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EXTENDED METHODOLOGY FOR WATER RESOURCES AND WATER-RELATED ENERGY ASSESSMENT ADDRESSING WATER QUALITY

ROZŠÍŘENÁ METODIKA PRO HODNOCENÍ VODNÍCH ZDROJŮ A JEJICH ENERGETICKÉ NÁROČNOSTI S OHLEDEM NA KVALITU VODY

DOCTORAL THESIS

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Abstract

Water issues, especially water scarcity and water pollution, have been affecting human lives and economic developments for a long time. Global climate changes exacerbate the probability and frequency of extreme events such as water scarcity and severe floods. The increasing irregular water supply and water pollution issues require more advanced water resources assessment methodologies to guide practical water use and management. This thesis presents the extended methods for water quantity-quality assessment and water-related energy consumption and emissions. Three major methodologies are proposed based on the Water Footprint concept and Water Pinch Analysis frameworks to assess the quantity and quality impact of water use. These methods are also demonstrated with numerical and empirical case studies targeting regional and industrial water resource assessment and optimisation. In addition, the Water-Energy Nexus is discussed to investigate the water issues from a broader perspective. An initial assessment of the water-related energy and GHG emissions of the seawater desalination industries is carried out.

The studies in this thesis convey several contributions to the current water resource assessment methodologies. The proposed Water Availability Footprint made an initial effort to cover the water quality degradation impact into the existing water scarcity assessment frameworks, which was not addressed previously. The second contribution of this work is the proposal of the Quantitative-Qualitative Water Footprint (QQWFP), where a cost-based water footprint is defined and determined with the total cost of water consumption and removing contaminants generated during the water use process. The cost-based water footprint provides results which are more intuitive for water managers and the public and can better guide industrial and regional water use and management. The third contribution is the development of the Water Scarcity Pinch Analysis (WSPA), which applied the Water Pinch Analysis at a macro level for regional water use assessment and optimisation. All three proposed methods determine the water use impact in terms of water quantity and quality, and the QQWFP and WSPA also cover the impact of multiple contaminants.

In addition to seeking solutions, this thesis also proposes potential directions for future investigations. Significant potential aspects to be further discussed include 1) a more advanced quantification method of the impact of multiple contaminants, and 2) an implementation and economic feasibility analysis of the WSPA and QQWFP with localised data, which seek a customised solution to regional and industrial water use optimisation.

Abstrakt

Problémy s vodou, zejména její nedostatek a znečištění, ovlivňují každodenní lidský život a hospodářský vývoj. Globální změny klimatu zvyšují pravděpodobnost a četnost extrémních událostí jako jsou sucho a záplavy. Rostoucí problémy s nepravidelnou dostupností a znečištěním vody vyžadují pokročilejší metodiky hodnocení vodních zdrojů, které povedou k efektivnímu využití a hospodaření s vodou. Tato práce se zabývá rozšířenými metodikami pro hodnocení vody z pohledu její kvality a kvantity a pro hodnocení spotřeby energie a produkce emisí souvisejících s vodou. Tři hlavní metodiky jsou navrženy na základě konceptu vodní stopy (Water Footprint) a pinch analýzy vody (Water Pinch Analysis) pro posouzení kvantitativních a kvalitativních hledisek využití a spotřeby vody. Použití těchto metod je rovněž demonstrováno pomocí numerických a empirických případových studií zaměřených na hodnocení a optimalizaci využití regionálních a průmyslových vodních zdrojůDále jsou diskutovány souvislosti mezi vodou a energií (Water-Energy Nexus) za účelem analýzy problémů týkající se vody z širší perspektivy. Z pohledu vody a vodních zdrojů je provedeno počáteční zhodnocení energetické náročnosti a produkce emisí skleníkových plynů v problematice odsolování mořské vody.

Výsledky prezentované v této práci navazují na současné metodiky hodnocení vodních zdrojů. Stopa dostupnosti vody (Water Availability Footprint) byla navržena pro zohlednění dopadu degradace kvality vody ve stávajících postupech pro posuzování nedostatku vody, ve kterých nebyla dříve řešena. Druhým přínosem této práce je návrh konceptu kvantitativní-kvalitativní vodní stopy (Quantitative-Qualitative Water Footprint - QQWFP), ve kterém je definována vodní stopa z pohledu nákladů a následně je stanovena v souvislosti s celkovými náklady na spotřebu vody a odstraňování kontaminantů, které se do vody dostávají v průběhu jejího využití. Vodní stopa založená na nákladech poskytuje výsledky, které jsou intuitivnější jak pro management vodních zdrojů tak i pro veřejnost. Tento přístup umožňuje lépe kontrolovat a řídit průmyslové a regionální využívání a správu vody. Třetím přínosem této práce je rozšíření pinch analýzy nedostatku vody (Water Scarcity Pinch Analysis - WSPA), ve které je aplikována pinch analýzy vody na makroúrovni se zaměřením na regionální hodnocení a optimalizaci zdrojů a využívání vody. Všechny tři navržené metody jsou zaměřeny na stanovení dopadů využití vody z hlediska jejího množství a kvality, analýzy QQWFP a WSPA také pokrývají dopady vícečetných kontaminantů.

Kromě hledání řešení se tato práce také pokouší naznačit potenciální směry pro budoucí výzkum v dané oblasti. Mezi významná potenciální témata k diskuzi patří 1) pokročilejší metoda kvantifikace vlivu více kontaminantů a 2) implementace a analýza ekonomické proveditelnosti přístupů WSPA a QQWFP s lokalizovanými daty, kteří hledají přizpůsobené řešení pro optimalizaci využití regionální a průmyslové vody.

Contributing Research Work Presented in Peer-Reviewed Publications

This thesis has been developed based on my publications in several distinguished international journals. In **Chapter 2**, the extended Water Availability Footprint Assessment framework and case studies are published in the Journal of Sustainable Development of Energy, Water and Environment Systems [1] and Resources, Conservation and Recycling [2]. Methodology development and applications of the Water Scarcity Pinch Analysis in **Chapter 3** are published in the journal of Resources, Conservation and Recycling [3]. The Water-Energy Nexus investigation presented in **Chapter 4** is based on the works published in Energies [4]. The review studies, and other developed assessments methods and results composing the thesis are published in other international journals, including the Journal of Cleaner Production, Applied Thermal Engineering, Chemical Engineering Transactions (Scopus Index). Major publications contributing to the thesis are listed as follows, and the complete publication list contributing to this PhD study can be found at the end of the full thesis.

1. **Jia, X.**, Klemeš, J.J., Alwi, S.R.W., Varbanov, P.S., 2020. Cost-based Quantitative-Qualitative water footprint Considering Multiple Contaminants, Resources, Conservation and Recycling (Under Review) **[IF = 8.086, CiteScore = 10.7]**
2. **Jia, X.,** Varbanov, P.S., Klemeš, J.J., Wan Alwi, S.R., 2019, Water Availability Footprint Addressing Water Quality, Journal of Sustainable Development of Energy, Water and Environment Systems, 7(1),72-86. **[CiteScore = 1.41]**
3. **Jia, X.**, Klemeš, J.J., Alwi, S.R.W., Varbanov, P.S., 2020. Regional Water Resources Assessment using Water Scarcity Pinch Analysis. Resources, Conservation and Recycling, 157, p.104749. **[IF = 8.806, CiteScore = 10.7]**
4. **Jia, X.**, Klemeš, J.J.; Varbanov, P.S.; Wan Alwi, S.R., 2019. Analysing the Energy Consumption, GHG Emission, and Cost of Seawater Desalination in China. Energies, 12, 463. **[IF = 2.702, CiteScore = 3.8]**

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CHAPTER 1 **Introduction**

1.1 General Introduction

The significant issues of water –too less (water scarcity), too much (emergency flood), and pollution – have been increasingly server and threatening people's living and industrial development. According to UNESCO and UN-Water (2020), about 74 % of natural disasters between 2001- 2018 are water-related. Irregular water supply issues (drought and flows) caused a total number of deaths of more than 1.6 million, and total economic damage of almost € 700 billion (UNESCO and UN-Water, 2020). As illustrated in Figure 1-1, the most water-related disasters including droughts, floods, landslides, and storms occurred in large countries and regions with a high population such as China (428), the US (343), India (254), and also in geographically small countries and regions such as Philippines (255). These water-related disasters and caused enormous damages to human lives and economic development.

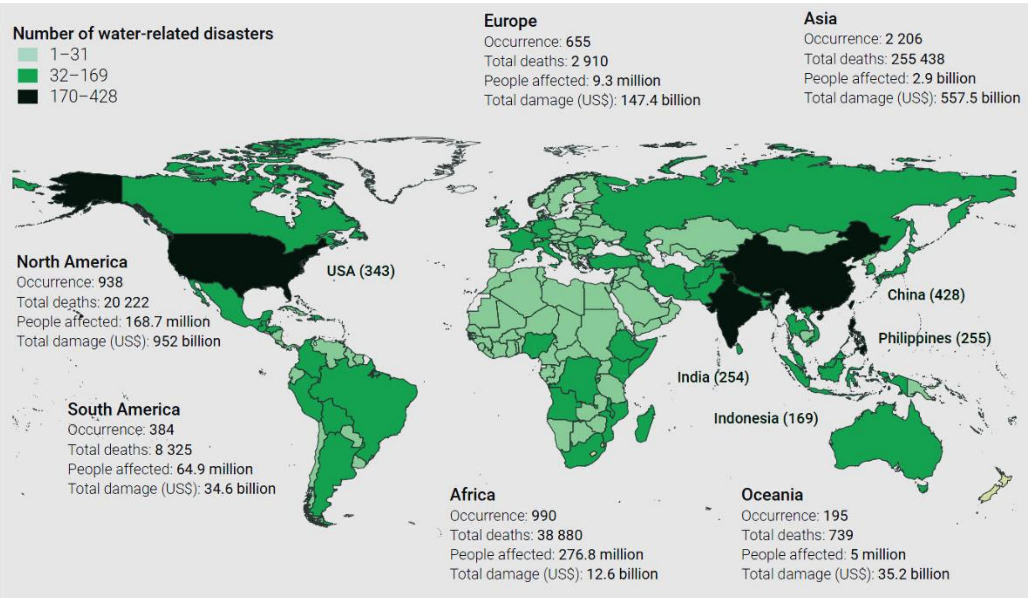


Figure 1-1: Spatial distribution of water-related disasters during 2001-2018 (UNESCO and UN-Water, 2020)

Water scarcity caused by the quantitative shortage and qualitative degradation has been increasingly severe in various regions globally. According to the UN-Water (2018), over 2 billion (10^9) people live in countries experiencing high water stress, and 700 million people worldwide could be displaced by intense water scarcity by 2030 (Hameeteman, 2013). Water scarcity does not always come as serious as yearly issues, but it can occur and affect our lives in a moderate form. According to (Mekonnen and Hoekstra, 2016), about 4 billion (10^9) people experience severe water scarcity during at least one month of the year. Except for surface water, studies show that a third of the world's biggest groundwater systems are facing scarcity issues (Richey et al., 2015). Figure 1-2 shows the projected water stress by countries projected in 2040. The water stress in this map is determined as the ratio of water withdraw and the water availability. Various regions, especially Asia, Northern Africa, North America and Europe, have been facing and would continue with medium to severe water scarcity issues.

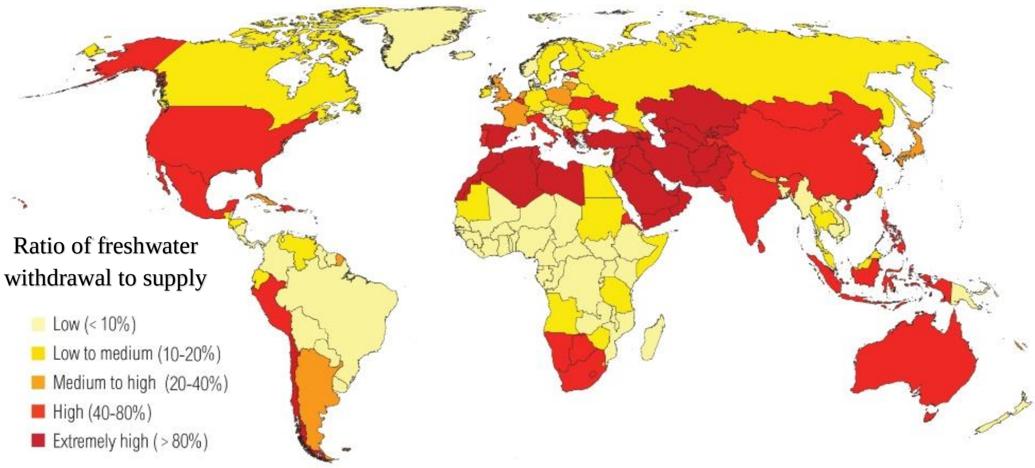


Figure 1-2: Water stress by country projected in 2040 (World Resources Institute, 2015)

On the other hand, the quantity and quality of the water supplies have been affected by climate change and land use, leading to an increasing frequency and intensity of extreme events such as storms and floods (UNESCO and UN-Water, 2020). Global floods and extreme rainfall events have dramatically increased by more than 50% during 2008-2018 with an increased rate four times higher than in 1980 (EASAC, 2018).

Figure 1-3 presents the spatial distribution of floods during 2001-2018 and more recent years. A large number of floods occurred in large countries such as China (184) and the US (82), as well as Europe (397). For example, severe flooding occurred across the UK from 2019 to 2020, and the flood in February 2020 led to an initial insured loss of more than €330 million (Insurance Journal, 2020). Another example is that more than 80 % of the territory in the Czech Republic experienced medium to severe water scarcity in 24 out 54 weeks in 2018, and 11/54 weeks in 2019 (Intersucho, 2020). In 2020, more than 82% of the country's territory experienced medium to extreme drought 5 out of the first 26 weeks. In the 25th and 26th week (15th to 28th June), the precipitation in the Czech Republic dramatically increased with intensive storms (Intersucho, 2020), and the drought level almost decreased to 0 after the two-weeks intensive precipitation. However, the abrupt increase of precipitation also challenged the capacity of the sewer system and led to serious floods and damages in the northern part of the country (Fox News, 2020).

