Past, present and future energy demands for clean water provision and water scarcity alleviation

PhD research proposal

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Contents

Abstract

Water scarcity currently affects at least 40% of the world population annually and is projected to worsen due to climate change, increases in the frequency of extreme weather events and socioeconomic developments (e.g. growing world population, industrialization and overall higher standards of life). These factors will modify the global spatiotemporal patterns of supply and demand of clean water resources.

The provision of clean water requires large amounts of energy, which is involved in all phases of abstraction, treatment, distribution, end-use, as well as the collection and treatment of wastewater. The expansion of water technologies, e.g. desalination and wastewater reuse, is considered a key option to alleviate water scarcity, in line with Sustainable Development Goals 6.1, 6.3. and 6.4. These are however energy-intense technologies, which might aggravate global warming if not properly integrated within renewable or circular energetic frameworks.

The purpose of this PhD project is to quantify historical (1970-2020) and future (2030-2100) global energy requirements to provide clean water and alleviate water scarcity, considering scenarios of climate change and socioeconomic developments. Special attention will be given to the energetic use of expanding both conventional and unconventional water technologies.

1 Introduction

1.1 Water scarcity in the Anthropocene

The Anthropocene[1] is characterized by the increasing influence of human activities on the hydrological cycle[2,3], which may trigger various tipping points in the Earth system[4]. In the current epoch, humans have modified water availability with the construction of dams[5,6], the extraction of water for human use[2,7], and the amplification of weather extremes due to human-water interactions[8–10] and land use change[11,12].

The hydrological cycle is also being disrupted by anthropogenic climate change, which is modifying river flows[13–15], increasing the frequency and intensity of heatwaves, rainfall events[16–18] and droughts[19–23], in addition to changes in the dynamics of groundwater[24] and soil moisture[25]. Furthermore, freshwater quality is degrading, due to climate change[26], worldwide salinization[27] and eutrophication[28–30], thermal pollution[14,31–33] and chemical pollution from poorly treated wastewaters[34,35], pharmaceuticals[36–38], microplastics[39–41] and other emerging contaminants[42–45].

All these factors contribute to varying degrees to water scarcity[46–49], as the most recent estimates show that about 4 billion people face severe water scarcity for at least one month per year[50] and about 40% of the world population suffers from water scarcity annually when including water quality[51]. Water scarcity is projected to increase[50,52,53], due to a combination of climate change effects, socioeconomic developments and poor management practices[54–57]. Nonetheless, water scarcity assessments may still be incomplete, as most studies do not properly include environmental flow requirements[58–61].

The expansion of unconventional water resources such as desalination[62,63] and wastewater reuse[64–67], coupled to the development of more conventional water sources, i.e. pumping and piping, and general enhancements to water productivity[68,69], could prove essential in alleviating water scarcity[51,70–72]. However, these technologies and the water sector at large are characterized by intensive energy use[73], which may result in potential conflicts[74,75] or synergies[76–79] between efforts to improve the provision of clean water and policies that aim to mitigate the effects of global warming[80,81]. It is thus necessary to first identify the energy use engrained in the water sector to understand the energetic implications of reducing future water scarcity[82].

The energy sector is also vulnerable to climate change[83–86], and feedbacks with the water sector may cascade non-linearly in time and space during drought/heatwave events[87–91]. For instance, water demands may already be higher under these weather extremes[92], putting additional strain on the energy sector and activating a series of feedbacks with the planetary hydrology as well[4,93–96]. Understanding historical energy use in the water sector during average and extreme conditions will thus enable further analysis on the future evolution of the water-energy nexus[97–102].

1.2 Energy for water

The provision of water to large communities is made possible through the use of considerable amounts of energy, which is required at all steps of the water supply chain[73,74,103–106] (fig. 1). Rothausen & Conway (2011)[74] stress the importance of defining clear boundaries to properly assess the energy use (kWh) engrained in the water sector. In this research, we follow the definition of *energy for water* delineated by Kyle et al. (2016)[107], as we strive to quantify the energy used for processes *whose primary output* is water. These consist in: a) *pre-use*, i.e. water abstraction, raw water treatment (including desalination) and distribution; and b) *post-use*, i.e. wastewater collection, treatment and discharge or reuse. Energy consumption related to *end use* in the water sector[104,108], e.g. water heating and cooling or energy consumed in household appliances and production of steam in industrial processes, is excluded from this definition[107].

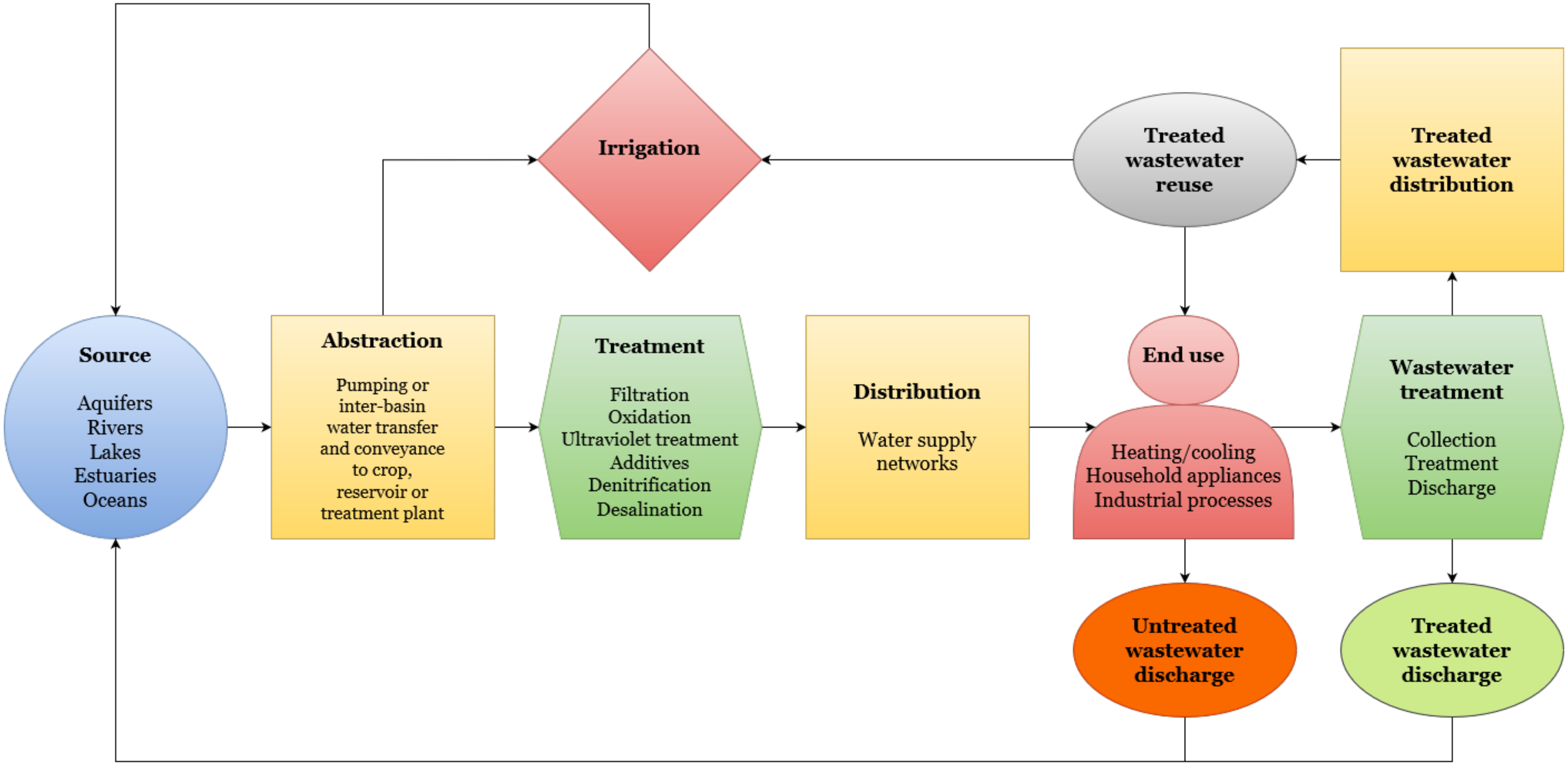

Figure 1. *A conceptual model of processes in the water use cycle involving energy consumption (modified after [74, 106, 108]).*

1.2.1 Abstraction

The first step in the water use cycle is the abstraction of water from various sources (i.e. groundwater, rivers, lakes, estuaries, oceans) by pumping it and conveying it either to farmlands for crop irrigation, to a reservoir for future use or to a treatment plant[74,106]. Pumping water involves using energy to move it from high depths and/or over long distances towards where it is needed (fig. 2). Prior to the discovery of fossil fuels, water works in human civilizations usually relied on energy provided by gravity[103].

Pump efficiency commonly determines the energy used for pumping, as the product of the efficiency of each component in a pumping system, i.e. type of pump, engine (electric vs. diesel-powered), transmission and pipe material[74,104,108–111]. Additional energy is needed to accommodate pressure requirements and the end point[112], e.g. for irrigation sprinklers[113] (fig. 2), to overcome machinery obsoletion and aging[114] and inefficiencies related to energy losses in the power supply[111]. Overall pump efficiencies may range between 0.5-27% for diesel-powered pumping systems and 30-60% for electrical ones[111,115], and have generally improved in the recent past (fig. 3).

