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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

DIZERTAČNÍ PRÁCE

AUTHOR Xuexiu JIA, MSc

AUTOR PRÁCE

SUPERVISOR: Doc. Dr-Habil. Ing. Petar Sabev Varbanov, Ph.D

ŠKOLITEL

CO-SUPERVISORS:

Prof. Dr-Habil. Ing. Jiří KLEMEŠ, DSc., Dr. H. C. (mult)

Prof. Dr. Sharifah Wan ALWI (Universiti Teknologi Malaysia, MY)

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Declaration

I declare that I am the author of this doctoral thesis. It has been prepared under the guidance of my supervisors. The reported results are original research which developed based on my knowledge gained during PhD study and consultation with experts. I have quoted all the sources including my own publications. The related references are provided at the end of this thesis

Brno, 2020 Ms. Xuexiu JIA

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 s cílem nalézt přizpůsobené řešení pro optimální využití regionální a průmyslové vody.

Acknowledgement

This thesis is a milestone of my study and research in the four years of work in the SPIL group. Throughout this journey, my passion has been focused on investigating novel tools to provide solutions for water-related issues. This thesis presents the lessons and knowledge learned in developing the assessment tools, and also the results of many experiences I have encountered from those remarkable individuals whom I wish to acknowledge.

First and foremost, I wish to thank Prof Jiří Jaromír Klemeš and Dr Petar Varbanov for being my major supervisors. Prof Klemeš and Dr Varbanov have been more than supportive in my studies and life since the days I began working and studying in the group. Prof Klemeš has always been encouraging me to focus in my field and broaden my mind in research, and his passion and active performance in scientific research have been such an encouragement for me to keep the passion in seeking solutions for practical environmental issues. I have been given unique opportunities and experience to participate in and organise conferences, work as guest editor and reviewer for several international journals. He has been supportive not only in scientific research but also helping me to fit in the local life. Dr Petar Varbanov has always been encouraging me to explore innovative thinking. There have been many inspiring discussions and suggestions contributed to the improvement of my research. His dedication to research and guidance have ensured the progress of my study and the development of this thesis. I would also like to thank my co-supervisor Prof Sharifah R. Wan Alwi, who has always been reachable and supporting with insightful suggestions to uplift my work.

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Poděkování

Tato disertační práce je milníkem mého studia a výzkumu za čtyři roky práce ve skupině SPIL. V průběhu této cesty se moje vášeň soustředila na zkoumání nových nástrojů k poskytování řešení problémů souvisejících s vodou. Tato práce představuje poznatky a poznatky získané při vývoji nástrojů hodnocení a také výsledky mnoha zkušeností, se kterými jsem se setkala od těch pozoruhodných osob, které chci ocenit.

Především bych ráda poděkovala prof. Jiřímu Jaromírovi Klemešovi a Dr. Petrovi Vrbanovovi za to, že byli mými hlavními supervizory. Prof. Klemeš a Dr. Vrbanov se od dob, kdy jsem ve skupině začal pracovat a studovat, více než podporovali v mém studiu a životě. Prof Klemeš mě vždy povzbuzoval, abych se zaměřila ve svém oboru a rozšířil svou mysl ve výzkumu, a jeho obetavost a aktivní výkon ve vědeckém výzkumu pro mě byly takovým podnětem, abych si udržela nadseni při hledání řešení praktických problémů životního prostředí. Dostala jsem jedinečné příležitosti a zkušenosti, abych se účastnila a organizovala konference, pracovala jako redaktorka Special Issues a recenzentka pro několik mezinárodních časopisů. Podpořil nejen muj vědecký výzkum, ale také mi pomohl prispusobit se místnímu životu. Dr. Petr Vrbanov mě vždy povzbuzoval k badani inovativním myšlením. Ke rozsireni mého výzkumu probehlo mnoho inspirativních diskusí a návrhů. Jeho obetavost k výzkumu a vedení podporilo pokrok v mém studiu a vývoj této práce. Také bych ráda poděkovala svému spolu vedouci disertace profesorce Sharifah R. Wan Alwi, ktera byla vždy dosažitelný a podporovala mne inspirativnimi návrhy a povzbuzovala moji práci.

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Děkuji vám mnohokrát.

Contributing Research Work Presented in Peer-Reviewed Publications

This thesis has been developed based on my publications in several distinguished international journals. In **Chapter 3**, 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 4** are published in the journal of Renewable and Sustainable Energy Reviews [3] and Resources, Conservation and Recycling [4]. The Water-Energy Nexus investigation presented in **Chapter 5** is based on the works published in Energies [5]. 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 thesis.

1. **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]**
2. **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]**
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5. **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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8. Ren X.Y., Jia **X.**, Varbanov P.S., Klemeš J.J., Liu Z.Y., 2018. Targeting the

Cogeneration Potential for Total Site Utility Systems, Journal of Cleaner Production, 170, 625-635. **[IF = 6.395, CiteScore = 10.9]**

Journal Articles –Scopus

9. **Jia, X.,** Varbanov, P.S., Wan Alwi, S.R., Klemeš, J.J., 2020. Total Site Water Main Concentration Selection: A Case Study, Chemical Engineering Transactions, 81, 259-264. DOI: 10.3303/CET2081044. **[CiteScore = 1.3]**
10. **Jia, X.**, Klemeš, J.J., Wan Alwi, S.R., Varbanov, P.S., 2019. Blue Water Footprint of the Czech Republic. Chemical Engineering Transactions, 76, 1063-1068. DOI: 10.3303/CET1976178. **[CiteScore = 1.3]**
11. **Jia, X.**, Klemeš, J.J.; Varbanov, P.S.; Wan Alwi, S.R., 2018. Energy-Emission-Waste Nexus of Food Deliveries in China, Chemical Engineering Transactions, 70, 661-666, DOI: 10.3303/CET1870111. **[CiteScore = 1.3]**
12. Varbanov, P.S., Walmsley, T.G., Klemes, J.J., Wang, Y., **Jia, X.**, 2018. Footprint Reduction Strategy for Industrial Site Operation. Chemical Engineering Transactions, 67, 607-612. DOI: 10.3303/CET1867102. **[CiteScore = 1.3]**
13. Walmsley, T.G., **Jia, X.**, Nemet, A., Liew, P.Y., Klemeš, J.J., Varbanov, P.S., 2018. Total Site Utility System Structural Design Using P-graph, Chemical Engineering Transactions, 63, 31-35. DOI: 10.3303/CET1863006. **[CiteScore = 1.3]**
14. **Jia, X.**, Varbanov, P.S., Walmsley, T.G., Klemeš, J.J., Ren, X.Y., Liu, Z.Y., 2018. Extended Indicators for Total Site Targeting. Chemical Engineering Transactions, 63, 211-216. DOI: 10.3303/CET1863036. **[CiteScore = 1.3]**
15. Walmsley, T.G., **Jia, X.**, Varbanov, P.S., Klemeš, J.J., Wang, Y., 2018. Total Site Utility Systems Structural Design Considering Environmental Impacts. Computer Aided Chemical Engineering, 43, 1305-1310.
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17. Ren, X.Y., **Jia, X.**, Varbanov, P.S., Klemeš, J.J., Liu, Z.-Y, 2017. Calculation of Cogeneration Potential of Total Site Utility Systems with Commercial Simulator, Chemical Engineering Transactions 61, 1231-1236. DOI: 10.3303/CET1761203. **[CiteScore = 1.3]**

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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.