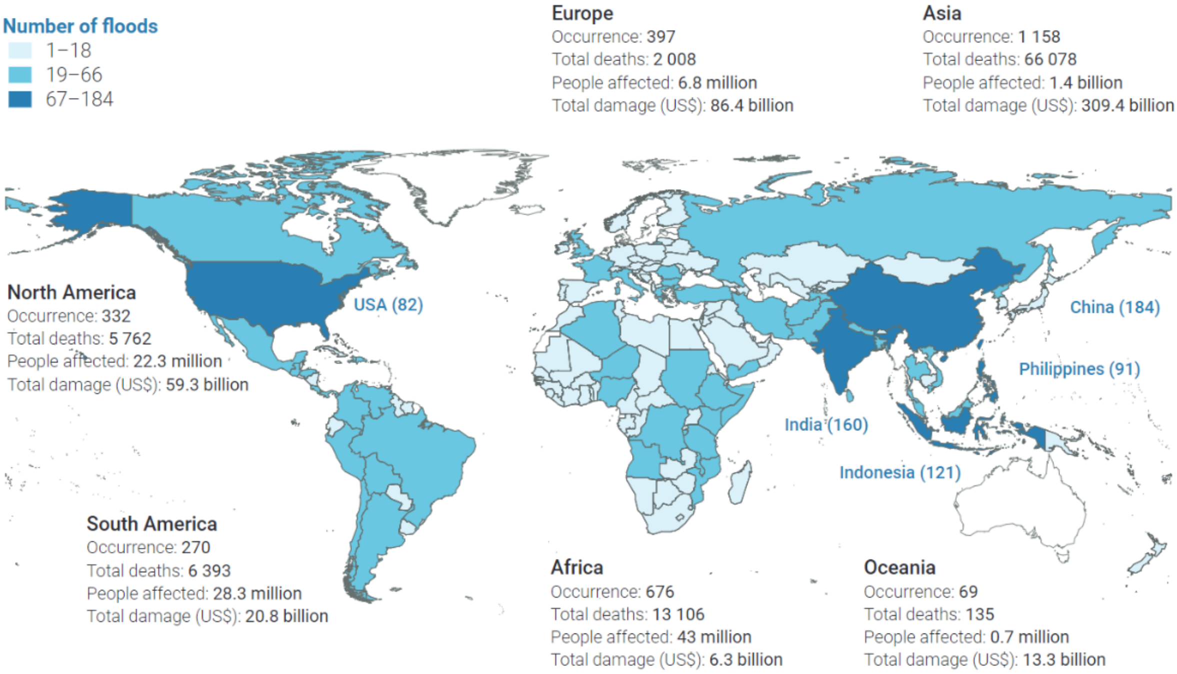


Figure 1-3: Spatial distributions of floods during 2001-2018 (UNESCO and UN-Water, 2020)

Besides the irregular water supply in quantity, surface and groundwater pollution have also been increasing in many countries, including China (Wang et al., 2008). The shortage of available freshwater and the increase in water pollution have increased the economic cost of water treatment and transportation, as well as its environmental impacts.

Even though water is a global resource, water production, use and management are still regional issues. Alternative water supplies are not always accessible to all regions around the world. Geographic location, economic status, climate, etc. can limit access to alternative water supplies at regional levels. Irregular water supplies and water pollution issues have been continuously increasing and restricting the development of the agricultural and industrial sectors and threatening human lives. In addition, water is one of the major elements in the resources nexus, and the scarcity and pollution of water also increase the water-related energy consumption and corresponding emissions. There is an urgent need to enhance and improve the water use assessment and design tools based on existing contributions. The impact of water quality degradation on water scarcity deserves exceptional attention and sufficient determination. Except for assessment tools for benchmarking, more decision-making tools are needed to guide practical water use and management.

1.2 Research Aim and Objectives

This PhD research targets at extending and improving the methodology development and benchmark of water use and water use impacts in terms of quantity and quality. The water-related energy consumption and emission are also discussed as the continuation of the water resource assessment. The research aim is to facilitate the improvement of water use efficiency and reduce water use impacts. A condensed summary of recently reported water issues and thorough literature review of the state-of-the-art (refer to Chapter 2 in the full thesis) initiates the study and identifies the following research gaps:

i) Existing water resource assessment methods mainly focus on volumetric consumption. The impact of water use on water quality deserves further investigation as water pollution becomes an essential contributor to water scarcity.

ii) Decision-making oriented tools are urgently needed for regional water management to tackle water scarcity. Post-assessment is only able to provide the current water scarcity level but can hardly guide regional water use optimisation in practice.

iii) Water-related energy consumption and emissions should be determined to facilitate decision making in regional water resource management.

Extended resources assessment methods addressing water quality using water footprint and Water Pinch Analysis are proposed and applied to case studies at both micro and macro levels. The core of the thesis consists of the following sections:

i) Extended water footprint assessment methods to determine the water quality degradation impact of water use

ii) Water Scarcity Pinch Analysis to minimise regional water scarcity and provide supporting information to decision making in regional water resource management.

iii) An initial determination of the energy use and emissions in seawater desalination plants

1.3 Thesis Outline

To summarise, water and water-related issues have been increasingly complex, especially under the background of climate changes. Various concepts and indicators and tools have been proposed to evaluate and guide the performance and environmental impact of industrial water use. However, some questions, including 1) how does water quality degradation affect water scarcity and how to quantify these impacts, 3) how to elevate the assessment tools to provide more decision-making oriented results and guide practical water use and assessment, and 3) how are water and other resources (e.g. energy) and emissions interconnected in large scale water use, still deserves further investigation. The complete version of the literature review chapter has been presented in the full PhD thesis, while this excutivev version thesis extracts the major research works of the PhD study. The following chapters provide an attempt to answer these questions by proposing extended Water Footprint Assessment (**Chapter 2**) and Water Pinch Analysis methodologies (**Chapter 3**) and presenting an initial assessment of the water-energy nexus in the seawater desalination industries (**Chapter 4**).

CHAPTER 2 **Extended Water Footprint Methodology in Water Quantity and Quality Assessment**

This chapter presents a Water Availability Footprint framework addressing water quality Section 2.1) and a Cost-based Qualitative and Quantitative Water Footprint (QQWFP) method in Section 2.2. The Water Availability Footprint framework is based on the author's publication on the Journal of Sustainable Development of Energy, Water and Environment Systems (Jia et al., 2019). The QQWFP is based on the work submitted to the journal of Resources, Conservation & Recycling, which is still under review.

2.1 Water availability footprint

2.1.1 Introduction

Water quality has an increasing impact on the availability of water sources. However, it has rarely been analysed in practical water resource assessments. Since the water footprinting concept and method has been well developed with various implementations, it would be beneficial to integrate the water quality into the current assessment framework. Based on the existing concepts and frameworks, the definition of water availability (WA) should be extended to consider the impact of water quality on water availability, and the determination of water availability footprint (WAF) should be adapted to reach an integrating result. In this study, water availability is defined as the quantitative and qualitative extent of a certain body of water which meets the needs of a particular purpose of water use. Comparing this definition to the existing water availability, the water availability proposed in this study integrates water quality and quantity and can be defined as the Effective Water Availability (EWA). Based on this definition, water availability footprint is defined as the water availability consumption of a certain water use process. A three-step water availability footprint (WAF) assessment framework is proposed and shown in Figure 2-1.

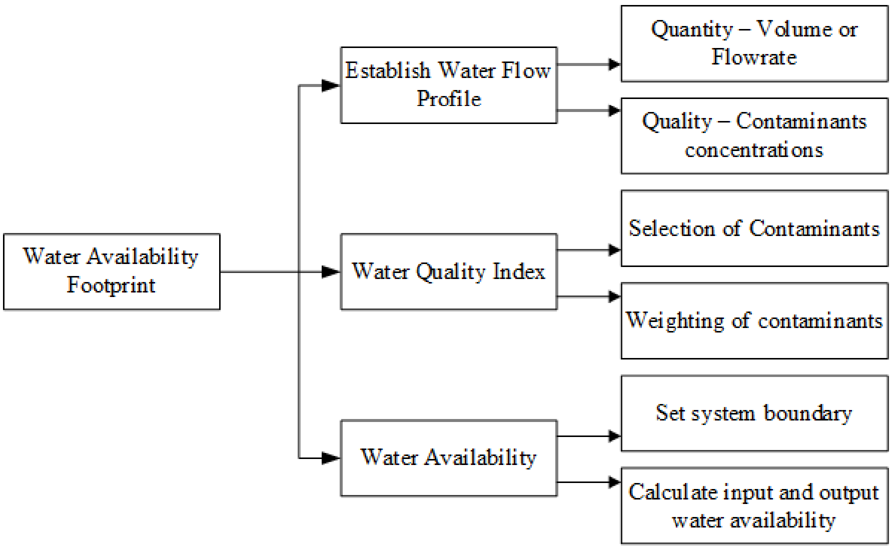


Figure 2-1: Water Availability Footprint Assessment Framework

Note that water quality is not a single and absolute value, but an indicator consisting of various physical and chemical indices. The development of the WQI becomes the most critical step. Considering the contaminants in different flow might vary, which will be challenging to use the same single contaminants as the criteria for all flows. It is beneficial to apply a WQI of relative value as the weighting factor, which would enable the comparability of the impact of water quality of different flows. Inspired by the Water Stress Index (WSI) (Pfister et al., 2009), which is a ratio of water consumption (demand) and water availability (supply), this study proposes a ratio of water quality demands and water quality supplies as the WQI.

2.1.2 Method

Water Quality Index

Following this consideration, the definition of the WQI proposed in this study is given: For a certain flow (body of water), WQI is the ratio between remaining allowance of pollutant discharge and the maximum acceptable pollutant allowance, which can be calculated as in Eq(2-1). It is based on the purpose of water use and the specific situation of the targeted region/area. The idea of WQI is to scale all the inflow and outflow of the system to be comparable. By defining the upper and lower bounds of the contaminants, the range of allowed concentrations in certain water bodies is given. Knowing the water profiles of the flows, the "credit" of each water flow in this region can be calculated, as a representation of water quality:

$$\mathrm{WQI}_i = \frac{X_{\mathrm{max},i} - X_i}{X_{\mathrm{max},i} - X_{\mathrm{min},i}} \tag{2-1}$$

where for pollutant i, WQI_i is the water quality index of specific water flow, X_i is the concentration of pollutant i, $X_{\mathrm{max},i}$ is the upper bound of acceptable the concentration of this pollutant, and $X_{\mathrm{min},i}$ is the lower bound of the acceptable concentration of pollutant i. The upper and lower bounds of the concentration of contaminants can be selected from national/regional water quality standards or defined according to the current water quality levels in the studied region.

In this study, two possible approaches are explored to quantify the overall water quality. One approach is to consider the most stringent pollutant as the bottleneck of water utilisation, as shown in Eq(2-2), which can be useful for water use with higher water quality requirement. For example, if the concentration of Lead (Pb) in a water flow exceeds the requirement for drinking water, then the WQI of this water flow for drinking water is 0. Consequently, the EWA of this drinking water body for drinking would be 0:

$$\mathrm{WQI}_{\mathrm{min}} = \min(\mathrm{WQI}_1, \mathrm{WQI}_2, \dots, \mathrm{WQI}_i) \tag{2-2}$$

where $\mathrm{WQI}_{\mathrm{min}}$ is the water quality index of the water flow and WQI_i is the WQI of contaminant i.

Another option is to calculate the average of the WQIs of all contaminants as shown in Eq(2-

3). In this case, it is assumed that each contaminant has the same impact on water usability. The average WQI can reflect the overall distribution of the pollutant concentrations and can be used for the situation that does not have strict water quality requirement, e.g. industrial cooling water, etc.:

$$\mathrm{WQI}_{\mathrm{avg}} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{WQI}_i \qquad (2\text{-}3)$$

Where, $\mathrm{WQI}_{\mathrm{avg}}$ is the WQI of the water flow and is calculated with the average of the WQI of all the contaminants. The applications of these two options are discussed in the case study in the following sections.

Water Availability Footprint calculation

For various purposes of water use, both water quantity and quality affect the extent of the availability of the water supply. Considering the correlation between water quality and water quantity, as well as their impact on the water usability, WQI can be considered as a weighting factor of water quantity, and the EWA can be calculated by Eq(2-4):

$$\mathrm{EWA} = A_{\mathrm{W}} \times \mathrm{WQI} \qquad (2\text{-}4)$$

where EWA is the effective water availability of a water body [m^3], A_{W} is the amount of water (input or output) [m^3], and WQI is the water quality index, which is a dimensionless quantity.

As water availability is defined as the changes of water availability during the water use process, for each water use unit process, the WAF can be calculated as the difference between all inputs and outputs of a certain process, as shown in Eq(2-5):

$$\mathrm{WAF} = \mathrm{EWA}_i - \mathrm{EWA}_{\mathrm{o}} \qquad (2\text{-}5)$$

where WAF is the water availability footprint of the water use process [m^3], EWA_i is the effective water availability of the input water flow [m^3], and $\mathrm{EWA}_{\mathrm{o}}$ is the effective water availability of the output water flow [m^3].

The WAF is calculated to reflect the usability changes before and after the water use process. The estimation of WQI is more difficult for the determination of water availability. Dealing with the multi-contaminants issues, the selection of the pollutants should be based on the practical situation of the assessing region, and the purpose of water use should be considered to determine the upper and lower bound of the pollutant. The following case study shows the potential implementation of the WAF assessment framework.

The water quality should be accounted for jointly with the water availability because this can provide the additional insights for water managers into improving water quality and water availability of the systems.

2.1.3 Results and Discussion

The system boundary of the case study shown in Figure 2-2. The input flow is from a water supply with certain volume and quality (F_1, WQI_1), and outflow (F_2, WQI_2) is discharged into the same water supply system. Within the water use system, some flows might be reused directly (F_3) or recycled (F_4) or exist between the treatment unit (F_5). Considering F_5 does not have direct impacts on the outside system, they are not considered during the WAF assessment.

