystem and water availability on freshwater ecosystem. Differently for humans, ecosystems do not have compensatory measures. Water use affects directly terrestrial and freshwater ecosystem water availability indicators. Terrestrial ecosystems are affected by wells water use whereas freshwater ecosystems, by wells, rivers, and lakes water uses.

Impacts on freshwater for ecosystem due to water use are currently not regionalized by country in the existing impact methodology. Additionally, only specific basins have been assessed. More comprehensive impact factors with worldwide coverage were published in 2023 [38]. However, these were not utilized in this study due to non-compatibility units to IMPACTWorld+ results and a lack of validation. To evaluate the regional influence on freshwater use, maximum, global average, and minimum coefficients were selected for water availability in freshwater and terrestrial ecosystems coefficients and are presented in Table 6. It's important to note that, although maximums and minimums were combined to assess the variability range, they are not necessarily concurrent in the same location.

Table 8 Chosen coefficients for freshwater use impacts in Ecosystem Quality corresponding to worst and best scarce scenario and world average.

Coefficients	Terrestrial ecosystem	Location	Freshwater ecosystem	Location
Worst case	2.10E-01	Andorra	8.96E-02	Kinniconick river (a. Ohio)
World average	2.18E-02	-	3.06E-04	-
Best case	1.85E-05	Tajikistan	1.70E-05	Sucio (a. Lempa) (San Salvador)

CHAPTER 3 RESULTS AND INTERPRETATION

Results are primarily focused on freshwater use scenarios to better analyze the trade-off among water management options in terms of water recovery. Then other scenarios regarding water quality and locations are explored in mid and endpoint levels.

3.1 Onsite freshwater consumption

On-site freshwater withdrawal, release and consumption (this latter calculated as the difference between withdrawal and release), per MWh of electricity production are presented in Figure 3.1. For the base case, 0.79 m^3/MWh is withdrawn, 0.61m^3/MWh is consumed, and 0.18 m^3/MWh is released. In the partial recovery scenario, the withdrawal is 0.70 m^3/MWh of electricity produced, consumption is 0.61 m^3/MWh, and release is 0.09 m^3/MWh. The zero liquid discharge scenario involves the consumption of the entire 0.61 m^3/MWh, resulting in no release of water into the river body. Since the required heat removed is the same for all scenarios, evaporation (i.e. consumed water) in the cooling tower remains identical. On the other hand, withdrawal and release values are lower as the recovery rate increases. Withdrawal tends towards the consumed value, and release approaches zero.

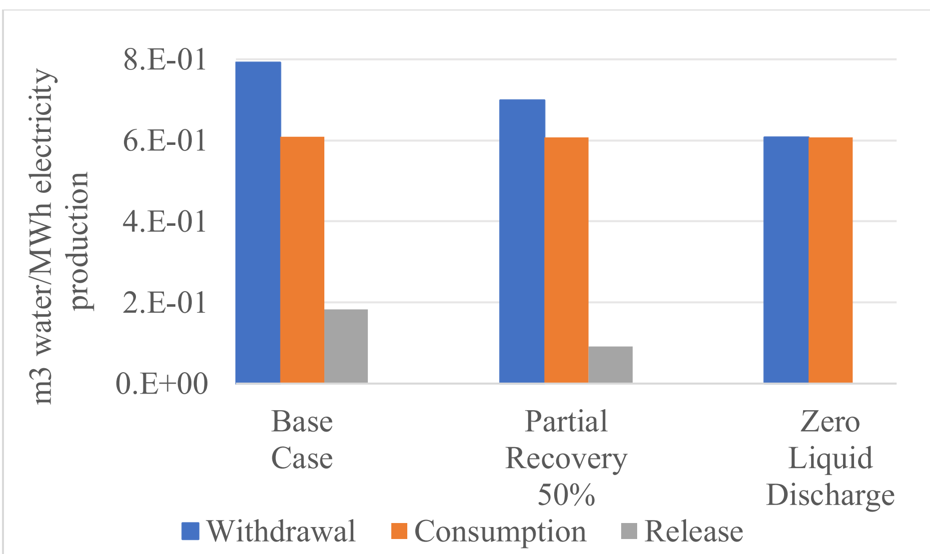

Figure 3.1 On-site water use for 1 MWh electrity production.

The Figure 3.1 does not account for the onsite surplus water consumption due to feedback effect resulting from additional energy consumption for recovery technologies. To every additional MWh of electricity to be produced due to high energy consumption for the water management system, around 0.6 m^3 of water is consumed. However, this increase in water consumption due to surplus electricity requirements is not representative. Table 7 provides the onsite energy consumption for the three main freshwater use scenarios. In the base case, partial recovery, and ZLD option 1, this energy consumption represents less than 1% of the total energy produced.

Table 9 Onsite electricity consumption for three main water management scenarios.

Electricity	Main freshwater use scenarios		
	Base case	50% Partial recovery	ZLD option 1
MWh produced	1	1	1
MWh consumed	8.01E-03	8.13E-03	9.38E-03
% diff MWh consumed from base case	-	2%	17%
MWh consumed representativeness in total production	0.80%	0.81%	0.94%

3.2 Areas of concern: water and carbon footprint

LCA results are initially presented for two impact categories representing the main areas of concerns for TOTAL Energies: carbon footprint and waster scarcity footprint.

3.2.1 Potential impact for the production of 1 MWh electricity (in French context).

Figure 3.2 indicates that relative contributions from water management are consistent across all scenarios, accounting for 0.06% of the total CO2-equivalent emissions and approximately 44% of the water scarcity footprint. Detailed impacts regarding 1MWh of electricity production is disponible in Appendix D.

Combined cycle is the primary source of CO-eq emissions for 1 MWh of electricity production. This is attributed to the combustion of natural gas in this process unit required for electricity production. Impacts on climate change for the water management system are two orders of magnitude lower than for the production of 1MWh (Figure 3.2 a).

Around 54% of the water footprint for the production of 1MWh comes from energy consumption. This is attributed to the substantial water quantities in the upstream process for natural gas production. The combined cycle process unit is the largest unit that consumes energy in the form of natural gas to produce electricity. The fact that this unit is not accounted within the boundaries of the functional unit referring only to water management explains the difference in water footprint magnitudes when comparing the water system in the entire electricity production.

Detailed analysis of water management for 1 MWh of electricity production is explored in the following section.

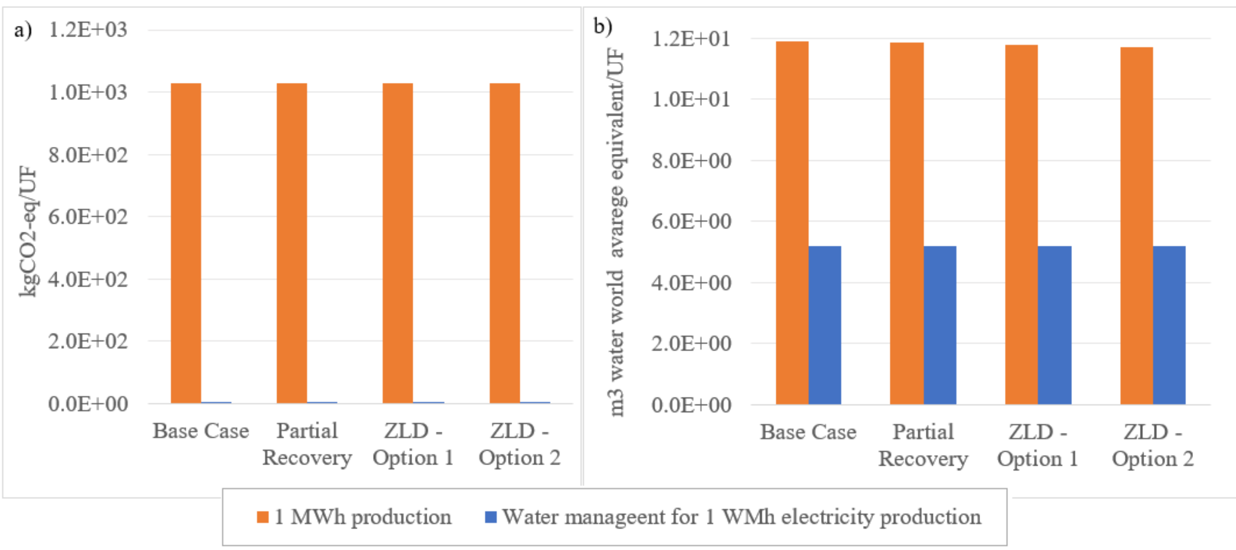

Figure 3.2 water management relative contribution to total 1 MWh electricity production impacts for a) CO2-eq emissions and b) AWARE impact category

3.2.2 Potential impact for the Water management required to support the production of 1 MWh electricity (in French context).

Figure 3.3. present the carbon footprint in CO2-equivalent per process unit in a) and per input category in b). Water footprint from the AWARE method is plotted per process unit is presented in c) and per input category in d). All scenario shows higher carbon footprint compared to the base case, contrary to the water footprint results of the alternative scenarios, where impacts are slightly better.

The base case has a water scarcity footprint of 5.20E0 m^3, partial recovery 5.17E0 m^3, ZLD option 1 5.10E0 m^3, and ZLD option 2 5.05E0 m^3 of H20 world average equivalent. Cooling tower contribution ranges from 93% to 99%. Onsite water consumption contribution varies from 95% to 98%. The AWARE indicator suggests lower potential impacts when water is recycled. Partial recovery presents similar results to the base case, but ZLD has lower impacts, especially for option 2.

By focusing solely on water management contributions, the differences between scenarios become apparent. In (a), transitioning from the base case to partial recovery, CO2-eq emissions increase due to the additional processes involved in reverse osmosis. The softening process unit (ST) experiences a reduction in its absolute water scarcity footprint as recycled water partially replaces withdrawals, helping to offset the emissions caused by recovery technologies. The demineralization system, despite having lower recovery rates when using recycled water, does not significantly impact total emissions. Biological wastewater treatment exhibits similar contributions in both the base case and partial recovery scenarios because its function is based on pollutant quantity rather than water volume. The CC and CT processes show no significant differences between scenarios as they are associated with energy production rather than water volumes. ZLD option 1 leads to a substantial increase in emissions, primarily due to the evaporation process. This increase is not offset by the non-biological wastewater treatment. However, ZLD option 2 reduces total recovery emissions by compensating for increased RO emissions with lower evaporator use.

In b), it is noteworthy that the contributions of chemical additives show a decreasing trend with higher recovery rates. Biological wastewater treatment involves the consumption of chemicals with high environmental impact. Conversely, electricity use exhibits an increasing trend with higher recovery rates. The contributions from other input categories are relatively lower.

In c), it is evident that the cooling tower is the primary contributor to this category of impact. This is understandable given that 75-97% of the inlet water is evaporated in this process unit. Additionally, as the impacts for recycling water were attributed to the wastewater function, cooling tower impacts are higher for recycling systems, and demineralization unit impacts are lower. However, one should be aware that this does not represent that more water is being evaporated and should therefore focus on the combination of the cooling tower and demineralization unit results.

From d), the primary contribution to the water scarcity footprint is onsite water use. As previously presented in Figure 3.1 , onsite water consumption is independent of recycling rates but rather dependent on the characteristics of the equipment. Consequently, on-site water use impacts remain similar for all scenarios using freshwater for withdrawal and release. The observed differences are mainly caused by variations in chemical additives.

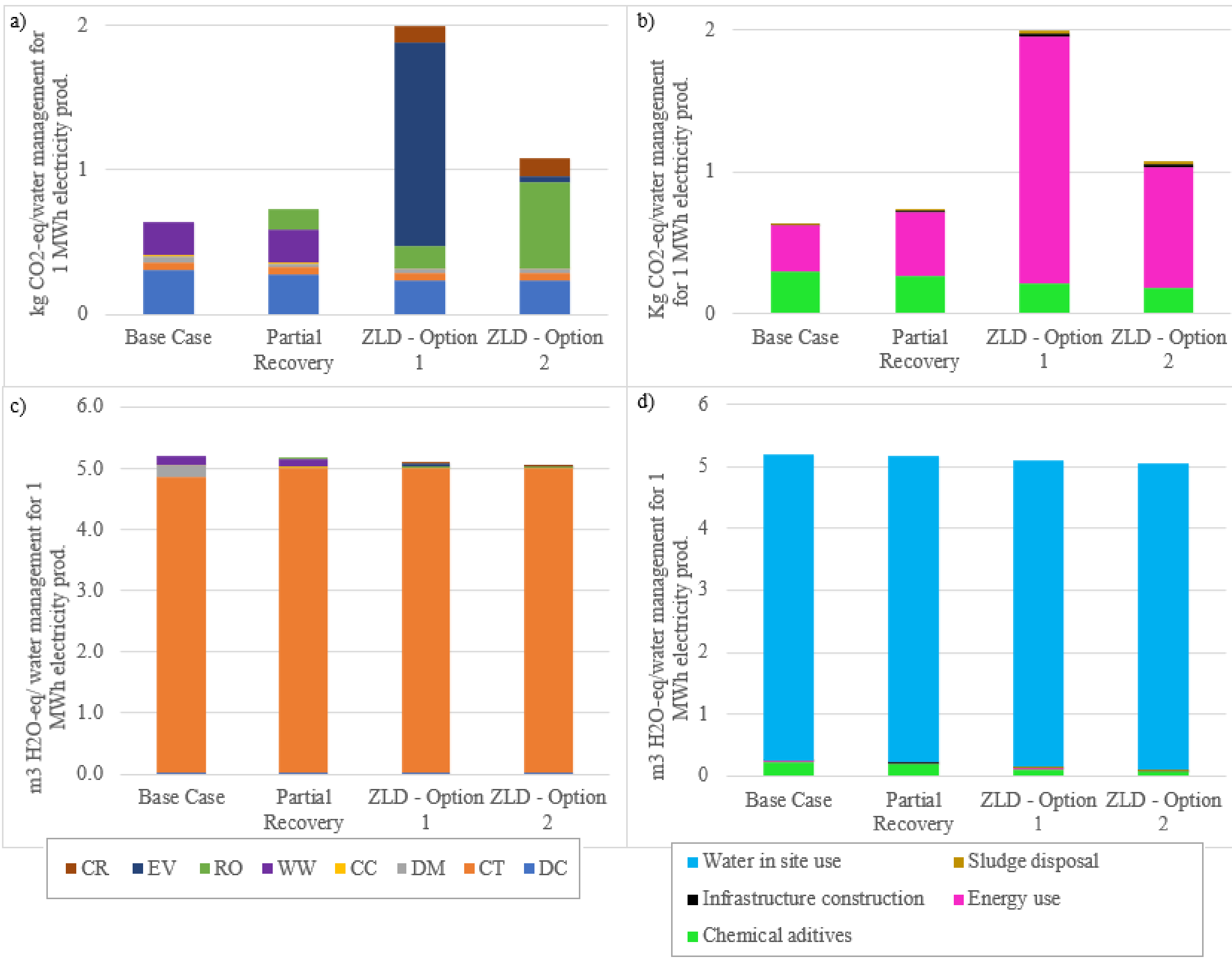

Figure 3.3 water management to produce 1 MWh electricity at mid-point impacts. In a) CO2-eq emissions per process unit; b) CO2-eq emissions per input category; c) AWARE per process unit; and d) AWARE per input category.

Figure 3.4 shows that the main contributors to the water scarcity footprint are sulfuric acid, sodium hydroxide, phosphoric acid, acetic acid, Performax DC5801, and sodium hypochlorite. Acetic acid is used in the biological wastewater treatment and, therefore, is the main factor responsible for lower impacts in ZLD scenarios. Even though the cooling tower also involves high-impact chemical use, its contributions remain similar in all scenarios. The demineralization system also contributes to reducing impacts when using recycled water due to its lower regeneration frequency.

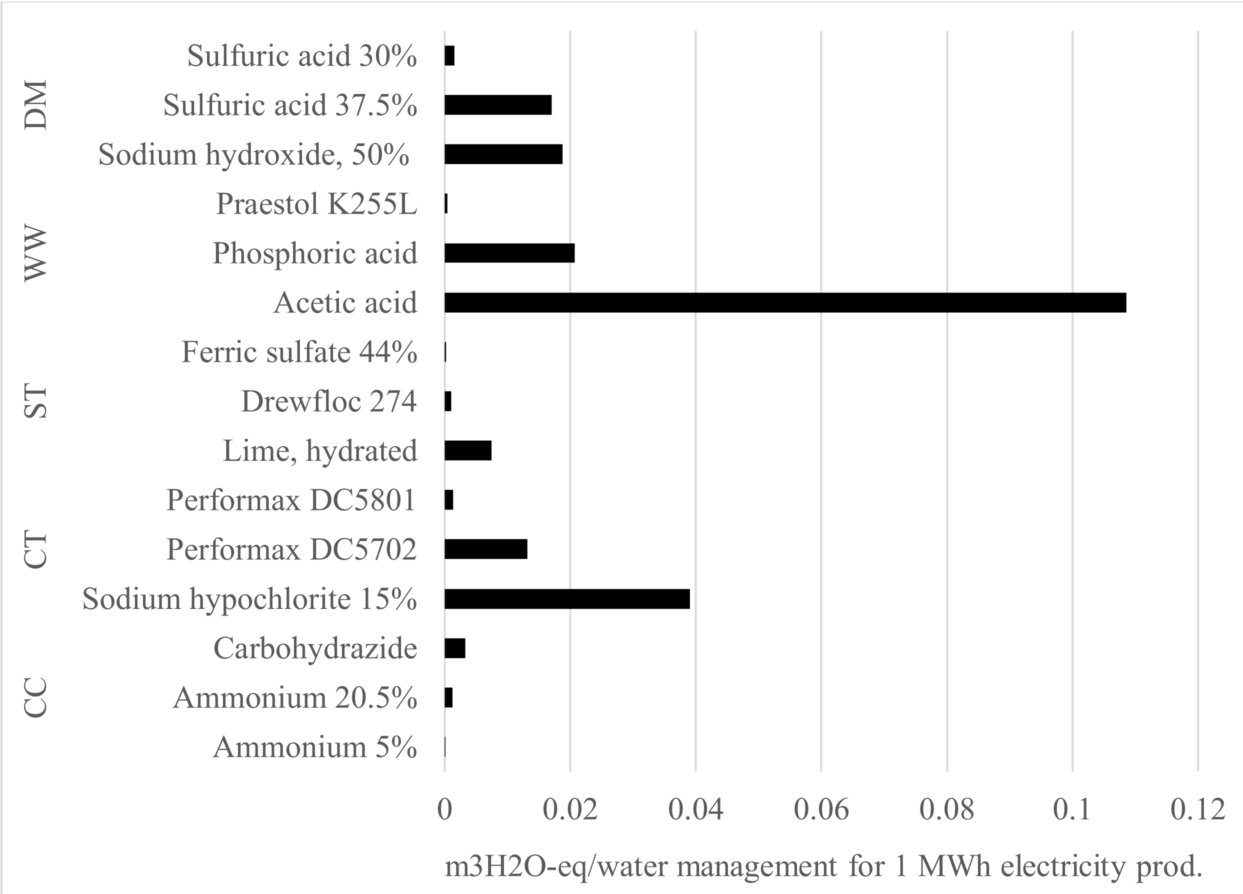

Figure 3.4 Chemicals additives contributions for total water scarcity footprint for water management for 1 MWh electricity production considering base case.

3.2.3 Sensitivity of sourcing from different water bodies

The same scenarios were tested for different water sourcing and releasing contexts: freshwater withdrawal and ocean release, withdrawal and release from and to ocean, ocean withdrawal and freshwater release. The scenario of freshwater withdrawal and release was also included in the following graphs to facilitate the comparison of all scenarios.

In Figure 3.5 a), in terms of CO_2-eq emissions, desalination presents higher impacts compared to softening. This leads to the impacts of partial recovery and ZLD option 2 being compensated by the lower use of desalination pretreatment. Due to high energy consumption in ZLD option 1, this scenario still presents higher potential impacts compared to the base case. However, its difference is 0.85 kgCO2-eq compared to 1.362 kgCO2-eq when freshwater is withdrawn and released.

Still from a), freshwater withdrawal and ocean release have the same impacts for the base case as for freshwater withdrawal and release. Thus, because there is no difference in processes and technologies. Water discharged in the ocean has the same composition as the one rejected in the river body. For partial recovery, it presents higher impacts compared to the base case due to surplus energy use. In this case, the recovery is about 96%, and it consumes more energy than recycling 50% (partial recovery freshwater withdrawal and release).

Also, from a), in case of ocean withdrawal and release, partial recovery presents similar results terms of CO2-eq emissions to ZLD option 2. This is because RO process achieves similar recovery to the RO unit used in ZDL option 2 and therefore similar energy consumption.

In terms of water scarcity footprint shown in b), ocean desalinization and subsequent freshwater release create water credits. As recycling rates go up, the water credits decrease because less freshwater is being created when freshwater is released into the river body.

Continuing from b), when freshwater is withdrawn and subsequently released into the ocean, all intake water is considered consumed, given that ocean water is not characterized as freshwater and is not considered scarce. Therefore, every increase in recovery lowers the total water footprint caused by a reduction in water withdrawal.

Ocean withdrawal and release do not have any onsite direct impacts in the water scarcity footprint because no freshwater is being used. In this scenario, only upstream water flows cause an impact, which are mainly due to chemicals production.

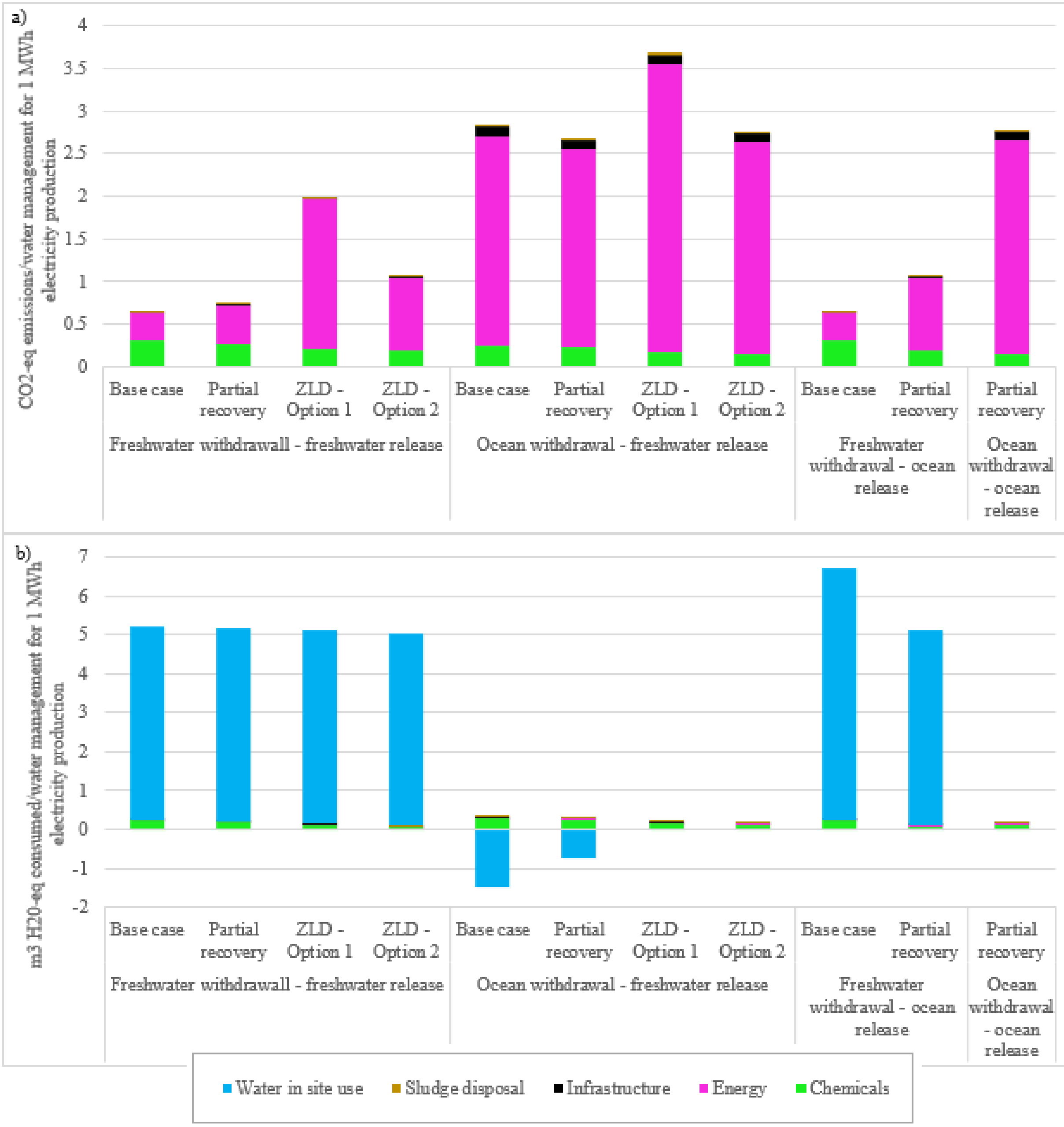

Figure 3.5 carbon footprint and water footprint profile for water management to produce 1 MWh electricity for different water source and discharge. In a) CO2-eq emissions, in b) AWARE

If seawater is used instead of freshwater, the required pretreatment changes from softening (ST) to desalination (TW). Figure 3.6 illustrates the differences between these unit operations in terms of CO2-eq in a; and for water scarcity footprint in b. Considering CO2-eq, desalination presents higher contributions compared to softening due to higher electricity demand. On the other hand, for the water scarcity footprint, desalination impacts are dominated by the use of chemical additives, leading to higher overall impacts. For desalination, water onsite consumption does not present associated impacts because there is no freshwater consumption. Also, only water consumption associated with pretreatment (softening and desalination) is counted.