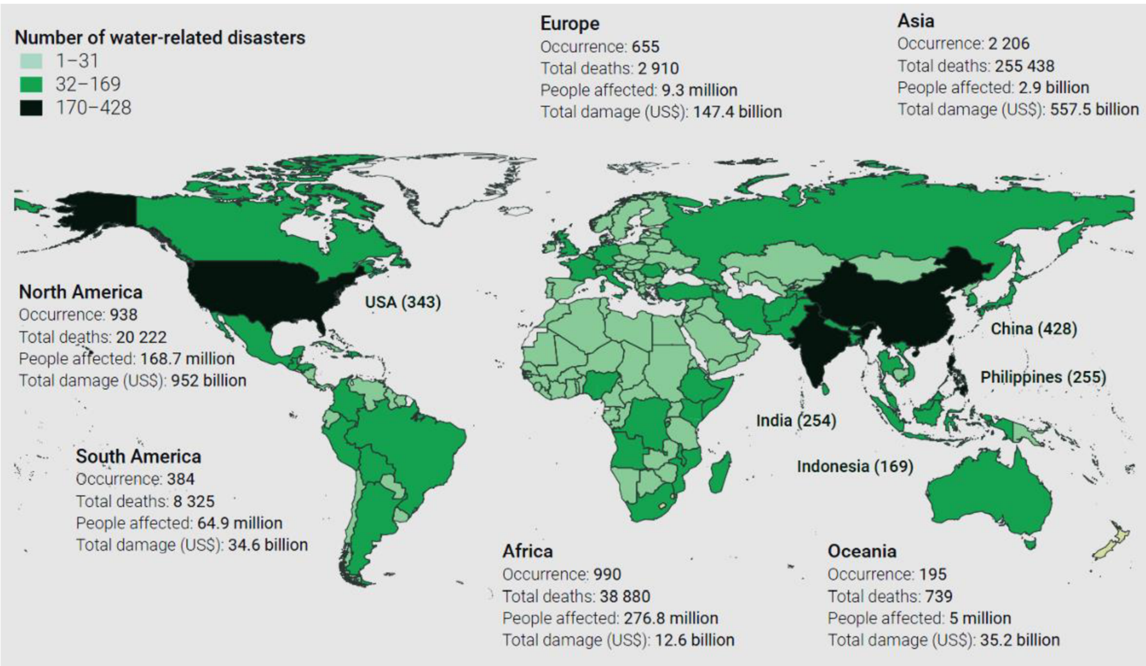

Figure 1-1: Spatial distribution of water-related disasters during 2001-2018 (UNESCO and UN-Water, 2020)

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.

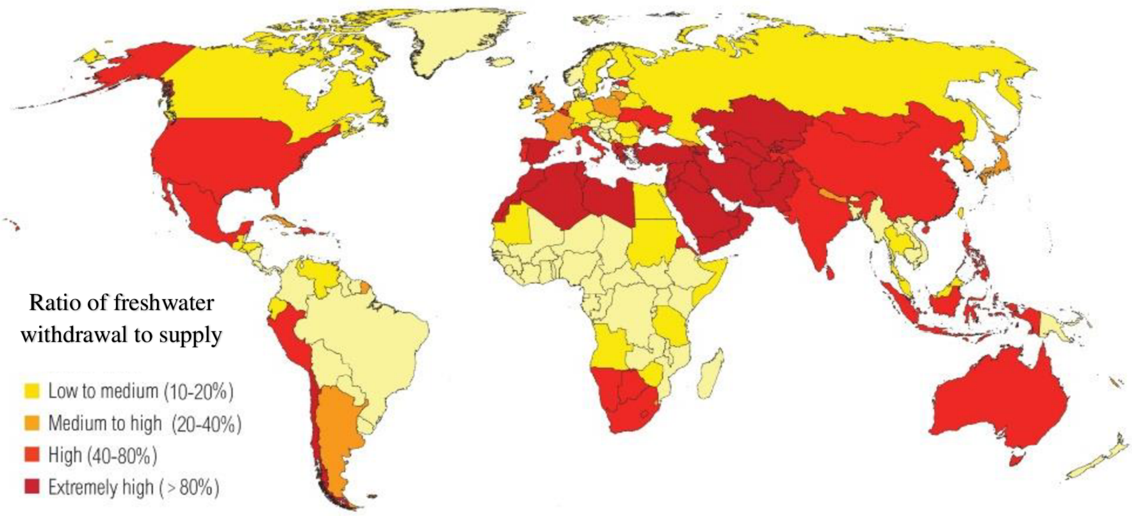

Figure 1-2: Water stress by country projected in 2040 (World Resources Institute, 2015)

Water covers about 71 % of the earth, and about 2.5 % of the earth's water is covered with freshwater, among which two-thirds have not been accessed due to their form (e.g. glacier) and geographical location limited assessment (World Bank, 2019). Oceans hold about 96.5 % of the earth's water, and with the development of seawater desalination technologies, water scarcity seems not a critical issue due to the natural abundance of water resources. However, 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. Water scarcity is essentially the shortage of freshwater and freshwater with a certain quality level for usage.

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).