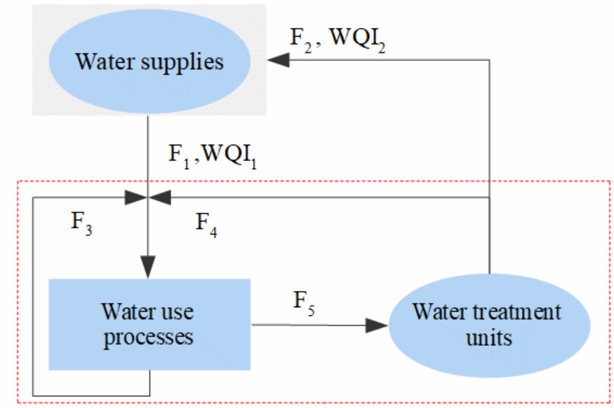


Figure 2-2: Case study: WAF framework and system boundaries

The WQI is presented in Figure 2-3.

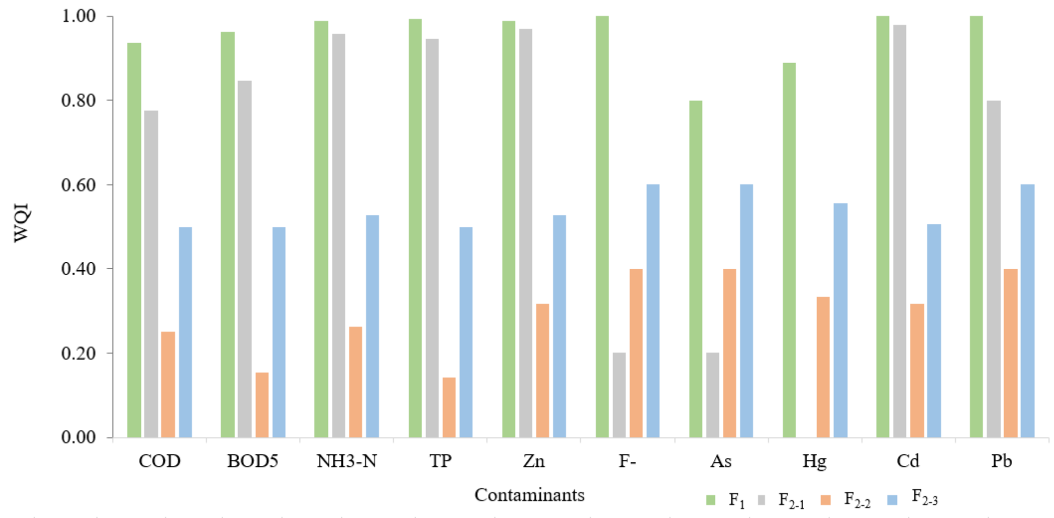


Figure 2-3: WQI of 10 selected contaminants

The green bar is the WQI for F_1, which is the inflow. $F_{2\text{-}1}$, $F_{2\text{-}2}$, and $F_{2\text{-}3}$ are the different flows with a different water quality pattern to test the impact of water quality on WAF. $F_{2\text{-}1}$ is the water flow with relatively higher overall water quality, but the levels of different contaminants are not distributed evenly. $F_{2\text{-}2}$ is a water flow with the lower overall quality, and the levels of the contaminants are quite even. $F_{2\text{-}3}$ is a water flow with medium overall water quality, and the levels of the contaminants are also distributed evenly.

To consider the two options for determining the overall WQI mentioned in the methodology section, the overall WQI based on $WQI_{min,i}$ and $WQI_{avg,i}$ are calculated. The EWA of the inflow (F_1) and outflow under three different situations ($F_{2\text{-}1}$, $F_{2\text{-}2}$, and $F_{2\text{-}3}$) are determined. The WAF can be calculated by EWA_i minus the EWA_o. The EWA of all the flows and the and WAF of the system are shown in Table 2-1.

Table 2-1: Overall WQI and EWA of the flows and the WAF of the system

Indicators	F_1	F_{2-1}	F_{2-2}	F_{2-3}
Volume [m^3]	2,000	1,000	1,000	1,000
WQI_{min}	0.80	0.00	0.14	0.50
WQI_{avg}	0.97	0.67	0.30	0.54
EWA_i [m^3] based on WQI_{min}	1,600	0.00	142.86	500
WAF_{min} [m^3]		1,600	1,457	1,100
EWA_o [m^3] based on WQI_{avg}	1,944	667	297	541
WAF_{avg} [m^3]		1,277	1,646	1,402
Volumetric WAF [m^3]			1,000	

The WAF of the water use process can be calculated as:

- With $WQI_{min,i}$, the WAF is: WAF = $EWA_1 - EWA_2$ = 1,600 m^3;
- With $WQI_{avg,i}$, the WAF is: WAF = $EWA_1 - EWA_2$ = 1,291 m^3.
- While if only water quantity is considered, the water consumption during this process is $F_1 - F_3$ = 1,000 m^3.

The results of WAF_{min} showed that water bodies with more evenly distributed WQIs have a smaller footprint and thus have higher EWA. For the results WAF_{avg}, as the average values revealed, the higher overall WQI, the smaller footprints. For F_{2-1}, the EWA based on WQI_{min} becomes 0 and independent on the volume of discharge. It indicates that the minimum WQI approach is not applicable for industrial water use but can be applicable for stricter water uses, such as drinking water. On the other hand, the averaged WQI can continuously represent the water availability changes. In addition, the averaging determination compromises the impact of all the contaminants, which indicates that this approach is more suitable for the assessment of water flows with moderate quality profiles. Applying weighting factors to different contaminants is one of the possible ways to improve the application of the average WQI. Conclusions

The proposed WAF framework tries to involve water quality into the WF assessment framework that is widely used. The involvement of water quality describes the usability change of the water flow beyond water quantity in order to provide more solution-oriented results. Defining water availability from the demand side and taking water quality into consideration, can contribute to a more specific measurement for WF assessment, and provide more support for improving the allocation to become closer to the optimal water and wastewater resources.

That the framework still has some limitations needs to be considered in the future works:

- A WQI that can be applied to more general situations has not been suggested in this study. The two approaches considered are limited to certain situations. The minimum WQI can be used for water flows that require higher water quality, and the average WQI can be used for flows that have more moderate quality;
- The different environmental impacts of all contaminants and the interactions among

contaminants are not considered;

- Only one type of water use is considered. When applying to a larger scale (e.g., region or country), with more than one kind of water use categories (e.g., industrial, agricultural, municipal, etc.), the baselines of the multiple contaminants would depend on the purpose of water use. With the results calculated with different baselines, it needs a further discussion of whether they can be added directly.

The proposed method still has limitations on the comprehensive determination of multiple contaminants, which should be further investigated in future studies. The indication of water quality and effective availability are not yet robust enough for practical application. In addition, the impact of secondary pollutions should be considered in future developments.

2.2 Cost-based Qualitative and Quantitative Water Footprint (QQWFP)

2.2.1 Introduction

Following the initial development of the water availability footprint addressing water quantity, this study provides a different perspective of determining the water use impact in terms of quality and quantity. The results of the existing water footprint assessments, which are represented with the volume of water needed for diluting (m^3) and pollutant equivalents (e.g. kg SO_2eq) are relatively difficult to be widely accepted for the public and water managers. Besides, the results could not provide a clear answer to "what should be done and how much would be the cost", which is essential for users and water resource managers. Another limit is that the greywater assessments allows the selection of one representative pollutant (Kounina et al., 2013) for calculation, which could lead to a different greywater footprint result when selecting different pollutants. The concept of Life cycle costing provides a perspective to determine the qualitative and quantitative impact of water use with the cost.

2.2.2 Methodology

Figure 2-4 presents the framework of the QQWFP.

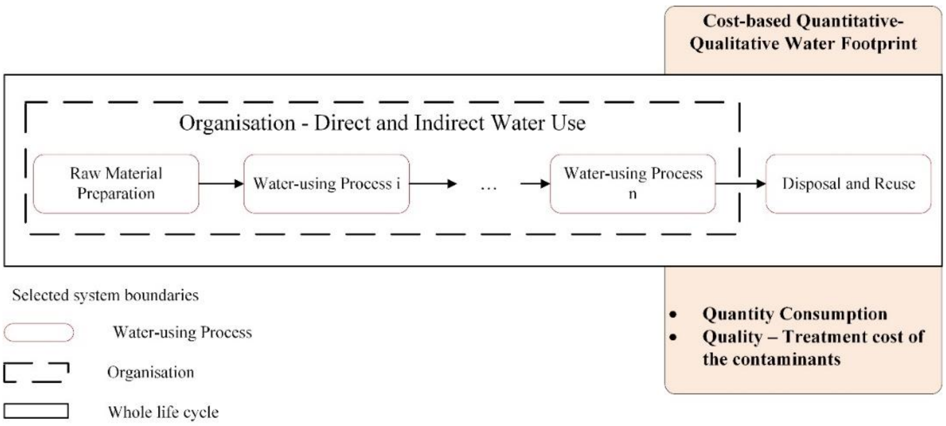


Figure 2-4: Assessment framework of the QQWFP

The system boundary of the QQWFP can be defined based on research objectives and data availability. The assessment should cover the whole life cycle of water use when data is available. When with limited data, the setting of system boundary should be justified. The Quantitative Water Footprint (WFqt) and Qualitative Water Footprint (WFql) are introduced in detail in the following sections.

2.2.2.1 Quantitative Water Footprint

The Quantitative Water Footprint is defined as the cost of net water consumption of producing 1 t of product. The net water input and consumption is determined as based on the mass balance of the water-using unit. Figure 2-5 is an illustration of water use in an industrial plant with n water-using units.

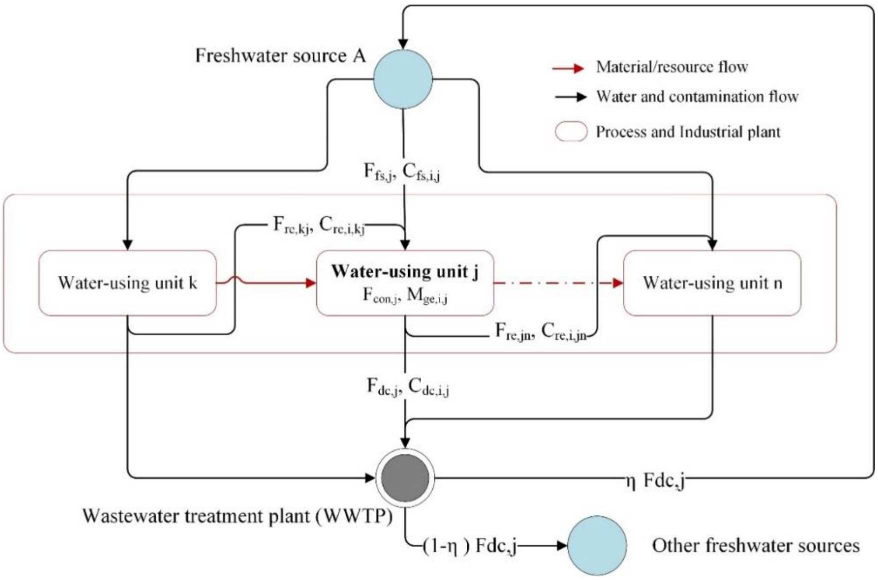


Figure 2-5: Illustration of the industrial water use

Take a typical water-using unit j as an example. The input water can be supplied from freshwater sources (e.g. municipal water network, underground water, etc.) or reuse water from other water-using units, and the different water supplies would have a different cost. After the water use inside the process, the effluents can be sent to other processes for reuse, or directly discharged to the wastewater treatment plant (WWTP) for treatment and finally sent back to nature.

The Quantitative Water Footprint (WF_{qt}) is defined as the cost of total net water input and the net cost of discharging water. The total water supplies include the input of freshwater and the net volume of reused water within the plant. The cost of discharged water is added to the Quantitative Water Footprint as an attempt to encourage the plant discharge as little as possible, and prevent the case of using freshwater (or cleaner water) to dilute the discharged water just to meet the requirements. The discharged water sent to the WWTP will be returned to the environment after treatment. A proportion of this volume of water enters another water use cycle with an economic value, and this part of the value should be deducted from the cost of water discharge of the water-using unit.

For the water-using unit j, the Quantitative Water Footprint is calculated as:

$$WF_{qt,j} = \mathrm{EC}_{fs} \times (F_{fs,j} - \eta F_{dc,j}) + \mathrm{EC}_{re} \times (F_{re,kj} - F_{re,jn}) + EC_{dc} \times F_{dc,j} \quad (2\text{-}6)$$

where, $WF_{qt,j}$ is the Quantitative Water Footprint of water using unit j, €/t product. EC_{fs} and EC_{re} are the unit cost of 1 m^3 of freshwater and reuse water, €/m^3. EC_{dc} is the unit cost of discharging 1 m^3 of water. η is the proportional coefficient of the volume of water sent to treatment and returned to the environment, $\eta F_{dc,j}$ represents the volume of water returned to the environment after treatment, m^3/t product.

The cost of infrastructure and operation is not considered, as the aim of the study is to quantify the cost of water quality and quantity exploitation.

2.2.2.2 Qualitative Water Footprint

The Qualitative Water Footprint (WFql) is defined as the total net cost to remove the contamination generated during the water using process. Figure 2-6 is an illustration of the mass load of contaminants in water-using unit j.