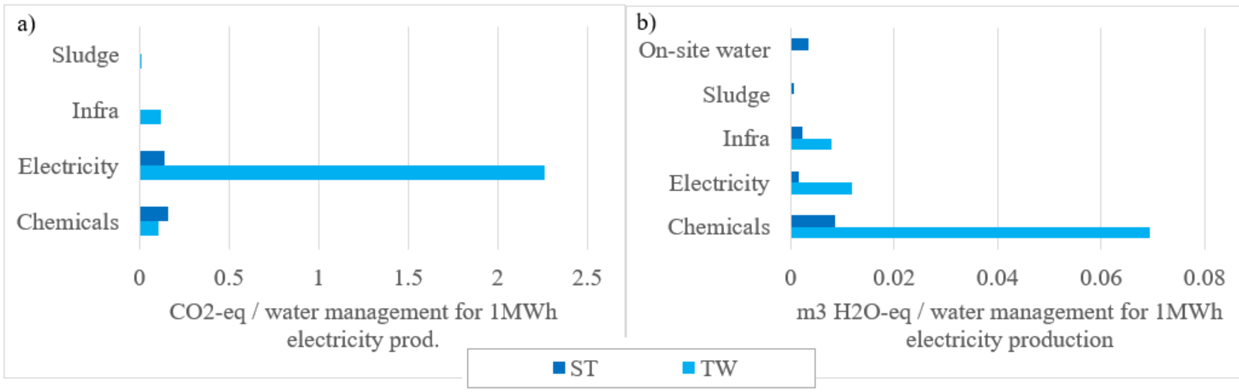

Figure 3.6 ST and TW differences contributions for CO_2-eq emissions and AWARE indicator for Base case.

3.2.4 Sensitivity from different water scarcity contexts

In Figure 3.7 the different options of water management were plotted for 3 different water scarcity locations. CO_2-eq emissions remain the same independently from the location because no upstream provider was changed in the LCA model. The orange bars are total AWARE score for France context, whereas gray and yellow for Algeria and USA respectively. The difference in water scarcity footprint evidence that water scarcity related impact can vary massively according to the location of the production site.

These findings were expected due to high influence of the on-site water use for the total water management water scarcity footprint. Higher the water scarcity context, less expressive the upstream associated impacts.

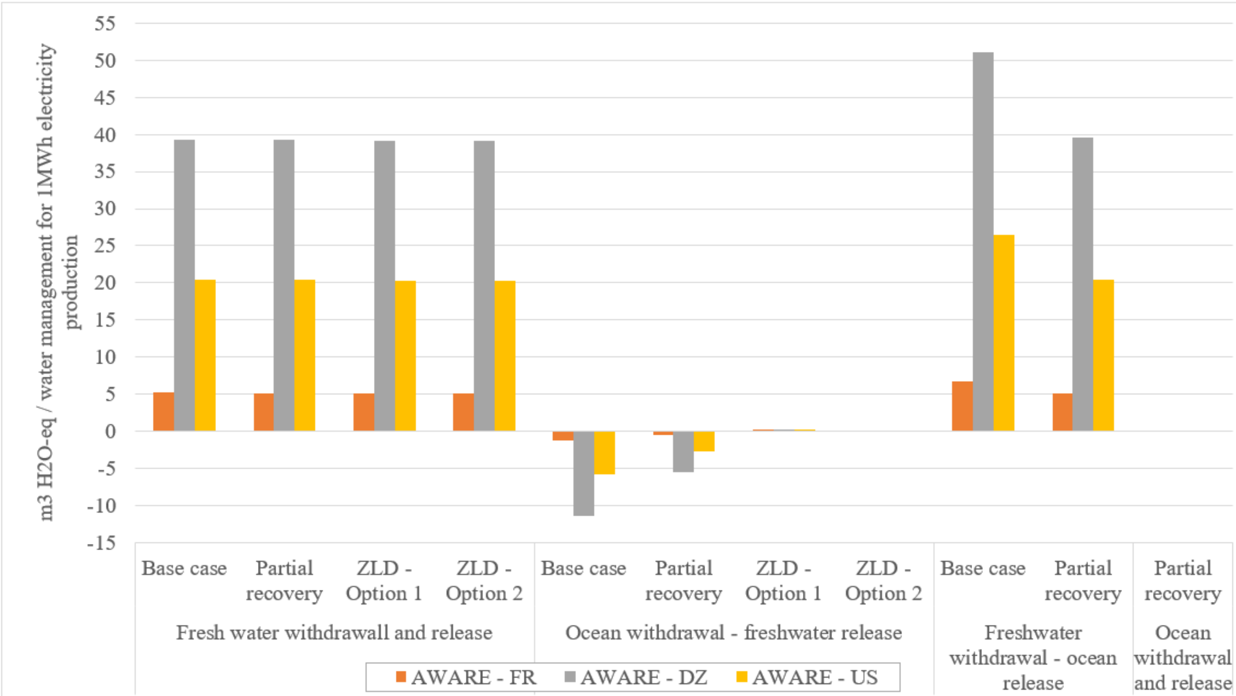

Figure 3.7 AWARE midpoint indicator for different water scarce context for all studied scenarios

Figure 3.8 illustrates that the relative significance of inputs based on the water scarcity context for 1MWh electricity production. In France, energy use holds a greater contribution than onsite water use. In more water-scarce locations, onsite water use can become the dominant impact source. However, as depicted in Figure 3.7, the overall trends remain consistent across scenarios.

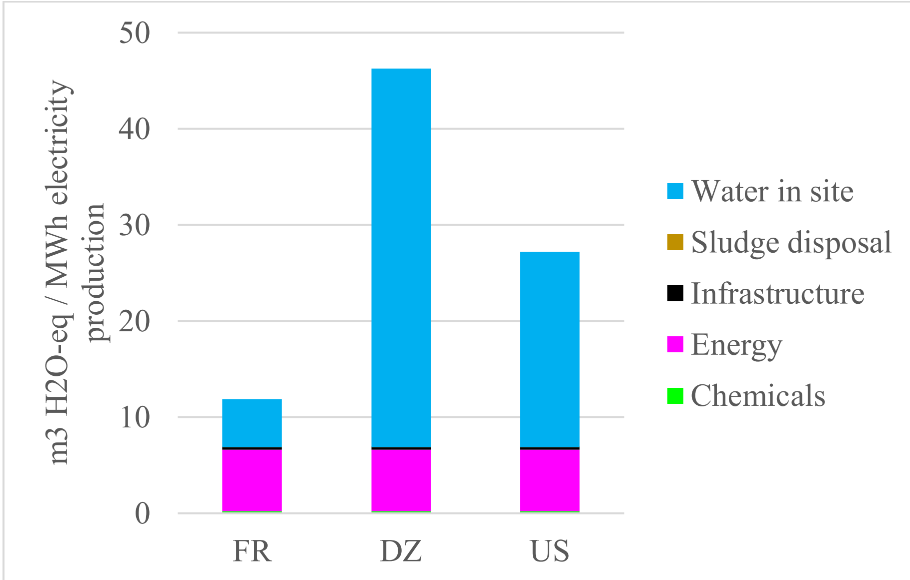

Figure 3.8 Base case with groundwater source use water scarcity footprint for different water scarce country context for 1MWh electricity production.

3.3 Area of protection: impact profile with the relative contribution of carbon and water scarcity footprint

3.3.1 Human Health

To understand the trade-offs between carbon footprint and water scarcity footprint, an evaluation of their influence and location sensitivity on the human health area of protection was conducted and plotted in Figure 3.9. Climate change is the most relevant problem in all develop countries (which that can compensate for human water deprivation) and for countries without water scarcity. Water scarcity becomes by far the most relevant problem in Algeria (and likely on other less developed countries located in high water scarcity areas).

Water use impacts on human health are associated with the presence of water scarcity and with the inability of users to compensate. If there is no water scarcity, zero are the impacts for Human Health related to the local water use. As a consequence, water consumption in Canada and Brazil, for example, won't result in any impacts. Additionally, in presence of water scarcity but also of compensatory measures, it is also considerable to not cause water-related impacts on human health. France, the USA and Spain are examples of water scarcity countries presenting zero local water consumption impacts because of its capacity to compensate for water use. These two situations where local water consumption presents zero impacts on Human Health is presented in a; whereas in b, aims to represents the trade-offs in Algeria as an example of less developed and high-water scarce place where local water consumption has associated impacts.

From Figure 3.9 a), partial recovery and ZLD option 2 present similar results to the base case when freshwater is used. In desalination cases, partial recovery and ZLD option 2 can even yield better results than the base case. This is because only upstream water related use cause impacts, and those are lower when water recovery is presents due to minor desalination demand. However, ZLD option 1 has higher impacts regardless of the water source due to its high energy requirements.

From Figure 3.9 b) onsite water related impacts dominates the HH impacts profile for non-developed and in a water-scarce context country. However, as consumption remains quite similar for freshwater use and release, there is no considerable differences in recycling water in this case.

For desalination, water credits are presents if water discharged in freshwater body and impacts can be largely reduce if recovery practices for water to be release in ocean are applied.

Climate change is still the largest source of impacts to Human Health for developed or not water scarce countries. If water scarcity is present, it can be overcome by compensatory measures. This is the case for USA. Even though the AWARE midpoint indicator presented in Figure 3.7 presented higher water scarcity for USA compared to France, for HH endpoint, water related impacts results similar. However, for non-developed countries facing water scarcity, in this case, Algeria, reduce freshwater consumption is more relevant than reductions in CO2-eq emissions for Human Health impacts. This is especially visible for cases with desalination followed by ocean release. Every freshwater recovery represents a big difference in terms of DALY impacts.

The differences in relative contribution of potential climate change and water scarcity in the final human health area of protections causes differences in conclusions regarding scenarios comparison. If desalination is not the best water management option in developed countries due to its high energy consumption, it is in a good option for less developed countries due to non freshwater use. ZLD option 1 can present a discrepant higher impact for freshwater use in developed countries, whereas for less developed, its impacts are in the same magnitude as other recovery practices.

It is important to state that the impacts categorized in climate change and in remaining impact categories are the same independent of the location because only the onsite water use was regionalized. The water scarcity dominance for Algeria is due to its onsite impacts being considered, thus increasing in two orders of magnitude the total HH impacts.

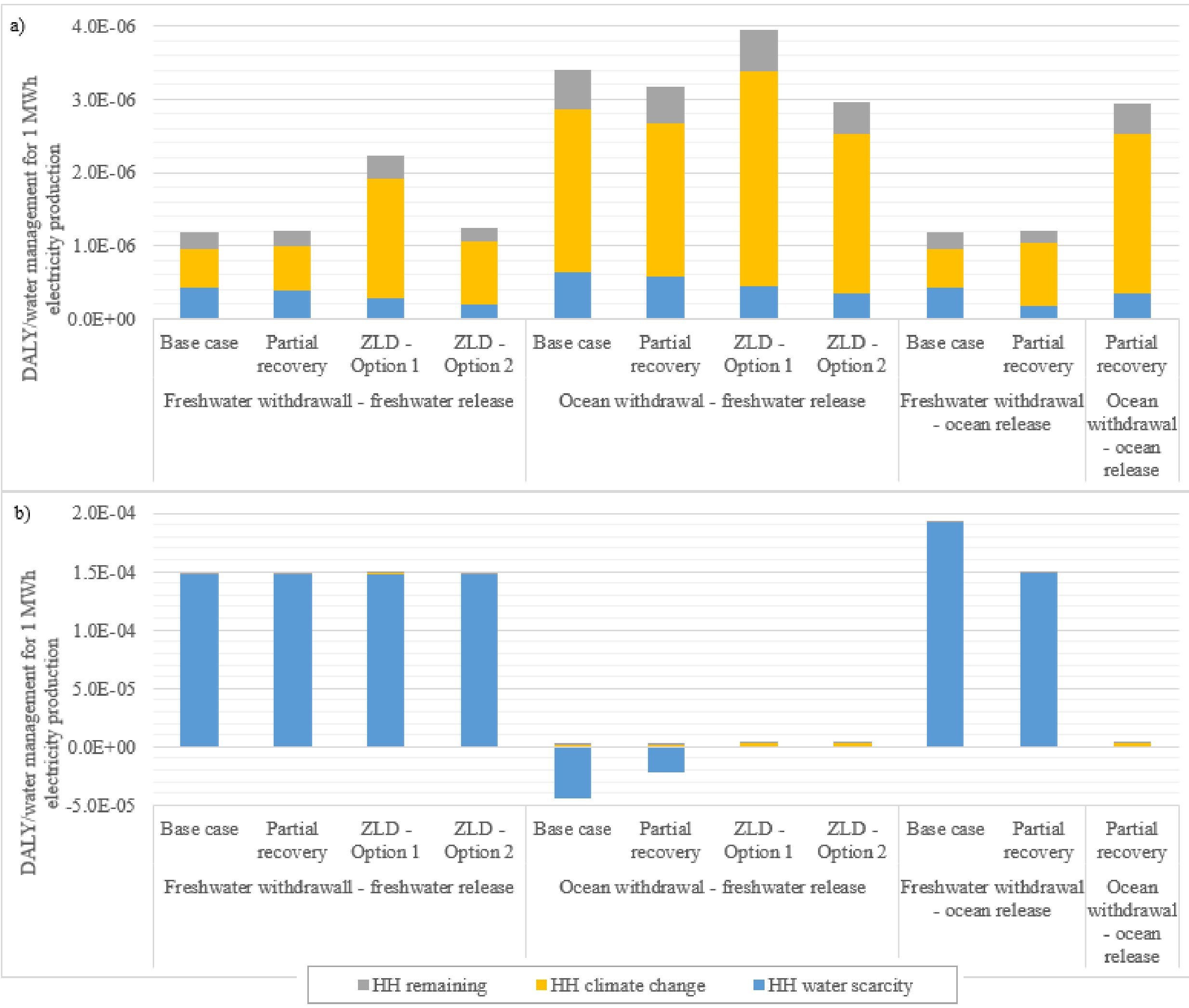

Figure 3.9 Human Health area of impact results for all scenarios in a) developed or/and non water scarce countries and b) for less developed and water scarce country, Algeria.

3.3.2 Ecosystem Quality

Figure 3.10 represents the total impacts for Ecosystem quality area of protection. First statement is that world average results are closer to the best-case scenario than the worst-case scenario. In this context, climate change has higher environmental relevance (i.e. higher contribution) to Ecosystem

Quality Area of Protection than freshwater consumption for most locations. Therefore, water management should prioritize low carbon emission procedures.

In the worst scarce scenario presented in c), which may be fictive as they combine the worst freshwater rivers use with the worst freshwater from groundwater (and those are not in the same place), it is demonstrated that freshwater use also has a relevant contribution alongside climate change.

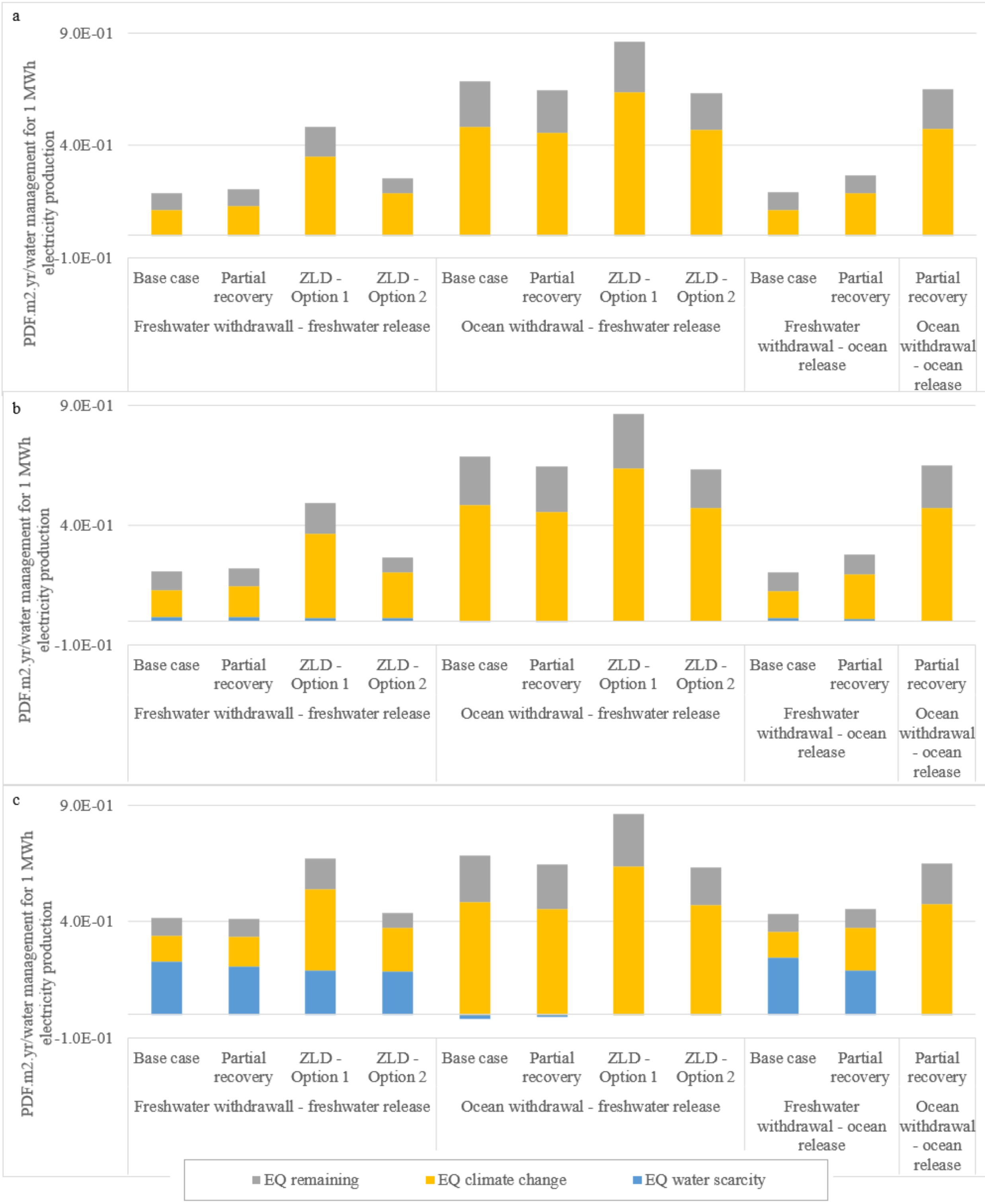

Figure 3.10 Ecosystem Quality impacts for water management for 1 MWh electricity production is a) lowest water scarcity context; b) world average water scarcity and c) highest water scarcity place combination.

3.4 Data quality

The highest level of data quality was achieved for the base-case scenario, benefiting from its physical presence at the power plant. In contrast, the data quality for all other scenarios is compromised as they were constructed, making local measurements unfeasible. TotalEnergies' internal projects were instrumental in providing specific data for the power plant, such as the case for 50% recovery reverse osmosis. For scenarios involving desalination and ZLD option 1, a combination of literature and TotalEnergies' internal projects from other production sites was used, resulting in a lower data quality. Zero liquid discharge option 2 and all scenarios with high reverse osmosis recovery rates were extrapolated from previous scenarios using literature and expert analysis, representing the worst level of data quality.

In foreground modeling, several assumptions were made regarding chemical compositions when not already available in the Ecoinvent database. This was particularly notable for commercial anti-scaling and biocide commercial names used as chemical additives. Infrastructure posed challenges due to a lack of data. For base case equipment, the technology provider manual was consulted, and estimations were made based on local measurements. The reverse osmosis equipment used literature and previous information from internal studies. Zero liquid discharge (ZLD) scenarios were solely based on literature for similar technology.

Data quality for the process unites were evaluated using indices and presented in the Table 11. Reliability refers to the numerical value (amount) of the intermediary flows required by process, while representativeness to the process modeling. Indices vary from 1 to 4 according to the data quality. The value of 1 is attributed to in site measurements and very data for flows and modeling process; 2 when data comes from documents and literature without local verified data, also modeling process is considered well represented; 3 for data originated and process modeling may consider similar technologies; 4 rough data estimation and non-adequate technology. For the contribution to the overall impact score, negligible is attributed when the process unit is responsible for less than 5% of the total impacts considering a specific area of concern; moderate when 5% up to 20%; important when between 20% and 50%, and dominant for more than 50%.

From Table 8, it is evident that results present low confidence in terms of CO2-eq emissions specially for freshwater withdrawn involving ZLD technologies. Dominant impacts are associated with low reliability or/and low representativeness of the evaporator and crystallizer units. This is expected due to its data collection possibility only using literature instead of local data. Therefore, confidence could be improved using site data from similar power plant technology using ZLD practices in sufficient close water related factors influencing water consumption.

Water footprint contribution for scenarios involving desalination and subsequent water release in freshwater body were not expressed in Table 11 due to difficult choices when addressing water footprint credits. However, it is evident that the cooling tower and desalination are the two main process keys for the water footprint score.

Table 10 Data quality evaluations for process units per scenario used in water management for 1 MWh electricity production.

Process unit	Data quality		Contribution																		
			freshwater withdrawn and release								ocean withdrawn, freshwater release				freshwater withdrawn and ocean release				ocean withdrawn and release	
	Reliability	Representativeness	CO2-eq				Water scarcity footprint				CO2-eq				CO2-eq		Water scarcity footprint		CO2-eq	Water scarcity footprint
			Base case	Partial recovery	ZLD opt. 1	ZLD opt. 2	Base case	Partial recovery	ZLD opt. 1	ZLD opt. 2	Base case	Partial recovery	ZLD opt. 1	ZLD opt. 2	Base case	Partial recovery	Base case	Partial recovery	Partial recovery	Partial recovery
TW	**1**	**3**	-	-	-	-	-	-	-	-	dominant	dominant	dominant	dominant	-	-	-	-	dominant	important
ST	**1**	**1**	important	important	moderate	important	negligible	negligible	negligible	negligible	-	-	-	-	important	important	negligible	negligible	-	-
CT	**1**	**1**	moderate	moderate	negligible	negligible	dominant	dominant	dominant	dominant	negligible	negligible	negligible	negligible	moderate	moderate	dominant	dominant	negligible	important
DM	**1**	**1**	moderate	moderate	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	moderate	negligible	negligible	negligible	negligible	negligible
RO 50% recovery	**2**	**2**	-	important	moderate	-	-	negligible	negligible	-	-	moderate	negligible	-	-	-	-	-	-	-
RO 96.5%-97.55% recovery	**3**	**3**	-	-	-	dominant	-	-	-	negligible	-	-	-	important	-	dominant	-	negligible	important	moderate
CC	**1**	**1**	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible	negligible
WW base case	**1**	**1**	important	-	-	-	moderate	-	-	-	moderate	-	-	-	important	moderate		-	-	-
WW RO 50% recovery	**2**	**3**	-	important	-	-	-	negligible	-	-	-	moderate	-	-	-	-	-	-	-	-
WW RO 96.5% recovery	**4**	**3**	-	-	-	-	-	-	-	-	-	-	-	-	-	moderate	-	negligible	moderate	negligible
EV	**3**	**3**	-	-	dominant	negligible	-	-	negligible	negligible	-	-	important	negligible	-	-	-	-	-	-
CR	**3**	**3**	-	-	moderate	negligible	-	-	negligible	negligible	-	-	negligible	negligible	-	-	-	-	-	-

CHAPTER 4 DISCUSSION

Despite meeting stricter policies regarding water use, the reuse of water may not necessarily lead to overall water savings, because it doesn't result in a direct reduction in water consumption as already demonstrated by Markus Berger and Sebastian Thiede in 2023 [39]. Important to restate that the indicator based on AWARE methodology uses water consumption (withdrawals – release) to calculate water footprint. Evaporate water is considered consumed because its precipitation may not occur in a way that could be directly incorporated in freshwater bodies, however a 2021 study from Link et al [40] explore the possibility to integrate evaporated water in the water footprint metrics. Water recovery technologies reduce withdraws and release water volumes as showed by Plata et al, in which recycling water can reduce withdrawals by 18% [30]. In this case study it was calculated that ZLD achieved a 23% reduction, while partial recovery led to a 12% reduction; however, consumption is inherent to the process of production (in this case mainly due to cooling tower evaporation) and not with the water treatment system. Direct water consumption was already demonstrated to be associated with evaporation rates, which are independent of recycling rates [29]. In this context, other cooling technologies or water condensation from wet cooling towers could result in lower water consumption.

Analyzing only water management contributions reveals trade-offs between CO_2-eq emissions and water footprint. Energy consumption is the main CO_2-equivalent source of impacts while the major contribution for water footprint if freshwater is consumed. Partial recovery and ZLD scenarios exhibit from similar to higher CO_2-eq emissions compared to baseline scenarios respectively, therefore reinforcing the idea that partial recovery could be seen as an advantage over the ZLD route [32] and therefore helpful to meet stricter policies in terms of water use volumes without compromising its overall environmental performance; however, there is only negligible differences in water scarcity footprints for cases with direct freshwater consumption. In this case the variations in water footprint are dependent on the upstream chemical's additive production process because onsite freshwater consumption remains unaltered. The significance of chemicals and energy consumption has already been underscored as critical elements in environmental impacts for wastewater systems [15, 41]. ZLD salts landfill disposal, sludge management and infrastructure were found to have a minor impact. Near Zero Liquid Discharge for brine resulting from CO_2 injection study found that landfill impacts and evaporation equipment contributed to around 13%, while energy requirements were 83% to overall impact score [42]. Except for waste generation, sludge disposal from desalinization plant contributes from 3% to 5% to environmental profile [43]. Salts can also generate credits as by-products, but it does not compensate for the higher ZLD impacts [41].