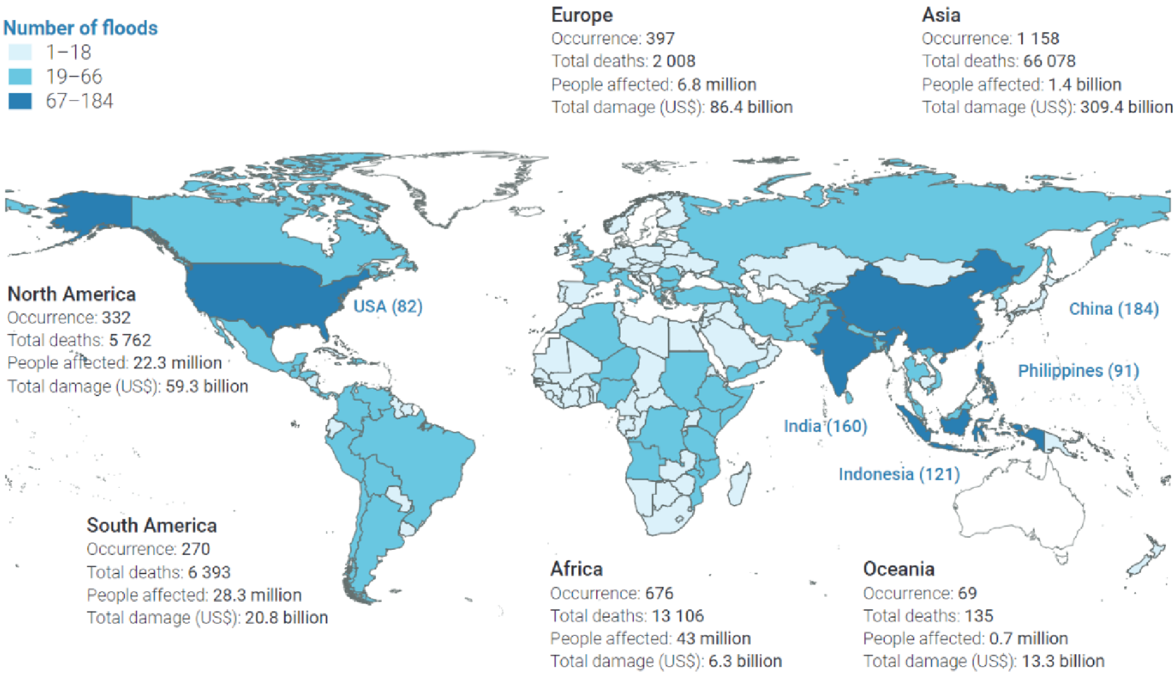

Figure 1-3: Spatial distributions of floods during 2001-2018 (UNESCO and UN-Water, 2020)

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).

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.

The transfer of water also increases the environmental burden of water pollution. As showed in Figure 1-4, the industrial goods imported to the EU by international trade caused water pollution in the original production country. It indicates that China, the Russian Federation, as well as the USA, are the major countries that have severe water pressure caused by international trade of industrial goods with the EU.

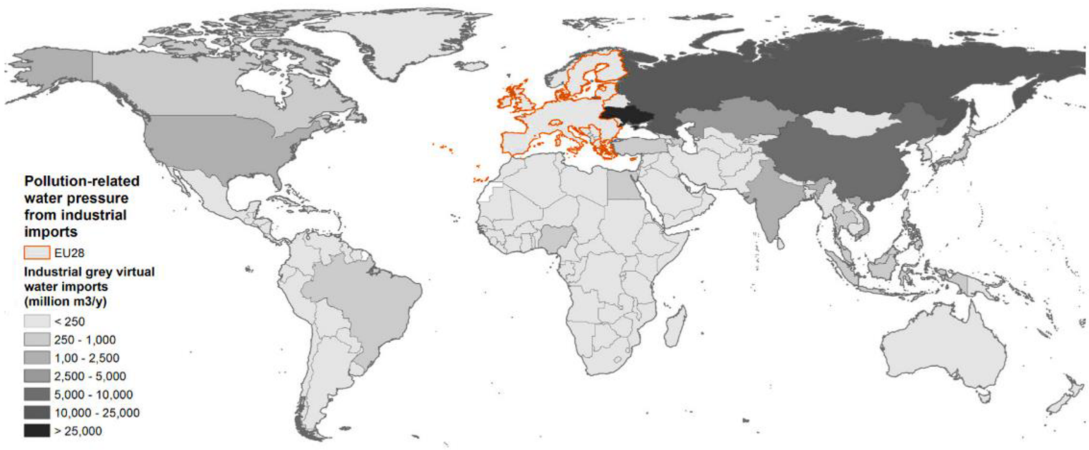

Figure 1-4: Pollution-related water pressure caused by the production of industrial goods imported to the EU (Ercin et al., 2016)

The resources consumed and embedded in the products are transferred to the consumer country in international trade, but the environmental impacts and issues caused by resource exploitation occur at the regional level in the production country. The water pollutants discharged from one country can have a significant impact on the countries on the other side of the globe.

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. Water scarcity and quality degradation issues. 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 (Chapter 2) 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

- **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]**
- **Jia, X.,** Klemeš, J.J., Wan Alwi, S.R., Varbanov, P.S., 2020. Cost-based Quantitative-Qualitative water footprint Considering Multiple Contaminants, RCR. **[IF = 8.086, CiteScore = 10.7]** (Under Review)
- **Jia, X.,** Klemeš, J.J., Wan Alwi, S.R., Varbanov, P.S., 2019, Blue Water Footprint of the Czech Republic. Chemical Engineering Transactions, 76, 1063-1068. DOI: 10.3303/CET1976178. **[CiteScore = 1.3]**
- **Jia X.,** Varbanov P.S., Walmsley T.G., Yan Y., 2017, Water Pollution Impact Assessment of Beijing from 2011 to 2015: Implication for Degradation Reduction. Chemical Engineering Transactions 61, 1525-1531. DOI: 10.3303/CET1761252. **[CiteScore = 1.3]**

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

- Klemeš, J.J., Varbanov, P.V., Walmsley, T.G., **Jia, X.,** 2018. New Directions in the Implementation of Pinch Methodology (PM). Renewable and Sustainable Energy Reviews, 98, 439-468. **[IF = 10.556, CiteScore = 25.5]**
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- Fan, X.Y., Klemeš, J.J., **Jia, X.,** Liu, Z.Y., 2019. An Iterative Method for Design of Total Water Networks with Multiple Contaminants. Journal of Cleaner Production, 240, p.118098. **[IF = 6.395, CiteScore = 10.9]**

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

- **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]**

1.3 Thesis Outline

Chapter 1 introduces the research scope of the thesis, summarise the research gaps, and presents the research aims and objectives. Chapter 2 presents a thorough literature review of water resources assessments, Water Footprint Assessment, Water Pinch Analysis, as well as the Water-Energy Nexus. The primary research work and achievements of the thesis are introduced with three chapters (Chapter 3, 4, and 5). Chapter 3 introduces the extended water footprint assessments methods as well as the case studies. Chapter 4 introduces the Water Scarcity Pinch Analysis and implementations. Chapter 5 presents the initial determination of the national wide water-related energy consumption as well as its emissions in seawater desalination plants. Chapter 6 concludes the whole research work and outlooks the potentials for future works. Following are the references and appendix providing supplementary data.

CHAPTER 2 LITERATURE REVIEW

2.1 Irregular water supplies and water pollution

Irregular water supply issues (e.g. water scarcity, emergency floods, and water pollution) have been increasing especially in urban areas, which severely threaten human lives and economic developments. Nowadays, water scarcity does not only exist in the near-desert regions but covering more and more regions. Climate changes bring contrasting challenges to water management in these regions (Otto et al., 2018). Various regions reported the water shortage/scarcity/stress and drought issues and these issues had been highly concerned by the policymakers and the public. For example, the water-scarce regions include large countries such as India, China and small countries in Europe. Ma et al. (2020) determined the water scarcity at the grid cell level in China and claimed that over half of the population are affected by water scarcity. On the other side of the globe, the Czech Republic went through the driest summer season in 2018 (Data.Brno, 2018). While the UK experienced the wettest February in 2020 and the floods caused a direct economic loss of more than € 328 million and flooded high-quality farmland of more than 30 thousand hectares (Energy & Climate Intelligence Unit, 2020). On top of water quantity issues, the study proved that inadequate water quality exacerbates water scarcity (Ma et al., 2020).