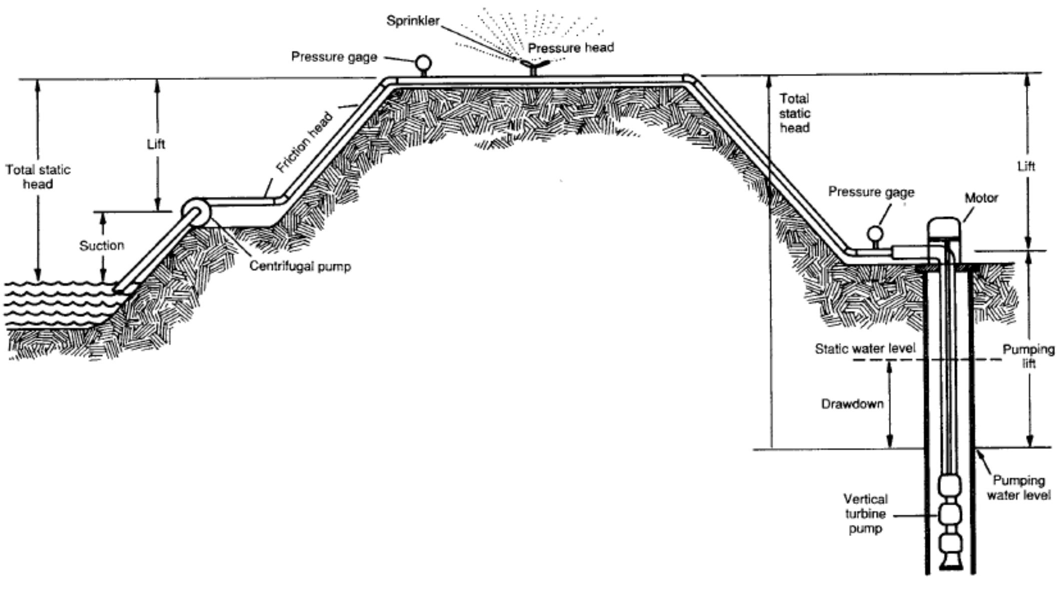

Figure 2. *The total head is the sum of the static head, friction head and pressure head. The components of the total static head for a surface water and well water pumping system are shown*[116]*.*

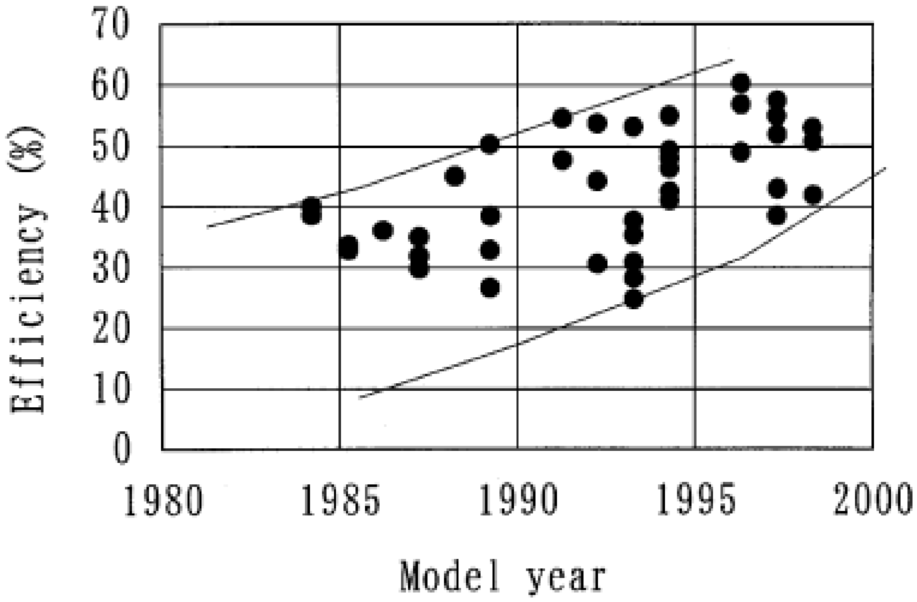

Figure 3. *Benchmark of water pump efficiency*[115].

Energy consumed in groundwater abstraction is additionally dependent on aquifer depth, abstraction rate, water table drawdown and groundwater depletion[110,111,117,118]. Analogically, energy used in pumping of surface water is related to the length and elevation changes involved in water routing, depending on the design of the specific supply network (i.e. the distance between the water source and the location of intended use) and the local topography[103,104,119]. The energy used to pump water over hills and mountains can be partially recovered with turbines that capture the kinetic energy from the water coming down the other side[103,120]. Some energy is however lost due to water leaks in distribution networks[74,111,120].

Depending on the depth of the water table and flow rate in the well, energy consumed for groundwater pumping may require between 0.15 and 3.02 kWh/m^3, with a specific energy consumption of 0.004-0.006 kWh/m^3 per m of lift[104], which is about two to three times the theoretical minimum of 0.0027 kWh/m^3 m [74]. For water supply systems, energy consumption may range anywhere from 0.2 to 4.07 kWh/m^3 [104, 106, 120], depending on the distances and elevation changes between the water source and the location of use. The specific energy requirements to supply water are however in the order of 0.002-0.007 kWh/m^3 per km of pumping distance[104,106].

1.2.2 Raw water treatment

The next step in the water supply is the treatment of water prior to distribution and end-use. The amount of energy used in this phase will depend on the quality of the water source and its intended end-use[121]. Treatment of abstracted water consists in the removal of dissolved gases, salts, nutrients, pathogens and organic and inorganic compounds[104,106]. Groundwater usually requires less intensive treatment[104] due to the filtering capacity of soils, which is determined by the concentration of the considered pollutant and their relative transport and adsorption processes in the soil itself[122]. Overall, it is reported that conventional water treatment consumes 0.01-1.44 kWh per m^3 of water treated[104,105,121].

Brackish water and seawater, however, require desalination, i.e. the removal of dissolved salts, to produce freshwater, in addition to pre-treatment. Production of desalinated water has been growing exponentially in the past few decades[62,63,123], from about 20 million m^3 in 1995 to the current 95.37 million m^3/day [62]. Desalination is now seen as a valuable tool to address water scarcity[51,71,124], being the only technology that can augment freshwater resources beyond natural availability. Yet, desalination poses great environmental concerns[125–128] and is a highly energy-intensive process, with the potential to worsen current greenhouse-gas (GHG) emissions if it is not integrated with renewable energy sources[78,129,130].

Al-Karaghouli & Kazmerski (2013)[131] provide an overview and schematic functioning of the main desalination technologies and their energy use. Currently, desalination can be essentially categorized as thermal and membrane processes[62,123,131]. Early expansion of desalination in the 20th century is mostly related to the use of thermal technologies, especially Multi-Stage Flash (MSF) (fig. 4A) and Multi-Effect Distillation (MED), in water-scarce oil-rich countries of the Middle East[62,103,129]. However, these are extremely energy-intensive processes and their development is associated with the use of cheap fossil fuels[103], potentially rendering them unsustainable in the long-term. Reported energy use for MSF ranges between 19 and 97 kWh/m^3, while MED processes require between 14 and 72 kWh/m^3 [105, 131, 132], with no difference in energy intensity for brackish water and seawater[105].

Today, the most widespread desalination technique is reverse osmosis (RO) (fig. 4B)[62,129,133,134], a highly energy-efficient process that is currently used as a benchmark for new technologies[129]. Reported energy use for RO ranges from 3.7 to 8 kWh/m^3 for seawater and between 1.5 and 2.5 kWh/m^3 for brackish water[131,135]. Since RO plants only require electricity to function[131], this technology has a high potential for coupled renewable energy supply[78,123,136,137]. Some energy can also be recovered in the process by integrating turbines that capture the kinetic energy from the freshwater exiting the membrane[130,134].

As of 2020, RO, MSF and MED account for 94% of the total desalinated water produced worldwide (69%, 18% and 7%, respectively) , followed by nanofiltration (NF, 3%), electrodialysis (ED, 2%) and electrodeionization (EDI, <1%)[62]. RO capacity has been growing exponentially in the past two decades[62,63] , and is currently projected to lead the overall expansion in seawater desalination due to its energy efficiency and overall inherent simplicity and elegance[63,134]. However, additional considerations on feedwater, end-use purpose, plant capacity and technological advances are needed when evaluating new plant construction[63,131].

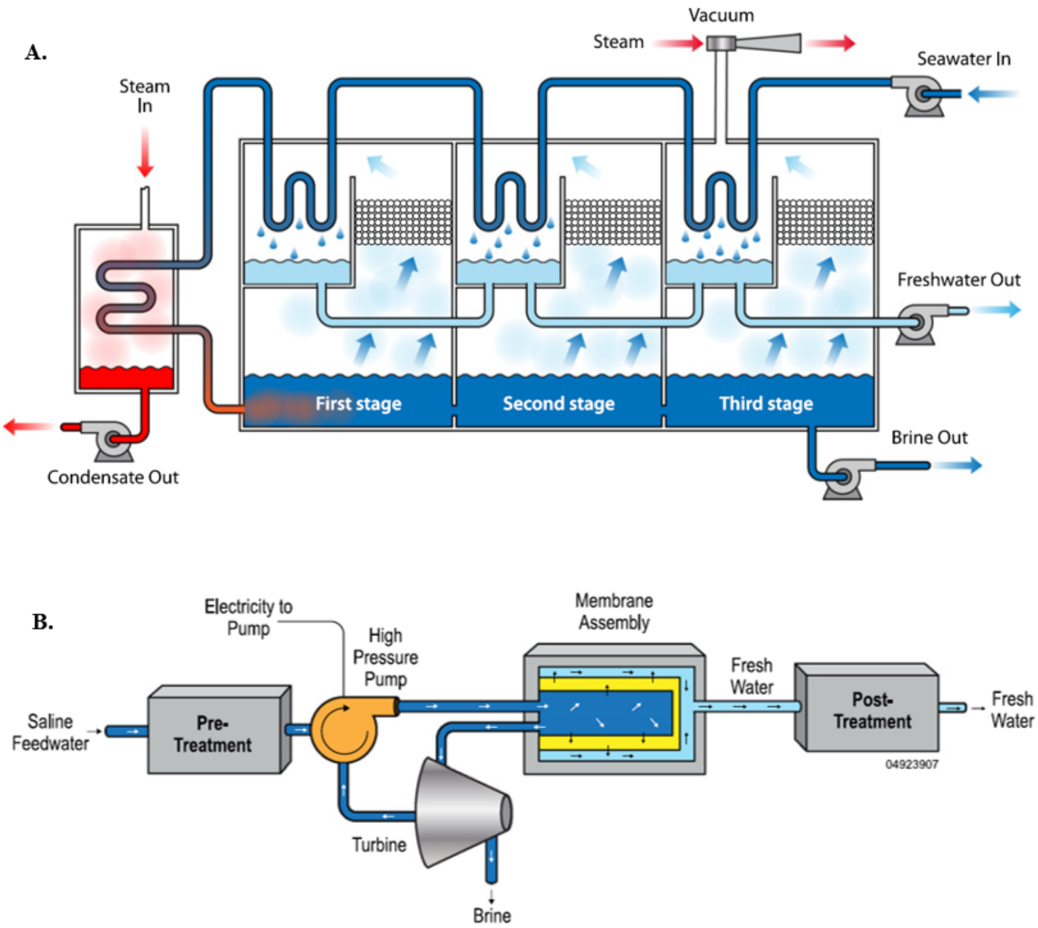

Figure 4. *Schematic diagram of (A) MSF unit and (B) RO system*[131].