Considering another water qualities combination than freshwater withdrawal and release, partial recovery has lower CO2-eq emissions impacts compared to the base case if desalinization is employed, different than if softening is used as pretreatment. A recent study suggests that the GWP impact for different recycling rates is dependent on the characteristics of the baseline technology [29]. Also, freshwater savings due to recycling are relevant and beneficial in reducing the water scarcity footprint in situations where water is withdrawn from freshwater sources with subsequent release into a saline water body. In this case, achieving maximum recovery is beneficial for reducing overall water consumption.

By analyzing the relative's contribution of the global warming potential by CO2-eq emissions and water availability into the areas of protection, it is evident that location plays a significant role. GWP is the most important contribution to the Human Health impacts for countries not facing water scarcity or for those with compensatory water use measures present for developed countries. This happens because the onsite water use does not lead to any impacts, and only upstream water uses in less developed, and water-scarce countries cause impacts. For those, the water availability relative contributions to human health impacts increase, potentially reaching almost the totality of the impacts. For ecosystem quality location changes the relative contribution of the two areas of concern, however, it doesn't change overall conclusions, being GWP the most relevant impact to be focused on.

Regarding the water management impacts in the 1 MWh of electricity production, this study found that it is irrelevant in terms of total CO2-eq emissions variation and important for water scarcity footprint. This was expected because burning natural gas in the combined cycle to produce electricity is by far the principal contributor for CO2-eq emissions. Consequently, the carbon footprint of water recovery scenario increases by less than 0.5% in respect to the overall impact score of producing 1 MWh of electricity. This finding is in accordance with 0.1% required facility energy generation to be used for ZLD [30]. Even though in relative values of CO2-eq variations between recovery scenarios are not perceptive, in absolute amount it represents substantial quantities. In terms of water scarcity footprint, less than 50% of water-related impacts when consuming freshwater comes from on site water use. This is because upstream natural gas-related processes contribute to high water footprint. For this study specific case, it is necessary around 0.6 m^3 in site water per MWh produced, which is close to estimations of 0.79 m^3/MWh for combined cycle power plants using recirculating cooling towers [44]. However, in the same research, it was found that natural gas cycle consumes only 0.015 m^3/MWh [44]. Water footprint for natural gas production varies over the world. Shale gas may cause minor water impact in certain regions as South America, and substantial impacts in others, as North Africa and Australia [45]. Natural gas provider selection could also contribute to lower water associated impacts.

Different configurations and technologies used in ZLD configurations were explored to reach lower energy requirements. Heat integration was a promising energy optimization that was not achievable because the selected evaporator technology, mechanical vapor compression, already optimize its energy use. Additionally, low heat grade use is not always energetic interesting if heat pumps need to be applied in circumstances where it requires high energy consumption. Also, additional cooling to condensation offsets possible water saving when applying heat integration in membrane distillation and combined cycle. However, exploring membrane osmosis at its maximum before the use of thermo-technologies reduces the amount of total electricity use, therefore, lower CO2-eq associated impacts. Pretreatment can considerably increase RO recovery before further thermo-based recovery, thus reducing total GWP impacts [46]; however, the option 2 is only possible for brackish water. If a facility presents high salinity in the output flow, it would be difficult to achieve the higher RO recovery.

Results should be considered with caution and focused on quality analysis only due to scenarios presenting different data quality. As the created scenarios were developed using assumptions from literature, the real performance of the required technologies may be considerably different from what was used in this study. Also, the sensitivity analysis of the results related to the location of the power plant only considered changes in the direct freshwater use (foreground system). All upstream flows remained unaltered, as did the water volume consumption. However, in reality cooling tower-associated impacts change from one location to another due to climate variation, causing variations in evaporation rates, and, consequently, energy use [47].

In this work, an attributional analysis was stated. This means that all impacts were calculated considering no consequential changes in a facility to migrate to another water management technology. Decommissioning and new equipment construction and installation would increase impacts associated to infrastructure. However, as those are already presented to be in lower importance regarding overall impacts, this may not change this study main conclusions.

There is also impact model's characteristic to be pointed out. First, the allocation of water scarcity credits due to desalination followed by freshwater release into the river may raise questions. It is noteworthy that the environmental value of the release point, especially when close to the river mouth, may differ if the release occurred upstream. Potential users decrease along the course, resulting in a cascade effect in water use impacts [48]. The AWARE indicator does not account for this effect in its methodology, and therefore considers a uniform watershed. Hence, one might argue that using downstream freshwater should have a lower water footprint impact. Conversely, the outflow of water may have potential industrial users, adding to release flow value. Second, additional impacts due to compensation water use measures were not quantified. Human health water use impacts are considered to be zero if water consumption occurs in high-income countries [49]. However, to overcome scarcity scenarios, compensation practices can end up emitting additional CO2-eq quantities, thus, affecting Human Health. Third, ecosystem quality sensibility use Hanafiah [50] and Van Zelm [51] extreme factors. More complete location sensibility can be made with last freshwater use impact in freshwater ecosystem coefficients published recently by Pierrat [38] once robustness established. And fourth, even though partial recycling was presented as a promising commitment with regulations and environmental performance, it implies higher pollutants concentration in the released water by maintaining the same mass of pollutants in a smaller water volume. This constraint also needs to be analyzed in terms of dilution effect, which was not considerable in the pertinent impact factors modeling routes.

This work contributes to a better understanding of the potential impacts associated with different industrial water management options. Studies had not yet been carried out considering the entire interaction of water treatment based on an LCA analysis for a real study comparing different water treatment configurations. Industrial water management options were modeled considering the same function to be delivered as a part of a production system. This allows the integration of pre-and post-treatment, which was not possible if water volume was chosen as comparable function. Additionally, regional and water quality variability were explored to better understand the limits of results both at the area of concern and area of protection levels. Although limited to a power plant, the results of this study can be a first step towards understanding the potential environmental impacts considering other types of industrial production if a cooling tower is the largest water consumer. However, for better results, it would be interesting to explore other production chains as well as potential updated versions of the impact model used.

CHAPTER 5 CONCLUSION AND RECOMMENDATIONS

Given the demand for better use of water resources, some different water management practices are presented. To better help decision-making, a question was settled: *What are the environmental impacts associated with industrial water management options?* To answer this question, this work evaluated the environmental performance through LCA approach, different industrial water management scenarios based on a power plant case study. Different recycling rates scenarios, base case with no recycling, partial recovery using reverse osmosis and total recovery under zero liquid discharge, were analyzed and then subsequent sensitivity analysis regarding water quality and water scarcity contexts were made. Also, the importance of water management in the total power plant impacts was also assessed. Indicators such as CO2-eq emissions and water scarcity footprints were chosen based on its relevance to the case; and human health and ecosystem quality protection areas to assess the relative contributions of water and carbon in a broad framework of impacts.

Recycling water is dissociated from freshwater consumption, which is the input for freshwater scarcity footprint. It reduces water withdrawals and release; however, water consumption is dictated by the process of production characteristics and not by the water management system. There are freshwater scarcity and carbon footprint trade-offs between different scenarios dependent on the quality of the resource used. If for groundwater use recycling can slightly reduce water scarcity footprints and increase CO2-eq emissions, for ocean water, recycling increases water scarcity while carbon footprint can be reduced depending on the recycling rate and configuration. Also, carbon and water footprint relative contribution are dependent on the context. In less developed countries facing severe water scarcity Human Health impacts are predominantly water use. However, regions with the capacity for compensatory measures or without water scarcity stress will have impacts governed by the CO-eq emissions profile, and therefore should prioritize low-emission technologies. In contrast, ecosystem quality impacts are less sensible in terms of location, and, in general, potential climate change has more significance than water scarcity impacts. Despite all trade-offs, water management have irrelevant contribution to the total power plant carbon footprint and represents less than 50% of the power plant water footprint.

These findings are subject to wide data quality and therefore should be taken with caution. Also, location variability applies only to onsite freshwater use and all other flows remains the same. The chosen impact model presents some limitations in terms of accuracy and regionalization.

Additionally, those results consider a specific powerplant water management system, meaning that for other process productions the required treatment may differ.

This study innovates by integrating pre- and post treatment technologies for different recycling rates for a real study case. Additionally, the comprehensive water scarcity and carbon footprints relative contributions to the areas of protections alongside different locations characteristics were not found up to date for industrial water treatment systems.

It would be interesting to analyze water management options impacts for other production processes that requires different water treatments. Though, this evaluation should consider water treatment in its full chain using real cases to better assess the potential trade-offs. Environmental policies should take a holistic view, considering the water context and present technologies. Environmental trade-offs can vary widely between countries. Protecting water resources to ensure human and ecosystem health risks being inefficient if not enough aspects are considered to determine a solution.

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APPENDIX A INVENTORY

A.1 General parameters

Table A.1 Inputs values for variables according to scenario

Process unit	Scenarios										
	Freshwater withdrawal and release				Ocean withdrawal, freshwater release				Ocean withdrawal and release	Freshwater withdrawal and ocean release	
	Base case	Partial rec.	Total recovery, option 1	Total recovery, option 2	Base case	Partial rec.	Total recovery, option 1	Total recovery, option 2	Partial rec.	Base case	Partial rec.
SC1	1	0	0	0	1	0	0	0	0	1	0
SC2	0	1	0	0	0	1	0	0	1	0	1
SC3	0	0	1	1	0	0	1	1	0	0	0
TW	0	0	0	0	1	1	1	1	1	0	0
ST	1	1	1	1	0	0	0	0	0	1	1
ro_recovery_rate	-	0.50	0.50	0.98	-	0.50	0.50	0.98	0.97	-	0.97
ro_energy_con	-	1.50E-03	1.50E-03	3.10E-03	-	1.50E-03	1.50E-03	3.10E-03	3.10E-03	-	3.10E-03
NF	0	0	0	1	0	0	0	1	1	0	1
FW_emi	1	1	1	1	1	1	1	1	0	0	0
OC_emi	0	0	0	0	0	0	0	0	1	1	1
ev_recovery_rate	-	-	0.98	0.62	-	-	0.98	0.62	-	-	-

A.2 Desalination Process Unit

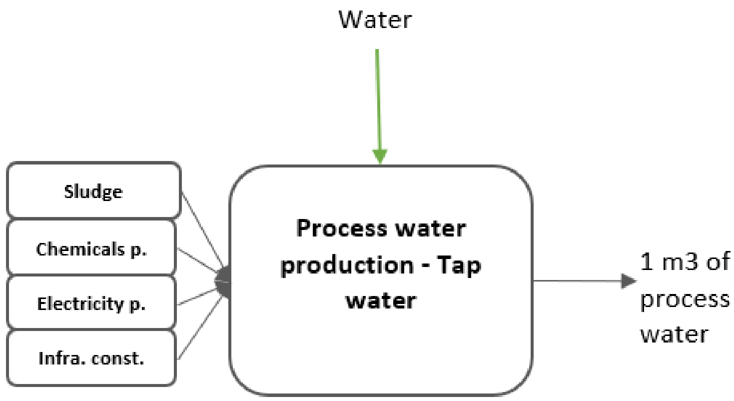

Figure A.1 Process water production for tap water quality from desalination process unit

Table A.2 Input and output modeling for desalination process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	Confidential	Confidential	Confidential	Confidential
Energy prod.	electricity, high voltage	Confidential	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	Confidential	Confidential	Confidential	Confidential
Sludge manag.	Confidential	Confidential	Confidential	Confidential
Water	Water, well, FR	Confidential	Confidential	Confidential
Output				
UF	Process water	1	m3	

A.3 Cooling Tower Process Unit

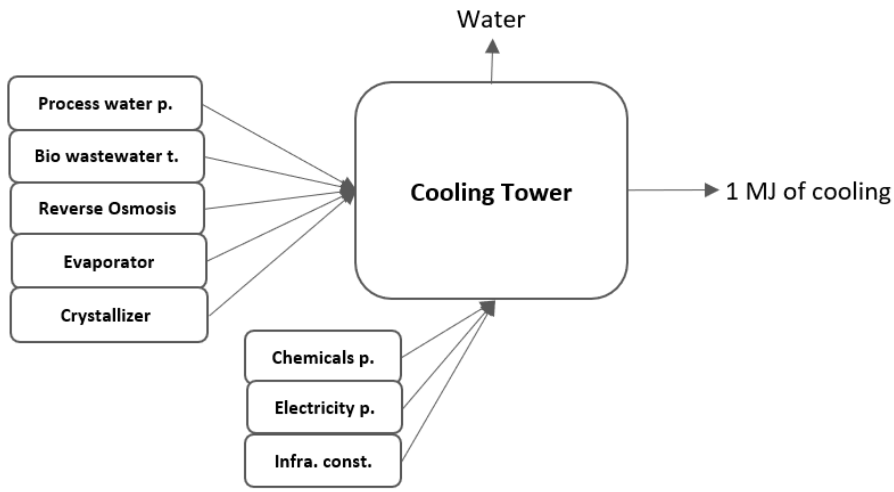

Figure A.2 Cooling Tower process unit system

Table A.3 Input parameters for cooling tower process unit

Input parameters			
Name	Value	Description	Data source
capacity_cooling_pss	234	MW	Site data
electrcal_energy_pss	33400	MWh	Site data
electrical_energy	864	MWh	Site data
life_years	20	years	estimation
blow_down_cc_water	5.91E-03	m3/MWh prod	Site data
factor_MJ_cooling_MW	1914.545454	MJ/MWh prod	Site calculation
make_up_ct_water	4.05E-04	m3/MJ	Site calculation
water_vapor_ct	3.10E-04	m3/MJ	Site calculation
blow_down_ct_water	9.54546E-05	m3/MJ	Site calculation

Table A.4 Dependent parameters for cooling tower process unit

Dependent parameters			
Name	Formula	Value	unit
cooling_capacity	electrical_energy *capacity_cooling_pss /electrcal_energy_pss	6.053173653	MW
cooling_capacity_life	cooling_capacity_MJ *life_years *365*24	3817857686	MJ
cooling_capacity_MJ	Cooling_capacity *3600	21791.42515	MJ
UNIT	1/COOLing_capacity_life	2.61927E-10	unit
valorized_water	blow_down_cc_water/factor_MJ_cooling_MW	3.09E-06	m3
ST_water	make_up_ct_water-valorized_water	4.02E-04	m3
water_vapor_emissions_ct	water_vapor_ct	0.000309991	m3
wastewater_management_ct	blow_down_ct_water	9.54546E-05	m3
DM_transfer	(((inlet_dm_water-(((recycle_ro_dm)*sc2)))*make_up_cc_water)/factor_MJ_cooling_MW*sc2)+(((inlet_dm_water-(((recycle_ro_dm+recycle_ev_dm +recycle_cr_dm)*sc3)))*make_up_cc_water)/factor_MJ_cooling_MW*sc3)	0	m3

Table A.5 Input and output modeling for cooling tower process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	Performax DC5702	0.002088043	g	Performax DC5702 production - created process - FR
	Performax DC5801	6.28E-05	gr	Performax DC5801 production - created process - FR
	sodium hypochlorite, without water, in 15% solution state	0.008683286	g	sodium hypochlorite production, product in 15% solution state | sodium hypochlorite, without water, in 15% solution state | Cutoff, U - RER
Energy prod.	electricity, high voltage	3.96E-06	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	Cooling tower	unit	Item(s)	Cooling tower construction
Water	Process water	ST_water	m3	Softened water production, internal unit, TotalEnergies - PSS
	valorised water	valorized_water	m3	CC water valorization
	Wastewater treatment from power energy generation	wastewater_management_ct	m3	wastewater treatment, internal unit for water treatment, TotalEnergies - PSS

Table A.5 Input and output modeling for cooling tower process unit (continuation)

Output				
UF	Refrigeration	1	MJ	
Water	Emission to air/unspecified	water_vapor_emissions_ct	m3	
	Transfer for DM	DM_transfer	m3	

A.4 Water management for Cooling Tower Process Unit

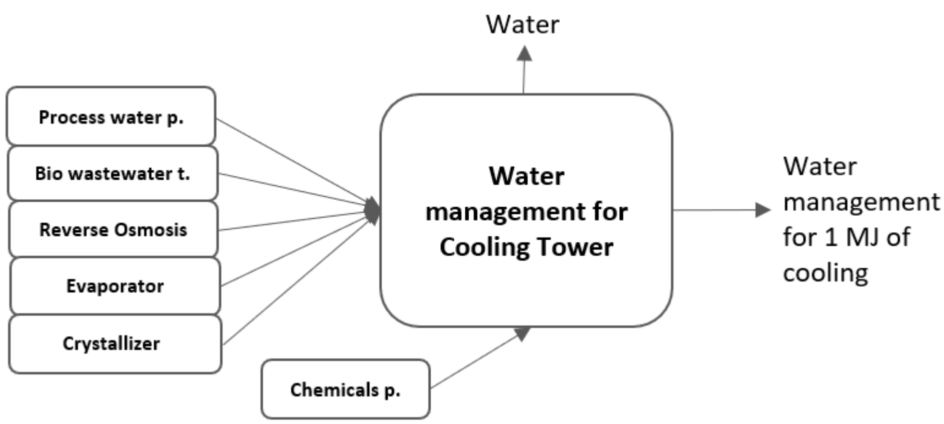

Figure A.3 Water management for cooling tower process unit system

Table A.6 Input and output modeling for water management for cooling tower process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	Performax DC5702	0.002088043	g	Performax DC5702 production - created process - FR
	Performax DC5801	6.28E-05	gr	Performax DC5801 production - created process - FR
	sodium hypochlorite, without water, in 15% solution state	0.008683286	g	sodium hypochlorite production, product in 15% solution state | sodium hypochlorite, without water, in 15% solution state | Cutoff, U - RER
Water	Process water	ST_water	m3	Softened water production, internal unit, TotalEnergies - PSS
	valorised water	valorized_water	m3	CC water valorization
	Wastewater treatment from power energy generation	wastewater_management_ct	m3	wastewater treatment, internal unit for water treatment, TotalEnergies - PSS
Output				
UF	Water management for 1 MJ cooling	1	MJ	
Water	Emission to air/unspecified	water_vapor_emissions_ct	m3	
	Transfer for DM	DM_transfer	M3	

A.5 Combined Cycle Process Unit

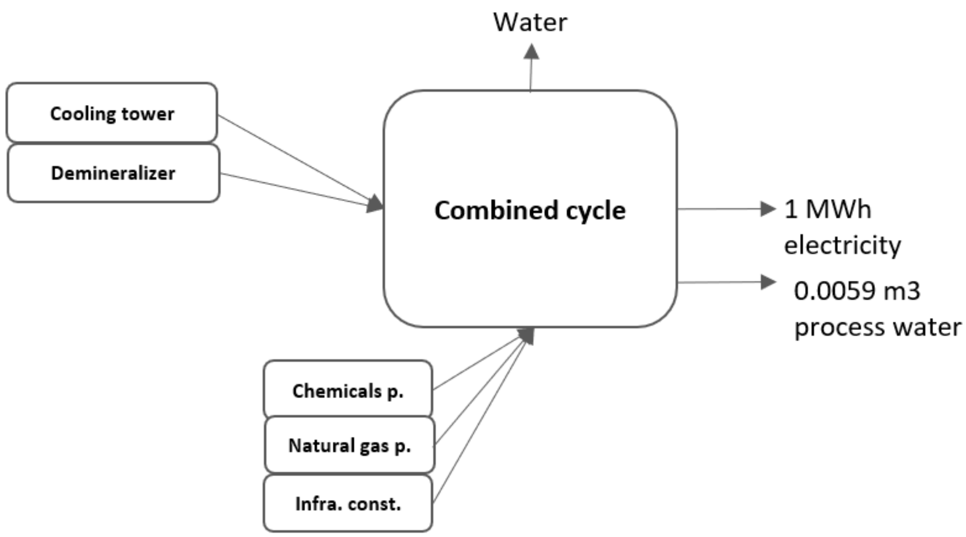

Figure A.4 Combined Cycle process unit system

Polluants emissions were calculated using ecoinvent database for similar combined cycle power plant.

Table A.7 Input parameters for combined cycle process unit

Input parameters			
Name	Value	Description	Data source
plant_capacity	440	MWh/h	Site data
cc_lifetime	180000	hours	Estimation
water_vapor_cc	1.36E-02	m3/MWh	Site data
av_electricity_production	369	MWh/h	Site data
demine_water	7.19E+00	m3/h	Site data

Table A.8 Dependent parameters for combined cycle process unit

Dependent parameters			
Name	Formula	Value	unit
power_plant_unit	1/(plant_capacity*cc_lifetime)	1.26E-08	unit
blow_down_cc_water	(factor_water_soft_MWh-water_vapor_cc)	5.91E-03	m3
water_completely_softned	demine_water/av_electricity_production	1.95E-02	m3
water_vapor_emissions_cc	water_vapor_cc	0.01363636	m3
factor_water_soft_MWh	demine_water/av_electricity_production	1.95E-02	m3/MWh

Table A.9 Input and output modeling for combined cycle process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	Ammonium 20.5%	3.25	g	Ammonium 20.5% production - created process - FR
	Ammonium 5%	0.975	g	Ammonium 5% production - created process - FR
	Carbohydrazide	3.24E-04	g	Carbohydrazide production - created process - FR
Fuel	natural gas, high pressure	405.2288707	m3	market for natural gas, high pressure | natural gas, high pressure | Cutoff, U - FR
Infra. Const.	gas power plant, combined cycle, 400MW electrical	power_plant_unit	Item(s)	gas power plant construction, combined cycle, 400MW electrical | gas power plant, combined cycle, 400MW electrical | Cutoff, U - RER

Table A.9 Input and output modeling for combined cycle process unit (continuation 1)

Water	Refrigeration	1914.545454	MJ	Cooling Tower refrigeration, recirculation, internal unit, TotalEnergies - PSS
	water, completely softened	1.95E-02	t	Demineralised water production, internal process TotalEnergies - PSS
Output				
UF	electricity, high voltage	1	MWh	
Water	Emission to air/unspecified	water_vapor_emissions_ct	m3	
	Transfer for CT, process water	blow_down_cc_water	m3	
Polluants	Acenaphthene	1.25E-08	kg	
	Acetaldehyde	1.26E-05	kg	
	Acetic acid	0.001912275	kg	
	Arsenic	6.50E-07	kg	
	Benzene	1.43E-05	kg	
	Benzo(a)pyrene	8.36E-09	kg	
	Beryllium	3.90E-08	kg	
	Butane	0.014634435	kg	
	Cadmium	3.57E-06	kg	
	Carbon dioxide, fossil	843.9296462	kg	
	Carbon monoxide, fossil	0.034768637	kg	
	Chromium	4.54E-06	kg	
	Cobalt	2.72E-07	kg	
	Dinitrogen monoxide	0.015440436	kg	

Table A.9 Input and output modeling for combined cycle process unit (continuation 2)

	Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin	4.58E-13	kg	
	Ethane	0.021651379	kg	
	Formaldehyde	5.10E-04	kg	
	Hexane	0.012532513	kg	
	Lead	1.63E-06	kg	
	Manganese	1.23E-06	kg	
	Mercury	1.09E-06	kg	
	Methane, fossil	0.015345612	kg	
	Nickel	6.81E-06	kg	
	Nitrogen oxides	0.403000112	kg	
	PAH, polycyclic aromatic hydrocarbons	1.26E-04	kg	
	Particulates, < 2.5 um	0.007759728	kg	
	Pentane	0.018174515	kg	
	Propane	0.011141768	kg	
	Propionic acid	2.53E-04	kg	
	Selenium	7.76E-08	kg	
	Sulfur dioxide	0.009039846	kg	
	Toluene	2.37E-05	kg	

A.6 Water management for Combined Cycle Process Unit

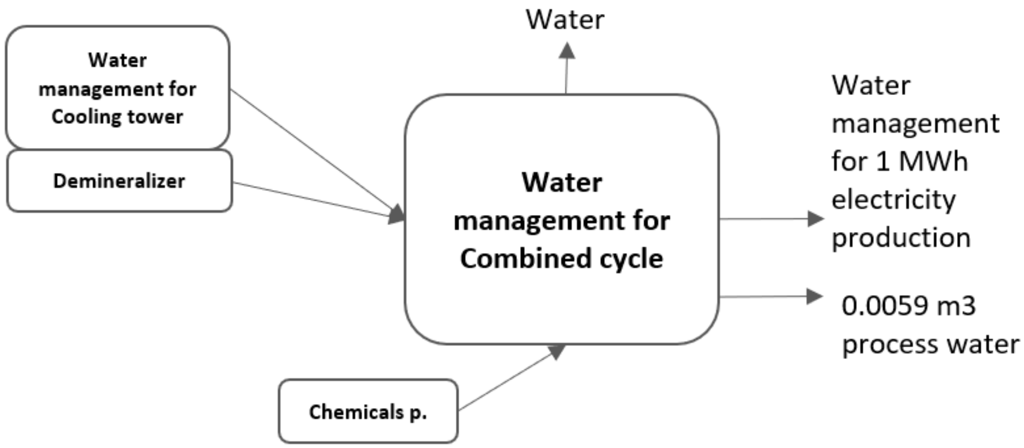

Figure A.5 Water management for Combined Cycle process unit system

Table A.10 Input and output modeling for water management for combined cycle process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	Ammonium 20.5%	3.25	g	Ammonium 20.5% production - created process - FR
	Ammonium 5%	0.975	g	Ammonium 5% production - created process - FR
	Carbohydrazide	3.24E-04	g	Carbohydrazide production - created process - FR

Table A.10 Input and output modeling for water management for combined cycle process unit (continuation)

Wate r	Refrigeration	1914.545454	MJ	Cooling Tower refrigeration, recirculation, internal unit, TotalEnergies - PSS
	water, completely softened	1.95E-02	t	Demineralise d water production, internal process TotalEnergies - PSS
Output				
UF	Water management for 1 MWh prouction	1	Uni t	
Wate r	Emission to air/unspecified	water_vapor_emissions_c t	m3	
	Transfer for CT, process water	blow_down_cc_water	m3	