Water resources assessment is enssential to support and guide regional water management. Tackling the irregular water supply and water pollution issues, various methods and tools have been developed to explore and determine the origins and impacts of water use. For example, the concept of Sponge city has been widely adopted to instruct the improvement of rainwater harvesting and conservation to improve the cities' water resilience (He et al., 2019). Assessment and optimisation tools, e.g. water footprint (Hoekstra, 2003) and Water Pinch Analysis (Wang and Smith, 1995), are designed to monitor and improve the performance of water use, aiming to maximise the water use efficiency.

This Chapter provides a thorough review of the water resources assessment methods. The literature review discussed the methods and tools in the following three sections regarding the consideration of water quality and guidance in practical water management. Chapter 2.2 introduces the post-assessment tools of water resources assessment, including the water scarcity assessment and water footprint. Chapter 2.3 discussed the optimisation tools of Water Integration and Water Pinch Analysis. Cahpter 2.4 presents the literature review of the Water-Energy Nexus.

2.2 Water Resources Assessment

2.2.1 Water Scarcity Assessment

Water scarcity issues have been highly discussed and analysed, and a series of metrics have been developed to assess the extent of water shortage. Table 2-1 presented a summary of the widely used indicators for water scarcity/stress assessment.

Table 2-1: Comparison of water resources assessment methods

Method	Definitions	Indication	Remark
Surface Water Supply Index (Shafer and Dezman, 1982)	$\text{SWSI} = (aP_{snow}+bP_{prec} + cP_{stream} + dP_{resv} - 50)/12$ P represents precipitation.	Extremely Dry: -4.2 to -3.0; Moderately Dry: -2.9 to -2.0; Slightly Dry: -1.9 to -1.0; Near Average: -0.9 to 1.0; Slightly Wet: 1.1 to 2.0; Moderately Wet: 2.1 to 3.0; Extremely Wet: 3.1 to 4.2.	-Non-supply-demand comparison. -Does not specify regional and time characterises. -Does not consider water quality
Water Stress Index Falkenmark and Widstrand, 1992)	The average amount of renewable water resources per capita per year	Water stress: WSI < 1700 m^3 Water scarcity: WSI < 1000 m^3 Absolute water scarcity: WSI < 500 m^3	
Water Resource Vulnerability Index (Raskin et al., 1997)	$\text{WRVI} = \frac{TWW}{TAW}$ TWW: Total water withdraw; TAW: Total available water	Highly vulnerable: 0 Moderately vulnerable: 0.25 Threshold: 0.5 Moderately resilient: 0.75 Highly resilient: 1.00	-Does not specify regional and time characterises. -Does not consider water quality. -Difficult to determine the water availability
Critically ratio (Alcamo et al., 2000)	$\text{CR} = \frac{TWU}{TAW}$ TWU: Total water use; TAW: Total available water	No water stress: CR < 0.1 Low water stress: 0.1 < CR < 0.2 Middle water stress: 0.2 < CR <0.4 High water stress: 0.4 < CR < 0.8 Very high water stress: 0.8 < CR < 1.0	
Water Poverty Index (Sullivan, 2002)	Weighted average of five dimensions: access to water; water quantity, quality and variability; water use; water management capacity; environmental aspects.	The higher WPI, the higher water stress.	-Eexpert experience is required. -Non-supply-demand comparison. -Does not consider water quality

Table 2-1 (Continued): Comparison of water resources assessment methods

Method	**Definitions**	**Indication**	**Remark**
Water Exploitation Index (EEA, 2005)	WEI = Mean annual total demand for freshwater / Mean annual freshwater resources	No water stress: 0 – 20 % Water stress: 20% – 40 % High water stress: > 40 %	-Non-supply-demand comparison. -Does not specify regional and time characterises. -Does not consider water quality
Water Stress Index (Pfister et al., 2009)	$\mathrm{WSI} = \frac{1}{1+e^{-6.4WTA}(\frac{1}{0.01}-1)}$ $\mathrm{WTA} = \frac{TWU}{TAW}$ TWU: Total water use TAW: Total available water	Minimal water stress: WSI < 0.01 Moderate water stress: 0.01 < WSI <0.5 Severe water stress: WSI > 0.5	-Does not consider water quality
Grey Water footprint (Hoekstra, 2003)	$WF_{grey} = \frac{C_{effl} - C_{act}}{C_{\max} - C_{nat}} \times E_{ffl}$ C_{effl}, C_{act}, C_{max}, and C_{nat} are the concentrations of the pollutant in the effluent, the intake water, the maximum acceptable and natural concentration of the water bodies. E_{ffl} is the effluent volume.	Indicates the volume of water required to assimilate pollutants entering freshwater bodies.	-Calculates the intensity of water pollution discharged by the user
Water Scarcity Index (Zeng et al., 2013)	WSI $= (BWF + GWF)/TAW$ BWF: Blue water footprint; GWF: Grey water footprint; TAW: Total available water	-Indicates the ratio between water use and water availability -The larger the WSI value, the higher water scarcity	- Lack of physical meaning. -Non-supply-demand comparison. -Considers the intensity of pollutant rather than the water quality of water supply and demand
Quantity-Quality water scarcity indicator (Liu et al., 2016)	$\mathrm{S_{quantity}} = \mathrm{W} \times \mathrm{R}(\mathrm{BWA} - \mathrm{EFR})$ $\mathrm{S_{quality}} = \mathrm{GWF}/\mathrm{BWR}$ BWF: Blue water footprint BWA: Blue water availability GWF: Grey water footprint EFR: environmental flow requirement. W (m^3) is the blue water withdrawal; R is the water consumption ratio		

Since the very early stage, indices such as the Falkenmark Indicator (FI) (Falkenmark and Widstrand, 1992), Social Water Stress Index (SWSI) (Ohlsson, 2000) and Water Poverty Index (WPI) (Sullivan, 2002) have been developed to quantify water shortage issues. FI and SWSI are based on the water requirements from socio-economic perspectives without considering water quality (Jia et al., 2016).

WPI is a comprehensive socioeconomic indicator and consists of five major components (resources, access, capacity, use, and environment), each with several sub-components. All these sub-components consist of several sub-sub-components, and some of them are qualitative variables (Lawrence et al., 2002). WPI is not often used due to the complex assessment procedures and data requirement. It started to consider water quality, but it is difficult to identify the impact of water quality in this highly integrated indicator, and thus can hardly provide indicating results of improving water use.