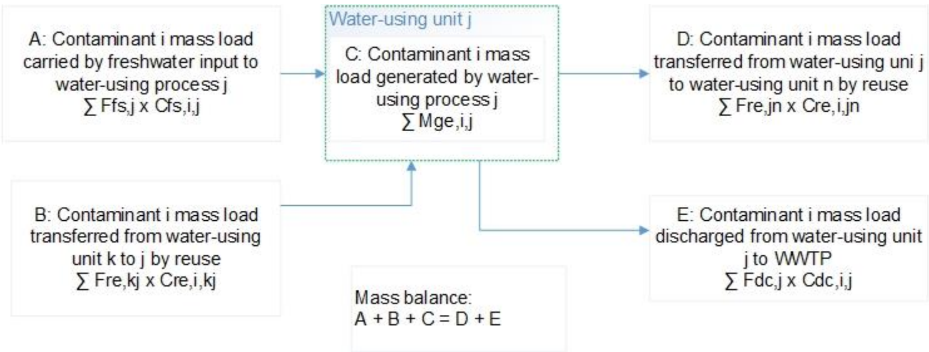


Figure 2-6: Illustration of the contaminants mass balance in water-using unit j

There are two contamination inputs to the process, which are the contamination from the freshwater (A) and reuse water (B). In the production process, a certain amount of contamination is generated due to the use of raw and auxiliary materials and the reactions between the materials (C). After the water-using unit, part of the contamination is transferred to another water-using unit with the reuse-flow (D), and the major portion of the contaminants will be sent to the WWTP with the discharged water (E). The mass load balance of the contaminations in process j is:

$$\sum_i (F_{fs,j} \times C_{fs,i,j}) + \sum_i (F_{re,kj} \times C_{re,i,kj}) + \sum_i M_{ge,i,j} = \sum_i (F_{re,jn} \times C_{re,i,jn}) + \sum_i (F_{dc,j} \times C_{dc,i,j}) \quad (2\text{-}7)$$

where, $C_{fs,i,j}$ and $C_{dc,i,j}$ are the concentration of pollutant i of the freshwater inflow and discharge water of process j. $C_{re,i,kj}$ is the concentration of pollutant i of the reuse flow from process k to process j, and $C_{re,i,jn}$ is the concentration (pollutant i) of the reuse flow from process j. The unit of concentrations is mg/L. $M_{ge,i,j}$ is the mass of contamination i generated in process j, kg/ t product.

From Eq(2-8) it is easy to obtain:

$$\sum_i (F_{dc,j} \times C_{dc,i,j}) - \sum_i \left(F_{fs,j} \times C_{fs,i,j}\right) = \sum_i M_{ge,i,j} + \left[\sum_i (F_{re,kj} \times C_{re,i,kj}) - \sum_i (F_{re,jn} \times C_{re,i,jn})\right] \tag{2-8}$$

The left side of the equation represents the contaminant mass load that needs to be removed from the discharge water to meet the contamination level of the freshwater. The mass load of local freshwater supply is set as the discharge standard because governmental standards are not the same for all countries and even cities. Selecting a fixed standard value will lead to the incomparability of the water footprint results. The right side is the sum of the contaminants generation in water-using unit j ($M_{ge,i,j}$) and the net contaminants transferred to water-using unit j by water reuse between the water-using units. It indicates that improving the process performance and increasing water reuse can reduce the net mass load generation of contaminant *i* in water-using unit j.

In this study, the Qualitative Water Footprint of *process j* ($WF_{ql,j}$) is defined as the cost of treating the contaminants mass load of discharged water to the contamination level of freshwater sources, when producing per unit of product, €/t product. The Qualitative Water Footprint of water-using unit *j* (Figure 2-6) can be calculated by the mass of contaminants multiplying the cost of treating per kg of contaminants:

$$WF_{ql,j} = \sum_i (F_{dc,j} \times C_{dc,i,j} - F_{fs,j} \times C_{fs,i,j}) \times TC_i \tag{2-9}$$

Where $WF_{ql,j}$ is the Qualitative Water Footprint of the water using unit *j*, €/t product. TC_i is the cost of treating 1 kg of contaminant *i* in a centralised wastewater treatment plant (WWTP), €/kg contaminant *i*. The values of TC_i can vary due to the various types of wastewater treatment plants, but it is essential to make sure to use localised data to improve the accuracy of the water footprint results.

The selection of contaminants should be made considering the characteristics of the water using processes and the wastewater treatment. In this way, it guarantees the evaluation of the contamination generation of the plant and excludes the unimportant pollutants for the local aquatic system.

2.2.2.3 Quantitative-Qualitative Water Footprint

The Quantitative-Qualitative Water Footprint of water using unit j is defined as the sum of Qualitative Water Footprint and Quantitative Water Footprint of this water-using unit:

$$QQWFP_j = WF_{qt,j} + WF_{ql,j} \tag{2-10}$$

where, $QQWFP_j$ is the Quantitative-Qualitative Water Footprint of the water-using unit j, €/t product. The total QQWFP of the industrial plant can be calculated by aggregating the footprints of all the water-using units:

$$QQWFP = \sum_j WF_{q-q,j} \tag{2-11}$$

where, QQWFP is the total Quantitative-Qualitative Water Footprint of the plant, €/t product.

Figure 2-7 presents the procedure of the QQWFP assessment.

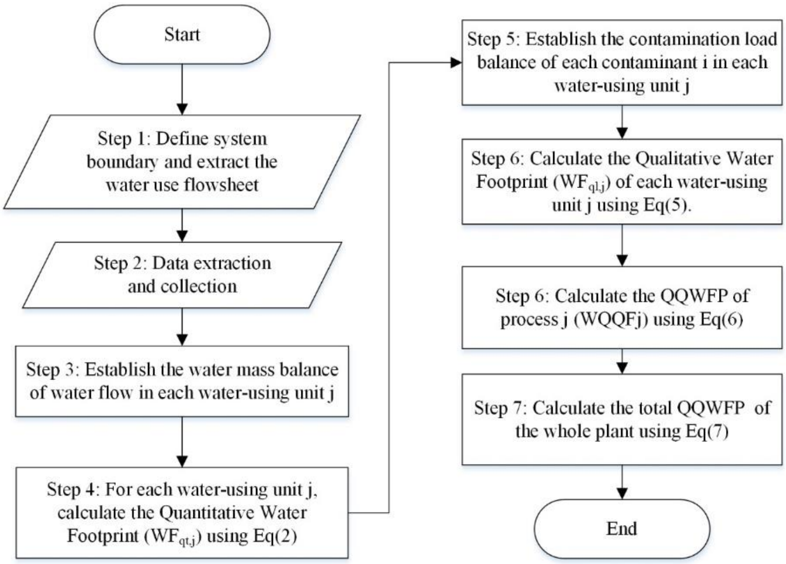


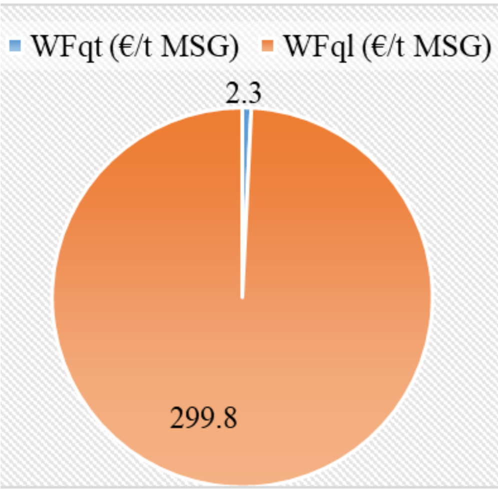
Figure 2-7: Quantitative-Qualitative Water Footprint assessment flowchart

Following the method description and the procedure of the Quantitative-Qualitative Water Footprint assessment, a case study of a monosodium glutamate plant is used to validate the method and investigate the performance of the method.

2.2.3 Results and Discussion

The water use network of a monosodium glutamate plant is used as a case to illustrate the implementation of the proposed Quantitative-Qualitative Water Footprint assessment method. The total QQWDP of producing 1 t MSG in the studied plant is 302.1 € (Figure 2-8a). The Qualitative Water Footprint (WFql) takes 99 % of the total footprint, with 299.8 €/t MSG, and Quantitative Water Footprint (WFqt) takes less than 1%. It indicates that in MSG production, water pollution is the major issue instead of water consumption. A much greater effort is needed to put in contaminants treatment than freshwater consumption.

(a)



(b)

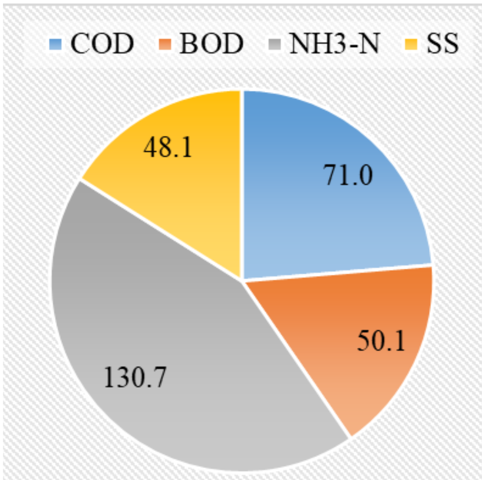


Figure 2-8: a) Breakdown of the QQWFP, and b) Detailed breakdown of the Qualitative Water Footprint (WFql) [€/t MSG]

Figure 2-8b presents the contributions of different contaminants in MSG production. As liquid ammonia is one of the most important raw materials to produce MSG ($C_5H_8NO_4Na$), the NH_3-N in the wastewater requires the most effort to be treated. The Quantitative Water Footprint (WFql) of NH_3-N of producing 1 t MSG is 130.7 €, taking 44 % of the total WFql of producing 1 t MSG. Following are BOD and COD, indicating the high contamination of biodegradable and non-biodegradable organic matters. BOD and COD contribute 40 % to the total Quantitative Water Footprint. Suspended solids (SS) contributes the least (48.1 €/t MSG) as it's relatively easier to remove from the polluted water.

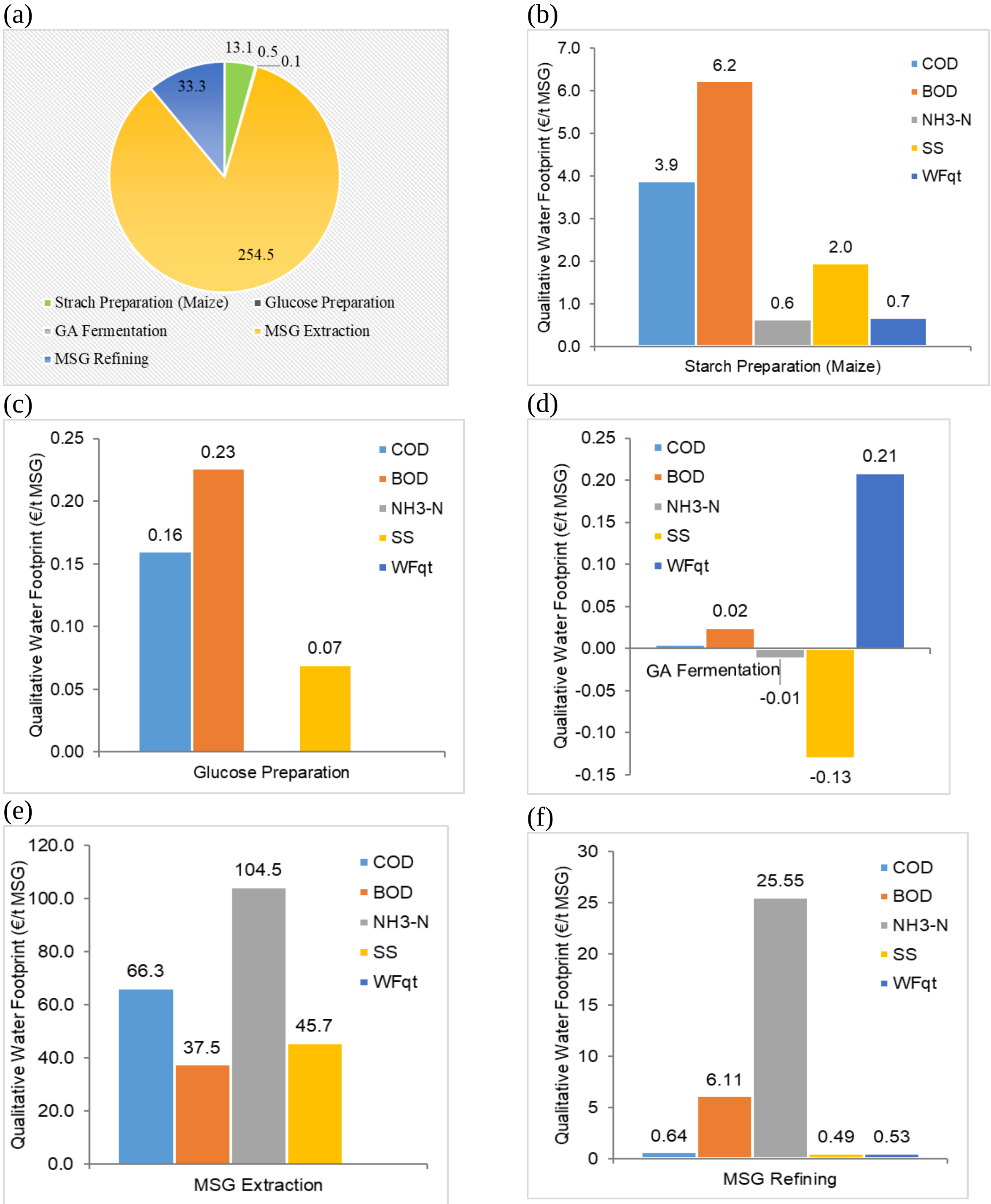


Figure 2-9: QQWFP breakdown of different processes

Figure 2-9a is the breakdown of the QQWFP of different processes. MSG Extraction has a QQWFP of 254.8 €/t MSG, with the largest contribution of 84 %. In this process, the Glutamate acid is crystallised in the concentration process, and reacts with sodium salt and generate sodium glutamate. A large amount of mother liquor with a high concentration of COD, SS, and NH_3-N, is generated in the process of MSG Extraction and Refining.

Figure 2-9b-f compares the detailed breakdown of different contaminants in each process. In the Starch Preparation and Glutamate Acid (GA) Preparation process, BOD is identified as the largest contributor, with the WFql of 6.2 €/t MSG (47 %) and 0.2 €/t MSG (49 %). COD is the second-largest contributor, with a WFql of 3.9 €/t MSG (29 %) and 0.2 €/t MSG (35 %) in the two processes. The GA Fermentation process is a more "static" process where mainly the fermentation occurs, and there is no major raw/auxiliary materials and resources consumption. In this process, there is a small volume of freshwater consumption, and the WFql of NH_3-N and BOD are negative. This is because there is only a very small wastewater discharge (from washing), and no other contaminants are generated. The low amount of contaminants in the freshwater are inputted into the process, but a less mass load of contaminants is generated and outputted.