A.7 Biological Wastewater Treatment Process Unit

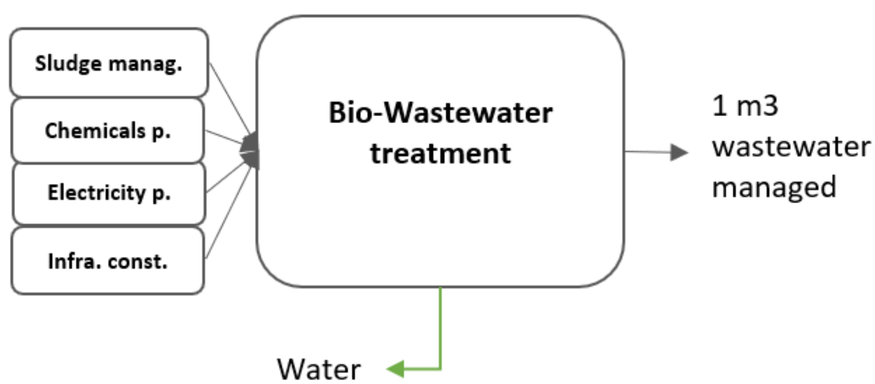

Figure A.6 Biological wastewater treatment process unit system

Table A.11 Input parameters for biological wastewater treatment process unit

Input parameters			
Name	Value	Description	Data source
acetic_acid_ww_con	161.3	g/m3	Site data
phosphoric_acid_ww_con	24.03	g/m3	Site data
floculant_ww_con	1.545	g/m3	Site data
ww_energy_con	8.42E-04	MWh/m3	Site data
unit_pss_capacity	100	m3/h	Technology provider
bod5_conc_ww	4.4	g/m3	Site data
chloride_conc_ww	112	g/m3	Site data
cod_conc_ww	7.5	g/m3	Site data
nitrogen_conc_ww	8.9	g/m3	Site data
phosphate_conc_ww	7.7	g/m3	Site data
sulfate_conc_ww	445	g/m3	Site data
ss_conc_ww	1.8	g/m3	Site data
WW_water_vapor	0.0066	m3/m3	Estimation
WW_water_sludge	0.05	%	Site data
sludge_ww_con	0.7105	kg/m3	Estimation

Table A.12 Dependent parameters for biological wastewater treatment process unit

Dependent parameters			
Name	Formula	Value	unit
acetic_acid_ww	(acetic_acid_ww_con*SC1)+(acetic_acid_ww_con*sc2*(1/RO_recovery_rate))	322.6	g
phosphoric_acid_ww	(phosphoric_acid_ww_con*SC1)+(phosphoric_acid_ww_con*sc2*(1/RO_recovery_rate))	48.06	g
praestol_k255l_ww	(floculant_ww_con*SC1)+(floculant_ww_con*sc2*(1/RO_recovery_rate))	3.09	g
electricity_pss_ww	(ww_energy_con*SC1)+(ww_energy_con*SC2*(1/(1-ro_recovery_rate)))	0.0016846	MWh
total_capacity	unit_pss_capacity *24*365*20	17520000	m3
unit	1/total_capacity	5.70776E-08	unit
BOD_emissions_water_ww	bod5_conc_ww*water_emissions_water_ww*sc1+(bod5_conc_ww/(1-ro_recovery_rate))*water_emissions_water_ww*sc2	8.74160738	g/m3
chloride_emissions_water_ww	chloride_conc_ww*water_emissions_water_ww*sc1+(chloride_conc_ww/(1-ro_recovery_rate))*water_emissions_water_ww*sc2	222.5136424	g/m3
COD_emissions_water_ww	cod_conc_ww*water_emissions_water_ww*sc1+(cod_conc_ww/(1-ro_recovery_rate))*water_emissions_water_ww*sc2	14.90046712	g/m3
FW_BOD5	BOD_emissions_water_ww*FW_emi	8.74160738	g/m3
FW_chloride	chloride_emissions_water_ww*fw_emi	222.5136424	g/m3
FW_COD	COD_emissions_water_ww*FW_emi	14.90046712	g/m3
FW_nitrogen	nitrogen_emissions_water_ww*FW_emi	17.68188766	g/m3
FW_phosphate	phosphate_emissions_water_ww*fw_emi	15.29781292	g/m3
FW_sulfate	sulfate_emissions_water_ww*fw_emi	884.0943827	g/m3

Table A.12 Dependent parameters for biological wastewater treatment process unit (continuation 1)

FW_TDS	TDS_emissions_water_ww*FW_emi	3.57611211	g/m3
nitrogen_emissions_water_ww	nitrogen_conc_ww*water_emissions_water_ww*sc1+(nitrogen_conc_ww/(1-ro_recovery_rate))*water_emissions_water_ww*sc2	17.68188766	g/m3
Oc_BOD5	BOD_emissions_water_ww*OC_emi	0	g/m3
OC_chloride	chloride_emissions_water_ww*oc_emi	0	g/m3
OC_COD	COD_emissions_water_ww*OC_emi	0	g/m3
OC_nitrogen	nitrogen_emissions_water_ww*OC_emi	0	g/m3
OC_phosphate	phosphate_emissions_water_ww*oc_emi	0	g/m3
OC_sulfate	sulfate_emissions_water_ww*oc_emi	0	g/m3
OC_TDS	TDS_emissions_water_ww*OC_emi	0	g/m3
phosphate_emissions_water_ww	phosphate_conc_ww*water_emissions_water_ww*sc1+(phosphate_conc_ww/(1-ro_recovery_rate))*water_emissions_water_ww*sc2	15.29781292	g/m3
sulfate_emissions_water_ww	sulfate_conc_ww*water_emissions_water_ww*sc1+(sulfate_conc_ww/(1-ro_recovery_rate))*water_emissions_water_ww*sc2	884.0943827	g/m3
TDS_emissions_water_ww	ss_conc_ww*water_emissions_water_ww*sc1+(ss_conc_ww/(1-ro_recovery_rate))*water_emissions_water_ww*sc2	3.57611211	g/m3
water_emissions_air_ww	WW_water_vapor	0.0066	m3
water_emissions_water_ww	1-water_emissions_air_ww-water_sludge	0.993364475	m3
water_sludge	(WW_water_sludge*sludge_ww_con)/1000	0.000035525	m3
Water_river_ww	water_emissions_water_ww-1	-0.00664	m3
Water_river_ct_dm	water_emissions_water_ww-Water_river_ww	1.00E+00	m3

Table A.13 Input and output modeling for biological wastewater treatment process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	acetic acid, without water, in 98% solution state	acetic_acid_ww	g	acetaldehyde oxidation | acetic acid, without water, in 98% solution state | Cutoff, U - RER
	phosphoric acid, industrial grade, without water, in 85% solution state	phosphoric_acid_ww	g	purification of wet-process phosphoric acid to industrial grade, product in 85% solution state | phosphoric acid, industrial grade, without water, in 85% solution state | Cutoff, U - RER
	Praestol K255L	praestol_k255l_ww	g	Praestol K255L production - created process - FR
Energy prod.	electricity, high voltage	electricity_pss_ww	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	watewater facility	unit	Item(s)	WW unit construction
Sludge manag.	sludge	1	Item(s)	wastewater treatment, internal unit for water treatment, TotalEnergies - Sludge
Output				
UF	wastwater treatmwnt for power wnwergy	1	m3	
Polluants	BOD5, Biological Oxygen Demand - ocean	Oc_BOD5	g	

Table A.13 Input and output modeling for biological wastewater treatment process unit (continuation)

	BOD5, Biological Oxygen Demand - freshwater	FW_BOD5	g	
	Chloride - ocean	OC_chloride	g	
	Chloride - freshwater	FW_chloride	g	
	COD, Chemical Oxygen Demand - ocean	OC_COD	g	
	COD, Chemical Oxygen Demand - freshwater	FW_COD	g	
	Nitrogen - ocean	OC_nitrogen	g	
	Nitrogen - freshwater	FW_nitrogen	g	
	Phosphate - ocean	OC_phosphate	g	
	Phosphate - freshwater	FW_phosphate	g	
	Sulfate - ocean	OC_sulfate	g	
	Sulfate - freshwater	FW_sulfate	g	
	Suspended solids, unspecified - ocean	OC_TDS	g	
	Suspended solids, unspecified - freshwater	FW_TDS	g	
Water	Water - air	water_emissions_air_ww	m3	
	Water, country, river	Water_river_ww	m3	
	Water, country, river	Water_river_ct_dm	m3	

A.8 Demineralization Process Unit

Table A.14 Input parameters for demineralization process unit

Input parameters			
Name	Value	Description	Source
infra_capacity	2.80E+06	m3	Membrane manufacturer estimation. 20 years life expectation.
sodium_hydroxide_dm_con	9.45E+02	g/m3	Site data
red_reg_dm_SC2	5.50E+00	dimensionless	Estimation
red_reg_dm_SC3	8.31E+00	dimensionless	Estimation
sulfuric_acid_30_dm_con	2.78E+02	g/m3	Site data
sulfuric_acid_37_dm_con	2.53E+03	g/m3	Site data
electricity_pss_dm_cons	1.02E+01	kW	Site data
demine_water_production	8.60E+00	m3/h	Site data
demine_water_regen	6.00E-01	m3/h	Site data

Table A.15 Dependent parameters for demineralization process unit

Dependent parameters			
Name	Formula	Value	unit
infra	1/infra_capacity	3.58E-07	unit
electricity_pss_dm	(electricity_pss_dm_cons/demine_water_production)/1000	1.18E-03	MWh
sodium_hydroxide_dm	(sodium_hydroxide_dm_con*sc1)+(sodium_hydroxide_dm_con*sc2/red_reg_dm_SC2)+(sodium_hydroxide_dm_con*sc3/red_reg_dm_SC3)	1.72E+02	g

Table A.15 Dependent parameters for demineralization process unit (continuation 1)

sulfuric_acid_30_dm	(sulfuric_acid_30_dm_con*sc1)+(sulfuric_acid_30_dm_con*sc2/red_reg_dm_sc2)+(sulfuric_acid_30_dm_con*sc3/red_reg_dm_sc3)	5.05E+01	g
sulfuric_acid_37_dm	(sulfuric_acid_37_dm_con*sc1)+(sulfuric_acid_37_dm_con*sc2/red_reg_dm_sc2)+(sulfuric_acid_37_dm_con*sc3/red_reg_dm_sc3)	4.59E+02	g
processwater_recovery_cr_dm	(recycle_cr_dm)*sc3	0.00E+00	m3
processwater_recovery_ev_dm	(recycle_ev_dm)*sc3	0.00E+00	m3
processwater_recovery_ro_dm	(((recycle_ro_dm)*sc2)+(recycle_ro_dm)*sc3)	0.00E+00	m3
ST_water_reg	water_softened_dm_reg*st	6.98E-02	m3
ST_water_prod	water_softened_dm_prod*st	1.00E+00	m3
water_softened_dm_prod	1*sc1	1.00E+00	m3
water_softened_dm_reg	(inlet_dm_water-1)*sc1	6.98E-02	m3
TW_water_prod	water_softened_dm_prod*TW	0.00E+00	m3
TW_water_reg	water_softened_dm_reg*TW	0.00E+00	m3
wastewater_management_dm	((outlet_dm_water*sc1)+(wastewater_ro_dm*sc2)-(0*sc3))	6.98E-02	m3
inlet_dm_water	((demine_water_production+demine_water_regen)/demine_water_production)*SC1+((demine_water_production+demine_water_regen_red)/demine_water_production)*(SC2+SC3)	1.07E+00	m3/m3
outlet_dm_water	((demine_water_regen)/demine_water_production)*SC1+((demine_water_regen_red)/demine_water_production)*(SC2+SC3)	6.98E-02	m3/m3
demine_water_regen_red	demine_water_regen/(SC1+(red_reg_dm_sc2*SC2)+(red_reg_dm_sc3*SC3))	6.00E-01	-

Table A.15 Dependent parameters for demineralization process unit (continuation 2)

recycle_cr_dm	(wastewater_ev_dm*cr_recovery_rate)	6.13E-04	m3/m3
recycle_ev_dm	(wastewater_ro_dm*ev_recovery_rate)	3.42E-02	m3/m3
recycle_ro_dm	(outlet_dm_water*ro_recovery_rate)	3.49E-02	m3/m3
wastewater_cr_dm	wastewater_ev_dm-(wastewater_ev_dm*cr_recovery_rate)	4.12E-05	m3/m3
wastewater_ev_dm	wastewater_ro_dm-(wastewater_ro_dm*ev_recovery_rate)	6.55E-04	m3/m3
wastewater_ro_dm	outlet_dm_water-(outlet_dm_water*ro_recovery_rate)	3.49E-02	m3/m3
water_transfer_prod	(inlet_dm_water-processwater_recovery_ro_dm)*sc2+(inlet_dm_water -processwater_recovery_ro_dm -processwater_recovery_ev_dm -processwater_recovery_cr_dm)*sc3	0.00E+00	m3/m3
water_transfer_rec	(inlet_dm_water-processwater_recovery_ro_dm-1)*sc2+(inlet_dm_water -processwater_recovery_ro_dm -processwater_recovery_ev_dm -processwater_recovery_cr_dm -1)*sc3	0.00E+00	m3/m3

Table A.16 Input and output modeling for demineralization unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	sodium hydroxide, without water, in 50% solution state	sodium_hydroxide_dm	g	chlor-alkali electrolysis, membrane cell | sodium hydroxide, without water, in 50% solution state | Cutoff, U - RER
	Sulfuric acid 30%	sulfuric_acid_30_dm	g	Sulfuric acid 30% production - created process - FR
	Sulfuric acid 37.5%	sulfuric_acid_37_dm	g	Sulfuric acid 37.5% production - created process - FR
Energy prod.	electricity, high voltage	electricity_pss_dm	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	Infrastructure	infra	Item(s)	Demineralised water production, internal process TotalEnergies - Infra
Water	Process water, recovered	processwater_recovery_ev_dm	m3	Evaporateur, internal unit, TotalEnergies
	Process water, recovered	processwater_recovery_ro_dm	m3	Reverse osmosis, internal unit, TotalEnergies
	Process water, recovered	processwater_recovery_cr_dm	m3	Crystalliser, internal unit, TotalEnergies
	Process water, desalination	TW_water_prod	t	Tap water production - GLO
	Process water, desalination	TW_water_reg	t	Tap water production - GLO

Table A.16 Input and output modeling for demineralization unit (continuation)

	Wastewater treatment from power energy generation	wastewater_management_dm	m3	wastewater treatment, internal unit for water treatment, TotalEnergies - PSS
	Transfer water from CT	water_transfer_prod	m3	RO recovered water
	Transfer water from CT	water_transfer_rec	m3	RO recovered water
	Process water, softened	ST_water_reg	t	Softened water production, internal unit, TotalEnergies - PSS
	Process water, softened	ST_water_prod	t	Softened water production, internal unit, TotalEnergies - PSS
Output				
UF	water, completely softened	1000	kg	

A.9 Reverse Osmosis Process Unit

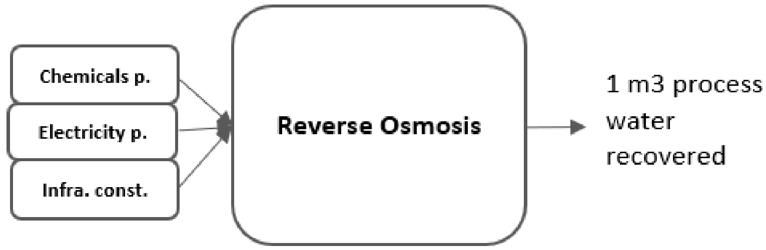

Figure A.7 Reverse osmosis process unit system

Table A.17 Input parameters for Reverse Osmosis process unit

Input parameters			
Name	Value	Description	Data source
antiscale_ro_con	5	g/m3	Internal study
bissulfite_ro_con	5	g/m3	Internal study
sulfuric_acid_30_ro_co	0	g/m3	Internal study

Table A.18 Dependent parameters for Reverse Osmosis process unit

Dependent parameters			
Name	Formula	Value	unit
DC5702_ro	antiscale_ro_con/ro_recovery_rate	10	g
sulfite	bissulfite_ro_con/ro_recovery_rate	10	g
sulfuric_acid_30	sulfuric_acid_30_ro_con/ro_recovery_rate	0	g
electricity_pss_ro	ro_energy_con	variable	MWh

Table A.19 Input and output modeling for Reverse Osmosis process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	Hypersense MSI310	DC5702_ro	g	Hypersense MSI310 production - created process - FR
	sodium hydrogen sulfite	sulfite	g	sodium hydrogen sulfite production | sodium hydrogen sulfite | Cutoff, U - RER
	Sulfuric acid 30%	sulfuric_acid_30	g	Sulfuric acid 30% production - created process - FR
Energy prod.	electricity, high voltage	electricity_pss_ro	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	RO infrastructure	1.00E+00	Item(s)	Reversis osmosis, internal unit, TotalEnergies - Infra
Output				
UF	process water recovered	1	m3	

A.10 Evaporator Process Unit

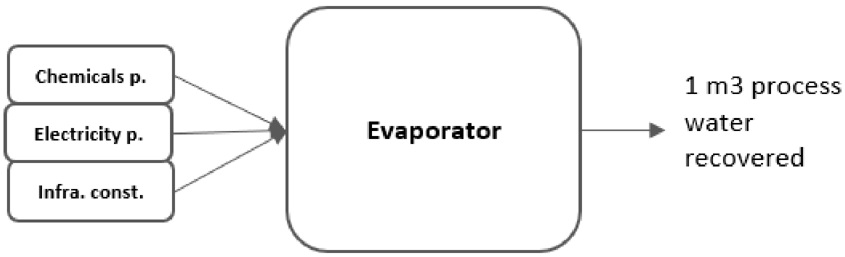

Figure A.8 Evaporator process unit system

Table A.20 Input parameters for Evaporator process unit

Input parameters			
Name	Value	Description	Data source
antifoam_conc_ev	0.024	kg/m3	Internal study
antiscale_conc_ev	0.01	kg/m3	Internal study
hcl_conc_ev	0.53	kg/m3	Internal study
electricity_pss_ev	0.01486	MWh/m3	[26]
building_machine_lifetime_capacity	3.75E+08	m3	[52]

Table A.21 Dependent parameters for Evaporator process unit

Dependent parameters			
Name	Formula	Value	unit
antifoam	antifoam_conc_ev/ev_recovery_rate	0.0244589	kg/m3
antiscale	antiscale_conc_ev/ev_recovery_rate	0.0101912	kg/m3
hydrochloric_acid	hcl_conc_ev/ev_recovery_rate	0.5401343	kg/m3
building_machine_ev	1/building_machine_lifetime_capacity	2.67E-09	1/m3

Table A.22 Input and output modeling for Evaporator process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Chemicals prod.	antifoam	antifoam	kg	Antifoam production, created process for Total energies
	hydrochloric acid, without water, in 30% solution state	hydrochloric_acid	kg	allyl chloride production, reaction of propylene and chlorine | hydrochloric acid, without water, in 30% solution state | Cutoff, U - RER
	Performax DC5702	antiscale	kg	Performax DC5702 production - created process - FR
Energy prod.	electricity, high voltage	electricity_pss_ev	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	RO infrastructure	building_machine_ev	Item(s)	building machine production | MED | Cutoff, U
Output				
UF	process water recovered	1	m3	

A.11 Crystallizer Process Unit

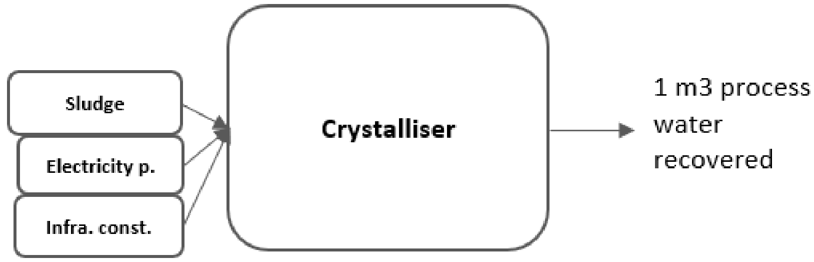

Figure A.9 Crystallizer process unit system

Table A.23 Input parameters for Crystallizer process unit

Input parameters			
Name	Value	Description	Data source
electricity_pss_cr	0.06	MWh/m3	[14]
building_machine_lifetime_capacity	375000000	m3	[52]

Table A.24 Dependent parameters for Crystallizer process unit

Dependent parameters			
Name	Formula	Value	unit
building_machine_cr	1/building_machine_lifetime_capacity	2.67E-09	Unit

Table A.25 Input and output modeling for Crystallizer process unit

Inputs				
Category	Flow	Amount	Unit	Provider ecoinvent
Energy prod.	electricity, high voltage	electricity_pss_cr	MWh	Electricity production, combined cycle, natural gas, TotalEnergies - Electricity
Infra. Const.	Building machine MED	building_machine_cr	Item(s)	building machine production | MED | Cutoff, U
Sludge		1	Item(s)	Crystallizer internal unit, TotalEnergies - Sludge
Output				
UF	process water recovered	1	m3	

A.12 Drewfloc 274

Drewfloc 274 is a commercial name for flocculant-aid agent. 100% polyacrilamida concentration was assumed based on the product flowsheet [53].

Table A.26 Input and output modeling for Drewfloc 274 production

Input			
Flow	Amount	Unit	Provider ecoinvent
Polyacrylamide	1	kg	market for polyacrylamide | polyacrylamide | Cutoff, U - GLO
Output			
Drewfloc 274	1	kg	Drewfloc 274 production - created process - FR

A.13 Ferric sulfate 44%

Ferric sulfate is a coagulant-aid chemical. Due to its concentration, a created process was chosen to best represent the specie.

Table A.27 Input and output modeling for Ferric sulfate 44% production

Input			
Flow	Amount	Unit	Provider ecoinvent
iron sulfate	0.44	kg	market for iron sulfate | iron sulfate | Cutoff, U - RER
water, deionised	0.56	kg	water production, deionised | water, deionised | Cutoff, U - Europe without Switzerland
Output			
Ferric sulfate 44%	1	kg	Ferric sulfate 44% production- created process - FR

A.14 Quicklime

Already provided by Ecoinvent database.

Table A.28 Input and output modeling for Quicklime production

Process used to describe	
Flow	Provider ecoinvent
lime, hydrated, packed	market for lime, hydrated, packed | lime, hydrated, packed | Cutoff, U - RER

A.15 Performax DC5702

Performax DC5702 is a commercial name for anti scaling agent. Due to insufficient data, a process was created to represent the solution using the main components. An 50-50% mixture was chosen based on the product flowsheet [54].

Table A.29 Input and output modeling for Performax DC5702 production

Input			
Flow	Amount	Unit	Provider ecoinvent
organophosphorus-compound, unspecified	0.5	kg	organophosphorus-compound production, unspecified | organophosphorus-compound, unspecified | Cutoff, U - RER
polycarboxylates, 40% active substance	0.5	kg	market for polycarboxylates, 40% active substance | polycarboxylates, 40% active substance | Cutoff, U - RER
Output			
Performax DC5702	1	kg	Performax DC5702 production - created process - FR

A.16 Performax DC5801

This chemical additive is a mixture of complex compounds that were not founded in ecoinvent database. As consequence, they were substitute by precursors or similar compounds describes in the product flowsheet [55].

Table A.30 Input and output modeling for Performax DC5801 production

Input			
Flow	Amount	Unit	Provider ecoinvent
benzo[thia]diazole-compound	1.50E-05	kg	benzo[thia]diazole-compound production | benzo[thia]diazole-compound | Cutoff, U - RER
nitro-compound	1.00E-04	kg	nitro-compound production | nitro-compound | Cutoff, U - RER
vegetable oil, refined	0.999885	kg	market for vegetable oil, refined | vegetable oil, refined | Cutoff, U - GLO
Output			
Performax DC5801	1	kg	Performax DC5801 production - created process - FR

A.17 Sodium Hypochlorite

Table A.31 Input and output modeling for Sodium Hypochlorite production

Process used to describe	
Flow	Provider ecoinvent
sodium hypochlorite, without water, in 15% solution state	sodium hypochlorite production, product in 15% solution state | sodium hypochlorite, without water, in 15% solution state | Cutoff, U - RER

A.18 Sodium Hydroxide

Table A.32 Input and output modeling for Sodium Hydroxide production

Process used to describe	
Flow	Provider ecoinvent
sodium hydroxide, without water, in 50% solution state	chlor-alkali electrolysis, membrane cell | sodium hydroxide, without water, in 50% solution state | Cutoff, U - RER

A.19 Sulfuric Acid 30%

Sulfuric Acid was already modeled in Ecoinvent database; however, deionized water was added to best represent the used concentration.

Table A.33 Input and output modeling for Sulfuric Acid 30% production

Input			
Flow	Amount	Unit	Provider ecoinvent
sulfuric acid	0.3	kg	sulfuric acid production | sulfuric acid | Cutoff, U - RER
water, deionised	0.7	kg	water production, deionised | water, deionised | Cutoff, U - Europe without Switzerland
Output			
Sulfuric acid 30%	1	kg	Sulfuric acid 30% production - created process - FR

A.20 Sulfuric Acid 37.5%

Sulfuric Acid was already modeled in Ecoinvent database; however, deionized water was added to best represent the used concentration.