1.2.3 Wastewater treatment

After freshwater has been used, the polluted wastewater needs to be collected and ideally treated in wastewater treatment plants (WWTPs), prior to being discharged or potentially being reused. All these processes (fig. 5) require intense energy use[138], and the overall energetic demands of wastewater treatment are only expected to grow as a consequence of socioeconomic developments (e.g. population growth, industrialization, increased sanitation) and stricter water quality requirements[35,73,108,139]. WWTPs further contribute to GHG emissions owing to the decomposition of organic material in the treated waters[140,141]. Crini % Lichtfouse (2019)[142] provide an overview of the different steps in treatment of wastewaters, in addition to advantages and disadvantages of the different technologies.

The energy used in a WWTP is dependent on the nominal size of the specific plant (bigger plants are usually more energy-efficient due to economies of scale), the load intensity, its age, the population served, the targeted nutrients and the level of treatment[104,106,138,143,144]. It is relevant to know that not all WWTPs necessarily execute more advanced treatments (fig. 5), and that not all wastewaters are treated prior to discharge[145].

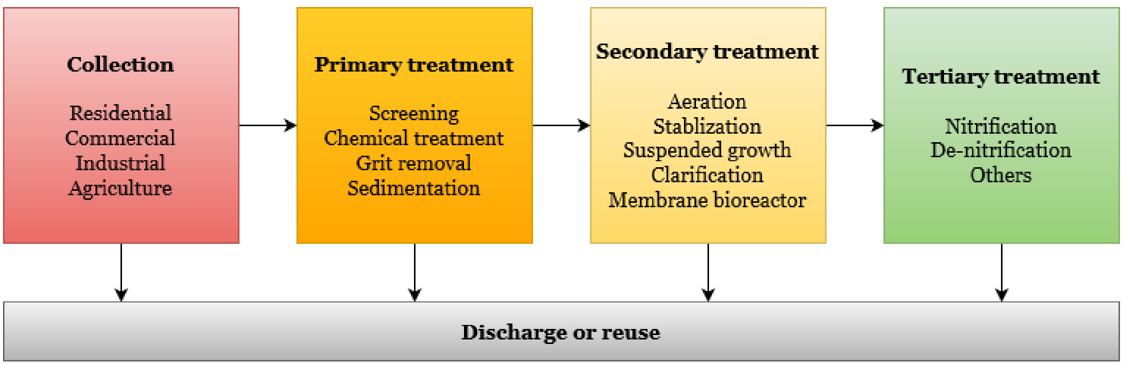

Figure 5. *Different wastewater treatment processes (modified after [106]).*

Assessments of energy use for WWTPs are further complicated by the fact that the strength of influent wastewater presents large spatiotemporal variations in quality[143,146]. For instance, rapid degradation of water quality during drought events[147] or increased inflows during floods may cause lower or higher energy use in WWTPs, respectively, due to opposite effects on dilution of contaminants[138,148]. Thus, it may be more adequate to characterize the energy intensity (EI) of a WWTP in kWh consumed to treat a population equivalent of wastewater (kWh/PE year), rather than in kWh/m^3 [138, 144]. The definition of PE may also differ between countries, and may be quantified as total nitrogen (gN/PE d), biochemical oxygen demand (g BOD/PE d) or chemical oxygen demand (g COD/PE d)[138]. In general, reported energy consumption for WWTPs ranges between 0.5-5 kWh/kg CODremoved [138].

The most energy-intensive process in the first phase of WWT is the pumping of sludge into the WWTP, requiring 0.003-0.19 kWh/m^3, and an overall 0.01-0.31 kWh/m^3 for the preliminary and primary treatment as a whole, including screening, grit removal and sedimentation[104,105]. Following this step, it is the type of technology employed for secondary treatment that determines most of the energy consumption in a WWTP[104,106,138,144], such as aerated lagoon or pond (AL), rotating biological contactor or biodisk (BD), biological nutrient removal (BNR), conventional aerated sludge (CAS), extended aeration (EA), membrane bioreactor (MB), oxidation ditch (OD) and trickling filter (TF).

An overview of energy intensities for different secondary treatment is given in Molinos-Senante & Sala-Garrido[144]. Overall, these techniques may consume on average between 0.57-2.91 kWh/kg CODremoved [138], with AL and MB being respectively the least and most energy-intensive ones[104,138,144]. Finally, the focus in tertiary treatment is the removal of nitrogen, which may require 0.4-0.5 kWh/m^3, and phosphorus, which consumes 0.06-1.6 kWh/m^3 in membrane processes[104].

1.3 Knowledge gaps

First and foremost, there is a pressing need to quantify the energy use of the water sector at the global scale. Quantifications are usually made at the scale of a physical process, local plant or country-aggregated, which may hinder proper representation of energy-for-water in Integrated Assessment Models (IAMs)[149]. Liu et al. (2016)[105] made a first-order estimation of global energy use of the water sector by merging historical data of water withdrawal with ranges of sectoral energy intensity collected from the literature. However, such an approach lacks physical consistency and is subject to a high degree of uncertainty due to bias on available data. The development of a hybrid process-based and data-driven model that is able to capture fine-scale spatio-temporal variations of energy consumption in the water sector will enable in-depth analysis and projections of future global energy use for the provision of clean water and alleviation of water scarcity.

Moreover, there is a limited understanding of the evolution in time and space of the cascading mechanisms between the water and energy sectors during droughts and heatwaves[85,88]. It is thus essential to explain how the energy use of the water sector responds to these extreme weather conditions (compared to average simulations) and to long-term climate change in order to balance the future provision of clean water and energy.

Thirdly, van Vliet et al. (2021)[51] quantified the potential for water scarcity alleviation by means of future expansion of clean water technologies. However, their model estimates were based on annual averages of present-day water scarcity, ignoring any impacts from extreme weather events. Furthermore, their study was limited to the analysis of the expansion of unconventional water resources, i.e. desalination and treated wastewater reuse. Thus, updates are needed in assessments of future water scarcity and expansion of technologies for future water supply.

Finally, the energetic implications of technological developments and expansion in the water supply are unknown. There is also a limited understanding of the potential trade-offs and synergies between water scarcity alleviation, clean energy provision and climate change mitigation[82,150]. By closing the previous knowledge gaps, it will be possible to tentatively quantify the consequences on GHG emissions due to the expansion of clean water technologies under various energy transitions and shared socio-economic pathways (SSPs)[151–153].

2 Objective and research questions

Reaching Sustainable Development Goal 6 of clean water for all[154] will have major implications on energy consumption by the water sector. Knowing the current energy use engrained in the supply of freshwater and wastewater treatment (and reuse) can further improve our understanding of the energetic implications of their future expansion. Projections of global energy consumption in the water sector will be affected by uncertainties in future water supply and demand, effects of global warming on long-term climate change and (compound) droughts and heatwaves, and socioeconomic scenarios (e.g. population, economy, industrialization, energy transitions). The overarching objective of this research thus concerns:

The quantification of global energy use for present and future clean water provision and water scarcity alleviation, considering changes in climate, weather extremes (droughts, heatwaves) and socioeconomic developments.

Our ability to make accurate projections of future energy use in the water sector will require closure of the knowledge gaps delineated in section 1.3. These can be associated to four main research questions (RQs) that will define the work outline (fig. 6). The proposed research questions are:

RQ 1. *What have been the spatiotemporal patterns and trends in global energy use of the water sector over recent decades?*

RQ 2. *What are the main drivers and mechanisms affecting energy use in the water sector during (compound) drought/heatwave events?*

RQ 3. *What are the energetic implications of expanding water technologies to provide clean water and mitigate future worldwide water scarcity (2030-2100)?*

RQ 4. *What are the potential trade-offs and synergies between providing clean water for all (SDG 6) and mitigating climate change (SDG 13)?*