MSG extraction process is the largest contributor to the total QQWFP of producing 1 t MSG. Different from other processes, NH_3-N is the bottleneck in the MSG extraction and refining process. The NH_3-N in MSG extraction and refining process has a WFql of 104.5 €/t MSG and 25.6 €/t MSG, taking 41 % and 78 % of the total QQWFP in these two processes. In all the processes, Quantitative Water Footprint is not the major contributor.

Comparing the results from QQWFP and ISO Water Footprint Assessment

The water footprint of producing 1 t MSG resulted from the proposed QQWFP and the water footprint assessment based on ISO (2014) are compared to address the emphasis and contributions of the method (Table 2-2).

Table 2-2: Results summary from QQWFP and Water Footprint Assessment by ISO (2014) (of producing 1 t MSG)

	Water Footprint (ISO, 2014)	QQWFP (This study)
Quantity	Water Availability Footprint: 0.05 m^3 (Calculated based on the same data)	Quantitative Water Footprint (WFqt): 2.3 €
Quality	Water Degradation Footprint: Aquatic acidification: 30.0 kg SO_{2eq} Aquatic eutrophication: 1.1 kg PO_4 P-lim_{eq} Aquatic ecotoxicity 787.0 t TEG $water_{eq}$ (Retrieved from (Yang et al., 2020))	Qualitative Water Footprint (WFql): 299.8 €
Total	Not Applicable	QQWFP: 302.1 €

Based on the ISO water footprint assessment, the water availability of producing 1 t MSG is 0.05 m^3, and the water degradation footprint, including the Aquatic Acidification footprint (30.0 kg SO_2eq), Aquatic Eutrophication (1.1 kg PO_4 P-limeq), and Aquatic Ecotoxicity (787.0 t TEG $water_{eq}$) (Yang et al., 2020). The quantity and quality aspects and different impact categories within the quality footprint are not comparable, and as a consequence, it is difficult to identify which (quantity/quality) is the bottleneck. The Quantitative Water Footprint (WFqt) and Qualitative Water Footprint (WFql) are determined by calculating the cost. The results can help the users and decisionmakers to identify the bottleneck of water use and guide the selection of alternative solutions, e.g. to improve water use efficiency or improve the process performance to reduce contaminant generation.

2.2.4 Conclusions

A Quantitative-Qualitative Water Footprint (QQWFP) is designed in this study to evaluate the negative impact of water use based on cost. The QQWFP is defined as the total cost of quantitative water consumption plus the cost of removing the contaminants generated during the water-using process. The QQWFP consists of two sub-indicators, Quantitative Water Footprint (WFqt) and Qualitative Water Footprint (WFql). A Monosodium Glutamate (MSG) plant is used as a case study to illustrate and validate the proposed method. The results showed that the WFql of producing 1 t MSG is 299.8 €, taking more than 99 % of the total QQWFP. The WFqt of producing 1 t MSG is only 2.3 €, with a proportion of less than 1 % of the total QQWFP. MSG extraction and refining process are the two major critical process, with a QQWFP of 254.8 €/ t MSG (84 %) and 33.1 €/ t MSG (11 %).

Comparing with existing water footprint assessment tools, the outcome of QQWFP, including the Quantitative Water Footprint (WFqt) and Qualitative Water Footprint (WFql), provides more insightful guidance for the users and manages to identify the bottleneck and provide insights for possible solutions to reduce the overall water use impact. Future studies should continue the investigation of the specific selection of contaminants and establishment of the database of the wastewater treatment cost.

CHAPTER 3 Water Pinch Analysis in Scarcity Assessment

3.1 Introduction

Based on the Pinch Analysis (Linnhoff and Flower, 1978) concept, Water Pinch Analysis (Manan et al., 2006) has been developed and widely used to use water cascade analysis (WCA) methodology to minimise the water targets. As summarised in the comprehensive review (Klemeš et al., 2018), WPA has been further developed and widely implemented (Manan et al., 2004) for various cases. Insight-based WPA and mathematical programming based targeting approaches are the two most used WPA methodologies (Ding et al., 2011). Insight-based WPA, also known as the graphical approach represented by the Composite Curve and Grand Composite Curve (Wang and Smith, 1994), can help to identify the water imbalances and the targets clearly. Water GCC also provides insights for water cascade as claimed by (Manan et al., 2004). All these advantages of the insight-based WPA, namely easy to use, graphical presentation, identification of targets and eligibility for water cascade, can be very helpful to improve the water scarcity assessment. Consequently, WPA is used as a basis to propose a modified Water Scarcity Pinch Analysis (WSPA) to identify the water scarcity targets and provide implications for water scarcity minimisation with water quality cascade.

3.2 Methodology – Water Scarcity Pinch Analysis

This study proposes a Water Scarcity Pinch Analysis (WSPA) to assess the water scarcity addressing water quantity and quality, based on the well-applied method of Water Pinch Analysis (WPA). The quality of water sources and demands are specified by setting water quality categorises, based on which the water quality of each water flow and constructing the staircase Grand Composite Curve. The proposed method has four steps. The first step is to define the system boundary. Step 2, which is critical for the whole process, is to categories the water resources in terms of quality. This step is to attach the water quality properties to each water body. Then the data can be collected to construct the water profile table, which provides the list of quantity and quality of water supplies and demands. The last step, Water Scarcity Pinch Analysis (WSPA), can assess the water scarcity and identify the target for scarcity minimisation.

3.2.1 System Boundary

A clear system boundary is helpful for data collection and better utilise the results for water scarcity minimisation in practical situations. The method is proposed for regional water scarcity assessment, e.g. a district, city, or a country, to be in line with the water use management. The overall method follows a bottom-up approach, which all data are summed from all water sources and users to get the regional data. The regional water supply and demand data can be annual/monthly an average data, rather than the supply and demand at a certain point of time.

3.2.2 Water Quality Categorisation

It is challenging to select a single contaminant or several selected contaminants to represent the water quality of a city or larger region. Water quality-related water scarcity can vary a lot when selecting different contaminants, which lowers the comparability among different regions or one region in different years. Many widely used water assessment indicators are difficult to be utilised in practical water resources management, mainly because the data is usually difficult to obtain, and the assessment results are not able to reveal the whole picture of the region. Water quality data, feasibility and insight-based results are critical points for the evaluating metrics to provide suggestions for water scarcity minimisation and guide regional water management.

Table 3-1: Water quality categories and recommended use (Ministry of Ecology and Environment of the PR of China, 2002)

Categories	Suggested user group
I	Natural reservation area
II	Natural reservation area
III	Drinking water (Residential)
IV	Industrial use
V	Agricultural Irrigation

In practical regional water resources management system, the natural water bodies are usually divided into different water quality categories, targeted at different purposes of water use. For example, in China, the surface water is divided into five categories (I-V in descending order) based on the evaluation of 23 types of contaminants, including pH, temperature, COD, BOD_5, heavy metals, etc. (for the full list of contaminants, please see Supplementary Table S1). The standard also provides suggested user group for each category, as shown in Table 3-1.

These groups are set based on matching their water quality requirement and the categories, and it is possible to use higher quality water for users with the lower requirement. For example, Category III is suggested for residential use, but it can also be used for industries and agricultural irrigation when needed. This indicates the possibility of water quality cascading for regional water use optimisation.

3.2.3 Water Profile Table

The Water Profile Table presents the water quality categories and water supply and demand data for the Water Scarcity Pinch Analysis (Table 3-2).

The volume of water in each water quality categories (N) is listed for both water supply and demand. It is assumed there are M grids (or sub-regions) in the assessed region, in order to provide the possibility of investigating the water scarcity distribution inside the region. The water supply matrix of each grid can be obtained as $\mathbf{V_s(M, N)}$, and the regional total water supply matrix is $\mathbf{V_s(N)}$. The water demand matrix of each grid is $\mathbf{V_d(M, N)}$, and the regional total water demand matrix is $\mathbf{V_d(N)}$.

Table 3-2: Water Profile Table of supply and demand

Grids	The volume of water in *N* water quality categories (m^3)									
	Supply					Demand				
	I	*II*	*III*	…	*N*	*I*	*II*	*III*	…	*N*
1	V_{s11}	V_{s12}	V_{s13}	…	V_{s1n}	V_{d11}	V_{d12}	V_{d13}	…	V_{d1n}
2	V_{s21}	V_{s22}	V_{s23}	…	V_{s2n}	V_{d21}	V_{d22}	V_{d23}	…	V_{d2n}
3	V_{s31}	V_{s32}	V_{s33}	…	V_{s3n}	V_{d31}	V_{d32}	V_{d33}	…	V_{d3n}
…	…	…	…	…	…	…	…	…	…	…
M	V_{sm1}	V_{sm2}	V_{sm3}	…	V_{smn}	V_{dm1}	V_{dm2}	V_{dm3}	…	V_{dmn}
Regional Total	V_{s1}	V_{s2}	V_{s3}	…	V_{sn}	V_{d1}	V_{d2}	V_{d3}	…	V_{dn}

The Water Profile Table provides the data needed for the Water Scarcity Pinch Analysis (WSPA).

3.2.4 Water Scarcity Pinch Analysis (WSPA)

The Composite Demand-Supply Curve is constructed based on the water profile, as illustrated in Figure 3-1. Regional data are used and the water categories 1-5 are used to represent I – V in Table 3-2.

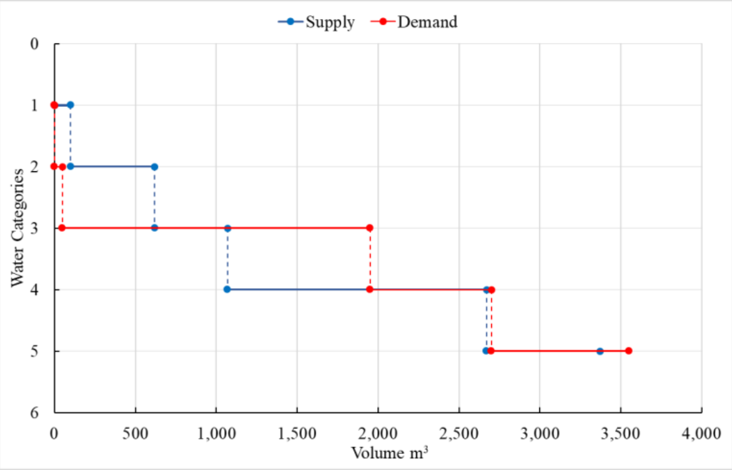


Figure 3-1: Illustration of the Composite Water Supply-Demand Curve

The Water Supply Curve is then shifted right until the water supply curve is on the right side of the water demand. The "Pinch Point" occurred with the volume of water quality Category III (Figure 3-2).

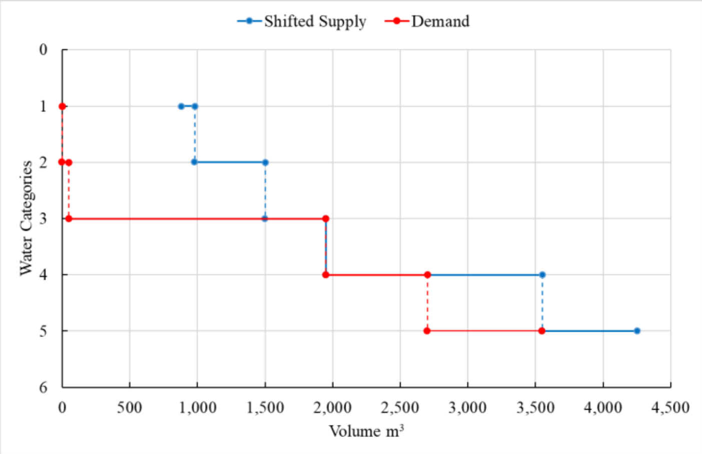


Figure 3-2: Illustration of the Pinched Composite Water Supply-Demand Curve

The "Pinch Point" has two dimensions – a volume with the quality category. There is a net water deficit above the Water Scarcity Pinch (WSP) and a net surplus below the WSP. Cross Pinch water utilisation should be avoided to reduce water scarcity. Based on the Composite Curves, the WS Grand Composite Curve (GCC) is constructed as illustrated in Figure 3-3.

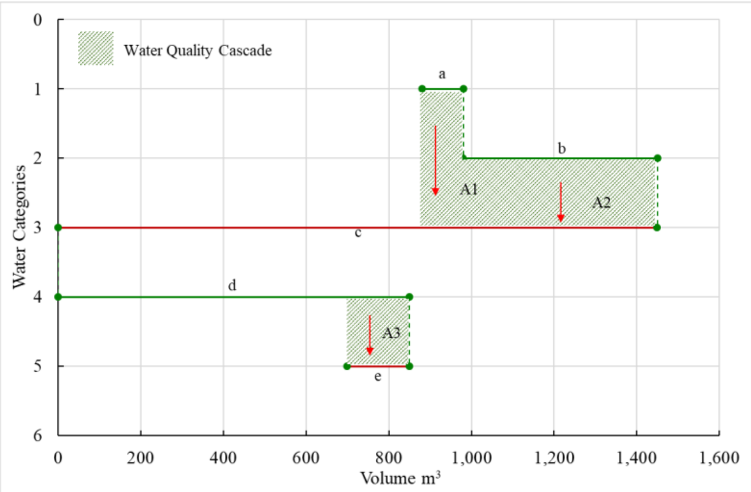


Figure 3-3: Water Scarcity GCC

As an analogy of the heat transfer Grand Composite Curve (GCC) (Varbanov, 2013), the WS GCC is a graph of net volume of water demand against shifted water demand provides a graphical representation of water volume and quality flow through the region.

In Figure 3-3, segment a, b, and d (water flows with Category I, II, and IV) have a net surplus of volume and contamination tolerance, and segment c and e (Category III and V) have a net deficit of volume. Three "Pinch Pockets" can be easily identified from the diagram (green shades A1, A2, and A3). Pockets A1 or A2 indicate the water Category I or II can be cascaded to replace the need of Category III. Pocket A3 indicates the surplus water flow Category IV can be used to fulfil the demand of Category V. In this situation, the cleaner water is "degraded" to replace less clean water.