Many other methods, on the other hand, integrate the water scarcity in terms of the comparison between water demand and available water. For example, the ratio of water withdrawal-to-availability (WTA) is used as a characterisation factor (Pfister et al., 2009) for water scarcity, quantifying the extent human water withdraw out of the hydrological available water resources. However, water withdrawn from the environment and released in the same watershed does not necessarily contribute to local water scarcity (Boulay et al. 2015).

As a continuation, methods based on water consumption-to-availability (CTA) ratio were developed. A series of ratio-based indicators have been similarly developed following this path, such as the demand-to-availability ratio (DTA), using water demand of the region instead of actual water consumption; DTAA, an indicator based on the DTA but includes a filter for arid regions (Boulay et al., 2015). DTAX is the product of two parameters: one representing the relative availability (DTA) and one representing absolute availability (AAv) per unit of surface (Boulay et al., 2015). 1/AMD, the inverse of availability minus demand, which are human water consumption (HWC), environmental water requirement (EWR) (Boulay et al., 2018). It is evident that these indicators and method follow the pattern of the demand-supply ratio (or consumption-available ratio) and uses mathematical transformations to improve and enrich the meaning of the indicator. The advantage of these indicators is that they are very easy to use and indicative enough to show the extent of scarcity by direct comparison. On the other hand, most of these indicators stop at the stage of problem representation, but not providing sufficient insights for the design stage or practical water scarcity solutions. The water scarcity index has been widely used in enormous publications and media reports to illustrate the situation of water shortage, but rarely used for providing solutions for a specific region. As the region-related factors, e.g. the number of natural water resources, economic situation, more importantly, the water quality in the region, are not considered in the comparison. The unification of these assessment leads to the inability of solution-oriented results, but rather informative results.

Various studies are then performed to seek a more systematic assessment of water use (Manan et al., 2009). One of the well-used indicators of water use assessment is the water footprint (WF) (Hoekstra 2003) initiated in the virtual water trade report in 2002, in which the water footprint assessment concept was introduced. The water footprint framework and calculation methods were further developed in the Water Footprint Assessment Manual (Hoekstra et al., 2011), aiming to set a global standard. In this framework, water footprints are defined with regard to water sources, e.g., blue water footprint, green water footprint, and grey water footprint, which represents the water consumption of fresh surface or groundwater, precipitation, and the volume of freshwater that is required to assimilate the load of pollutants based on natural background concentrations and existing ambient water quality standards (Hoekstra et al., 2011). The WFA method has been widely used and developed for water consumption analysis with various implementations. Most studies on product water footprint are contributed by Hoekstra and his research team (Zhang et al., 2017). Pellegrini et al. (2016) investigated the green, blue, and grey water footprints of different olive growing systems, and considered WFA as a useful tool for orchard system decision making. Deng et al. (2016) studied the water footprint changes of China in 2002 and 2007 with an input-output model and analysed virtual water trade patterns of China. Water footprint approaches require a robust database and concentrate mainly on the volumetric measurement of product/regional water use (Jia et al., 2017), and the analysis regarding green water was claimed incapable of revealing irrigation water use for food production. Applying to broader aspects (e.g. environmental impacts) of water-related assessment, the concept and calculation methods of WF have been further developed. Bluewater availability footprint, which is estimated by reducing total natural runoff by 80 % to account for presumed environmental flow requirements (Hoekstra et al., 2012), started to consider natural water availability. Ridoutt et al. (2009) addressed the combination of water footprint with Life Cycle Assessment (LCA) framework and later developed a method (Ridoutt and Pfister, 2013) for water footprint calculation, emphasising the environmental impacts of water use. Following this direction, the International Organisation for Standardisation (ISO) formed an international standard – ISO 14046 – for WF evaluation (ISO, 2014), and a comprehensive framework was built to evaluate all water-related environmental impacts. This framework aims to perform a comprehensive WFA and includes water availability footprint (WAF) and water footprints addressing water degradation (Ridoutt et al., 2010).

Several other indicators of water quality classification are also developed to address water degradation problems. Parparov et al. (2006) developed a water quality index (WQI) that takes the specific characteristics and uses of a given water resource into consideration and applied this method to water quality assessment of Lake Kinneret and Naroch Lake in Belarus. Huang et al. (2014) developed a water quality classification method based on a multi-classification support vector machine (SVM), and the results showed that this method is more concise when classification features are unclear. The WQI developed by the CCME (Canadian Council of Ministers of the Environment) and NSF (National Sanitation Foundation) (CCME, 2003) has also been well used in water quality quantification studies (Alexakis et al., 2016). Hanslík et al. (2016) investigated the influence of water flowrates on the water quality in natural water bodies and found that nitrates, suspended solids and dissolved oxygen are highly influenced.

The changes in water quality should be considered because it is becoming more important under a situation of water shortage. However, water quality and the environmental impact of water use has been less addressed in WFA framework, even though it is an essential factor for water use (Čuček et al., 2012). The concept of greywater footprint started to consider the environmental impact of water pollutants, while the condition and changes of water quality during water use processes were rarely considered both in theoretical frameworks and in practical assessments. The ISO water footprint approach (ISO, 2014) started to discuss water quality as an impact factor of water availability and noted that water quality should be considered, but the involvement of water quality in WFA in practical implementations has not been well interpreted yet. At present, most classification methods have been developed based on a single water quality metric (e.g. COD, BOD) and then are applied to a specific source of surface water. Most water quality indicators concern more on specific surface water bodies in terms of chemical or biological indicators, and the water quality indicators are rarely considered for a macro water use assessment. There has been still a need to extend the single water quality indices to multiple metrics to provide a complete picture of its usability. It is obvious that water quality degradation has an increasing contribution to the water scarcity, and it is yet sufficiently considered in the water scarcity assessment.

On the one hand, the degrading water quality in the natural water bodies decreases the water availability (supply), and the mismatching between water supply and water demand, limits the water use efficiency. On the other hand, Natural water supplies require pre-treatment before water use, discharge or recycle/reuse processes (Klemeš, 2012), which also means an increase of the economic cost to obtain a high-quality water supply/discharge (Wan Alwi and Manan, 2007). The overtreatment of wastewater, e.g. the various influents entering WWTP are all treated to one single quality level, which limits the opportunity of providing outflows with different water qualities for different user and reduces the cost at the same time.

It is evident that the lack of amount of water is not the only cause for water scarcity issues in various regions. Regions with a sufficient amount of water might have water scarcity issues due to the insufficient quality of the water supply, while regions with a limited amount of water, might have less serious problem thanks to the adequate supply-demand matching and water integration. Water quality degradation and the mismatch between water supplies and water demands in terms of quality, has been a critical cause in various regions. One research gap is identified from the literature review that modified methods need to be developed to address the water quality in water scarcity assessment. Another research gap is that the regional characteristics of decision-making oriented water scarcity (and water availability) have not been sufficiently investigated.