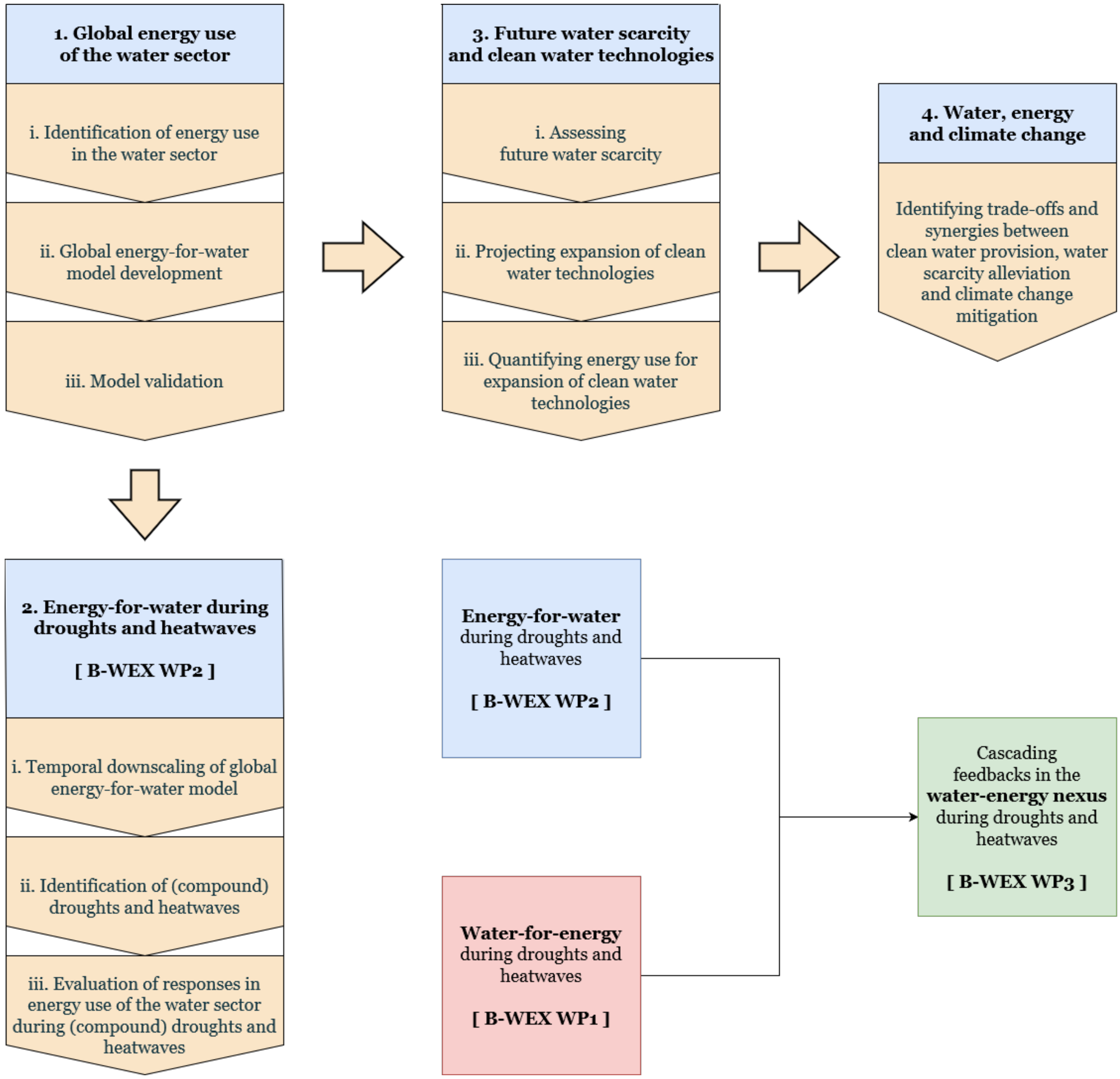

Figure 6. *Envisioned workflow of the PhD project and its position in the B-WEX project.*

3 Methods

3.1 Global energy use of the water sector

RQ 1. *What have been the spatiotemporal patterns and trends in global energy use of the water sector over recent decades (1970-2020)?*

a. Methodology

i. Identification of energy use in the water sector

A clear definition of *water sector* is of primary importance in developing our theories and models. We use the definition of *energy for water* delineated by Kyle et al. (2016)[107], which includes pumping and distribution (agricultural, municipal, industrial sectors), raw water treatment/desalination, collection and treatment of wastewaters, and their discharge or reuse. This phase is also dedicated to the collection of data regarding the energetic intensity of the various sectors, which will be used to calibrate and validate the model. Although it is not in the scope of this research, the framework can later be expanded to include additional hidden energy use in the water sector, e.g. the impacts of the bottled water industry[155], water heating/cooling and household or industrial appliances[74,103,108].

The water sector as defined thus implies the calculation of energy use at the following main levels in the water use cycle:

1. Water pumping from different sources (i.e. depth) and routing (i.e. distance between source and end-use point) for a) irrigation, b) municipal drinking water supply and c) industrial processes;

2. Raw water treatment, with a focus on disentangling energy use of the various desalination technologies;

3. Collection, treatment and reuse or discharge of wastewaters.

ii. Global energy-for-water model development

This phase consists in building the Global-scale model of ENErgy use of the Water Sector (GENEWS) that will enable quantification of the total energy use (kWh) in the water sector as defined. A conceptual scheme, parameters and assumptions for this model are shown in fig. 7. By using a bottom-up combination of process-based and statistical descriptions of energy use for various processes, we aim to quantify historical energy consumption in the water sector with parametric uncertainty. This will be done initially at a yearly scale, to identify long-term trends, and then at a monthly scale to describe seasonal variations. The model will rely on a combination of physically-based (whenever possible) and data-driven approaches, as described below.

- The following physical relation describes the energy consumed in water pumping[74,110]:

$$E = \frac{[g * h] * [\rho * Q * \Delta t]}{3.6 * 10^6 * \eta} \tag{1}$$

where E is the energy used (kWh), g is the acceleration of gravity (9.8 m s^{-2}), h is the pumping lift height (m), ρ is the density of water (1000 kg/m^3), Q is the abstraction rate (m^3 s^{-1}) over a time Δt (s), η is the efficiency of the pumping system (between 0 and 1) and $[3.6 * 10^6]^{-1}$ is the conversion factor from [J] to [kWh]. Lifting 1 m^3 of water to a height of 1 m for a system with 100% efficiency thus requires 0.0027 kWh/m^3 [74]. This relation has already been used in a few case studies to model the energy use related to groundwater abstraction in Northern China[111,118]. However, large-scale assessments and standardized comparisons across regions are currently lacking.

For groundwater pumping, a 5 arcmin global-scale transient groundwater model[156] can be employed to simulate transient historical groundwater heads (m) and groundwater depletion for the years 1970-2020 (fig. 8). Values of sectoral groundwater abstraction (m^3/d) can then be taken from PCR-GLOBWB[157]. By merging these two datasets and making assumptions on pump efficiencies, a global dataset of energy used in groundwater pumping can be built. PCR-GLOBWB also includes quantifications of surface water withdrawals. Water abstracted from either source is further divided amongst the main end-users, i.e. agriculture, municipalities and industry.

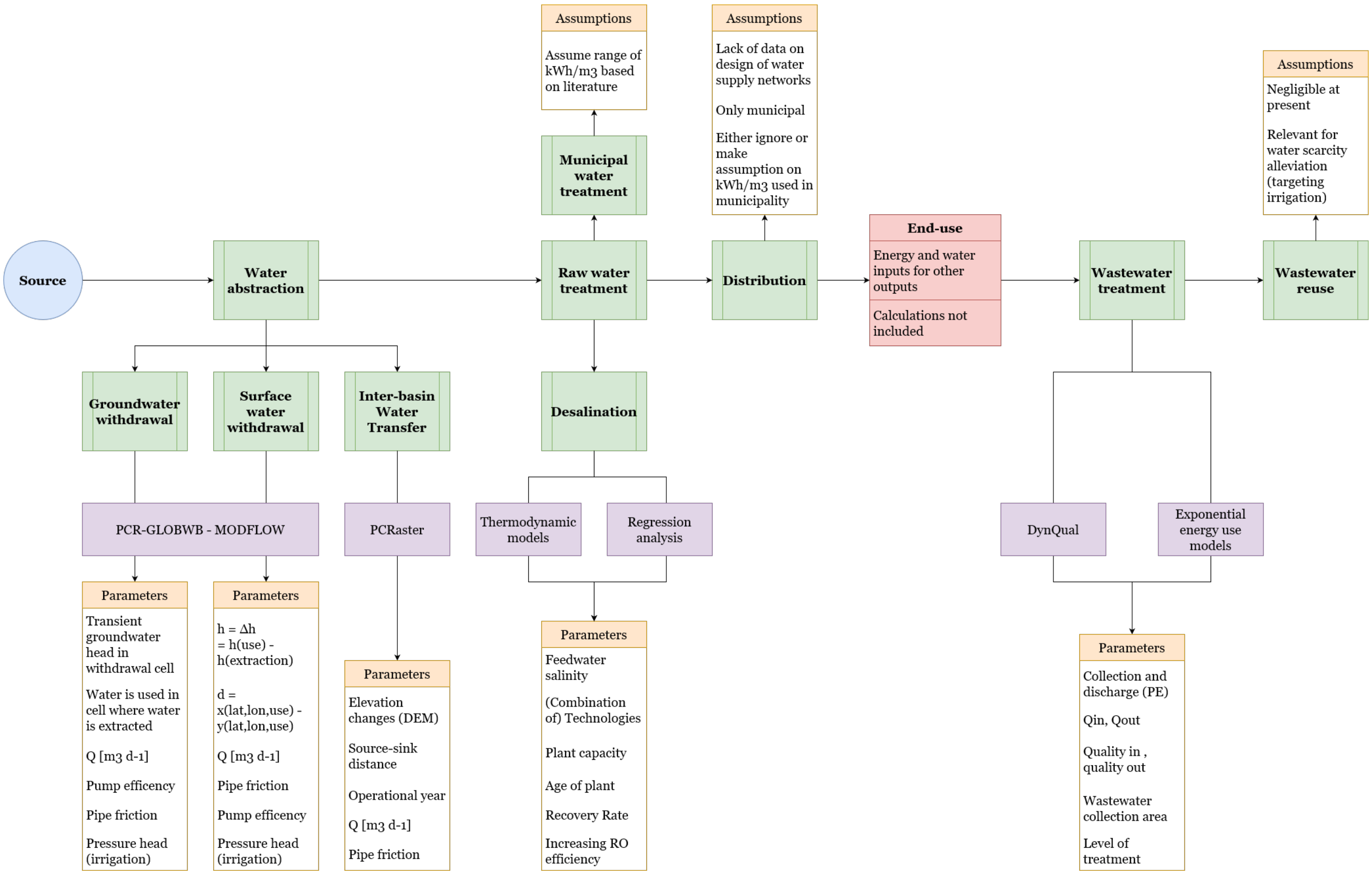

Figure 7. *Scheme of processes (green) represented in the energy-for-water model, possibly employed frameworks (purple) and their assumptions and/or parameters.*