After water cascade Category III still has a net deficit volume. Category IV has a net surplus, but it cannot be used because it failed to meet the water quality requirement (Category III).

The **regional water scarcity** can be defined as the deficit volume (m^3) of water of certain water quality (categories). In this situation, the assessed region has a water scarcity of c – (a + b) m^3 of Category III.

On the other hand, the WS GCC in Figure 3-3 also indicates the possibility of upgrading the water quality by mixing different water flows. For example, instead of utilising the "pinch pocket", the surplus of Category I and II can be mixed with Category IV to obtain Category III. The mixing volumes can be calculated based on the contamination concentrations given by the water category standard (Table S1) using dilution theories.

3.2.5 Water Quality Upgrading

Mixing two different water categories to upgrade the water quality can be realised by water dilution. Assume using Category X (clean) to upgrade 1 m^3 of water in Category Y to get the targeted Category Z, the volume of Category X (Vx) is the dilution factor, which can be calculated with Equation (3-1), (3-2) and (3-3).

$$V_{Xi} \times C_{Xi} + V_{Yi} \times C_{Yi} = (V_{Xi} + V_{Yi}) \times C_{Zi} \tag{3-1}$$

$$V_{Xi} = V_{Yi} \times \frac{(C_{Yi} - C_{Zi})}{(C_{Zi} - C_{Xi})} \tag{3-2}$$

Where V_X, and V_Y are the volume of the clean water, reference water flow and targeted water flow, m^3, and C_{Xi}, C_{Yi}, and C_{Zi} are the concentration of pollutant i. Based on the example of surface water quality categorisation in China (Ministry of Ecology and Environment of China, 2002), 23 contaminants are considered for the categorisation and i = 23. The concentration Ci can be found in Table S1. Among the 23 dilution factors, the maximum value is selected as the final dilution factor. This ensures that the concentrations of the rest 22 contaminants are diluted to the acceptable concentration.

$$V_X = Max(V_{Xi}) \tag{3-3}$$

The dilution factors of selected scenarios are presented in Figure 3-4.

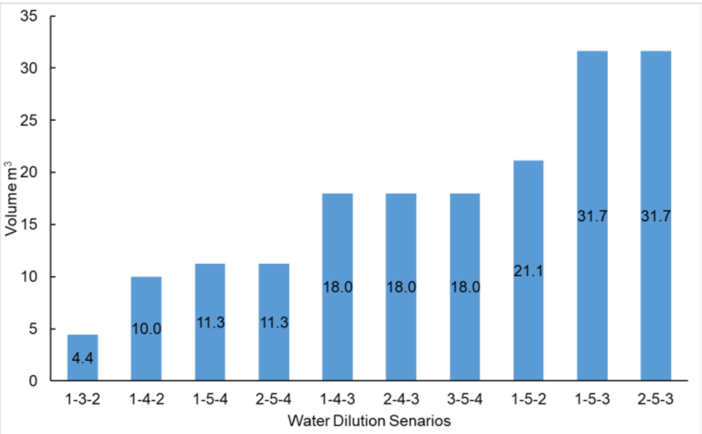


Figure 3-4: Water dilution factors of selected scenarios

The x-axis represents the dilution scenarios, and the y value is the volume of water is needed to dilute the current water to a target category. For example, 1-3-2 means using Category I to upgrade Category III to Category II, and 4.4 m^3 of Category I is needed upgrade 1 m^3 Category III to Category II. Similarly, the second bar indicates that 10 m^3 Category I is needed to dilute 1 m^3 Category IV to Category II. To get the same targeted water quality category, the dilution factor is different in different dilution scenarios. For example, using Category I to upgrade 1 m^3 Category V to Category IV (1-5-4) has the same dilution factor of 11.3 m^3 as using Category II (2-5-4), but much lower than using Category III (3-5-4, 18.0 m^3).

The dilution factors in Figure 3-4 can be used to select the optimal water quality categories for water quality upgrade. Note that in this study, only two categories mixing are considered, mixing involved more than two categories are left for investigation in future work.

3.3 Results and Discussion

Three numerical case studies are carried out to illustrate the proposed method. The water quality categorisation is referred to the data provided by the Chinese surface water standard (Ministry of Ecology and Environment of the People's Republic of China, 2002).

3.3.1 Case Study 1

The Water Scarcity GCC (WS GCC) OF Case 1 is constructed based on the net differences between supplies and demands, as shown in Figure 3-5.

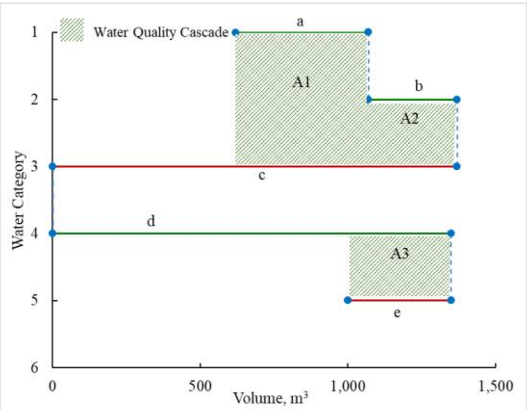


Figure 3-5: Water Scarcity GCC – Case 1

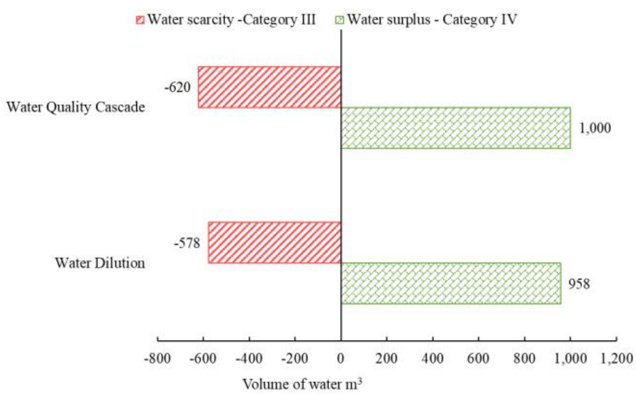


Figure 3-6: Water scarcity of Water Quality Cascade and Water Dilution - Case 1

The GCC represents the net water flow supply against the demand, thus from Category I to V, the segments along the x-axis direction indicates a net surplus volume of water and the segments in negative direction means a net deficit. The regional water scarcity, which is the overall deficit after applying the "Pinch Pockets" is 620 m^3 Category III, and there is still a surplus of 1,000 m^3 Category V.

The WS GCC in Figure 3-5 also indicates the possibility of using higher quality categories to upgrade the lower categories to reach minimal water scarcity. As shown in Figure 3-5, Category I and II can be used to upgrade Category IV to obtain more Category III to reduce the water scarcity. Using the dilution factors calculated in Section 3.2.5, the water scarcity of applying Water Dilution is calculated and compared with the result of applying Water Quality Cascade (Figure 3-6).

In the Water Dilution scenario, the surplus of Water categories I and II are mixed with Category IV to obtain the maximum volume of Category III. Even though the ratio of water supply to demand is bigger than 1 (indicates no single-volumetric water scarcity) in Case 1, the WSPA identifies the water scarcity caused by insufficient water quality. After applying the WQC, the regional water scarcity is 620 m^3 of Category III with a surplus of 1000 m^3 Category V. Water quality upgrading via dilution can improve water use efficiency and reduce the water scarcity to 578 m^3 (Category III) with a surplus of Category IV (958 m^3).

3.3.2 Case Study 2

Case Study 2 is set to investigate the performance of the WSPA with identifying regional water scarcity and potential in implicating suggestions for water scarcity minimisation. The Water Scarcity GCC can be constructed in Figure 3-7, and the "Pinch Pockets" are marked in the green shade. The segment marked in Green solid lines (+450 m^3), (+300 m^3), and (+850 m^3) present the net surplus and Red solid lines (-770 m^3) and (-450 m^3) represents the net deficit volume of water. After applying the "Pinch Pockets", the overall water scarcity of region B is 20 m^3, Category III, with a surplus of 400 m^3 Category IV.

The water scarcity of applying WQC and WD are presented in Figure 3-8, and it showed the water scarcity could be eliminated by water dilution. In addition, instead of having a surplus of 400 m^3 Category IV, the WD scenario can still keep a small surplus of high-quality water (25 m^3, Category I).

An important implication from this case study is that WSPA can identify the water quality-quantity water scarcity, and proved potential solutions to minimise the water scarcity with a relatively low extra input

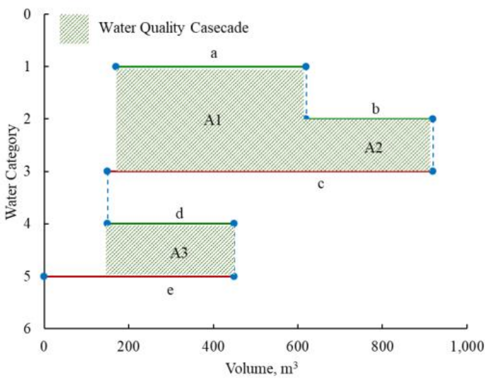


Figure 3-7: Water Scarcity GCC – Case 2

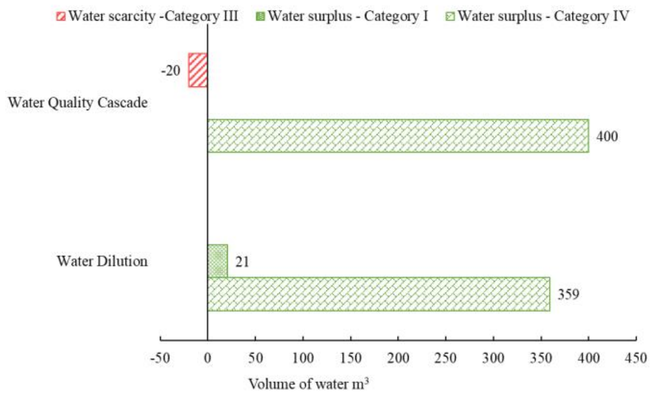


Figure 3-8: Water scarcity of Water Quality Cascade and Water Dilution - Case 2

3.3.3 Case Study 3

Region C has a higher water demand than supply, which indicates a physical water scarcity that cannot be eliminated without water import or regeneration. The GCC of Case 3 is constructed in Figure 3-9. The "Pinch Pocket" marked in the green shades means the Category I and II can be directly used to meet the demand of Category III, and Category IV can be directly used for Category V.

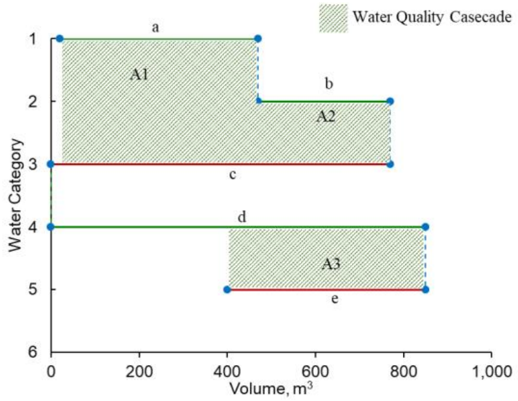


Figure 3-9: Water Scarcity GCC – Case 3

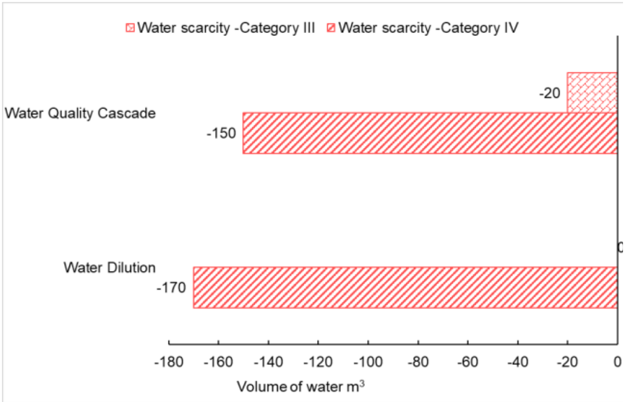


Figure 3-10: Water scarcity of Water Quality Cascade and Water Dilution - Case 3

The water scarcity after water quality cascade is 20 m^3 Category III and 150 m^3 Category V. Then the Water Dilution is applied, using Category I and II dilute Category IV to obtain Category III. The water scarcity result is compared with the WQC scenario in Figure 3-10.

Unlike in Case 2 where the water scarcity is eliminated by water quality upgrades, water scarcity is identified in all scenarios in Case 3. But WD still has the optimal result with water scarcity of lowest quality (170 m^3 Category V), comparing with WQC (20 m^3 Category III and 150 m^3 Category V). In other words, water quality upgrade reduces the water scarcity and shifted the scarcity from higher to lower quality water.

3.4 Conclusion

Water scarcity is redefined as the deficit of water volume of a certain quality. A graphical Water Scarcity Pinch Analysis (WSPA) is proposed to assess the regional water scarcity in terms of water quality and quantity. The staircase water scarcity supply-demand composite curves enables the quantification of water quality and quantity scarcity. Water scarcity is defined as the deficit volume of water with a water quality description, e.g. 170 m^{3,} Category III in case 3. The water scarcity Grand Composite Curve clearly demonstrates the "Pinch Pocket" (water quality cascade) and indicates the possibilities of water quality upgrading for water scarcity minimisation. The results showed that WSPA is able to identify the water quality scarcity together with quantity. Water quality upgrading can reduce and even eliminate water scarcity via water dilution.

CHAPTER 4 **Water-Energy Nexus: An Illustration of Seawater Desalination**

This chapter presents an initial assessment of the water-energy nexus illustrated with an example of the seawater desalination plants in China. This work is supported by the author's publication in the journal of Energies, with the title "Analysing the Energy Consumption, GHG Emission, and Cost of Seawater Desalination in China". In this study, the current development of seawater desalination in China, including the capacity, distribution, processes, as well as the desalted water use, are analysed and discussed. Energy consumption and GHG emissions of the nationwide seawater desalination industries are calculated covering the period of 2006–2016. The unit product cost of seawater desalination plants specifying processes is also estimated.