2.2.2 Water Footprint and Life Cycle Costing

Environmental footprints have emerged and been widely applied in environmental impact assessments (Čuček et al., 2012), and water footprint (Hoekstra, 2003) is one of the most commonly used indicators in water use assessment. Table 2-2 presents the characteristics of the water footprint and compares the water footprint with other post-assessment tools (Life Cycle Costing) and optimisation tools (Water Pinch Analysis), which is introduced in the next section.

Table 2-2: Comparison of water resource assessment and design tools

	Water Footprint (WFP) **(Hoekstra, 2015)** and (ISO, 2014)	Life Cycle Costing (LCC) **(Dara et al., 2019)**	Water Pinch Analysis (WPA) **(Wang and Smith, 1994)** and developments **(Wan Alwi and Manan, 2013)**
Assessment type	Post assessment	Post assessment	In-process targeting and design
Assessing object	Product, Process, Organization, Region	Products	Organisation, Region
Target	Water user, public	Public	Water user
Aim	Evaluation of quantitative water use and pollution generation	Determination of life cycle cost	Optimisation
Implementation	Product, process, organisation, region	Products	Process, organisation, region
Determination of water quantity	Water consumption (m^3)	No applications to water resources assessment yet	Water input and output flowrate (t/h)
Determination of water quality	The volume of water needed to dilute the concentration of single contaminant (m^3) (Hoekstra, 2015); Aquatic Eutrophication (PO_4 $P\text{-}_{limeq}$), Aquatic Acidification (kg SO_{2eq}), Aquatic Ecotoxicity (t TEG $water_{eq}$), (ISO, 2014)	Not specified	Contaminants are considered as the constraints of water integration; the impact of water pollution is not quantified.
Outcome Characterisation	The representative volume of water (m^3)	The total cost of the materials covering the whole life cycle of an item (e.g. €)	Freshwater input and/or wastewater discharge flowrate (t/h)
Limitations	“Black box” – count only the input and output, not helpful for water use within the process/organisation	Have not been applied to resources assessment	Challenging to consider multiple contaminants
	Incomparable between different users and regions: Hard to be used for government water monitoring:	No unified assessment framework in water sources assessment has been proposed	Virtual water is not considered in the current determination
	Requires comprehensive database	Requires comprehensive database	

The water footprint concept consists of three types of water footprints to cover the water consumed (green and blue water footprint) and contaminated (grey water footprint). The water consumption footprints, i.e. green and blue water footprint, distinguishes different water sources. For example, green water footprint evaluates the water from precipitation, and blue water footprint determines the consumption of surface and groundwater. The grey water footprint indicates the water pollution by calculating the water volume needed to assimilate the concentration load of a selected pollutant to reach a standard or acceptable value for a water body (Hoekstra et al., 2012). The result of the water footprint assessment is the sum of the water consumption volume and the indicating volume of water to dilute the pollutant concentration to a certain level, with a unit of m^3 or L. For example, the world-average water footprint of producing 250 mL of milk is 255 L, including a green water footprint of 216.8 L, a blue water footprint of 20.4 L, and grey water footprint of 17.8 L (Mekonnen and Hoekstra, 2012).

The water footprint concept was further developed by Ridoutt and Pfister (2010) by adopting a regional water stress index to indicate the regional characteristics of the environmental impact of water use. The International Organisation for Standardisation (ISO, 2014) adapted the water footprint assessment framework following the existing carbon footprint assessment framework (ISO, 2002), which further promotes the application of the concepts. The water footprint defined by the ISO standards uses the mass of pollutant equivalent (e.g. kg SO_{2eq}) to quantify the environmental impact of different categories (ISO, 2014). The water footprints in different environmental impact categories cannot be aggregated together as they have different units, e.g. for aquatic acidification is kg SO_{2eq}, and for aquatic eutrophication, the unit is kg $PO_{4P\text{-}lim}$. In addition, the summation of the water volumetric water footprint results provide limited insights in water quality caused scarcity in both global, regional, as well as industrial levels (Wichelns, 2017).

Jia et al. (2019b) proposed an effective water availability footprint framework and attempted to involve the quantification of water quality degradation in water use assessment. The effective water availability footprint represents the volumetric footprint weighted with a water quality index, which is calculated by locating the pollution concentration to some certain concentration criteria. Multiple pollutants are considered and averagely weighted in the assessment, and the outcome is a volume of water (m^3).

The water footprint framework is designed for post-assessment and benchmarking the environmental impact of water use. The assessment scheme is also comparatively straightforward and works well in increasing public awareness of the water appropriation of different products/activities in daily lives (Klemeš, 2012). Together with the GHG footprint (Carbon footprint) (Wiedmann and Minx, 2008), the water footprint concept has been adopted by organisations (mainly industries) as a performance evaluator to benchmark their environmental performance for publicity in social responsibility (Ridoutt and Pfister, 2010).

Simultaneously, the application of the existing water footprinting approaches has been restricted in guiding water use management and optimisation in practical applications. The precise boundaries among the three sub-indicators of green/blue/grey water footprints have been challenging for the manager to include the water footprint in practical condition. The quantifications using the representative volume of water (grey water footprint) or pollutant equivalents also limits the feasibility of implementation. For example, grey water footprint is calculated as the water volume needed to dilute a certain pollutant in the effluent to reach a certain standard or acceptable level. The outcome of grey water footprint is an indicative value of pollution generation but does not indicate the total effort that needed to treat all the pollutants generated during the water use (Pfister et al., 2017).

The concept of Life Cycle Costing (LCC) was initially developed by the US Department of Defence and applied in the UK and the US several decades ago (Sherif and Kolarik, 1981). The LCC was designed to account the total cost expended in support of the item from its conception and manufacture through its operation to the end of life (Woodward, 1997). The concept was mainly applied in the industrial segments for products/construction assessment (Korpi and Ala-Risku, 2008). Due to the comprehensiveness of the method, it was challenging to be implemented as it requires an enormous amount of data of the whole life cycle of an assessed item, therefore in practical implementation, most of the cases cover just part of the life cycle. Starting from recent years, with the development and wide application of Life Cycle Assessment (LCA), LCC began to be included in environmental studies (Trigaux et al., 2017). Most of the existing LCA+LCC assessments applied are only covering the cost of materials and energy. Water, either quantity and quality, has not been accounted in life cycle costing (Dara et al., 2019). The LCC evaluates but also optimises the total cost of asset ownership and can identify the critical expenditure of the asset (Woodward, 1997). The LCC concept and framework provide an implication to evaluate the water use impact quantitative and qualitative water use.

The existing post-assessment tools, such as the water footprint assessment has a widely accepted framework for water use impact benchmarking. However, the outcome of the assessment emphasises the quantitative water use and still needs more specific attention on the impact of water quality degradation. Another limit of the water footprint assessment that most of the applications only consider the input and output of water use, which overlooks the water use features inside the assessed targets. As a consequence, water footprint assessment results provide limited information to guide water use optimisation and water use impact minimisation. The design and optimisation-oriented method, such as Water Pinch Analysis, provides specific solutions for water use optimisation and water network design but does not assess the quantitative as well as the qualitative impact of water use. A comprehensive approach is needed to fulfil these gaps.