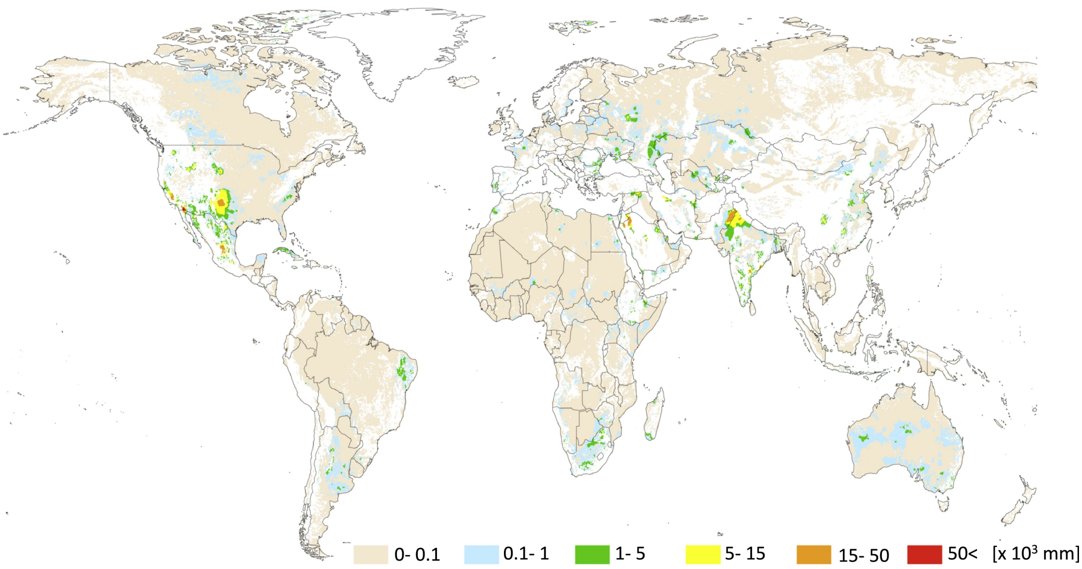

Figure 8. *Cumulative groundwater depletion (in mm over 1960–2010) resulting from human water use, modelled with a two-layer transient groundwater model*[156].

- Inter-basin water transfer megaprojects (WTMP) (fig. 9) are the most evident form of surface water pumping to resolve imbalances in water availability. WTMP are large-scale engineering operations that either exceed US$ 1 billion in cost, 190 km in distance or transfer more than 0.23 km^3 per year[158]. Even though their overall sustainability is being questioned[159,160] and their environmental impacts can be disruptive to ecosystems[161,162], there are currently 34 existing (fig. 9A) and 76 planned WTMP[158] (fig. 9B).

  It is highly likely that WTMP currently consume significant amounts of energy to move water between and within river basins[104]. If future projects are approved and developed, the contribution of WTMP to projections of energy use in the water supply will continue to increase. Modelling the energy use in WTMP can potentially be achieved with the Python PCRaster framework[163]. By integrating a Digital Elevation Model (DEM) with the spatial distribution of long-distance piping, and by making assumptions on pump efficiency, pipe friction and water leaks it might be possible to understand what is the energy use of these large-scale water engineering projects.

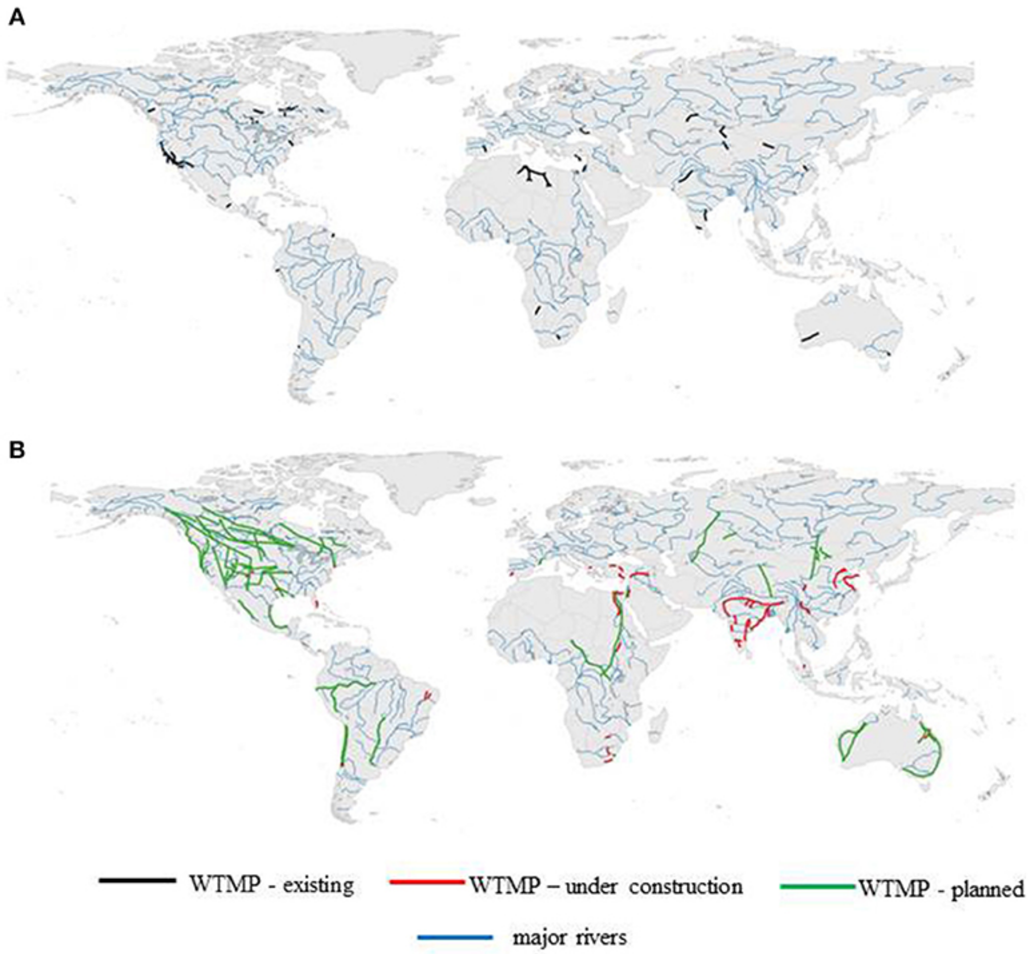

Figure 9. *Global distribution of (A) existing water transfer megaprojects (black lines) (N = 34) and (B) future water transfer megaprojects that are under construction (red lines) or in the planning phase (green lines)*[158].

- Evolutions of energy use for desalination in time and space will be simulated using inputs from DesalData[164], which provides the starting operational year of desalination plants worldwide, in addition to the feedwater type, the specific technology employed, i.e. thermal or membrane, plant capacity and intended end-use (fig. 10).

  The theoretical minimum energy to separate freshwater from seawater is independent of the desalination method, and is limited by the second law of thermodynamics[135,165]. Values of said minimum can be calculated as a function of the recovery rate (RR), i.e. the percentage of seawater converted to freshwater, and are dependent on the osmotic pressure of the feedwater[129,134,165] (i.e. its total dissolved solids (TDS)) (fig. 11A):

$$dW = \Pi_{os} * dv \tag{2}$$

  where dW is the work required for separation, Π_{os} is the osmotic pressure of the inlet water and dv is the volume of freshwater produced.

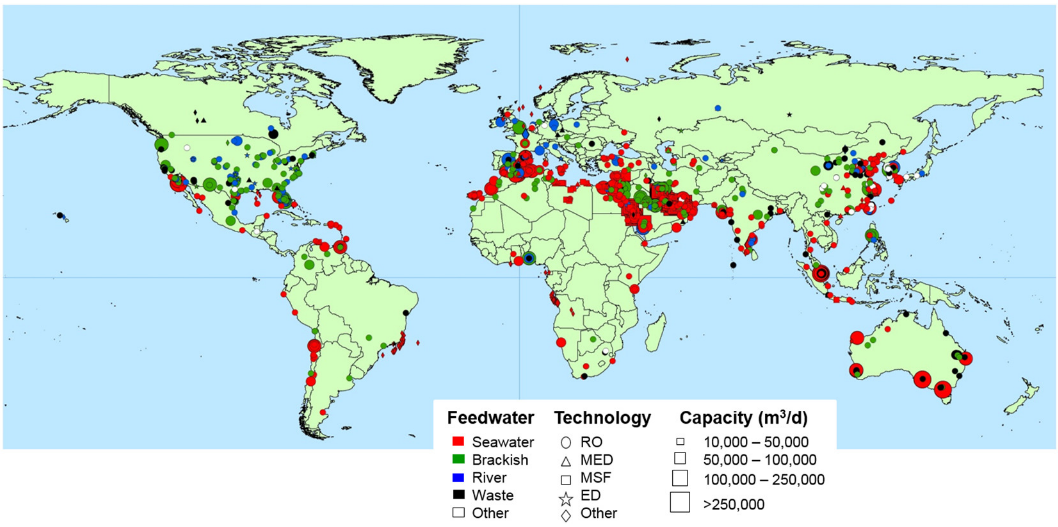

Figure 10. *Global distribution of large desalination plants by capacity, feedwater type and desalination technology*[62].

At 25 °C, the calculated values of the energy demand for desalination range from 0.77 kWh/m^3 with 0% RR at 33,000 ppm TDS[131]; 0.71, 0.81, 0.97 and 1.29 kWh/m^3 for 25%, 50% and 75% RR at 34,300 ppm TDS[134]; and 1.06 kWh/m^3 with 50% RR at 35,000 ppm TDS[129]. Most plants operate at an average 50% RR, ranging between 40% and 60%[62,129]. Plants that process brackish seawater require less minimum energy (due to lower inlet Π_{os}) and usually operate at higher RR[62,134].