Table A.34 Input and output modeling for Sulfuric Acid 37.5% production

Input			
Flow	Amount	Unit	Provider ecoinvent
sulfuric acid	0.375	kg	sulfuric acid production | sulfuric acid | Cutoff, U - RER
water, deionised	0.625	kg	water production, deionised | water, deionised | Cutoff, U - Europe without Switzerland
Output			
Sulfuric acid 37.5%	1	kg	Sulfuric acid 37.5% production - created process - FR

A.21 Ammonium 20.5%

Ammonium was already modeled in Ecoinvent database; however, deionized water was added to best represent the used concentration.

Table A.35 Input and output modeling for Ammonium 20.5% production

Input			
Flow	Amount	Unit	Provider ecoinvent
ammonia, anhydrous, liquid	0.205	kg	market for ammonia, anhydrous, liquid | ammonia, anhydrous, liquid | Cutoff, U - RER
water, deionised	0.795	kg	water production, deionised | water, deionised | Cutoff, U - Europe without Switzerland
Output			
Ammonium 20.5%	1	kg	Ammonium 20.5% production - created process - FR

A.22 Ammonium 5%

Ammonium was already modeled in Ecoinvent database; however, deionized water was added to best represent the used concentration.

Table A.36 Input and output modeling for Ammonium 5% production

Input			
Flow	Amount	Unit	Provider ecoinvent
ammonia, anhydrous, liquid	0.05	kg	market for ammonia, anhydrous, liquid | ammonia, anhydrous, liquid | Cutoff, U - RER
water, deionised	0.95	kg	water production, deionised | water, deionised | Cutoff, U - Europe without Switzerland
Output			
Ammonium 5%	1	kg	Ammonium 5% production - created process - FR

A.23 Carbohydrazide

Carbohydrazide (IUPAC 1,3-Diaminourea) production is based on the reaction $OC(NH2)2 + 2\ N2H4 \rightarrow OC(N2H3)2 + 2\ NH3$ [56]. As the substance was not in ecoinvent database, its precursors were selected. Ammonia production was not considered.

Table A.37 Input and output modeling for Carbohydrazide production

Input			
Flow	Amount	Unit	Provider ecoinvent
hydrazine	60	kg	market for hydrazine | hydrazine | Cutoff, U - RER
urea	64	kg	market for urea | urea | Cutoff, U - RER
Output			
Carbohydrazide	90	kg	Carbohydrazide production - created process - FR

A.24 Acetic Acid

Table A.38 Input and output modeling for Acetic Acid production

Process used to describe	
Flow	Provider ecoinvent
acetic acid, without water, in 98% solution state	acetaldehyde oxidation | acetic acid, without water, in 98% solution state | Cutoff, U - RER

A.25 Phosphoric Acid

Table A.39 Input and output modeling for Phosphoric Acid production

Process used to describe	
Flow	Provider ecoinvent
phosphoric acid, industrial grade, without water, in 85% solution state	purification of wet-process phosphoric acid to industrial grade, product in 85% solution state | phosphoric acid, industrial grade, without water, in 85% solution state | Cutoff, U - RER

A.26 Praestol K255L

It is a water-soluble polyelectrolytes flocculant. Due to no data source, it was modeled as polyacrylamide compound. [57]

Table A.40 Input and output modeling for Praestol K255L production

Input			
Flow	Amount	Unit	Provider ecoinvent
Polyacrylamide	1	kg	market for polyacrylamide | polyacrylamide | Cutoff, U - GLO
Output			
Praestol K255L	1	kg	Praestol K255L production - created process - FR

A.27 Hypersense MSI310

It is a polymer silica antiscaling [58]. However, its composition was not founded. Due to its function, it was assumed similar composition to Performax DC5702.

Table A.41 Input and output modeling for Hypersense MSI310 production

Input			
Flow	Amount	Unit	Provider ecoinvent
organophosphorus-compound, unspecified	0.5	kg	organophosphorus-compound production, unspecified | organophosphorus-compound, unspecified | Cutoff, U - RER
polycarboxylates, 40% active substance	0.5	kg	market for polycarboxylates, 40% active substance | polycarboxylates, 40% active substance | Cutoff, U - RER
Output			
Hypersense MSI310	1	kg	Hypersense MSI310 production - created process - FR

A.28 Sulfite

Table A.42 Input and output modeling for Sulfite production

Process used to describe	
Flow	Provider ecoinvent
sodium hydrogen sulfite	sodium hydrogen sulfite production | sodium hydrogen sulfite | Cutoff, U - RER

A.29 Antifoam

There was not a specific antifoam agent. A commercial product was chosen. Antifoam agents are silicone-based agents [59].

Table A.43 Input and output modeling for Antifoam production

Input			
Flow	Amount	Unit	Provider ecoinvent
silicone product	1	kg	market for silicone product | silicone product | Cutoff, U - RER
Output			
Antifoam	1	kg	Antifoam production, created process for Total energies

A.30 Hydrochloric acid

Table A.44 Input and output modeling for Hydrochloric acid production

Process used to describe	
Flow	Provider ecoinvent
hydrochloric acid, without water, in 30% solution state	allyl chloride production, reaction of propylene and chlorine | hydrochloric acid, without water, in 30% solution state | Cutoff, U - RER

A.31 Softening Unit infrastructure

The softening unit infrastructure was called decarbo due to decarbonatation process. Its data was estimated using provider technology data and local measurements. It was considered 20 years life expectation and 480 m3/h production capacity.

This infrastructure is mostly made by concrete, including treatment reservoirs and building. Chemicals stockage are composed by polymers as well as tubulation. However, the later was difficult to estimate and therefore was not considered. Pumps and valves were considered as stainless steel.

Table A.45 Input parameters for Softening Unit infrastructure production

Input parameters		
Name	Value	Description
concrete_density	2400	kg/m3
concrete_total	1087	m3
PE_density	900	kg/m3
PE_total	0.13	m3
PP_density	900	kg/m3
PP_total	0.19	m3
steel_density	7850	kg/m3
steel_total	1.24	m3

Table A.46 Dependent parameters for Softening Unit infrastructure production

Dependent parameters			
Name	Formula	Value	unit
concrete_total_mass	concrete_total *concrete_density	2608800	kg
PE_total_mass	PE_total *PE_density	117	kg
PP_total_mass	pp_total *pp_density	171	kg
steel_total_mass	steel_total *steel_density	9734	kg

Table A.47 Input and output modeling for Softening Unit infrastructure production

Input			
Flow	Amount	Unit	Provider ecoinvent
concrete, normal	1087	m3	market for concrete, normal | concrete, normal | Cutoff, U - RoW
polyethylene, high density, granulate	117	kg	market for polyethylene, high density, granulate | polyethylene, high density, granulate | Cutoff, U - GLO
polypropylene, granulate	171	kg	polypropylene production, granulate | polypropylene, granulate | Cutoff, U - RER
reinforcing steel	9734	kg	reinforcing steel production | reinforcing steel | Cutoff, U - Europe without Austria
Output			
Decarbo	1	Item	Decarbo construction
scrap steel	9734	kg	market for scrap steel | scrap steel | Cutoff, U - Europe without Switzerland
waste concrete	2608800	kg	market for waste concrete | waste concrete | Cutoff, U - Europe without Switzerland
waste polyethylene	117	kg	market group for waste polyethylene | waste polyethylene | Cutoff, U - Europe without Switzerland
waste polypropylene	171	kg	market group for waste polypropylene | waste polypropylene | Cutoff, U - Europe without Switzerland

A.32 Cooling Tower infrastructure

The necessary raw material was taken from literature [47, 60]. It was considered 20 years life expectation, and no capacity was found. Electric motors were substituted by heat pump production with same power capacity.

Table A.48 Input and output modeling for Cooling Tower infrastructure production

Input			
Flow	Amount	Unit	Provider ecoinvent
ferrochromium, high-carbon, 55% Cr	850	kg	market for ferrochromium, high-carbon, 55% Cr | ferrochromium, high-carbon, 55% Cr | Cutoff, U - GLO
heat pump, 30kW	0.6	item	heat pump production, 30kW | heat pump, 30kW | Cutoff, U - RER
heat pump, 30kW	0.5	item	heat pump production, 30kW | heat pump, 30kW | Cutoff, U - RER
polyvinylchloride, bulk polymerised	192.3	kg	market for polyvinylchloride, bulk polymerised | polyvinylchloride, bulk polymerised | Cutoff, U - GLO
Output			
Cooling tower	1	Item	Cooling tower construction
electronics scrap	735	kg	
scrap steel	850	kg	market for scrap steel | scrap steel | Cutoff, U - Europe without Switzerland
waste polyvinylchloride	192.3	kg	market for waste polyvinylchloride | waste polyvinylchloride | Cutoff, U - FR

A.33 Demineralization Unit infrastructure

Estimations were made using technical provider information.

Table A.49 Input parameters for Demineralization Unit infrastructure production

Input parameters		
Name	Value	Description
coal_density	2100	kg/m3
coal_volume	2.48719	m3
concrete_density	2400	kg/m3
concrete_volume	267.3	m3
pe_density	900	kg/m3
pe_volume	0.36322	m3
resin_an_density	820	kg/m3
resin_an_volume	1.39474	m3
resin_ca_density	820	kg/m3
resin_cat_volume	1.61769	m3
sand_density	1600	kg/m3
sand_volume	2.48719	m3
steel_density	8050	kg/m3
steel_volume	0.28516	m3

Table A.50 Dependent parameters for Demineralization Unit infrastructure production

Dependent parameters			
Name	Formula	Value	Unit
coal_mass	coal_volume *coal_density	5223.1074	kg
concrete_mass	concrete_volume *concrete_density	641520	kg
PE_mass	pe_volume *pe_density	326.894724	kg
resin_an_mass	resin_an_volume *resin_an_density	1143.687538	kg
resin_cat_mass	resin_cat_volume *resin_ca_density	1326.506062	kg
sand_mass	sand_volume *sand_density	3979.5104	kg
steel_mass	steel_volume *steel_density	2295.530755	kg

Table A.51 Input and output modeling for Demineralization Unit infrastructure production

Input			
Flow	Amount	Unit	Provider ecoinvent
activated carbon, granular	5223.11	kg	activated carbon production, granular from hard coal | activated carbon, granular | Cutoff, U - RER
anionic resin	1143.69	kg	market for anionic resin | anionic resin | Cutoff, U - RER
cationic resin	1326.51	kg	market for cationic resin | cationic resin | Cutoff, U - RER
concrete, normal	267.3	m3	market for concrete, normal | concrete, normal | Cutoff, U - RoW
polyethylene, low density, granulate	326.895	kg	market for polyethylene, low density, granulate | polyethylene, low density, granulate | Cutoff, U - GLO
reinforcing steel	2295.53	kg	reinforcing steel production | reinforcing steel | Cutoff, U - Europe without Austria
sand	3979.51	kg	market for sand | sand | Cutoff, U - RoW
Output			
Demineraliser	1	Item	Demineralised water production, internal process TotalEnergies - Infra
scrap steel	2295.53	kg	market for scrap steel | scrap steel | Cutoff, U - Europe without Switzerland
spent activated carbon, granular	5223.11	kg	
spent anion exchange resin from potable water production	1143.69	kg	market for spent anion exchange resin from potable water production | spent anion exchange resin from potable water production | Cutoff, U - RoW
spent cation exchange resin from potable water production	1326.51	kg	market for spent cation exchange resin from potable water production | spent cation exchange resin from potable water production | Cutoff, U - RoW
waste concrete	5223.11	kg	market for waste concrete | waste concrete | Cutoff, U - Europe without Switzerland
waste polyethylene	326.895	kg	market for waste polyethylene | waste polyethylene | Cutoff, U - FR

A.34 Combined Cycle infrastructure

It was not possible to estimate the required material to build the combined cycle structure. As consequence, this unit was approximated as a gas power plant of similar capacity already disponible in ecoinvent database.

Table A.52 Ecoinvent provider selected to Combined Cycle infrastructure production

Process used to describe	
Flow	Provider ecoinvent
gas power plant, combined cycle, 400MW electrical	gas power plant construction, combined cycle, 400MW electrical | gas power plant, combined cycle, 400MW electrical | Cutoff, U - RER

A.35 Bio-Wastewater Unit infrastructure

Estimations were made using local data and provider technical information. It is a 100 m3/h treatment capacity and considered 20 years life expectation.

Table A.53 Input parameters for Bio-wastewater Treatment Unit infrastructure production

Input parameters		
Name	Value	Description
concrete_density	2400	kg/m3
concrete_volume	786.28	m3
pp_density	900	kg/m3
pp_volume	6.087	m3
steel_density	8050	kg/m3
steel_volume	1.83	m3

Table A.54 Dependent parameters for Bio-wastewater Treatment Unit infrastructure production

Dependent parameters			
Name	Formula	Value	unit
concrete_mass	concrete_volume *concrete_density	1887072	kg
pp_mass	pp_volume *pp_density	5478.3	kg
steel_mass	steel_volume *steel_density	14731.5	kg

Table A.55 Input and output modeling for Bio-wastewater Treatment Unit infrastructure production

Input			
Flow	Amount	Unit	Provider ecoinvent
concrete, normal	786.28	m3	market for concrete, normal | concrete, normal | Cutoff, U - RoW
polypropylene, granulate	5478.3	kg	polypropylene production, granulate | polypropylene, granulate | Cutoff, U - RER
reinforcing steel	14731.5	kg	reinforcing steel production | reinforcing steel | Cutoff, U - Europe without Austria
sand	24	kg	market for sand | sand | Cutoff, U - RoW
Output			
wastewater facility	1	Item	WW unit construction
scrap steel	14731.5	kg	market for scrap steel | scrap steel | Cutoff, U - Europe without Switzerland
waste concrete	1887072	kg	market for waste concrete | waste concrete | Cutoff, U - Europe without Switzerland
waste polypropylene	117	kg	market group for waste polyethylene | waste polyethylene | Cutoff, U - Europe without Switzerland

A.36 Reverse Osmosis infrastructure

Reverse Osmose infrastructure has the particularity of being different according to the scenario. For 50% recovery scenarios, it is constituted by ultrafiltration followed by reverse osmosis membranes. To estimate this infrastructure, a TotalEnergies internal study was used. For higher RO recovery rates, an additional membrane module is necessary. This additional module is activated if NF variable has the value of 1 according to the Table A.1.

Table A.56 Input parameters for Reverse Osmosis infrastructure production

Input parameters		
Name	Value	Description
filtrate_flow_rate	8.8	m3/h
RO_membranes	18	units
RO_surface	41	m2
total_life	20	years
UF_LIQUIFLUX_area	75	m3
UF_modules	4	units
UF_provider_area	50	m2

Table A.57 Dependent parameters for Reverse Osmosis infrastructure production

Dependent parameters			
Name	Formula	Value	unit
RO2_module	RO_surf*NF	0	m2
ro_module	0.00000169*1000	0.00169	unit
RO_surf	ro_total_surface /total_capacity	0.000478674	m2
RO_total_surface	ro_membranes*ro_surface	738	m2
total_capacity	filtrate_flow_rate *24*365*total_life	1541760	m3
UF_mod	uf_total_module/total_capacity	3.89166E-06	unit
UF_total_module	uf_modules *uf_LIQUIFLUX_area /uf_provider_area	6	unit

Table A.58 Input and output modeling for Reverse Osmosis infrastructure production

Input			
Flow	Amount	Unit	Provider ecoinvent
seawater reverse osmosis module	0.00048	m2	market for seawater reverse osmosis module | seawater reverse osmosis module | Cutoff, U - GLO
seawater reverse osmosis module	0	m2	market for seawater reverse osmosis module | seawater reverse osmosis module | Cutoff, U - GLO
ultrafiltration module	3.9E-06	Item	market for ultrafiltration module | ultrafiltration module | Cutoff, U - GLO
Output			
RO infrastructure	1	Item	Reversis osmosis, internal unit, TotalEnergies - Infra

A.37 Evaporator infrastructure

Due to lack of data, this infrastructure was modeled according to Multi-stage flash evaporator from a previous study [61].

Table A.59 Input parameters for Evaporator infrastructure production

Input parameters		
Name	Value	Description
normal_concrete_density	2400	kg/m3
normal_concrete_mass	6000	ton
reinforced_concrete_density	2500	kg/m3
reinforced_concrete_mass	2500	ton
steel_dencity	4430	kg/m3
steel_sheet_thikness	0.002	m
ti_steel_mass	100	ton

Table A.60 Dependent parameters for Evaporator infrastructure production

Dependent parameters			
Name	Formula	Value	unit
normal_concrete	normal_concrete_mass*1000/normal_concrete_density	2500	m3
reinforced_concrete	reinforced_concrete_mass*1000/reinforced_concrete_density	1000	m3
ti_steel	(ti_steel_mass*1000/steel_dencity)/steel_sheet_thikness	11286.68172	m2

Table A.61 Input and output modeling for Evaporator infrastructure production

Input			
Flow	Amount	Unit	Provider ecoinvent
cast iron	30	t	cast iron production | cast iron | Cutoff, U - RER
concrete, high exacting requirements	1000	m3	concrete production, for building construction, with cement CEM II/A | concrete, high exacting requirements | Cutoff, U - CH
concrete, normal	2500	m3	concrete, all types to generic market for concrete, normal strength | concrete, normal | Cutoff, U - RoW
iron-nickel-chromium alloy	826	t	iron-nickel-chromium alloy production | iron-nickel-chromium alloy | Cutoff, U - RER
steel, chromium steel 18/8	3370	t	steel production, electric, chromium steel 18/8 | steel, chromium steel 18/8 | Cutoff, U - RER
steel, low-alloyed	740	t	steel production, converter, low-alloyed | steel, low-alloyed | Cutoff, U - RER
steel, unalloyed	300	t	steel production, converter, unalloyed | steel, unalloyed | Cutoff, U - RER
tin plated chromium steel sheet, 2 mm	11286.7	m2	market for tin plated chromium steel sheet, 2 mm | tin plated chromium steel sheet, 2 mm | Cutoff, U - GLO
Output			
Evaporator	1	Item	building machine production | MSF | Cutoff, U

A.38 Crystallizer structure

Similar to evaporator, this structure were modelized base on the multi effect distillation from a previous study [61]

Table A.62 Input parameters for Crystallizer infrastructure production

Input parameters		
Name	Value	Description
concrete_density	2400	kg/m3
normal_concrete_density	2400	kg/m3
normal_concrete_mass	6000	ton
reinforced_concrete_density	2500	kg/m3
reinforced_concrete_mass	2500	ton

Table A.63 Dependent parameters for Crystallizer infrastructure production

Dependent parameters			
Name	Formula	Value	unit
normal_concrete	normal_concrete_mass*1000/normal_concrete_density	2500	m3
reinforced_concrete	reinforced_concrete_mass*1000/reinforced_concrete_density	1000	m3
total_concrete	(normal_concrete +reinforced_concrete)*concrete_density	8400000	kg

Table A.64 Input and output modeling for Crystallizer infrastructure production

Input			
Flow	Amount	Unit	Provider ecoinvent
cast iron	30	t	cast iron production | cast iron | Cutoff, U - RER
concrete, high exacting requirements	1000	m3	concrete production, for building construction, with cement CEM II/A | concrete, high exacting requirements | Cutoff, U - CH
concrete, normal	2500	m3	concrete, all types to generic market for concrete, normal strength | concrete, normal | Cutoff, U - RoW
iron-nickel-chromium alloy	3200	t	iron-nickel-chromium alloy production | iron-nickel-chromium alloy | Cutoff, U - RER
steel, chromium steel 18/8	230	t	steel production, electric, chromium steel 18/8 | steel, chromium steel 18/8 | Cutoff, U - RER
steel, low-alloyed	740	t	steel production, converter, low-alloyed | steel, low-alloyed | Cutoff, U - RER
steel, unalloyed	300	t	steel production, converter, unalloyed | steel, unalloyed | Cutoff, U - RER
Output			
Evaporator	1	Item	building machine production | MED | Cutoff, U
scrap steel	4500	t	market for scrap steel | scrap steel | Cutoff, U - Europe without Switzerland
waste concrete	8400000	kg	market for waste concrete | waste concrete | Cutoff, U - Europe without Switzerland

APPENDIX B ZDL OPTIONS

B.1 ZLD option 1 energy integration

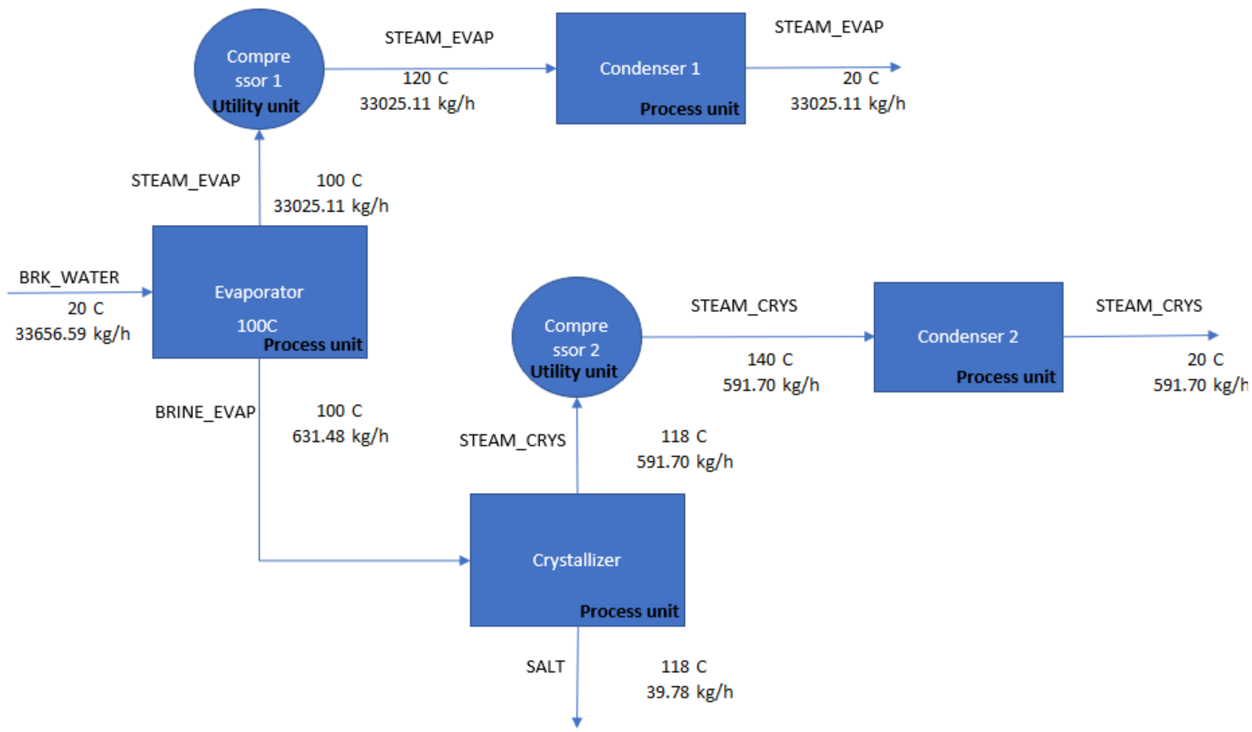

Figure B.1 ZLD option 1 hot streams for water recovery system used for energy integration.

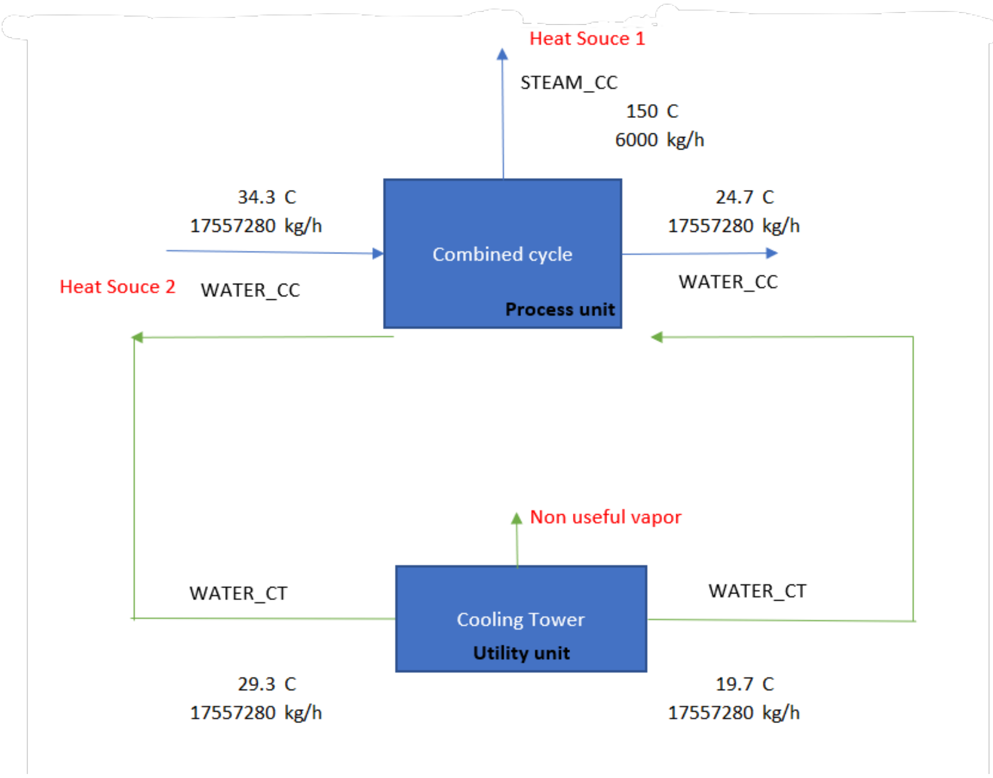

Figure B.2 Combined cycle and cooling tower hot streams used for energy integration.