2.3 Water Integration and Water Pinch Analysis

Pinch Analysis (PA) originates from systematic efforts to improve heat recovery in the industry through Process Integration (PI) (Linnhoff and Flower, 1978), Water Pinch (Wang and Smith, 1995) is one of the successful extensions. Comparing the post-assessment tools such as water footprint, Water Pinch Analysis (WPA) is a design and optimisation tool for industrial water use (Wang and Smith,1994). WPA is designed to integrate the water supplies and demands in industrial sites, aiming to target freshwater input and wastewater generation minimisation and water network design (Klemeš et al., 2018). WPA mainly includes two types of approaches, i.e. the insight-based Pinch Analysis and mathematical programming based targeting methods (Wan Alwi and Manan, 2013). The insight-based techniques mainly include graphical targeting techniques, i.e. Material Recovery Pinch Diagram (MRPD) developed by El-Halwagi et al. (2003), and algebraic targeting techniques, i.e. Material Cascade Analysis (MCA). Widespread studies have also been conducted on the topic of mathematical programming targeting (Mughees and Al-Ahmad, 2015). They have been reported in review papers (Foo, 2009) as well as the book (Foo, 2012). Industrial applications have also been reported, e.g. (El-Halwagi, 2017). Several chapters in the Handbook of Process Integration (Klemeš, 2013) further interpreted the approaches for water management and minimisation based on the WPA and introduced the Total Site concept. The application of WPA and superstructure-based optimisation techniques are described, and a new Process-based graphical approach is proposed for the simultaneous targeting and design of water networks.

A typical WPA solution has two steps of setting the water targets and followed by network design to achieve the targets (Manan et al., 2006). In the work of Wang and Smith (1994), the targets of using freshwater, maximise water re-use and water regeneration are discussed, and both single and multiple contaminants are addressed. Composite Curves are used to represent the water using process. The approach is able to identify the bottleneck of water minimisation in industrial processes, and the conceptual framework can help to specify the optimal type of regenerator and regenerator specification. Their work serves as one of the earliest contributions of graphical methods for water minimisation studies using WPA. In recent studies, the technique has been further discussed and developed. Tan et al. (2007) developed a new systematic method for the retrofit of water network with regeneration based on WPA. The procedure consists of two parts: retrofit targeting and design for a water network with regeneration unit(s). In the targeting stage, retrofit targets (utility savings and capital investment) were determined for a range of process parameters (total flowrate or outlet concentration of the regeneration unit) to obtain savings versus investment curve. Next, the existing water network was re-designed to meet the chosen targets.

Tan et al. (2009) started to combine water footprint and water pinch analysis. In their study, a Graphical Pinch approach for the analysis of water footprint constraints on biofuel production systems is presented. The methodology is based on the Composite Curve method, which was originally developed for carbon-constrained energy planning. The Pinch Analysis approach enables limiting water footprint conditions to be identified and provides insights that are useful for planning the large-scale cultivation of biofuel crops. An illustrative case study based on the bioethanol program of the Philippines is solved using the proposed approach. Jia et al. (2015) extended the Water Footprint Pinch analysis technique, which is based on the decomposition of total water footprint into external and internal footprint components. Results show that water is mainly consumed in the utility processes, and it achieves a goal for water-saving of 16 %.

Pinch Analysis has been implemented for multiple-contaminant water systems, and the approach for the determination of interim concentrations for concentration decomposition is explored. Mohammadnejad et al. (2012) applied WPA to analyse the water network of Tehran oil refinery and considered three key contaminants, including suspended solids, hardness as well as COD. Results show that water minimisation through single contaminant approach was more considerable, while the method based on the double contaminant gives more precise results rather than a single contaminant. Mughees and Al-Ahmad (2015) implemented the WPA of water minimisation at a refinery and set COD and hardness contaminants with single and double contaminants approach. The new technique was demonstrated to compare to previous studies favourably. The method resulted in a high percentage reduction of 43.8 % and 61.2 % of freshwater in three processes regarding COD and hardness. Skouteris et al. (2018) applied PA for the water management and optimisation in a brick-manufacturing industry and concluded that combined use of water footprint with Pinch Analysis could provide water-intensive manufacturing industries with a sound and a robust water management tool that can significantly improve their water consumption and consequently their long-term sustainability.

Graphical methods are practical to solve single-contaminant problems, but are complicated and sometimes impossible to apply to multiple-contaminant problems. Mathematical methods are more exact but sometimes complicated, especially in the case of multiple contaminants (Ataei and Yoo, 2010). Modelling such issues can be performed using an algebraic language and environment – such as those provided by GAMS (GAMS, 2018). The development and implementation of WPA have shown a great contribution to water minimisation analysis and significant potential in consideration of water quality, especially multiple contaminants, which still needs further effort. In existing Water Pinch Analysis, contaminants are considered as the constraint of water use and integration, but the impact of water pollution is not quantified. WPA targets at water use optimisation and design at the plant or site level and is not suitable for water use impact assessment of the product. Besides, the outcome of the analysis is specified for the assessed plant and provides limited information to guide decision-makers in regional water resource assessment.

2.4 Water-Energy Nexus

Water and energy are the essential resources to sustain life and fundamental to national, regional and global economies. These resources are interlinked in multiple ways, and the term "nexus" captures the interconnections. To benefit from the nexus approach in terms of resource use efficiency, it is essential to understand, operationalize and practice the nexus of all three resources. The correct understanding and interpretation of the "nexus" concept are crucial for the development of the quantification methods. The next step is to identify the issues that need solving. Looking at production or urban system holistically, minimising the intake of resources and emission release can be simultaneously affected by improving the system efficiency. The understanding and interpretation of the "nexus" concept are very important for proceeding the development of the quantify cation methods. The first step is to identify the issues that need to be solved. Looking at production or urban system holistically, minimising the intake of resources and emission release can be simultaneously affected by improving the system efficiency. As demand for these resources increases worldwide, using them sustainability is a critical concern for scientists and citizens, governments and policymakers. There have been many works is shedding light upon the links among water and energy use, as well as their connection with food production and consumption. This section analyses a selection of those works, grouping the analyses into several main nexus classifications: One important goal is to connect water-energy nexus with the circular economy, whose ultimate goals are to minimise the input and maximise the outcome of the system, at the same time to control the environmental impact to the ecosystem. Hamiche et al. (2016) classified the nature of the nexus from five dimensions, i.e. environmental, technological, economic, political and social dimension. His classification quantifies the impact of these five dimensions on the WFN. For example, on the Environmental aspect, climate change and natural drought would limit the utilisation of natural water and increase energy consumption for climate change mitigation; on the technological dimension, improving technology would increase energy/water intensity, etc. More commonly, the WFN is interpreted and assessed as two elements, water for energy and energy for water.