4.1 Introduction

Increasing water scarcity has become a global issue. Freshwater supply is limited and has been remarkably affected by the degradation of water quality in natural water bodies, while the demand for freshwater has continued to increase. Besides water consumption minimisation by improving water use efficiency, conventional water treatment and desalination are employed to reclaim the polluted water and freshwater to increase the supply. Especially in water-scarce regions, where the water source is mainly from precipitation, the water supply has been unreliable due to the influence of global climate change (Boulay et al., 2018). Seawater desalination is considered a technique with high water supply potential and has become an emerging alternative for freshwater supply in China. The increase of the capacity also increases energy consumption and greenhouse gases (GHG) emissions, which has not been well investigated in existing studies. Water desalination has been widely applied in the world.

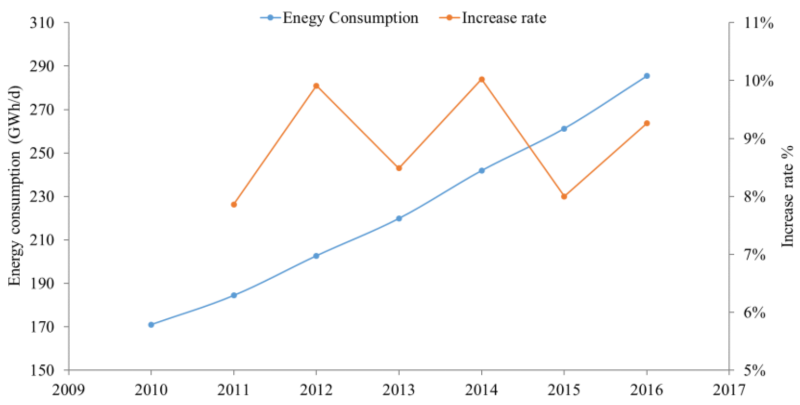


Figure 4-1: Water desalination energy consumption (electricity) from 2010 to 2016

Water desalination is an energy-intensive approach for freshwater production (Attarde et al., 2017), and the rapid increase of installed capacity has resulted in increasing resource (mainly energy) consumption and environmental impacts. Based on the water desalination capacities and the energy consumption factor provided by (Al-Karaghouli and Kazmerski, 2013), the energy consumption of the world overall water desalination is estimated and as shown in Figure 4-1.

The environmental impact of water desalination has been focused on theoretical and scenario analyses (Čuček et al., 2012). Cornejo et al. (2014) found that reverse osmosis (RO) technologies have lower GHG emissions than thermal desalination technologies. The estimated GHG emissions footprint of seawater RO desalination (0.4–6.7 kg CO_{2eq}/m^3) is generally larger than brackish water RO desalination (0.4–2.5 kg CO_{2eq}/m^3) and water reuse systems (0.1–2.4 kg CO_{2eq}/m^3). Shrestha et al. (2011) determined that the associated CO_2 emissions for seawater desalination (0.25 Mt/y) are 47.5 % higher than that for water conveyance (0.17 Mt/y). The GHG footprint values vary due to the variability of location, technologies, life cycle stages, parameters considered, etc.

Facing the water shortage issue, China is making a significant effort with increasing the water use efficiency and eliminating water waste. For the regions with severe water shortage, there are mainly two possibilities to increase the amount of available freshwater. One solution is water transfer projects, including the South-North Water Transfer Project and the Water Transfer from Yellow River to Qingdao Project (Sheng and Webber, 2017). These projects are carried out by constructing water channels to transfer freshwater from water-rich areas to water-scarce regions, mainly Beijing, Hebei, Henan, and Shandong. Another action is the promotion of seawater desalination projects (Figure 4-2). With the promotion and development of water desalination projects and more advanced technology, the total capacity of seawater desalination plants increased from 20×10^6 m^3/y to 390×10^6 m^3/y from 2006 to 2016 (Ministry of Natural Resources of the People's Republic of China, 2018).

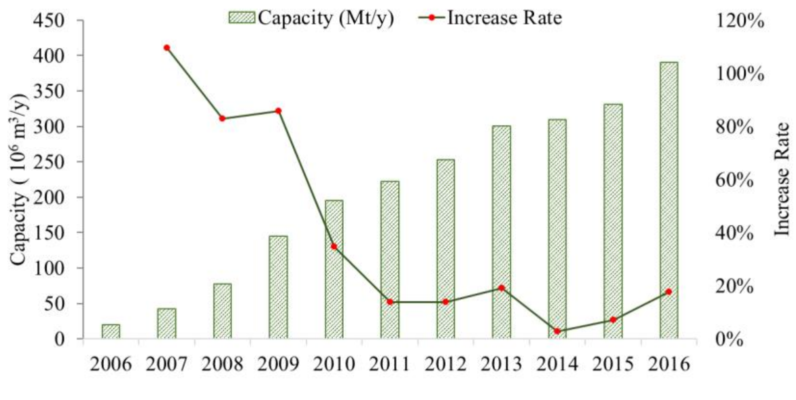


Figure 4-2: Total seawater desalination plant capacities in China from 2006 to 2016, derived from (Ministry of Natural Resources of the People's Republic of China, 2018)

Most of the literature references have focused on either the advancement of the desalination process or the specific case plants. The overall picture of the development and environmental performance, as well as the cost of seawater desalination in China, has not been thoroughly discussed. There is an urgent need to analyse the current development of the seawater desalination in China and to benchmark the energy consumption, emissions, as well as the cost. This can provide an overall picture of the environmental and economic performance, and facilitate energy consumption minimisation, GHG reduction, and efficiency improvement in seawater desalination implementations.

4.2 Methodology

The energy consumption, GHG emission, and the unit product cost of the seawater desalination plants in China are assessed for the year of 2006–2016. The seawater desalination capacity data of China overall and selected provinces in 2016 are mainly derived from Ministry of Natural Resources of the People's Republic of China (2018), and other data sources are explained where mentioned.

4.2.1 Energy Consumption

The energy consumption of seawater desalination plants in China can be calculated using mass balance equations along with the specific energy consumption (SEC) and the capacity of the plants. SEC in kWh/m^3 desalinated water, is one of the most critical factors characterizing the performance of the water supply (Caldera et al., 2016).

$$EC_a = \sum SEC_i \times C_i \times 365 \times P_a \qquad (4\text{-}1)$$

Where EC_a is the annual energy consumption of the plant, kWh/y; *SECi* is the specific energy consumption of seawater desalination plants with process i, kWh/m^3; the energy consumption of all desalination processes involved in this study (RO, MED, MSF, and ED) are converted to the form of electricity, kWh/m^3; C_i is the capacity of the desalination plants with process i, m^3/d. P_a is the availability of the plant when specific data is not available, P_a is set as 90% based on the study of (Wittholz et al., 2008).

The specific energy consumption of various desalination processes is listed in Table 4-1.

Table 4-1: Specific energy consumption (SEC) of different processes (Al-Karaghouli and Kazmerski, 2013)

Process	Specific Energy Consumption kWh/m^3
RO (seawater)	5.0
MED	17.9
MSF	23.4
ED	4.1

4.2.2 GHG Emissions

Since there are no major direct GHG emissions in water desalination, the estimation of GHG emissions mainly considers the emissions from energy consumption. The estimation method is based on the calculation method of GHG emission from processing proposed by ISCC (ISCC, 2017), which is shown as follows:

$$G_e = EM_e + EM_{in} + EM_{waste} \quad (4\text{-}2)$$

Where *Ge* is the annual GHG emissions of the desalination plants, t CO_{2eq}/y; EM_e is the emission of energy consumption, t CO_{2eq}/y; EM_{in} is the emission of material inputs, t CO_{2eq}/y; and EM_{waste}, is the indirect emission from treating the waste generated from the desalination processes, t CO_{2eq}/y. In this study, the GHG emission from energy consumption is estimated, and the emissions of material input (seawater) and waste (brine) are not considered due to the limit of data availability.

$$EM_e = EC_a \times E_f \quad (4\text{-}3)$$

Where EC_e is the annual energy consumption of process i, kWh/m^3; and Ef is the emission factors, t CO_{2eq}/kWh. In this study, the Ef is set as 1.04 t CO_{2eq}/kWh according to the reference (Brander et al., 2011).

4.2.3 Unit Product Cost

The cost of water desalination mainly includes capital cost and operating cost, with the latter mainly consisting of energy cost for plant operation and the cost for maintenance. In this study, the unit product cost, which is the cost per m^3 desalted water, is calculated based on the method proposed by (Wittholz et al., 2008).

Estimation of the unit product cost is calculated as follows:

$$UPC = \frac{CC/_{Pl} + OP_a}{Ca \times Pa} \quad (4\text{-}4)$$

Where *UPC* is the unit product cost, USD/m^3; *CC* is the capital cost of the plant over the lifespan, USD; *Pl* is the plant life, y; OP_a is the annual operating cost; USD; *Ca* is the capacity of the plant, USD; *Pa* is the plant availability, %.

Capital cost

The capital cost is calculated according to the power-law rule:

$$CC_x/CC_{rf} = [Ca_x/Ca_{rf}]^m \quad (4\text{-}5)$$

Where CC_x and Ca_x are the capacity (m^3/d) and capital cost (MUSD) of the studied plant; CC_{rf} and Ca_{rf} are the capacity (m^3/d) and capital cost (MUSD) of the reference plant, m is the power value. Consequently, the capital cost of plant x can be calculated as:

$$CC_x = e^{m \times ln(Ca_x) - m \times ln(Ca_{rf}) + ln(CC_{rf})} \quad (4\text{-}6)$$

According to (Wittholz et al., 2008), m is set as 0.8 for seawater desalinate plants. A dataset of the year 2016 from the Carlsbad Desalination Plant, in San Diego County, USA, is selected as the reference plant to estimate the overall capital cost of the desalination plants (shown in Table 4-2).

Table 4-2: Basic data of the Carlsbad Desalination Plant, in San Diego County (Wittholz et al., 2008).

Parameters	Value	Units
Total capacity	204,390	m^3/d
Feed water TDS	34,500	mg/L
Process	RO 4 stages	-
Capital cost of the plant	537 M	USD

Operating cost

The annual operating cost includes the energy consumption (electrical power), maintenance, labour, membrane replacement, as well as the cost for the chemicals. The operating cost is dependent on the operating process of the desalination plants, but in general, energy cost is the major component. Zhou and Tol (2004) studied the cost of thermal processes and found that energy cost is 87% of the total operating cost.

Table 4-3: Average cost breakdowns of different desalination processes, calculated based on (Wittholz et al., 2008)

Process	Fixed Cost Contribution	Operating Contribution	Energy Cost Contribution in Operating Cost	EOP
RO (seawater)	35 %	65 %	35 %	54 %
RO (brackish water)	35 %	65 %	30 %	46 %
MED	40 %	60 %	45 %	75 %
MSF	40 %	60 %	45 %	75 %

Wittholz et al. (2008) investigated the cost of water desalination and analyzed the breakdowns of the cost, including fixed cost (capital cost) and operating cost (maintenance, material and energy cost, etc). The contribution of energy cost to operating cost is also estimated (Table 4-3).

The operating cost can be calculated with energy cost and the energy/operating cost ratio as in Eq(4-7):

$$OP_a = Eco/EOP \tag{4-7}$$

Where *OPa* is the annual operating cost, MUSD, *Eco* is the energy cost, MUSD, and *EOP* is the ratio of energy cost and operating cost, %, which is shown in Table 4-3.

The cost of energy consumption can be calculated based on the specific energy consumption of different processes and the capacity as well as the price of the electric power, as shown in Eq(4-8):

$$Eco = SEC_i \times C_i \times P_e \quad (4\text{-}8)$$

Where SECi is the specific energy consumption, kWh/m^3; the energy consumption of all desalination processes involved in this study (RO, MED, MSF, and ED) is converted to the form of electricity, kWh/m^3; P_e is the price of the electricity supplied for desalination plant, USD, the price is estimated for the year of 2016.

The electricity price for water desalination plant is referred from reference (Price Bureau of Shandong, 2017). The cost is estimated from water input to the gate of the plant; water conveyance and distribution, as well as the brine disposal, are yet considered.

4.3 Results and Discussions

4.3.1 Energy Consumption and GHG Emissions

The energy consumption and GHG emissions of the Chinese seawater desalination are determined for the period of 2006–2016 (Figure 4-3).

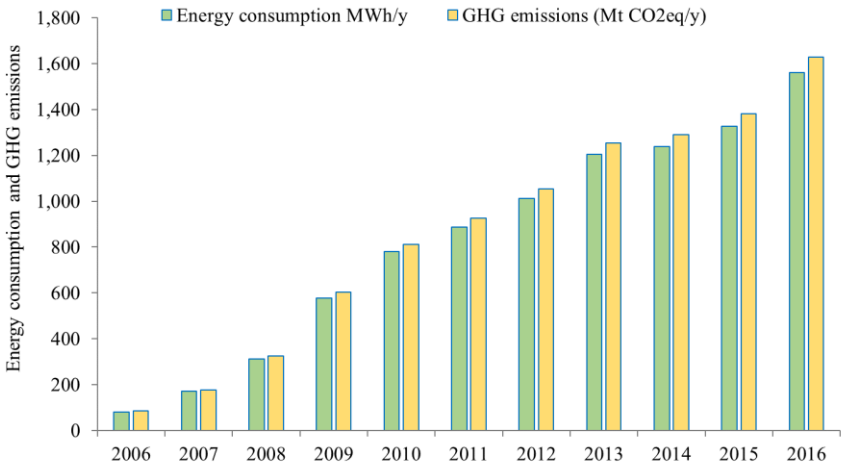


Figure 4-3: Overall seawater desalination energy consumption and GHG emissions from 2006–2016.

The annual energy consumption increased in the 11 y from 81 MWh/y to 1,561 MWh/y, with an increasing rate of 182%. The GHG emissions increased from 85 $MtCO_{2eq}$/y to 1,628 $MtCO_{2eq}$/y.The breakdowns of GHG emissions by province and desalination processes are estimated for the year 2016, as shown in Figure 4-4.