However, the actual energy consumption is larger since desalination plants are finite, i.e. the thermodynamics are irreversible[129,131,134,165]. In addition to the initial salinity of the feedwater and the RR, the energy demand for desalination is related to the operational scale of the plant itself (large plants are generally more efficient due to economies of scale[130,133]), water pre- and post-treatment and ultimately the employed technology[130,131]. Since its advent in the 1950s, energy consumption in reverse osmosis (RO) has decreased such that RO plants today work very close to theoretical minima[129] (fig. 11B). Thus, year-to-year improvements in energy efficiency will be considered for RO, while energy use in thermal technologies are to be considered constant as in Liu et al. (2016)[105].

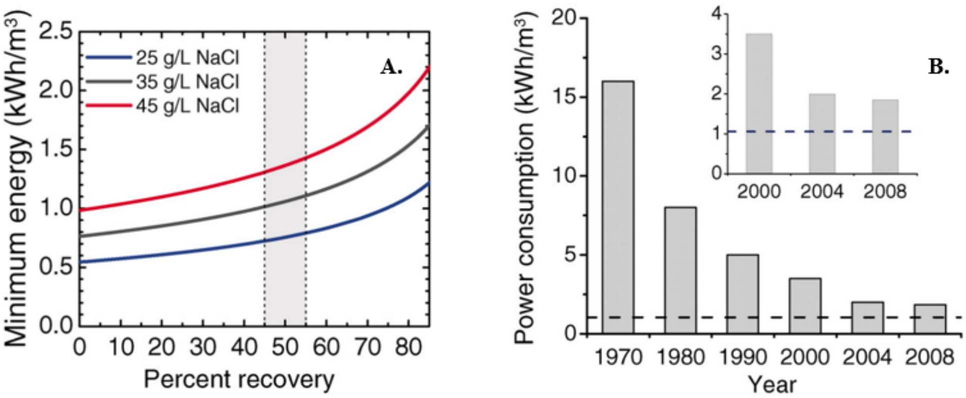

Figure 11. *(A) Theoretical minimum energy for desalination as a function of RR for common seawaters. Minimum energies for recoveries between 45 and 55% are highlighted. (B) Change in power consumption for the reverse osmosis stage from the 1970s to 2008. The horizontal dashed line corresponds to the theoretical minimum energy required for desalination of 35 g/litre seawater at 50% recovery (1.06 kWh/m^3). The data exclude the energy required for intake, pre-treatment, post-treatment, and brine discharge*[129].

- For what concerns the energy used in wastewater treatment plants (WWTPs), the rapid audit (RA) methodology will be used[166]. RA (fig. 12) consists of black-box modelling of energy use in a WWTP based on a) aggregated energy consumption from energy bills; and b) routine analysis of influent/effluent water quality.

  Additional parameters can be employed to account for inflow/outflow rates, age of the treatment plant, wastewater collection area and amount of sludge produced[148], in addition to the overall level of treatment (i.e. primary, secondary, tertiary) executed in the specific plant. Potential datasets to be explored to this end are hydroWASTE (fig. 13)[167] and data on wastewater production rates from Jones et al. (2021)[145] and Jones et al. (2022)[33].

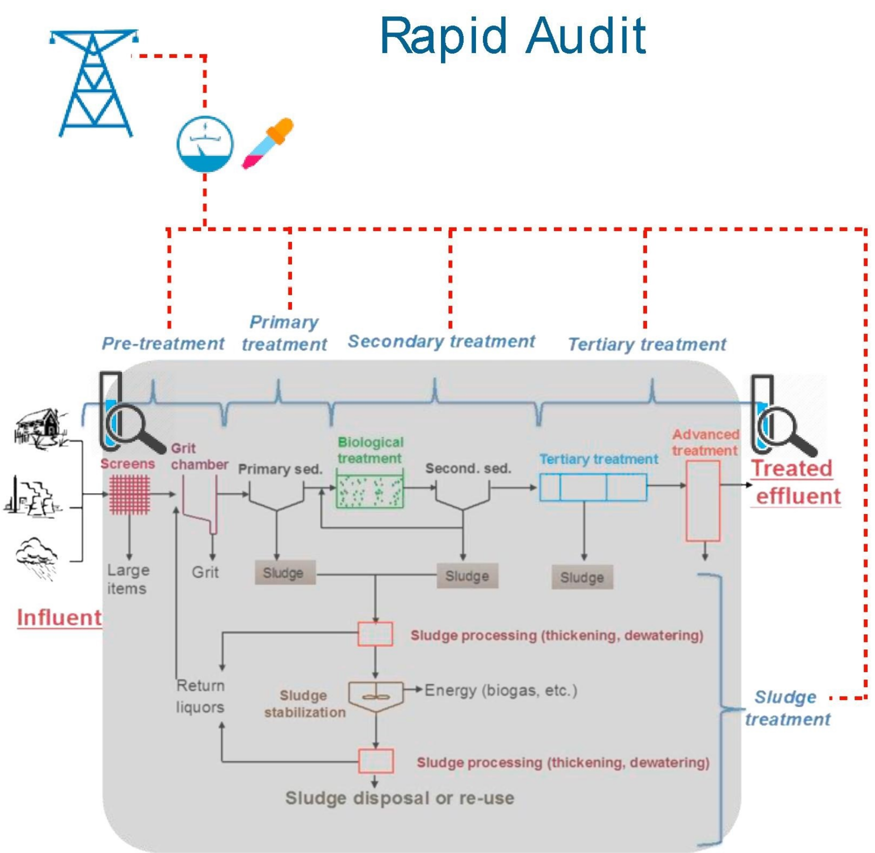

Figure 12. *Scheme of Rapid Audit (RA) ENERWATER methodology. The grey square indicates that in RA both the energy consumption and the operation data refer to the entire plant observed as black box*[166].

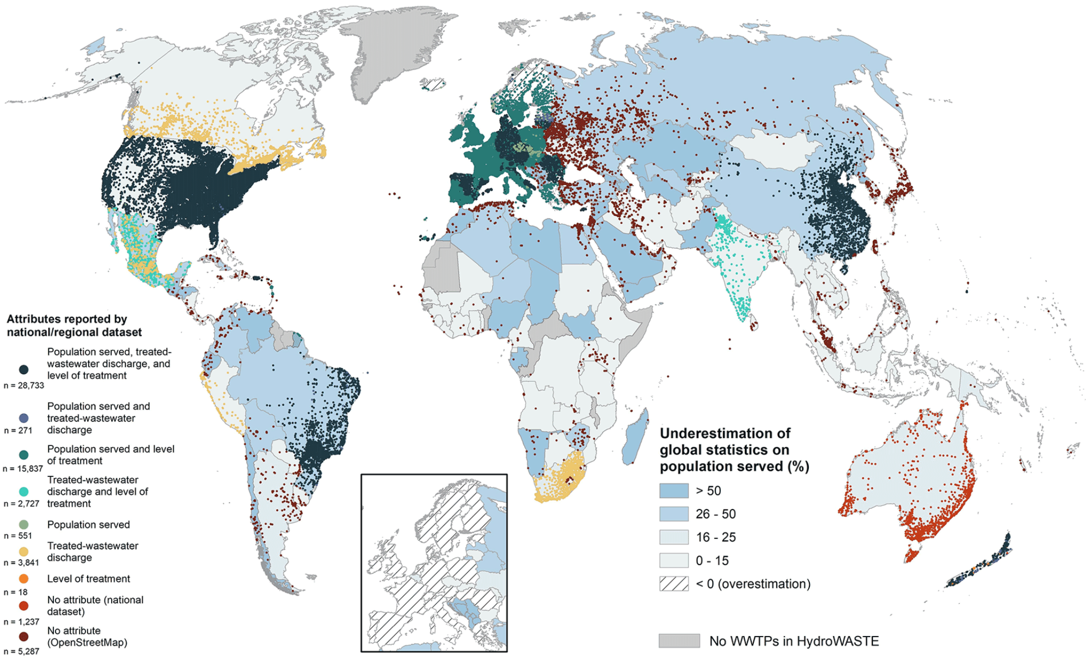

Figure 13. *WWTP locations, attributes, and completeness of population served in HydroWASTE*[167]*. Each point represents a WWTP, with colors depicting their reported attribute completeness with respect to the population served, treated-wastewater discharge, and level of treatment. Due to the high point density in Europe, an inset was added to show the underlying country shading.*

Exponential functions have been shown to work better than linear ones in describing the Energy Intensity (EI) of WWTPs[144,148]. Niu et al. (2019)[148] developed the following multi-parametric exponential model to assess the energy use of WWTPs in China:

$$E = e^{\alpha} * W^{\beta} * Y^{\delta} * S^{\omega} * M^{\theta} * P_{in}^{r_{in}} * P_{out}^{r_{out}} \tag{3}$$

where E is the electric energy consumption of a WWTP (kWh/y) and e, W, Y, S, M, P_{in}, and P_{out} are continuous variables: e is the base of the natural logarithm ($\approx$2.718); W is the flow rate and represents the treatment scale of the WWTP (m^3/year); Y is the age of the plant facility (years); S is the wastewater collection area of the pipe network (km^2); M is the amount of sludge produced and processed per unit wastewater treated (t/m^3); P_{in} is the concentration of pollutant in the influent (mg/L); P_{out} is the concentration of pollutant in the effluent (mg/L); β, δ, ω, θ, r_{out}, and r_{out} are all regression coefficients of the above variables that were derived through regression based on sample data.

iii. Model validation

Developing the model parallelly requires the building of a dataset that collects all the scattered data on energy use of various processes in the global water supply. This dataset will be used to calibrate/validate global simulations at regional scales. Global energy use of the water sector as defined is expected to be in the 1-5% range of total global energy consumption, with slight variations between countries[105].

b. Novelty

This research phase will bring to the creation of the first hybrid model of energy use in the water sector. The development of such a model will enable estimation of worldwide spatiotemporal evolution of energy use in the water supply in the past decades (1970-2020). The framework can potentially be used to improve quantitative analysis and future balance of the water-energy(-food-ecosystems) nexus at different scales. The outcome paper of this first phase will be either a reanalysis or a description of model development and results.