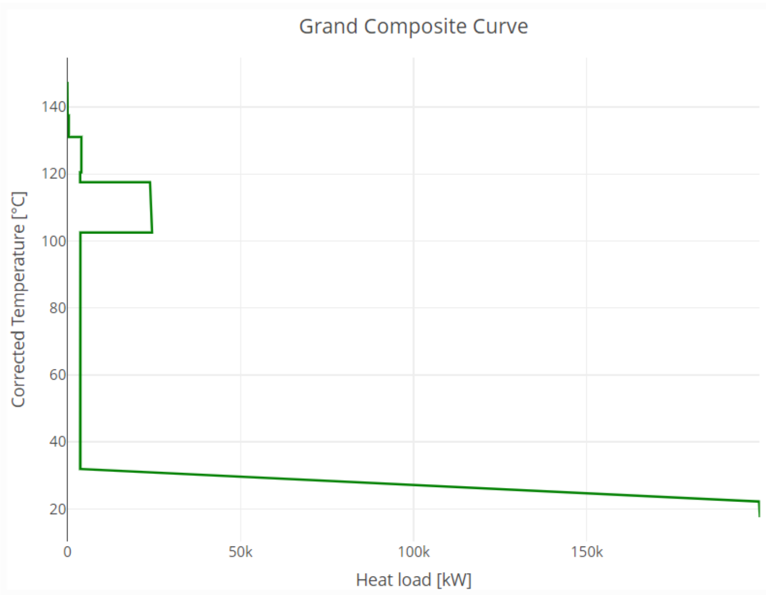

Figure B.3 Grand composite curve resulted from ROSMOSE simulation for ZLD option 1.

B.2 ZLD configuration 1 energy consumption

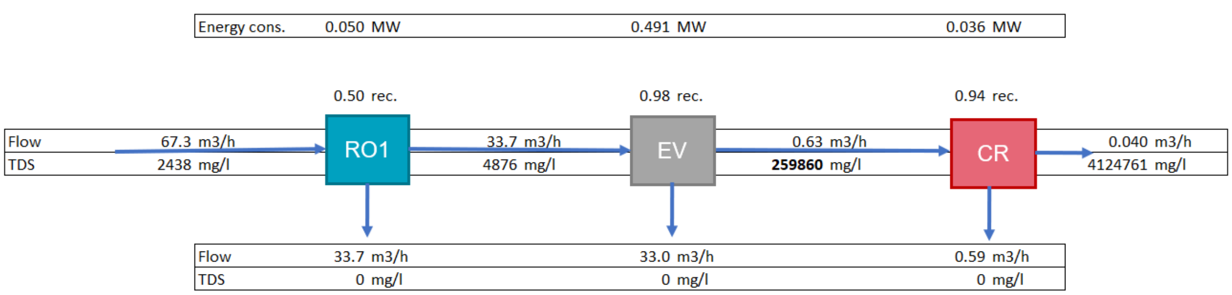

Figure B.4 ZLD option 1 flows and energy consumption for recovery system.

B.2 ZLD configuration 2 energy consumption

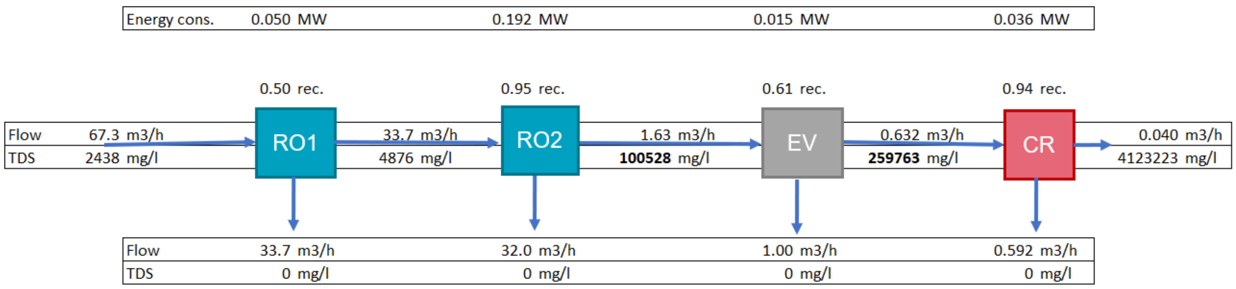

Figure B.5 ZLD option 2 flows and energy consumption for recovery system.

B.2 ZLD configuration 3 energy consumption

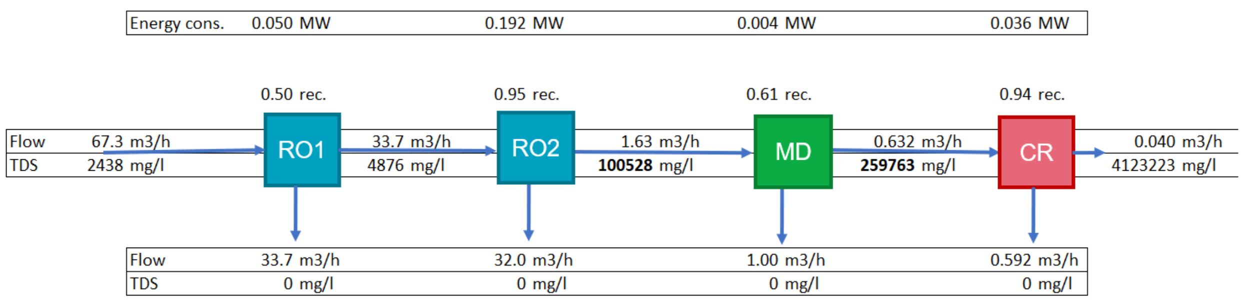

Figure B.6 ZLD option 3 flows and energy consumption for recovery system.

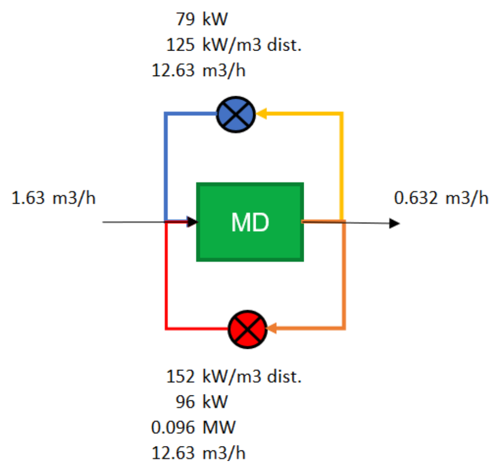

Figure B.7 Membrane distillation heat and cold flows for ZLD configuration 3

B.2 ZLD configuration 4 energy consumption

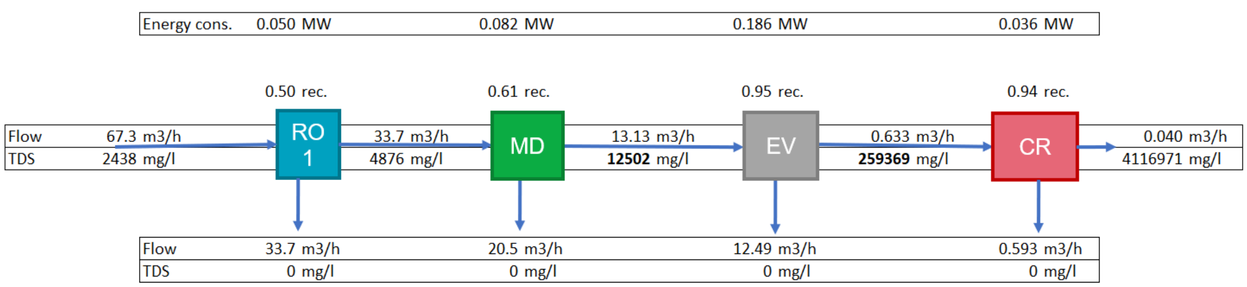

Figure B.8 ZLD option 4 flows and energy consumption for recovery system.

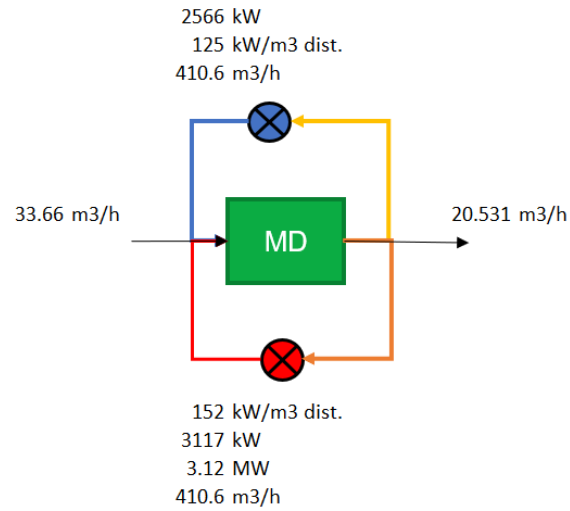

Figure B.9 Membrane distillation heat and cold flows for ZLD configuration 4

B.2 ZLD configuration 5 energy consumption

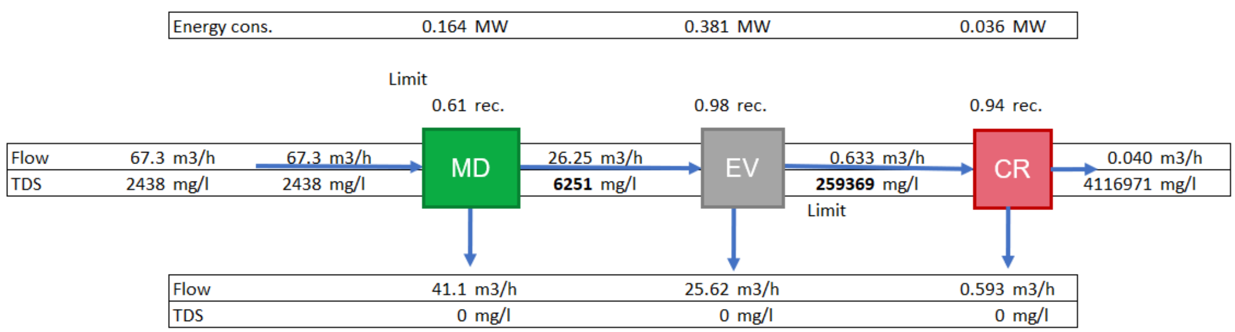

Figure B.10 ZLD option 5 flows and energy consumption for recovery system.

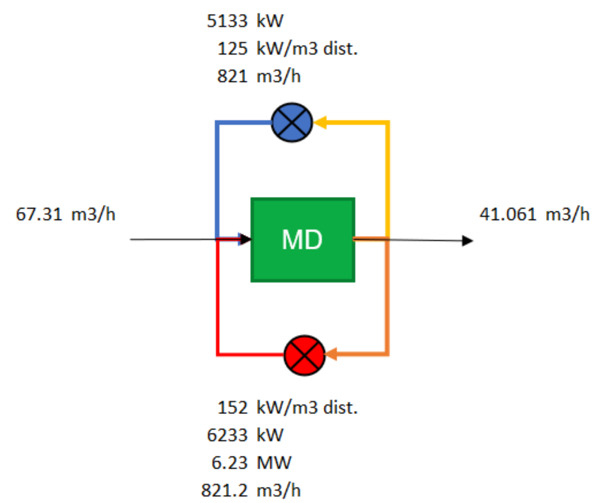

Figure B.11 Membrane distillation heat and cold flows for ZLD configuration 5

B.2 Heat pump principle

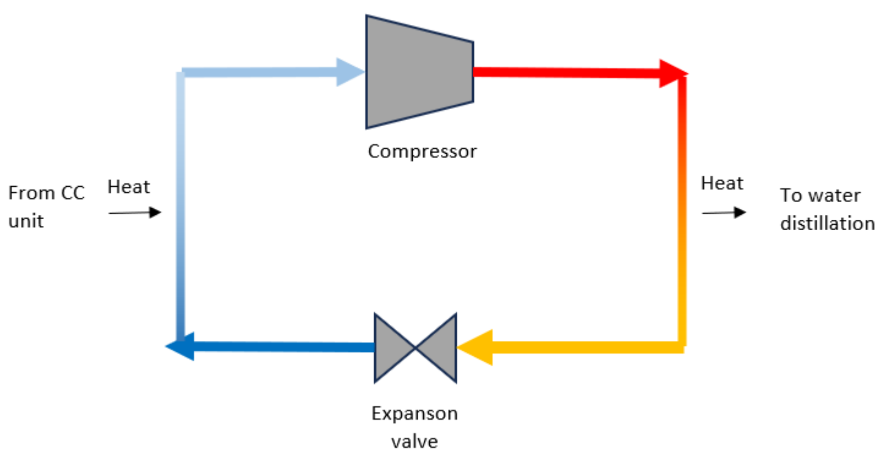

Figure B.12 Heat pump simplified diagram.

Figure B.12 presents as schematic of heat pump function. The hot fluid is exhausted from compressor and release heat to the water distillation. The resulted flow pass trough an expansion valve where its temperature is dropped. The cold flow receives low grade heat from the combined cycle unit and feed the compressor to close the system.

B.3 Heat pump and cooling tower energy equations and results

```
Heat pump equations
```
Evap_Tin = [C] # Evaporator temperature inlet
Evap_Tout = [C] # Evaporator temperature outlet
Cond_Tin = [C] # Condenser temperature inlet
Cond_Tout = [C] # Condenser temperature outlet
Cond_Qmax = [kW] # Condenser reference heat flow rate
exeff = 0.5 [-] # Second law efficiency
COPcarnot = (%Cond_Tin% + 273) / (%Cond_Tin% - %Evap_Tin%) [-] # Carnot COP
COP = %exeff% * %COPcarnot% [-] # Actual COP
W_heatpump = %Cond_Qmax% / %COP% [kW] # Heat pump power consumption
Evap_Qmax = %Cond_Qmax% * (%COP% - 1) / %COP% [kW] # Evaporator heat flow rate
```
```

Figure B.13 Heat pump equations extrait from ROSMOSE software

Table B.1 Heat Pump values for ZLD options 3, 4 and 5.