The map in Figure 4-4 showed the east coastal line in China with the provincial distribution of with seawater desalination plants. The deeper colour indicates higher provincial seawater desalination GHG emissions. The total GHG emissions of the seawater desalination plants in China in 2016 are 9,409 $MtCO_{2eq}$. The provinces of Tianjin, Hebei, and Shandong are the top three contributors. The GHG emissions of these three provinces are 7,359 $MtCO_{2eq}$, which is 78.2% of the total seawater desalination GHG emission in China.

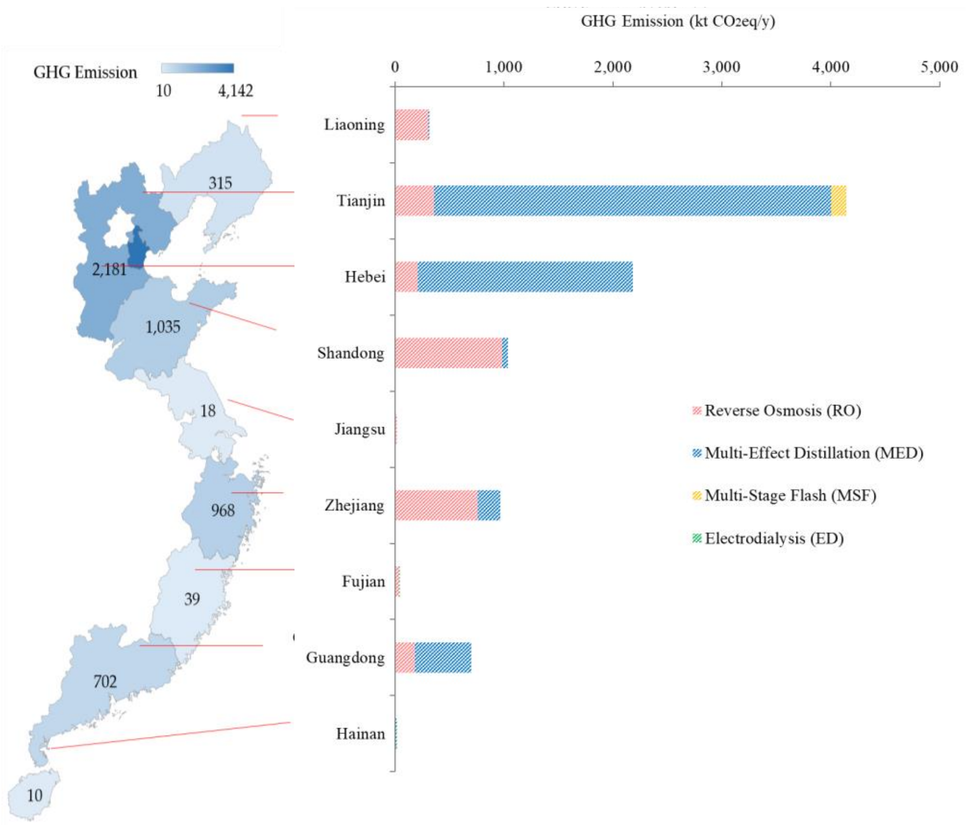


Figure 4-4: GHG emissions of seawater desalination: Regional distribution and breakdowns by processes.

Regarding the desalination process, MED plants contribute the most to the GHG emissions. Tianjin has the highest GHG emissions of 4,142 Mt CO_{2eq} in China, and the MED plants contributed more than 88.0% (3,645 Mt CO_{2eq}) of the total seawater desalination GHG emissions of Tianjin. Tianjin is a major contributor to the overall emissions of all seawater desalination plants in China in 2016.

4.3.2 Unit Product Cost

The Unit Product Cost (UPC) is correlated with the desalination processes, capacity of the plant, and the type of energy used for the plant, etc. (Pinto and Marques, 2017). In this study, the energy consumptions of all processes are converted to electricity, and the impact of energy source is not analysed. The UPC of seawater desalination plants in different provinces in 2016 is determined, as shown in Figure 4-5 and the desalination process is specified.

The UPC of MED, MSF, and ED is much higher than RO, which is inconsistent with the conclusion of other studies. For example, a case study of Qingdao (Hua et al., 2014), Shandong Province, China showed the average economic cost of seawater desalination process is 8 CNY/ m^3 (approx. 1.16 USD based on the current exchange rate 0.15), with an RO plant capacity of 3×10^3 m^3/d. Hainan has the highest UPC for RO seawater desalination of 1.3 USD, Shandong and Zhejiang have the lowest UPC for RO seawater desalination of 0.8 USD.

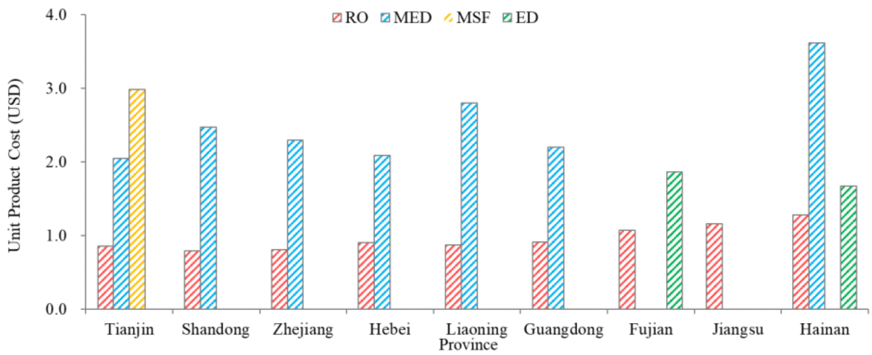


Figure 4-5: Unit product cost of water desalination by provinces in 2016.

For MED seawater desalination, Hainan has the highest UPC at 3.6 USD, while Tianjin has the lowest UPC of 2.0 USD. The only province with MSF process, Tianjin, has a UPC for MSF desalination of 3.0 USD. For the same process, the price varies within a reasonable range, e.g. the UPC of RO process desalination plants in the selected provinces in increasing order is: Shandong = Zhejiang < Tianjin = Hebei = Liaoning = Guangdong < Fujian < Jiangsu < Hainan.

4.4 Conclusions

This study analysed the water-related energy consumption and GHG emissions of the seawater desalination industries in China. The key results and conclusions are:

(1) With the increasing installed capacity of seawater desalination from 2006 to 2016, the energy consumption and GHG emission increased from 81 MWh/y to 1,561 MWh/y during the 11 years. The overall GHG emission increase from 85 Mt CO_{2eq}/y to 1,628 Mt CO_{2eq}/y, with an increasing rate of 180%. Tianjin has the largest GHG emissions, followed by Hebei and Shandong, with emissions of 4.1 Mt CO_{2eq}/y, 2.2 Mt CO_{2eq}/y. and 1.0 Mt CO_{2eq}/y.

(2) The unit product cost (UPC) of seawater desalination is higher than other water supply alternatives, and it differentiates the desalination processes. The UPC of the RO process varies from 0.8 USD to 1.3 USD in 2016, and the UPC of MED, MSF, and ED are 2.0 USD–3.6 USD, 3.0 USD, and 1.7 USD to 1.9 USD. Tianjin which has the largest overall seawater desalination capacity, has the relatively lowest UPC for RO and MED.

(3) Seawater desalination is becoming a critical water supply alternative for cities with serious water scarcity. The cost, energy demand and GHG emissions are still considerably higher than surface water supply. There is potential for energy consumption, GHG emission and cost reduction with the application of energy recovery units, the integration of desalination plants and renewable energies or low potential heat, as well as the development of new technologies.

CHAPTER 5 **Conclusions and Proposed Future Development**

5.1 Conclusions of the PhD study

Water pollution and irregular water supply issues, including water scarcity and floods have increased the challenges in water resource assessment and management. The increasing water scarcity and pollution have significantly affected agriculture and industrial development, and even drinking water. These complex issues require updated methodology developments to facilitate and guide practical water use and management.

The PhD study aims to investigate the water resource assessment methods and solutions to minimise water scarcity and water-use related energy consumption. Three major methodological studies and one major assessment work compose the core of this thesis.

The PhD thesis is initiated with an extension of the water availability footprint method with the aim to involve water quality impact into the existing water use assessment framework. Following the extended development of water footprint assessment method, a cost-based Quantitative-Qualitative Water Footprint (QQWFP) considering multiple contaminants is proposed and illustrated with a case study of a Monosodium Glutamate (MSG) plant in China. The cost-based method provides intuitive and insightful results to guide the decision-makers and users in water resources management and water use optimisation. Comparing with existing water footprint indicators, the water quality and quantity footprints of QQWFP are comparable, which enables the user and manager to identify the critical water use sector and the bottleneck of water use (i.e. water consumption or pollution). An added benefit is that the QQWFP can be labelled on the product package and increase the customer' awareness of water use and saving. The results of the case study indicate the significance of addressing water quality determination and the potential for water quality-oriented industrial water use optimisation. The major novel contributions of the methods include 1) Evaluation of the impact of quantity and quality in water use in the form of cost, and the water footprint comparison among different users that covers multiple contaminants. 2) Coverage of the treatment cost of multiple contaminants. 3) Cost-based and unified water footprint results that guide water users and managers to minimise water use impact and optimise water use efficiency

The QQWFP targets at process level and plant level user, the graphical method - Water Scarcity Pinch Analysis (WSPA) is a proposed as a significant improvement of the Water Pinch Analysis (WPA) targeting at regional water resources assessment. The impact of multiple contaminants is represented with the water quality categories, and the freshwater targeting is conducted with the staircased Grand Composite Curves. Water Quality Cascade and Water Quality Upgrading are investigated as alternative solutions to maximise the water use efficiency and minimise freshwater input. The proposed WSPA is illustrated and implemented with three case studies. The major conclusions and contributions of this work are 1) WSPA enables accounting for water quality together with quantity in water scarcity assessment and provides both quantity and quality targets for minimising regional water scarcity; 2) Applying the WSPA to a macro level elevates the ratio-based water scarcity assessment from single determination to insight-based assessment that can guide the regional water resource management. 3) water quality cascade and water quality upgrade via mixing can improve the water use efficiency and reduce the water scarcity. Future directions include the further development of WSPA covers water regeneration and the cost and energy consumption of inter-region water distribution.

Water issues are not only about water resource but also other elemental resources. The increase in water use and water treatment also increase water-related energy consumptions and emissions. An initial assessment of the water-energy nexus in seawater desalination plants in China is also conducted in this PhD study. The energy consumption, GHG emission, as well as the unit products cost of the seawater desalination plants in China are determined. The major results and conclusions of this study are 1) The installed capacity maintained increased from 2006 to 2016, and reverse osmosis is the major process used for seawater desalination in China. 2) The energy consumption increased from 81 MWh/y to 1,561 MWh/y during the 11 years. The overall GHG emission increase from 85 Mt CO_2eq/y to 1,628 Mt CO_2eq/y. Tianjin had the largest GHG emissions, following are Hebei and Shandong, with emissions of 4.1 Mt CO_2eq/y, 2.2 Mt CO_2eq/y, and 1.0 Mt CO_2eq/y. 3) The unit product cost of seawater desalination is higher than other water supply alternatives, and it differentiates the desalination processes. The average unit product cost of the reverse osmosis process is 0.96 USD and 2.5 USD for the multiple-effect distillation process.

5.2 Novel contributions

The novel contributions lie in the following four aspects. The first contribution is to quantify the impact of water quality degradation into the existing water scarcity assessment frameworks. This is supported by the work of the extended water availability footprint framework (Section 2.1). The second contribution of this work is the development of the Quantitative-Qualitative Water Footprint (QQWFP), which uses the total cost of water consumption and cost of treating the contaminant generated during the water use process to determine the quality and quantity impact of water use (Section 2.2). The third contribution is the coverage of multiple contaminants. The QQWFP covers multiple contaminants by accounting the total cost of treating different contaminants. In another work, Water Scarcity Pinch Analysis (WSPA) applied water quality categories to determine the impact of multiple contaminants (Chapter 3). The last contribution is that this study presented an initial assessment of the water-related energy consumption and GHG emissions in the seawater desalination plants in China during 2006-2016 (Chapter 4).

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Supplementary Data

Table S1: Water quality categories and the regulated items (Ministry of Ecology and Environment of the People's Republic of China, 2002)

Regulated Items		Unit	Categories				
			I	III	III	IV	V
Temperature	–	–	-2 <= ΔT(weekly) <= 1				
pH	–	–	6-9				
DO	>=	mg/L	7.5	6	5	3	2
Permanganate	<=	mg/L	2	4	6	10	15
COD	<=	mg/L	15	15	20	30	40
BOD5	<=	mg/L	3	3	4	6	10
NH3-N	<=	mg/L	0.15	0.5	1	1.5	2
TP	<=	mg/L	0.02	0.1	0.2	0.3	0.4
TN	<=	mg/L	0.2	0.5	1	1.5	2
Cu	<=	mg/L	0.01	1	1	1	1
Zn	<=	mg/L	0.05	1	1	2	2
F-	<=	mg/L	1	1	1	1.5	1.5
Sn	<=	mg/L	0.01	0.01	0.01	0.02	0.02
As	<=	mg/L	0.05	0.05	0.05	0.1	0.1
Hg	<=	mg/L	0.00005	0.00005	0.0001	0.001	0.001
Cd	<=	mg/L	0.001	0.005	0.005	0.005	0.01
Cr 6+	<=	mg/L	0.01	0.05	0.05	0.05	0.1
Pb	<=	mg/L	0.01	0.01	0.05	0.05	0.1
Cyanide	<=	mg/L	0.005	0.05	0.2	0.2	0.2
Volatile Phenols	<=	mg/L	0.002	0.002	0.005	0.01	0.1
Petroleum	<=	mg/L	0.05	0.05	0.05	0.5	1
Anionic surfactants	<=	mg/L	0.2	0.2	0.2	0.3	0.3
Sulphurs	<=	mg/L	0.05	0.1	0.2	0.5	1
Escherichia coli	<=	/L	200	2000	10000	20000	40000

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3. **Jia X.,** Klemeš J.J., Wan Alwi S.R., Varbanov P.S., 2020. Regional water resources assessment using water scarcity pinch analysis. Resources, Conservation and Recycling, 157, p.104749. **[IF = 8.086, CiteScore = 10.7]**
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