Paper 1. *Global energy use of the water sector*

c. Risks and feasibility

This phase likely represents the biggest challenge in the PhD project, as the energy-for-water model developed here will be the base for all other research steps. Challenges here are related to choosing appropriate models to describe energy consumption for different processes, identifying model parameters, gathering input and validation data, and understanding model run times. A sensitivity analysis should also be included to quantify the impacts of uncertainties in model parameters on the quantification of energy use at the global scale. After satisfactory validation, application in scenarios should technically be less cumbersome to implement.

Data is lacking for locations of raw water treatment plants (excluding desalination) and water distribution networks. This might make it difficult to spatially quantify the energy use for the treatment and supply of non-saline surface waters. If acceptable data is not found, energy use for these processes can be considered static in space at the locations of surface water withdrawal in PCR-GLOBWB.

d. Outcomes

Outcome 1.1. GENEWS: A novel hybrid model of energy use in the water sector.

Outcome 1.2. Historical reanalysis of energy use in the water sector (1970-2020), including long-term trends and seasonal variabilities.

3.2 Energy-for-water during droughts and heatwaves

> **RQ 2.** *What are the main drivers and mechanisms affecting energy use in the water sector during (compound) droughts and heatwaves?*

a. Methodology

i. Temporal downscaling of global energy-for-water model

Here, the developed and tested GENEWS model will be run at finer temporal scales (weeks at first, maybe days) to be able to identify potential correlations between (compound) drought/heatwaves events and the energy use of the water sector. This phase will be a foundational part for the **B-WEX** project, of which this PhD research is **Work Package 2**. Evaluation of the model at this finer temporal scale will enable coupling to the *water for energy* model developed in **Work Package 1**, to study the cascading feedbacks between the water and energy sectors under long-term climate change and increasing extremes.

ii. Identification of (compound) droughts and heatwaves

In addition to studying the effects of long-term climate change on the water-energy nexus, the B-WEX project focuses on droughts and heatwaves and potential compound drought/heatwave events[168–170], as the direct effects on the water and energy supply and demand may be more readily evident during these weather extremes. Thus, it is necessary that clear indexes are used for the definition of drought[20,92] and heatwave[171,172]. Quantifications of droughts (hydrological and agricultural) and heatwaves and their compound occurrence are part of the PhD research of Gabriel Antonio Cárdenas Belleza MSc, who will produce 'a set of timeframes and locations of interest', in addition to sectoral water use during these events. The GENEWS model can later be potentially used in the simulation of energy use in the water sector during other weather extremes[90].

iii. Evaluation of responses in energy use of the water sector during (compound) droughts and heatwaves

Once locations and timeframes of (compound) droughts and heatwaves are identified, the availability of water and the different sectoral water demands will determine the energy consumption to sustain the supply of clean water during these events. At this stage, outputs from the GENEWS model at these times and places will be visualized to identify short-term trends in energy use of the water sector during these events.

We hypothesize that the biggest role in energy use increase during droughts and heatwaves will be played by groundwater withdrawals (e.g. fig. 14), caused by the compounding effect of a lowered water table and the reduced availability of surface water, in addition to increased irrigation and conflict between water demands from different sectors. In contrast, wastewaters are usually more concentrated during droughts[147], which may increase the energy efficiency of WWTPs[138,148], as opposed to during rainfall events and extreme floods, which may cause higher energy use due to higher dilution of wastewaters by stormwater and their increased pumping to avoid surface overflows.

b. Novelty

The product of this research phase may be a short letter in which the GENEWS model is applied to a few case studies, i.e. showing concise results in selected locations of the behaviour of energy use in the water sector during (compound) droughts and heatwaves. A potential co-authorship could be considered with Gabriel Antonio Cárdenas Belleza MSc for his identification of droughts and heatwaves and sectoral water use during these events.

Paper 2. *Global impacts of droughts and heatwaves on energy use in the water sector*

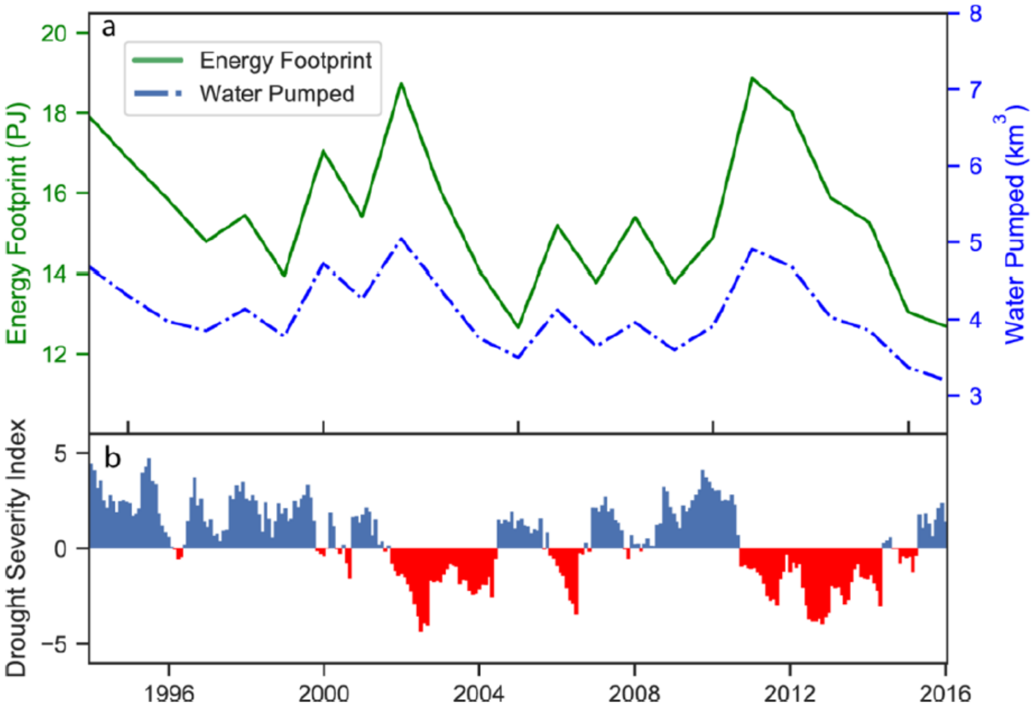

Figure 14. *(a) Energy footprint (PJ/total annual irrigation) and water use from irrigation from 1994 to 2016 for the High Plains Aquifer portion of Kansas. (b) Palmer drought severity index averaged for the Climate Divisions 1, 4, 7, and 8 of western Kansas, which shows two drought periods from 2002 to 2004 and 2011 to 2014 [173].*

c. Risks and feasibility

There may be a significant lack of data of energy use in the water sector during droughts and heatwaves to validate model performance under these weather extremes. Moreover, running the global model at sub-monthly scale may require intense memory use. A potential solution could be either to downscale only specific timeframes and/or run the model only for certain locations.

d. Outcomes

Outcome 2.1. Temporal downscaling of the GENEWS model.

Outcome 2.2. Analysis of responses of energy use in the water sector during droughts and heatwaves.

3.3 Future water scarcity and clean water technologies

RQ 3. *What are the energetic implications of expanding water technologies to provide clean water and mitigate future worldwide water scarcity (2030-2100)?*

a. Methodology

i. Assessing future water scarcity

The quantification and potential of future expansion of clean water technologies will build on novel assessments of future water scarcity (2030-2100). These will include additional water quality parameters in the DynQual model[33] and calculations of sectoral water use interactions and environmental flow requirements, to reflect seasonal variabilities in water availability and demands[59,60] and uncertainties in future SSP-RCP pathways[174]. Quantifications of future water quality will be provided by Edward Jones MSc and Duncan Graham MSc, while future sectoral water use will be provided by Gabriel Antonio Cárdenas Belleza MSc. Edward Jones MSc and Gabriel Antonio Cárdenas Belleza MSc will also provide future quantifications of water scarcity.

ii. Projecting expansion of clean water technologies

Model outputs from PCR-GLOBWB[157] (water quantity) and DynQual[33] (water quality) will therefore be used to make projections of the potential impact of future expansion of clean water technologies on water scarcity. These will require making assumptions or creating a predictive model to explore which technologies will be built and where, based on past developments (e.g. desalination close to the coast, wastewater treatment plants closer to urban or manufacturing environments, pumping in rural areas). Future hydroclimatic and socioeconomic developments will also generate potential hotspots where the expansion of different technologies will have the highest impact in reducing future water scarcity. Fig. 15 shows an example of probabilistic projections of future desalination plants.