Scenario	3	4	5
Variable			
Evap_Tin	29.297	29.18728	29.075
Evap_Tout	29.297	29.18728	29.075
Cond_Tin	85	85	85
Cond_Tout	85	85	85
Cond_Qmax	102.8611	3342.939	6685.878
exeff	0.5	0.5	0.5
COPcarnot	6.426943	6.414308	6.40143
COP	3.213471	3.207154	3.200715
W_heatpump	32.00935	1042.338	2088.87
Evap_Qmax	70.85179	2300.601	4597.008

~~~
Cooling tower equations
```
Cool_Elec = [kW/kW] #Cooling Tower electricity input kWel/kWth
E_ref_CT = %Cool_Elec%*%Cool_Qmax% [kW] # Electricity consumption
~~~

Figure B.14 Cooling Tower equations extrait from ROSMOSE software

Table B.2 Cooling Tower values for ZLD options 1,2 3, 4 and 5.

Scenarios	1 and 2	3	4	5	Unit
Cool_Elec	1.43E-02	1.43E-02	1.43E-02	1.43E-02	kW/kW
Cool_Qmax	1.96E+05	1.96E+05	1.96E+05	1.97E+05	kW
E_ref_CT	2.79E+03	2.79E+03	2.80E+03	2.80E+03	kW

B.4 Energy requirements per ZLD options

Table B.3 Energy requirements per equipment per ZLD option

ZLD Options	Option 1				Option 2				Option 3				Option 4				Option 5			
Equipment	Elec. Energy	Unit	Thermal e.	Unit	Elec. Energy	Unit	Thermal e.	Unit	Elec. Energy	Unit	Thermal e.	Unit	Elec. Energy	Unit	Thermal e.	Unit	Elec. Energy	Unit	Thermal e.	Unit
Cooling tower	2.795	MW	196.0	MW	2.795	MW	196.0	MW	2.795	MW	196.1	MW	2.798	MW	196.3	MW	2.802	MW	196.6	MW
RO1	0.05	MW	0	MW	0.05	MW	0	MW	0.05	MW	0	MW	0.05	MW	0	MW	0	MW	0	MW
RO2	0	MW	0	MW	0.19	MW	0	MW	0.19	MW	0	MW	0	MW	0	MW	0	MW	0	MW
EV	0.49	MW	0	MW	0.015	MW	0	MW	0	MW	0	MW	0.19	MW	0	MW	0.38	MW	0	MW
CR	0.036	MW	0	MW	0.036	MW	0	MW	0.036	MW	0	MW	0.036	MW	0	MW	0.036	MW	0	MW
MD	0	MW	0	MW	0	MW	0	MW	0.004	MW	0	MW	0.082	MW	0	MW	0.164	MW	0	MW
HP	0	MW	0	MW	0	MW	0	MW	0.032	MW	0.096	MW	1.042	MW	3.12	MW	2.089	MW	6.23	MW
Total	3.37	MW			3.09	MW			3.11	MW			4.19	MW			5.47	MW		

APPENDIX C GRAPHS DATA

C.1 Onsite freshwater consumption

Table C.1 Values for onsite freshwater consumption for 3 main scenarios

Flow m3 of water/1 MWh produced	Scenarios		
	Base Case	Partial Recovery 50%	Zero Liquid Discharge
Withdrawal	0.7917	0.699	0.6076
Release	0.1829	0.0909	0
Consumption	0.6088	0.6081	0.6076

C.2 1 MWh electricity production, freshwater use in French context

Table C.2 CO2-eq emissions for 1MWh of electricity production using freshwater in French context

Scenarios	Base Case	Partial Recovery	ZLD - Option 1	ZLD - Option 2
Per input category				
Chemical additives	2.99E-01	2.76E-01	2.17E-01	1.93E-01
Energy use	1.03E+03	1.03E+03	1.03E+03	1.03E+03
Infrastructure construction	8.53E-01	8.56E-01	8.62E-01	8.67E-01
Sludge disposal	6.98E-03	6.38E-03	2.11E-02	2.11E-02
Water in site use	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Per process unit				
ST	3.05E-01	2.76E-01	2.40E-01	2.40E-01
CT	7.92E+00	7.92E+00	7.94E+00	7.93E+00
DM	4.13E-02	2.79E-02	2.70E-02	2.70E-02
CC	1.02E+03	1.02E+03	1.02E+03	1.02E+03
WW	2.31E-01	2.28E-01	0.00E+00	0.00E+00
RO	0.00E+00	1.52E-01	1.52E-01	6.01E-01
EV	0.00E+00	0.00E+00	1.42E+00	4.41E-02
CR	0.00E+00	0.00E+00	1.17E-01	1.17E-01
TOTAL CO2 emissions				
1 MWh produced	1.0285E+03	1.0286E+03	1.0298E+03	1.0289E+03
Water management 1 MWh produced	6.38E-01	6.38E-01	6.38E-01	6.38E-01
Relative contribution				
% energy	99.89%	99.89%	99.89%	99.89%
% cc	99.17%	99.16%	99.04%	99.13%
% water management	0.06%	0.06%	0.06%	0.06%

Table C.3 AWARE for 1MWh of electricity production using freshwater in French context

Scenarios	Base Case	Partial Recovery	ZLD - Option 1	ZLD - Option 2
Per input category				
Chemical additives	2.36E-01	2.07E-01	9.76E-02	7.49E-02
Energy use	6.37E+00	6.38E+00	6.38E+00	6.38E+00
Infrastructure construction	2.65E-01	2.64E-01	2.83E-01	2.64E-01
Sludge disposal	8.41E-04	7.50E-04	7.17E-03	7.17E-03
Water in site use	5.00E+00	5.00E+00	5.00E+00	4.99E+00
Per process unit				
ST	1.69E-02	1.49E-02	1.30E-02	1.29E-02
CT	4.97E+00	5.14E+00	5.14E+00	5.14E+00
DM	3.84E-02	6.56E-03	5.26E-03	5.26E-03
CC	6.70E+00	6.54E+00	6.54E+00	6.54E+00
WW	1.45E-01	1.38E-01	0.00E+00	0.00E+00
RO	0.00E+00	5.59E-03	5.59E-03	1.07E-02
EV	0.00E+00	0.00E+00	5.90E-02	2.29E-03
CR	0.00E+00	0.00E+00	8.08E-03	8.07E-03
TOTAL AWARE footprint				
1 MWh produced	1.19E+01	1.18E+01	1.18E+01	1.17E+01
Water management 1 MWh produced	5.20E+00	5.20E+00	5.20E+00	5.20E+00
Relative contribution				
% energy	53.67%	53.83%	54.24%	54.43%
% cc	56.45%	55.25%	55.55%	55.83%
% ct	41.87%	43.36%	43.68%	43.83%
% water management	43.82%	43.95%	44.22%	44.42%

Table C.4 AWARE contributions for cooling tower and combined cycle process units 1 MWh of electricity production

Process Unit	Total	Chemicals	Energy	Infra	Sludge	Water onsite
CT	4.9732	0.05394	0.09077	0.00122	0	4.82727
CC	6.70452332	0.0046	6.27975332	0.25959	0	0.16058

C.3 Water management for 1 MWh electricity production when freshwater use in French context.

Table C.5 CO2-eq emissions for water management for 1 MWh electricity production when freshwater use in French context

Scenarios	Base Case	Partial Recovery	ZLD - Option 1	ZLD - Option 2
Per input category				
Chemical additives	3.01E-01	2.74E-01	2.15E-01	1.90E-01
Energy use	3.23E-01	4.47E-01	1.75E+00	8.47E-01
Infrastructure construction	7.29E-03	9.60E-03	1.47E-02	2.01E-02
Sludge disposal	7.07E-03	6.33E-03	2.09E-02	2.10E-02
Water onsite use	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Per process unit				
ST	3.10E-01	2.74E-01	2.38E-01	2.38E-01
CT	5.31E-02	5.31E-02	5.31E-02	5.31E-02
DM	4.10E-02	2.77E-02	2.67E-02	2.67E-02
CC	4.93E-03	4.93E-03	4.93E-03	4.93E-03
WW	2.29E-01	2.26E-01	0.00E+00	0.00E+00
RO	0.00E+00	1.51E-01	1.51E-01	5.96E-01
EV	0.00E+00	0.00E+00	1.41E+00	4.37E-02
CR	0.00E+00	0.00E+00	1.16E-01	1.16E-01
Total	6.38E-01	7.37E-01	2.00E+00	1.08E+00

Table C.6 AWARE for water management for 1 MWh electricity production when freshwater use in French context

Scenarios	Base Case	Partial Recovery	ZLD - Option 1	ZLD - Option 2
Per input category				
Chemical additives	2.34E-01	2.05E-01	9.67E-02	7.42E-02
Energy use	3.73E-03	5.13E-03	1.99E-02	9.65E-03
Infrastructure construction	4.56E-03	3.43E-03	2.17E-02	3.36E-03
Sludge disposal	8.40E-04	7.50E-04	7.10E-03	7.10E-03
Water onsite use	4.96E+00	4.96E+00	4.95E+00	4.95E+00
Per process unit				
ST	1.67E-02	1.48E-02	1.28E-02	1.28E-02
CT	4.84E+00	5.00E+00	5.00E+00	5.00E+00
DM	1.97E-01	6.50E-03	5.22E-03	5.22E-03
CC	4.57E-03	4.57E-03	4.57E-03	4.57E-03
WW	1.44E-01	1.37E-01	0.00E+00	0.00E+00
RO	0.00E+00	5.54E-03	5.52E-03	1.07E-02
EV	0.00E+00	0.00E+00	5.84E-02	2.23E-03
CR	0.00E+00	0.00E+00	7.99E-03	7.99E-03
Total	5.20E+00	5.17E+00	5.10E+00	5.05E+00
Relative contribution				
Water onsite use	95.33%	95.85%	97.15%	98.13%
CT	93.04%	96.75%	98.14%	99.14%

Table C.7 AWARE contribution from chemicals additives for different process units

Process Unit	Chemical additive	Value
CC	Ammonium 5%	0.00012
	Ammonium 20.5%	0.0012
	Carbohydrazide	0.00325
CT	Sodium hypochlorite 15%	0.03902
	Performax DC5702	0.01311
	Performax DC5801	0.00138
ST	Lime, hydrated	0.007463
	Drewfloc 274	0.001007
	Ferric sulfate 44%	0.000205
WW	Acetic acid	0.10862
	Phosphoric acid	0.02072
	Praestol K255L	0.000433
DM	Sodium hydroxide, 50%	0.01878
	Sulfuric acid 37.5%	0.01704
	Sulfuric acid 30%	0.00155

C.4 Differences in water type for 1 MWh electricity production when freshwater use in French context.

Table C.8 CO2-eq emissions and AWARE score for different water types for 1 MWh electricity production in French context

Scenarios	Fresh water withdrawal and release				Ocean withdrawal - freshwater release				Freshwater withdrawal - ocean release		Ocean withdrawal and release
	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	Partial recovery
CO2-eq emissions											
Total CO2-eq	1028.474	1028.577	1029.846	1028.923	1030.6844	1030.528	1031.546	1030.618	1028.478	1028.916	1030.63
Chemicals	0.29938	0.276147	0.217359	0.193065	0.24923	0.228457	0.175779	0.150146	0.30311	0.195131	0.153101
Energy	1027.314	1027.439	1028.746	1027.842	1029.4583	1029.332	1030.395	1029.489	1027.314	1027.848	1029.512
Infrastructure	0.853188	0.855688	0.86195	0.866795	0.9668327	0.958718	0.95163	0.956175	0.853183	0.866222	0.956742
Sludge disposal	0.006976	0.006381	0.021135	0.021125	0.0101251	0.009041	0.023465	0.023465	0.007125	0.005691	0.008021
AWARE											
Total AWARE	11.8777	11.84367	11.76936	11.71789	5.45151	6.1703	6.83295	6.78574	13.38027	11.76835	6.78502
Chemicals	0.235775	0.207005	0.097605	0.074875	0.29772	0.261665	0.144985	0.122155	0.235775	0.080792	0.128572
Energy	6.37428	6.37505	6.38316	6.37756	6.38758	6.3868	6.3934	6.38777	6.37428	6.3776	6.38792

Table C.8 CO2-eq emissions and AWARE score for different water types for 1 MWh electricity production in French context (continuation)

Infrastructure	0.265413	0.264302	0.283049	0.264348	0.2717782	0.269912	0.287969	0.269228	0.265413	0.263478	0.268408
Sludge disposal	0.000841	0.00075	0.007166	0.007166	0.000117	0.000112	0.006614	0.006614	0.000841	0.00067	0.000108
Water in site use	5.00139	4.99655	4.99839	4.994	-1.5057	-0.74819	0	0	6.50396	5.04582	0

C.5 Differences in water type for water management for 1 MWh electricity production when freshwater use in French context.

Table C.9 CO2-eq emissions and AWARE score for different water types for water management for 1 MWh electricity production in French context

Scenarios	Fresh water withdrawal and release				Ocean withdrawal - freshwater release				Freshwater withdrawal - ocean release		Ocean withdrawal and release
	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	Partial recovery
CO2-eq emissions											
Total CO2-eq	6.38E-01	7.37E-01	2.00E+00	1.08E+00	2.83E+00	2.67E+00	3.68E+00	2.76E+00	6.38E-01	1.07E+00	2.77E+00
Chemicals	3.01E-01	2.74E-01	2.15E-01	1.90E-01	2.47E-01	2.26E-01	1.74E-01	1.49E-01	3.01E-01	1.93E-01	1.52E-01

Table C.9 CO2-eq emissions and AWARE score for different water types for water management for 1 MWh electricity production in French context (continuation)

Energy	3.23 E-01	4.47E-01	1.75E+00	8.47E-01	2.45E+00	2.33E+00	3.38E+00	2.48E+00	3.23E-01	8.54E-01	2.51E+00
Infrastructure	7.29 E-03	9.60E-03	1.47E-02	2.01E-02	1.21E-01	1.10E-01	1.02E-01	1.07E-01	7.29E-03	1.97E-02	1.08E-01
Sludge disposal	7.07 E-03	6.33E-03	2.09E-02	2.10E-02	1.00E-02	8.94E-03	2.32E-02	2.32E-02	7.07E-03	5.64E-03	7.94E-03
AWARE											
Total AWARE	5.20 E+00	5.17E+00	5.10E+00	5.05E+00	-1.17E+00	-4.59E-01	1.98E-01	1.52E-01	6.70E+00	5.10E+00	1.51E-01
Total chemicals	2.34 E-01	2.05E-01	9.67E-02	7.42E-02	2.95E-01	2.59E-01	1.43E-01	1.21E-01	2.34E-01	8.01E-02	1.27E-01
Total electricity	3.73 E-03	5.13E-03	1.99E-02	9.65E-03	1.30E-02	1.39E-02	2.24E-02	1.64E-02	4.20E-03	9.76E-03	1.65E-02
Total infra	4.56 E-03	3.43E-03	2.17E-02	3.36E-03	1.03E-02	8.51E-03	2.61E-02	7.77E-03	4.56E-03	2.51E-03	6.98E-03
Total sludge	8.40 E-04	7.50E-04	7.10E-03	7.10E-03	1.16E-04	1.11E-04	6.54E-03	6.54E-03	8.40E-04	6.70E-04	1.07E-04
Total water in site	4.96 E+00	4.96E+00	4.95E+00	4.95E+00	-1.49E+00	-7.41E-01	0.00E+00	0.00E+00	6.45E+00	5.00E+00	0.00E+00

Table C.10 Differences in AWARE contributions per input category for softening and desalination units

Unit operation	Total	Chemicals	Electricity	Infra	Sludge	Onsite water
AWARE						
TW	0.08954	0.06954	0.012011	0.007954	3.59E-05	0
ST	0.016738	0.008675	0.001613	0.002198	0.00076	0.003492
CO2-equivalent						
TW	2.49854	0.10662	2.26569	0.11689	0.00934	0
ST	0.309602	0.16057	0.13935	0.003302	0.00638	0

C.6 Different water type for others country context

Table C.11 Comparison between freshwater footprint for other water scarcity context for water management to produce 1MWh electricity

Scenarios	Fresh water withdrawal and release				Ocean withdrawal - freshwater release				Freshwater withdrawal - ocean release		Ocean withdrawal and release
	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	Partial recovery
CO2-eq	0.637609	0.736515	1.99614	1.07849	2.826938	2.672885	3.68294	2.76234	0.637609	1.072403	2.77374
AWARE - FR	5.20	5.17	5.10	5.05	-1.17	-0.46	0.20	0.15	6.70	5.10	0.15
AWARE - DZ	39.32	39.25	39.19	39.11	-11.44	-5.56	0.20	0.15	51.06	39.51	0.15
AWARE - US	20.41	20.37	20.30	20.23	-5.75	-2.73	0.20	0.15	26.48	20.44	0.15

Table C.12 Differences in AWARE contributions for base case to produce 1MWh of electricity for 3 difference water scarce scenarios

Countries	Base case - Freshwater withdrawal and release		
	FR	DZ	US
CO2-eq	1028.474	1028.474	1028.474
Chemicals	0.29938	0.29938	0.29938
Energy	1027.314	1027.314	1027.314
Infrastructure	0.853188	0.853183	0.853183
Sludge disposal	0.006976	0.006976	0.006976
Water in site	0	0	0
AWARE	11.8777	46.25354	27.20375
Chemicals	0.235775	0.235775	0.235775
Energy	6.37428	6.37428	6.37428
Infrastructure	0.265413	0.265413	0.265413
Sludge disposal	0.000841	0.000841	0.000841
Water in site	5.00139	39.37723	20.32745

C.7 Human Health 1 MWh electricity production

Table C.13 Human Health 1 MWh electricity production

Scenarios	Fresh water withdrawals and release				Ocean withdrawal - freshwater release				Freshwater withdrawal - ocean release		Ocean withdrawal and release
	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	Partial recovery
Developed or non-water scarce country											
HH short term	9.27 E-04	9.27E-04	9.28E-04	9.27E-04	9.29 E-04	9.29E-04	9.30E-04	9.29E-04	9.27E-04	9.27E-04	9.29E-04
HH water scarcity	1.29 E-05	1.28E-05	1.27E-05	1.26E-05	1.31 E-05	1.30E-05	1.29E-05	1.28E-05	1.29E-05	1.26E-05	1.28E-05
HH climate change	8.41 E-04	8.41E-04	8.42E-04	8.42E-04	8.43 E-04	8.43E-04	8.44E-04	8.43E-04	8.41E-04	8.42E-04	8.43E-04
HH remaining	7.27 E-05	7.26E-05	7.27E-05	7.26E-05	7.30 E-05	7.29E-05	7.30E-05	7.29E-05	7.27E-05	7.26E-05	7.28E-05
Algeria											
HH short term	1.07 E-03	1.07E-03	1.08E-03	1.07E-03	8.84 E-04	9.07E-04	9.30E-04	9.29E-04	1.12E-03	1.08E-03	9.29E-04
HH water scarcity	1.61 E-04	1.61E-04	1.61E-04	1.61E-04	-3.15 E-05	-9.15E-06	1.29E-05	1.28E-05	2.06E-04	1.62E-04	1.28E-05
HH climate change	8.41 E-04	8.41E-04	8.42E-04	8.42E-04	8.43 E-04	8.43E-04	8.44E-04	8.43E-04	8.41E-04	8.42E-04	8.43E-04
HH remaining	7.27 E-05	7.26E-05	7.27E-05	7.26E-05	7.30 E-05	7.29E-05	7.30E-05	7.29E-05	7.27E-05	7.26E-05	7.28E-05

C.8 Human Health water management for 1 MWh electricity production

Table C.14 Human Health water management for 1 MWh electricity production

Scenarios	Fresh water withdrawal and release				Ocean withdrawal - freshwater release				Freshwater withdrawal - ocean release		Ocean withdrawal and release
	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	Partial recovery
Developed or non-water scarce country											
HH short term	1.18 E-06	1.21E-06	2.22E-06	1.24E-06	3.41 E-06	3.18E-06	3.94E-06	2.96E-06	1.18E-06	1.21E-06	2.94E-06
HH water scarcity	4.32 E-07	3.93E-07	2.88E-07	1.88E-07	6.35 E-07	5.72E-07	4.43E-07	3.43E-07	4.32E-07	1.78E-07	3.35E-07
HH climate change	5.22 E-07	5.99E-07	1.63E-06	8.69E-07	2.23 E-06	2.11E-06	2.94E-06	2.18E-06	5.22E-07	8.64E-07	2.19E-06
HH remaining	2.23 E-07	2.15E-07	3.07E-07	1.84E-07	5.45 E-07	4.99E-07	5.54E-07	4.30E-07	2.23E-07	1.64E-07	4.13E-07
Algeria											
HH short term	1.48 E-04	1.48E-04	1.49E-04	1.48E-04	-4.09 E-05	-1.88E-05	3.94E-06	2.96E-06	1.92E-04	1.50E-04	2.94E-06
HH water scarcity	1.48 E-04	1.47E-04	1.47E-04	1.47E-04	-4.37 E-05	-2.14E-05	4.43E-07	3.43E-07	1.92E-04	1.49E-04	3.35E-07
HH climate change	5.22 E-07	5.99E-07	1.63E-06	8.69E-07	2.23 E-06	2.11E-06	2.94E-06	2.18E-06	5.22E-07	8.64E-07	2.19E-06

Table C.14 Human Health water management for 1 MWh electricity production (continuation)

HH remaining	2.23E-07	2.15E-07	3.07E-07	1.84E-07	5.45E-07	4.99E-07	5.54E-07	4.30E-07	2.23E-07	1.62E-07	4.13E-07

C.9 Ecosystem Quality 1 MWh electricity production

Table C.15 Ecosystem Quality 1 MWh electricity production

	Fresh water withdrawal and release				Ocean withdrawal - freshwater release				Freshwater withdrawal - ocean release		Ocean withdrawal and release
Scenarios	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	Partial recovery
World average											
EQ short term	2.24 E+02	2.24E+02	2.24E+02	2.24E+02	2.24 E+02	2.24E+02	2.25E+02	2.24E+02	2.24E+02	2.24E+02	2.24E+02
EQ water scarcity	1.48 E-02	1.33E-02	1.19E-02	1.19E-02	1.89 E-03	1.91E-03	1.94E-03	1.94E-03	1.49E-02	1.20E-02	1.94E-03
EQ climate change	1.82 E+02	1.82E+02	1.82E+02	1.82E+02	1.82 E+02	1.82E+02	1.83E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02
EQ remaining	4.19 E+01	4.19E+01	4.19E+01	4.19E+01	4.20 E+01	4.20E+01	4.20E+01	4.20E+01	4.19E+01	4.19E+01	4.20E+01
Worst case											
EQ short term	2.24 E+02	2.24E+02	2.24E+02	2.24E+02	2.24 E+02	2.24E+02	2.25E+02	2.24E+02	2.24E+02	2.24E+02	2.24E+02

Table C.15 Ecosystem Quality 1 MWh electricity production (continuation)

EQ water scarcity	5.72E-02	5.71E-02	5.71E-02	5.71E-02	-1.46E-02	-6.29E-03	1.94E-03	1.94E-03	7.37E-02	5.76E-02	1.94E-03
EQ climate change	1.82E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02	1.83E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02
EQ remaining	4.19E+01	4.19E+01	4.19E+01	4.19E+01	4.20E+01	4.20E+01	4.20E+01	4.20E+01	4.19E+01	4.19E+01	4.20E+01
Best case											
EQ short term	1.36E+03	1.36E+03	1.36E+03	1.36E+03	-1.17E+02	5.45E+01	2.25E+02	2.24E+02	1.70E+03	1.37E+03	2.24E+02
EQ water scarcity	1.14E+03	1.13E+03	1.13E+03	1.13E+03	-3.42E+02	-1.70E+02	1.94E-03	1.94E-03	1.48E+03	1.15E+03	1.94E-03
EQ climate change	1.82E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02	1.83E+02	1.82E+02	1.82E+02	1.82E+02	1.82E+02
EQ remaining	4.19E+01	4.19E+01	4.19E+01	4.19E+01	4.20E+01	4.20E+01	4.20E+01	4.20E+01	4.19E+01	4.19E+01	4.20E+01

C.10 Ecosystem Quality water management for 1 MWh electricity production

Table C.16 Ecosystem Quality water management for 1 MWh electricity production

Scenarios	Fresh water withdrawal and release				Ocean withdrawal - freshwater release				Freshwater withdrawal - ocean release		Ocean withdrawal and release
	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	ZLD - Option 1	ZLD - Option 2	Base case	Partial recovery	Partial recovery
World average											
EQ short term	2.07E-01	2.22E-01	4.95E-01	2.66E-01	6.86E-01	6.45E-01	8.63E-01	6.34E-01	2.03E-01	2.77E-01	6.52E-01
EQ water scarcity	1.75E-02	1.54E-02	1.35E-02	1.35E-02	-3.58E-05	-9.74E-06	1.71E-05	1.38E-05	1.28E-02	9.97E-03	1.38E-05
EQ climate change	1.13E-01	1.30E-01	3.52E-01	1.88E-01	4.83E-01	4.57E-01	6.37E-01	4.72E-01	1.13E-01	1.87E-01	4.74E-01
EQ remaining	7.68E-02	7.69E-02	1.29E-01	6.48E-02	2.03E-01	1.88E-01	2.26E-01	1.62E-01	7.76E-02	7.98E-02	1.78E-01
Worst case											
EQ short term	4.17E-01	4.14E-01	6.70E-01	4.40E-01	6.70E-01	6.37E-01	8.63E-01	6.34E-01	3.71E-01	4.55E-01	6.52E-01
EQ water scarcity	2.28E-01	2.08E-01	1.89E-01	1.87E-01	-1.64E-02	-8.14E-03	1.71E-05	1.38E-05	2.44E-01	1.89E-01	1.38E-05
EQ climate change	1.13E-01	1.30E-01	3.52E-01	1.88E-01	4.83E-01	4.57E-01	6.37E-01	4.72E-01	1.13E-01	1.87E-01	4.74E-01

Table C.16 Ecosystem Quality water management for 1 MWh electricity production (continuation)

EQ remaining	7.68E-02	7.69E-02	1.29E-01	6.48E-02	2.03E-01	1.88E-01	2.26E-01	1.62E-01	7.76E-02	7.97E-02	1.78E-01
Best case											
EQ short term	0.189733	0.206515	0.481541	0.252884	0.6863689	0.64499689	0.86349856	0.634136	0.190564	0.266867	0.652104
EQ water scarcity	2.69E-05	2.5E-05	2.28E-05	2.23E-05	1.722E-05	1.661E-05	1.7091E-05	1.38E-05	3.01E-05	2.26E-05	1.38E-05
EQ climate change	0.112929	0.129631	0.352332	0.188078	0.4832463	0.45659277	0.63717243	0.472405	0.112929	0.187042	0.474322
EQ remaining	0.076776	0.076859	0.129186	0.064783	0.2031054	0.18838751	0.22630904	0.161718	0.077605	0.079802	0.177768

APPENDIX D 1MWH ELECTRICITY PRODUCTION

D.1 CO2-equivalnt emissions and AWARE midpoint, freshwater use in French context

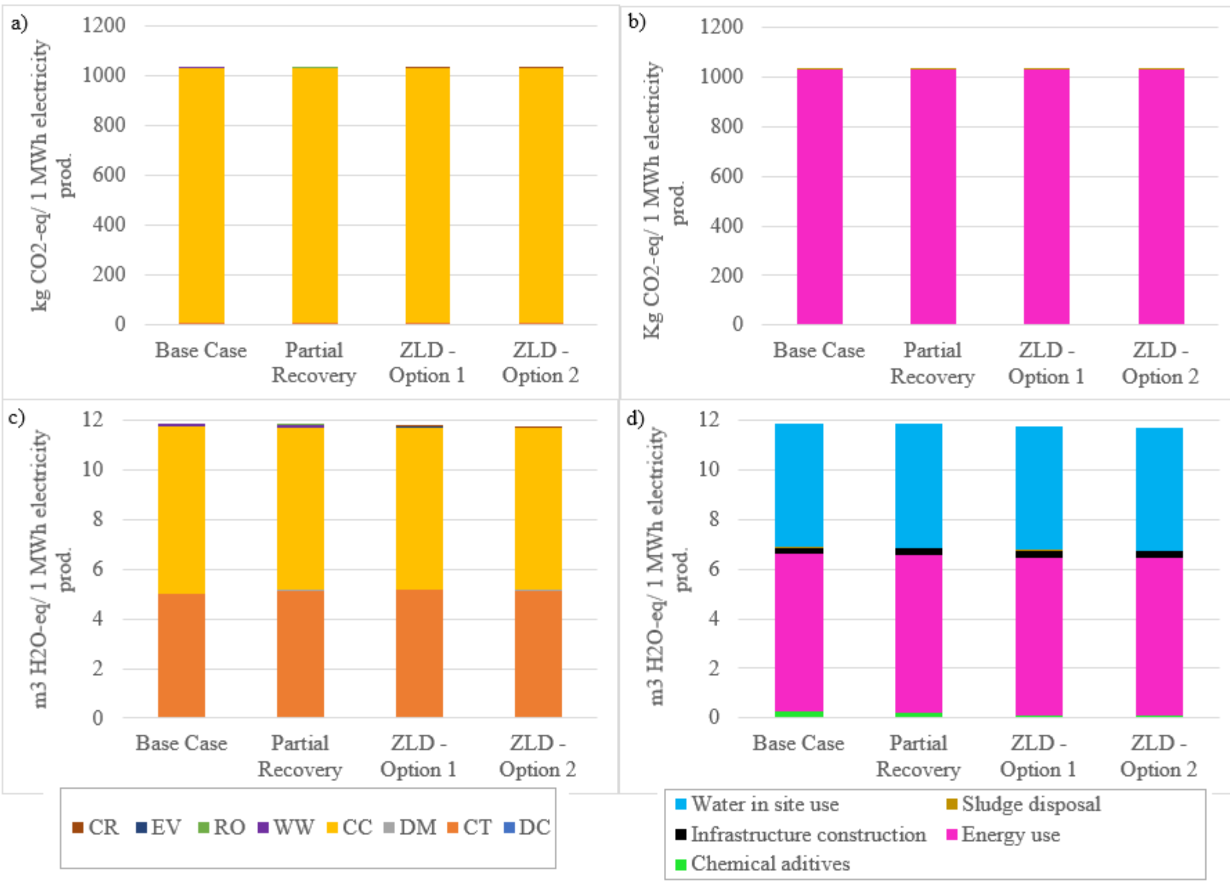

Figure D.1 CO2-eq emissions and AWARE for 1MWh of electricity production classified in a) CO2-eq emissions per process unit; b) CO2-eq emissions per input category; c) AWARE per process unit and d) AWARE per input category for different recovery scenarios when using freshwater only.

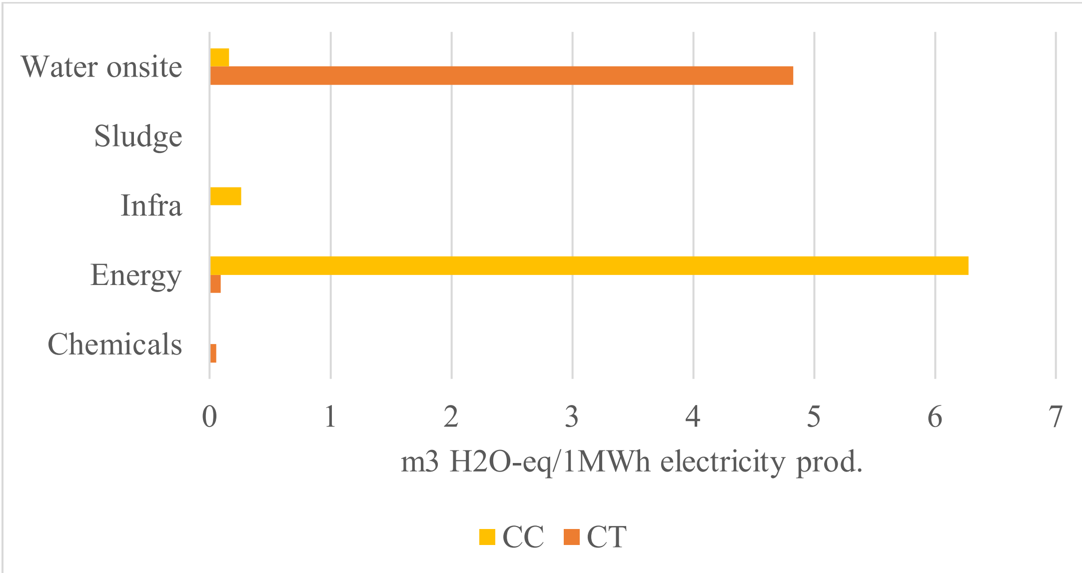

Figure D.2 Main process unit contribution to AWARE indicator for base case using freshwater for 1 MWh electricity production.

D.2 Different water type for French context

Figure D.3 Different scenarios performance presented in a) for CO2-eq emissions and b) for AWARE profile when changing water type for 1 MWh electricity production in French context.

D.3 Human Health impacts

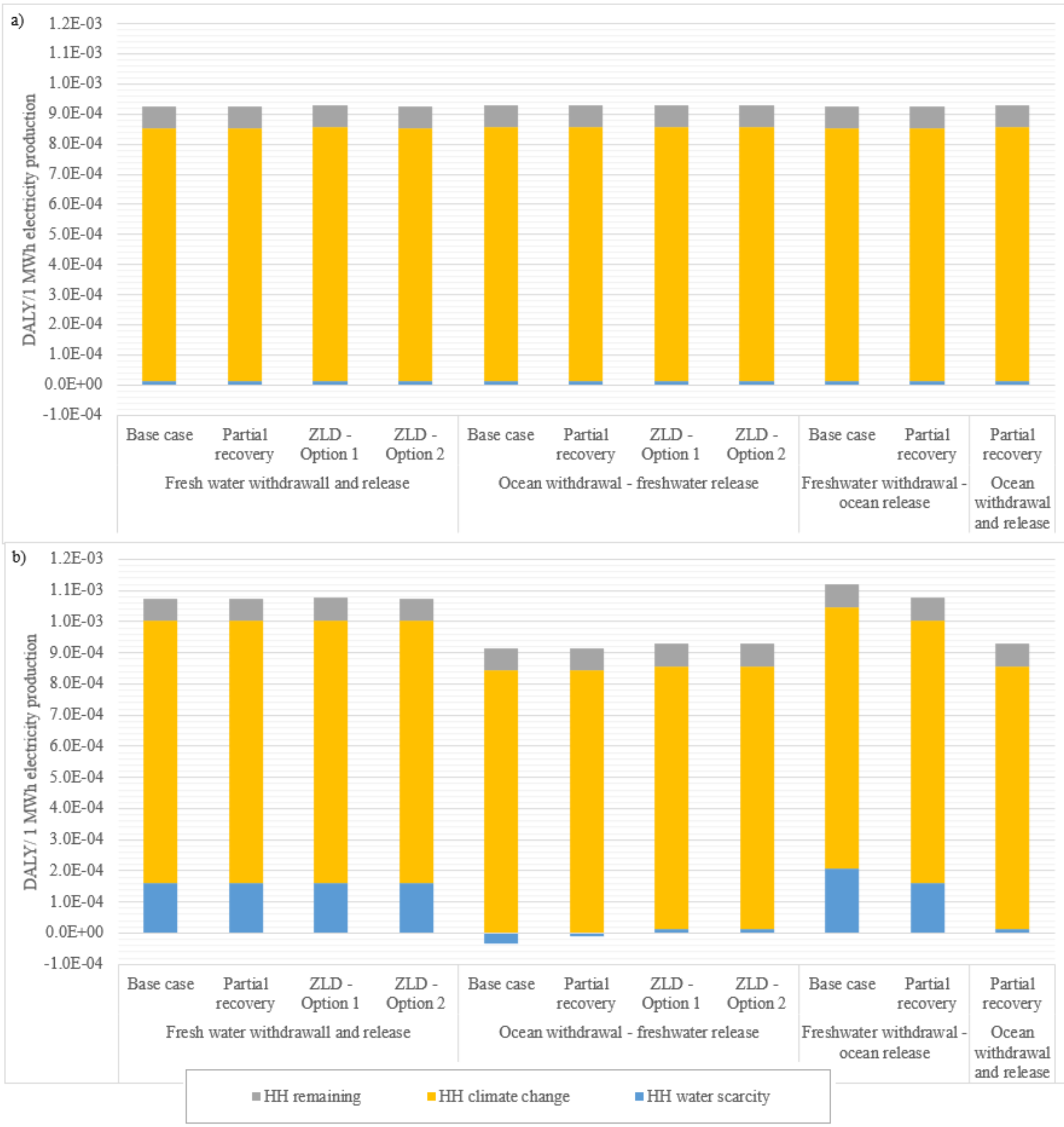

Figure D.4 Human Health impact for 1 MWh electricity production in a) non-scarce or developed countries and b) for non-developed and water scarce place using Algeria as example.

D.4 Ecosystem Quality impacts

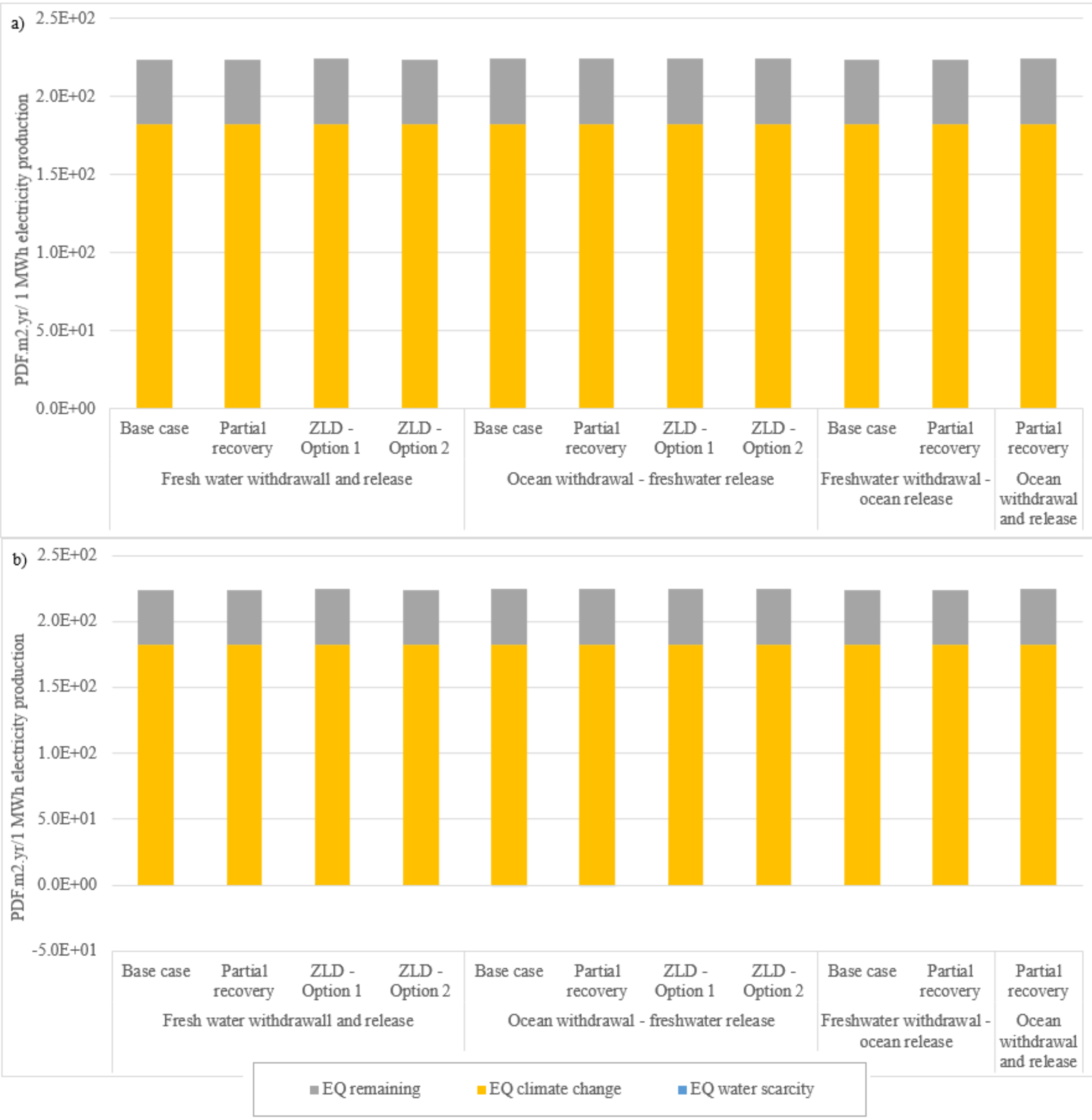

Figure D.5 Ecosystem Quality impacts for 1 MWh electricity production in a) world average water scarcity and b) worst case water scarcity

APPENDIX E SYSTEM PRODUCTS

E.1 Base case

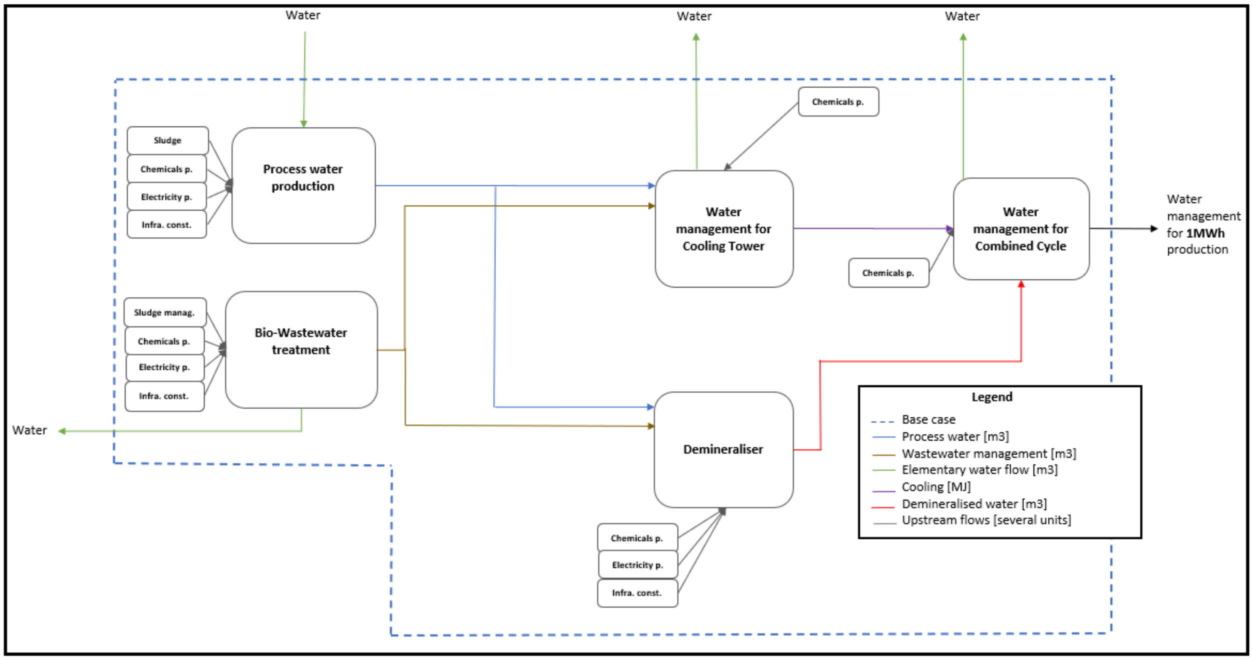

Figure E.1 Base case system product for water management function unit only.

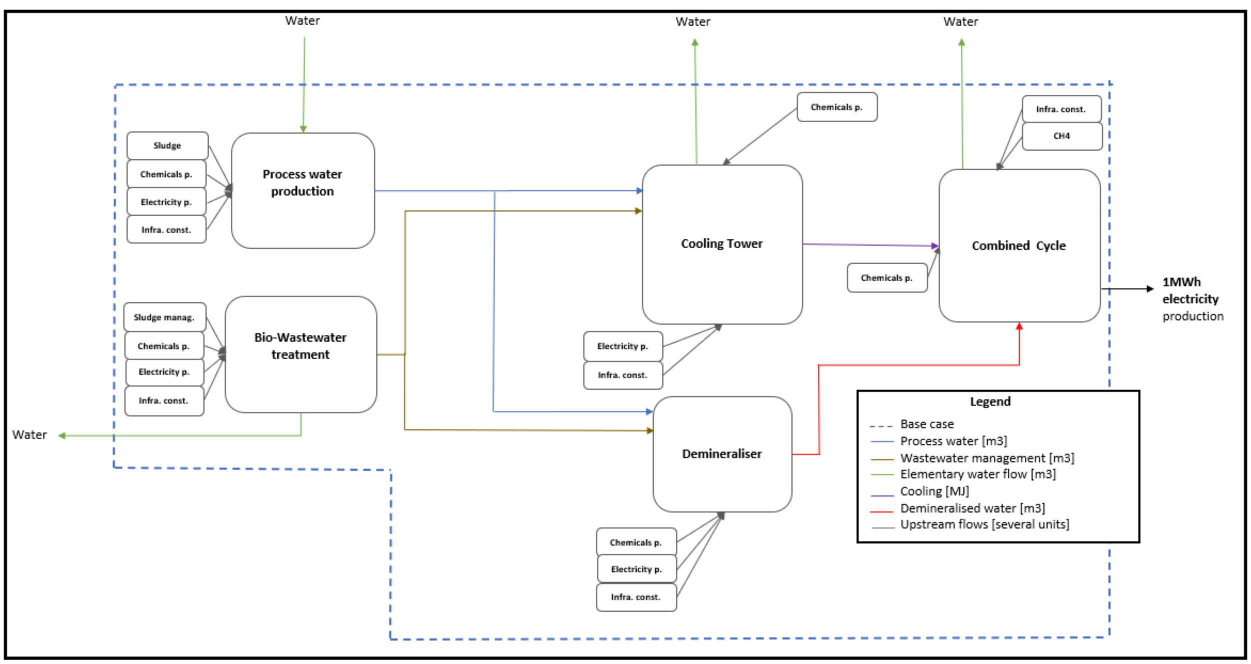

Figure E.2 Base case system product for 1 MWh electricity production unit only.

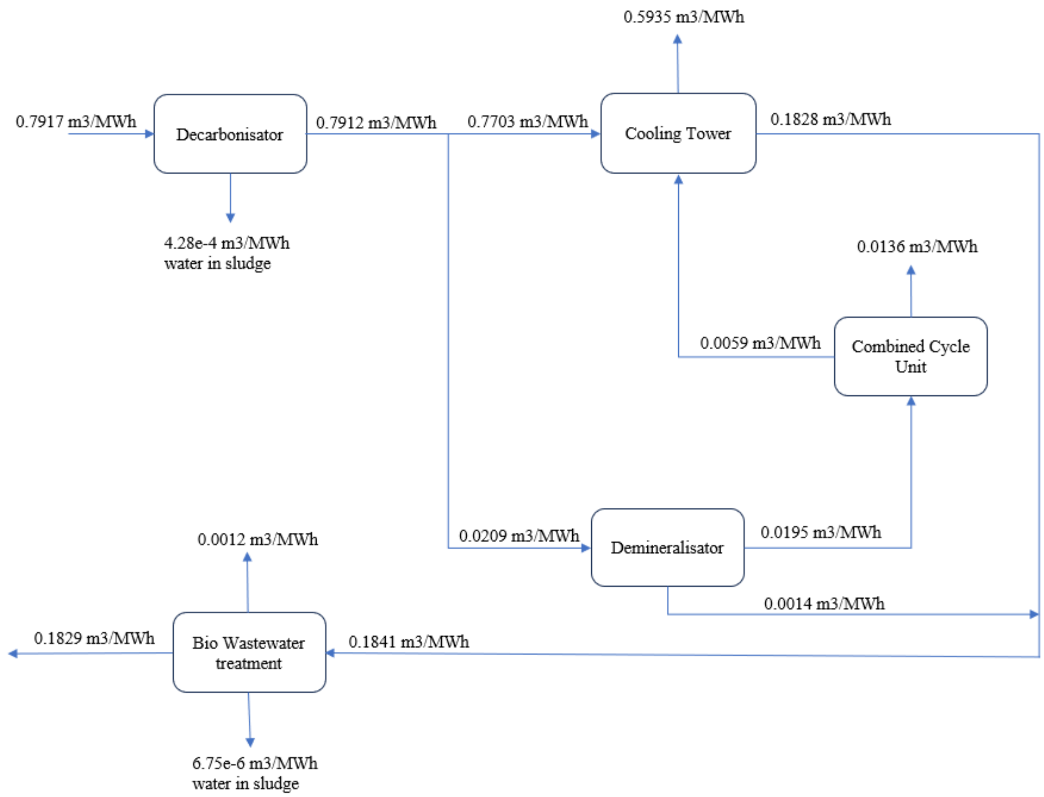

Figure E.3 Process view for main water flows and cooling requirements for base case scenario.

E.2 Partial recovery

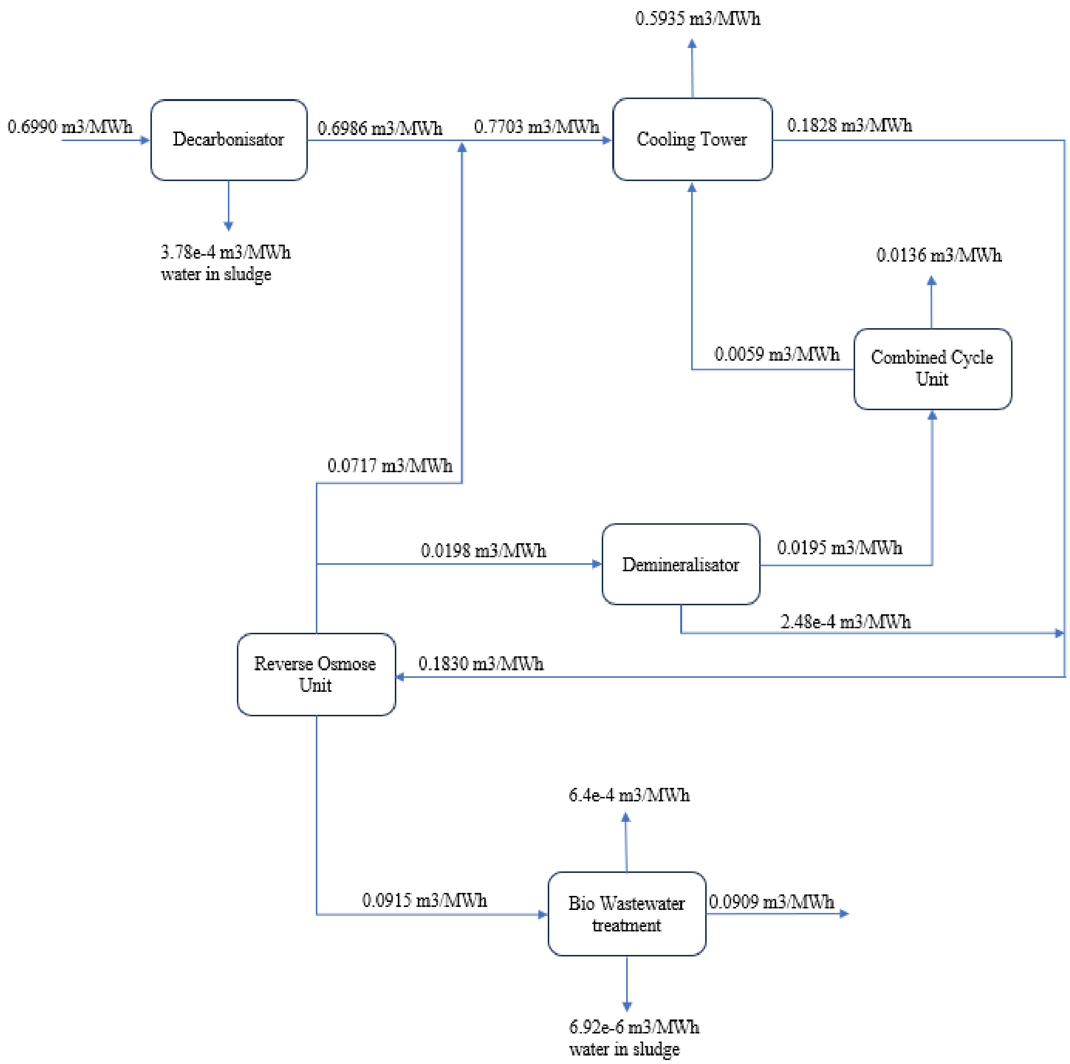

Figure E.4 Process view for main water flows and cooling requirements for 50% partial recovery scenario.

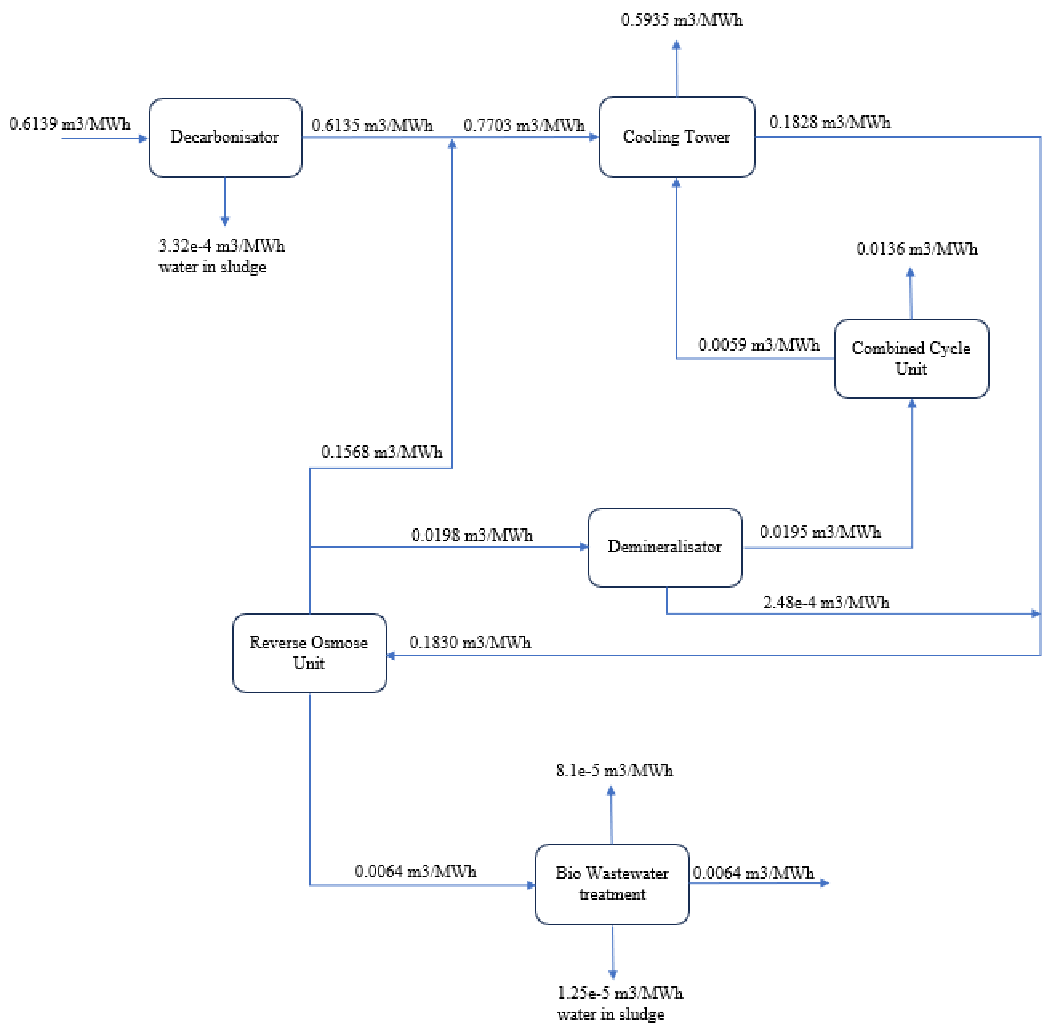

Figure E.5 Process view for main water flows and cooling requirements for 96.5% partial recovery scenario.

E.3 Zero liquid Discharge

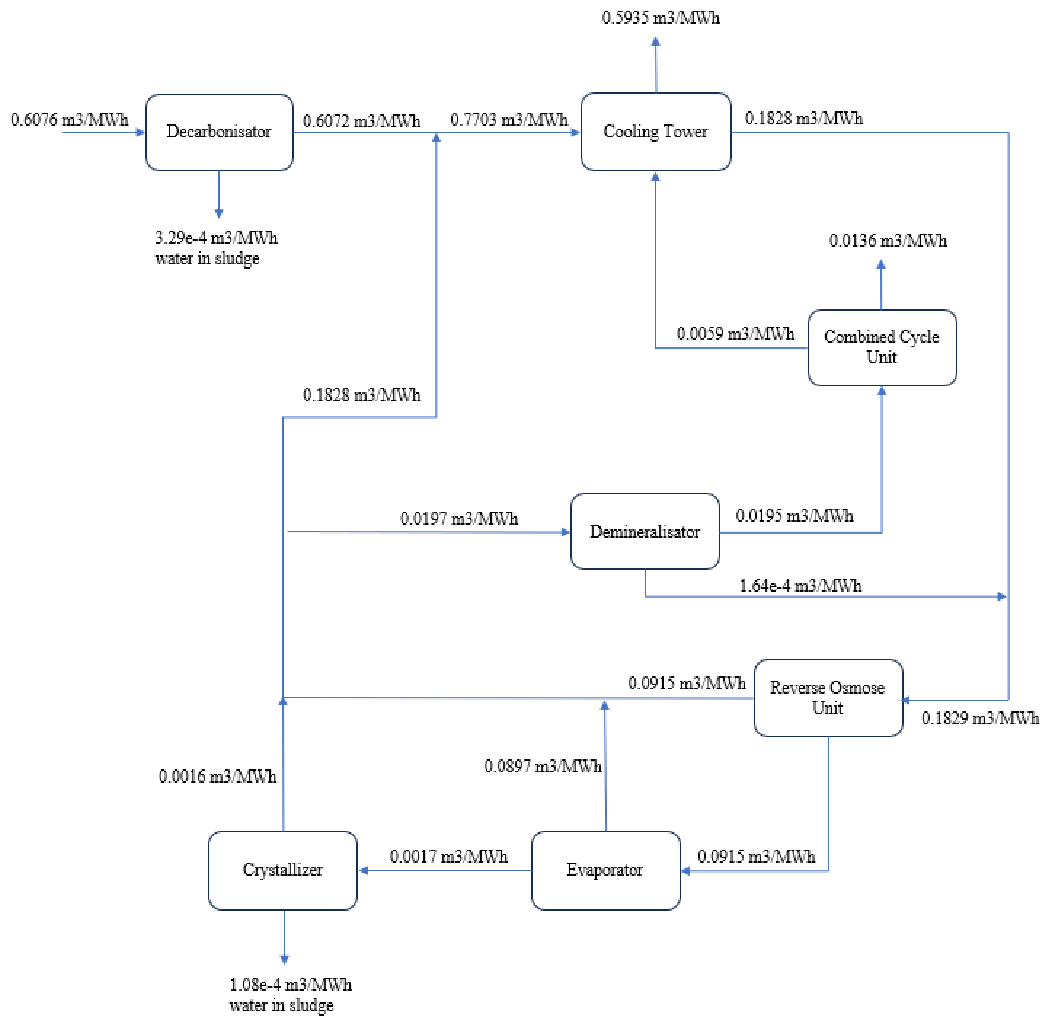

Figure E.6 Process view for main water flows and cooling requirements for zero liquid discharge option 1 scenario.

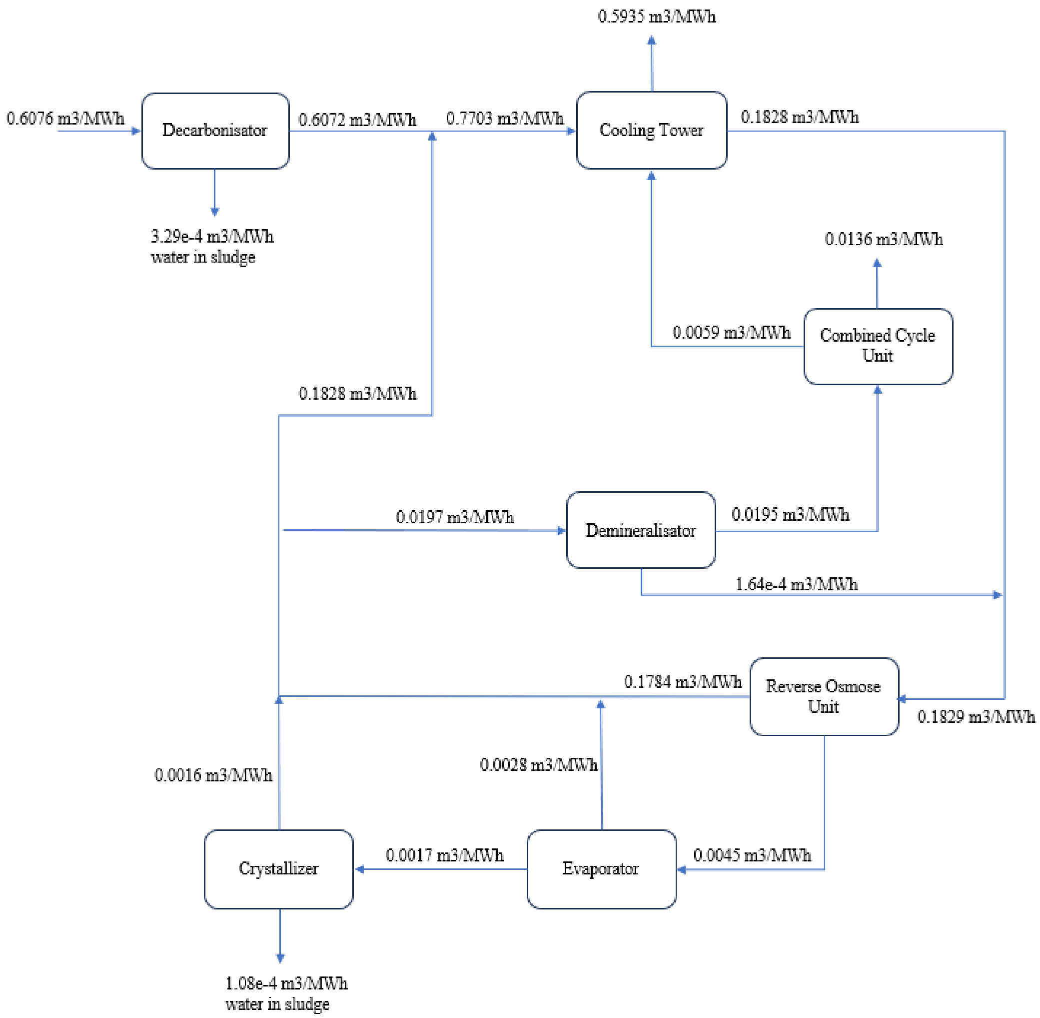

Figure E.7 Process view for main water flows and cooling requirements for zero liquid discharge option 2 scenario.