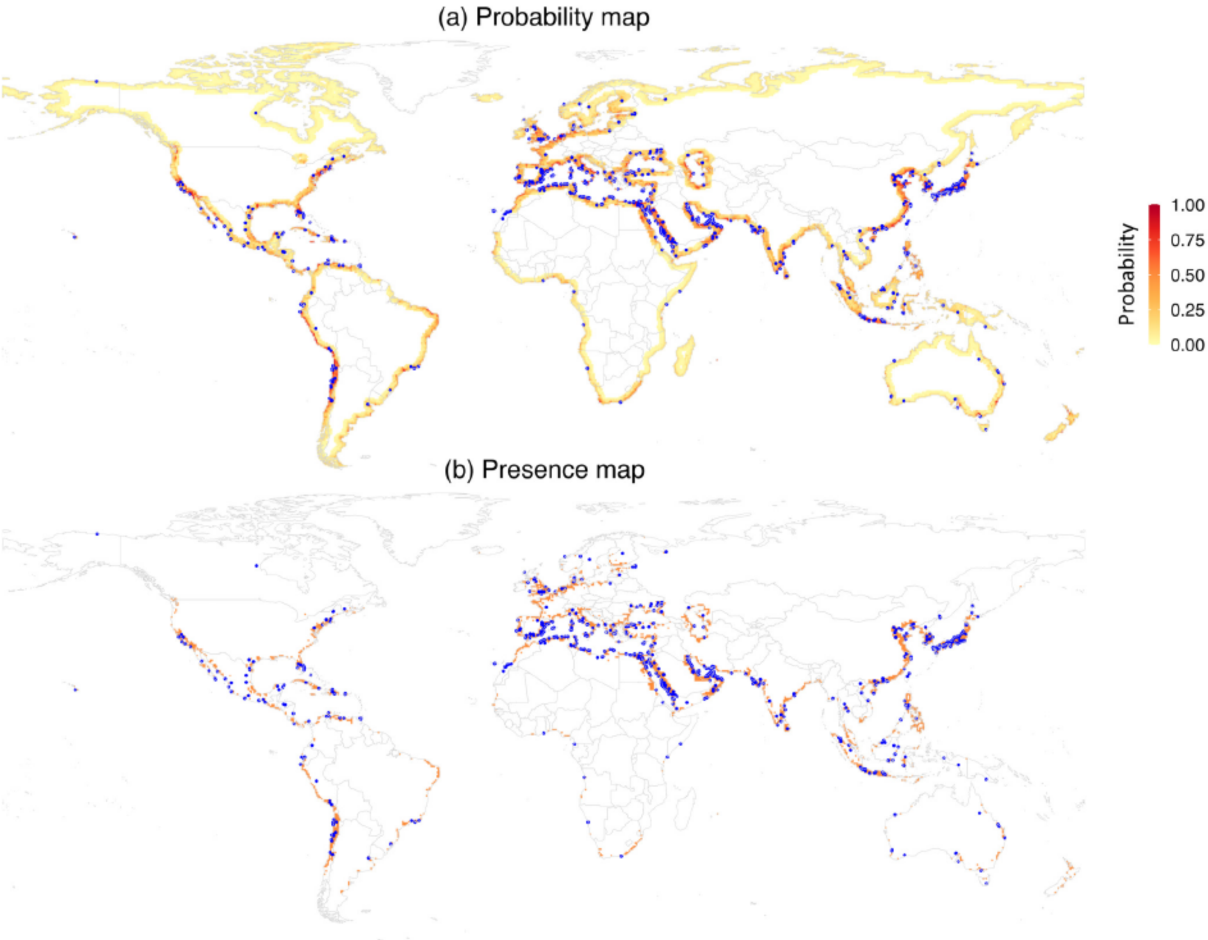

Figure 15. *Probabilistic modelling of future desalination plants*[175]*. The ensemble probability map (a), and the ensemble presence map (b) generated from the current predictions of the random forest and generalized boosted regression model. The blue dots denote the locations of the desalination plants by 2014. The legend in (a) shows the predicted probability of occurrence of seawater desalination plants with values ranging from 0 to 1.*

iii. Quantifying energy use for expansion of clean water technologies

Projections from section 3.3.ii will be used as inputs to the GENEWS model to calculate the energetic implications (kWh/year) of expanding clean water technologies to mitigate future water scarcity (2030-2100). Additional scenarios may be created by calculating in which places each specific technology (i.e. pumping, desalination, wastewater treatment) will be most energy-efficient at alleviating the most water scarcity, potentially with an optimization approach. Different projections that consider developments and potential improvements in energy efficiency of various clean water technologies may also be considered.

b. Novelty

Paper 3. *Energetic implications of expanding clean water technologies to mitigate future water scarcity worldwide*

c. Risks and feasibility

This phase is dependent on quantifications of water scarcity from other researchers. Different scenarios of technological expansion should be considered to have a better picture of uncertainties in future energy use.

d. Outcomes

Outcome 3.1. Future scenarios of spatiotemporal distribution of clean water technologies.

Outcome 3.2. Quantification (with uncertainties) of future energy use for expansion of clean water technologies.

3.4 Water, energy and climate change

RQ 4. *What are the potential trade-offs and synergies between providing clean water for all (SDG 6) and mitigating climate change (SDG 13)?*

a. Methodology

This final research phase will exploit the projections of future energetic demands calculated in paper 3 to quantify GHG emissions of expanding clean water technologies under various energy transitions and SSPs worldwide. This phase may require integration and/or coupling of projections of SSP-RCP scenarios from Integrated Assessment Models (IAMs)[176] with the novel energy-for-water model. Potential collaborations may include scientific communities involved with the IMAGE model[177] and the energy supply model MESSAGE[178]. This research phase might also require to quantify the effects of a changing climate and increasing droughts and heatwaves (i.e. baseline scenario with no technological expansion) on energy use in the water sector. Overall, the aim here is to identify trade-offs and synergies between clean water and energy provision, water scarcity alleviation and climate change mitigation[96].

Here, the potential to target multiple Sustainable Development Goals is considered through scenarios that integrate the water supply and the expansion of clean water technologies within renewable and/or circular energetic frameworks. For example, water pumping[76,179] and RO desalination[78,104,136] have the potential to provide clean water with little to no GHG emissions. On another note, wastewater treatment may be completely self-sufficient, as energy contained in the sludges far exceeds the energetic needs of WWTPs[121,180,181].

b. Novelty

There is potential for this research phase to achieve significant impact on how we perceive connections between some of the global challenges that lie ahead, as this work lies at the intersection of hydrology, energy science, biogeochemistry and (potentially) economy. In this paper we aim to demonstrate that reduction in water scarcity does not necessarily mean increasing our dependence on fossil fuels, as this would ultimately conspire to worsen the current efforts in climate action. For comparison, however, the resulting paper should also include results quantifying the impacts of expansion of water technologies in a 'business-as-usual' scenario[182,183].

Paper 4. *Simultaneous water scarcity alleviation and mitigation of GHG emissions*

c. Risks and feasibility

This is a highly risky research phase, as it is dependent on all previous steps, especially 3.1. and 3.3., i.e. model development and projections of future expansion in clean water technologies. Multiple models will also need to be used for climate change, energy transitions and socioeconomic developments, to give the best possible overview of the uncertainties inherent to our modelling approach.

d. Outcomes

Outcome 4.1. Quantification of GHG emissions for 2030-2100 due to expansion of clean water technologies, considering different scenarios of climate change, energy transitions and socioeconomic developments.

4 Timetable

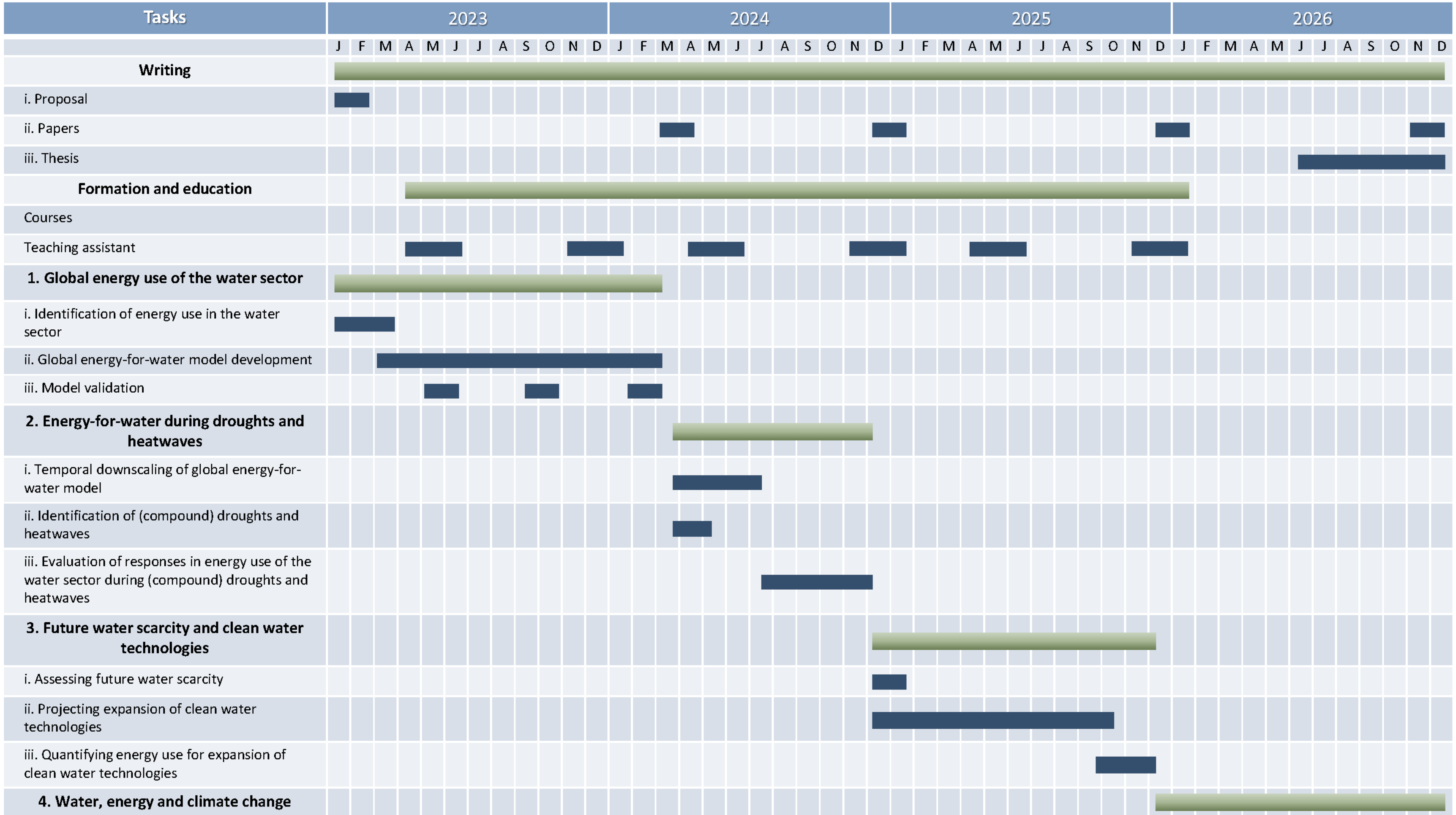

Figure 16. *Gantt chart of the PhD project.*

5 Collaborations

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6 Data management plan

All model source code will be shared on GitHub. Input and output files will be shared either on Zenodo, Yoda or Surf.

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