Enormous studies and reports have been investigating the impact of water supplies on energy production. Regular energy production e.g. fossil fuel electricity usually has high water consumption. Studies found that water is also a critical resource for the production of renewable energy. For example, the power generation of Kenya from hydro sources decreased as a result of poor hydrology and the dependence on expensive fossil fuel generation which saw electricity prices increase (African Trade Insurance Agency, 2017), and there was a continued decrease in hydropower generation (8.93 % decrease) as a result of poor hydrology. Nuclear capacity reduced from 7 % to 15 % for three weeks due to lack of cooling water in India (World Nuclear Association, 2017). Shale gas also has a high water consumption (Tidwell and Moreland, 2016) as the fracking fluid contains 80 % water and 19 % propane, which also makes possible water pollution issues. During the lifetime of a well, the shale gas production consumes 25,000 – 500,000 m^3 water (Tidwell and Moreland, 2016).

On the other hand, the withdraw, transportation, manufacturing (bottle water, desalination), treatment of water also consumes lots of energy, especially the electricity for pumping. Figure 2-1 shows the specific energy consumption of the water supply and treatment processes. Due to the increasing intensive nexus between the two resources, water resources management has a significant impact on the related energy consumption as well as GHG emissions. Water scarcity can lead to higher energy consumption due to the increase in wastewater treatment, water transportation, and water-saving measures, etc. Many studies have been carried out to investigate the water-energy nexus in terms of quantity, but the impact of water quality has not been well investigated. A scenario analysis should be carried out to examine the impact of patching the supply and demand of both quantity and quality, and comparison should be made to identify the contribution of water quality changes.

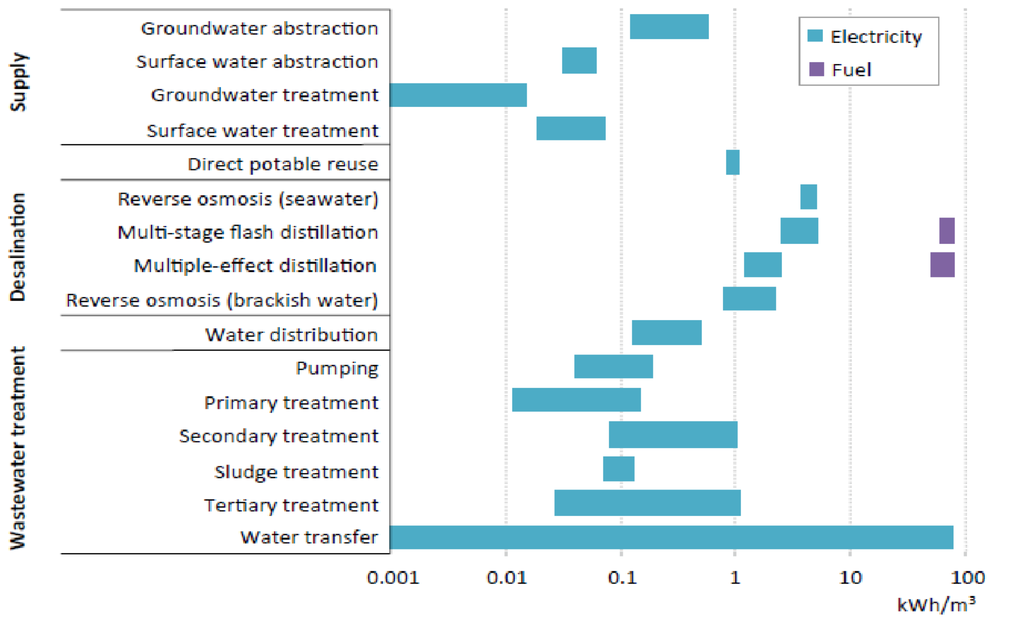

Figure 2-1: Energy consumption of the water supply and treatment processes (Smith and Liu, 2017)

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 following chapters provide an attempt to answer these questions by proposing extended Water Footprint Assessment (**Chapter 3**) and Water Pinch Analysis methodologies (**Chapter 4**) and presenting an initial assessment of the water-energy nexus in the seawater desalination industries (**Chapter 5**).

CHAPTER 3 EXTENDED WATER FOOTPRINT METHODOLOGY IN WATER QUANTITY AND QUALITY ASSESSMENT

This chapter presents a Water Availability Footprint framework addressing water quality Section 3.1) and a Cost-based Qualitative and Quantitative Water Footprint (QQWFP) method in Section 3.2. 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., 2019b). The QQWFP is based on the work submitted to the journal of Resources, Conservation & Recycling, which is still under review. Other related published works also supported this chapter, including the Water Pollution Impact Assessment of Beijing from 2011 to 2015: Implication for Degradation Reduction (Jia et al., 2017) and Blue Water Footprint of the Czech Republic (Jia et al., 2019a), which are both published in the journal of Chemical Engineering Transactions.

3.1 Water Availability Footprint Framework

As has been discussed in the Literature Review, 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 addition, water availability should also consider the purpose of water use, since the same body of water has different usability for various purposes, e.g., drinking or producing a piece of cloth. It becomes inappropriate to claim that for two different processes, consuming the same amount of water means the same WAF. Based on the WAF defined by ISO (2014), the present paper extends the definition of WAF integrating water quality and quantity and proposes a brief framework to illustrate its application.

Identifying the amount of water that is available from a given source is the first step for water use assessment, and it is necessary to quantify the quality of this water source. A clear definition and application framework are remarkably needed. Aiming to assess the quality-quantity consumption of water use, a WAF should focus on the following aspects:

1) Integrating water quality and water quantity. Water use process may change the

quantity or quality, or both quality and quantity simultaneously. The integrated consideration implies that for the same amount of available water volume, the water stream with higher quality provides larger availability.

2) Reflecting the purpose of water use. Water use sectors, such as industry, household (washing and drinking), and agriculture, usually have a different emphasis on water quality features. For most industrial water use, the requirement is more related to general physical and chemical properties, such as the concentration of SS, minerals, COD, BOD, etc. Residential water use usually has a higher water quality requirement than other purposes of water use, and irrigation water use usually requires water with lower quality category, but more stringent in (heavy metal) toxicity and alkalinity. In other words, a specific water source might have different availability/usability for different purposes of water use. When a water source with lower quality is used for a user with higher quality requirements, it may need other resources (e.g. energy) to improve the water quality and the usability.

3) Considering the availability of water discharge. Wastewater discharged from a water use process, or treatment plant may be used directly for processes with a lower quality requirement or discharged into river water after proper treatment. In both situations, the water becomes "newly" available and can be used for other users. Therefore, the availability of this part of water resources should be accounted for.

Combining the above-mentioned critical points, 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 3-1.

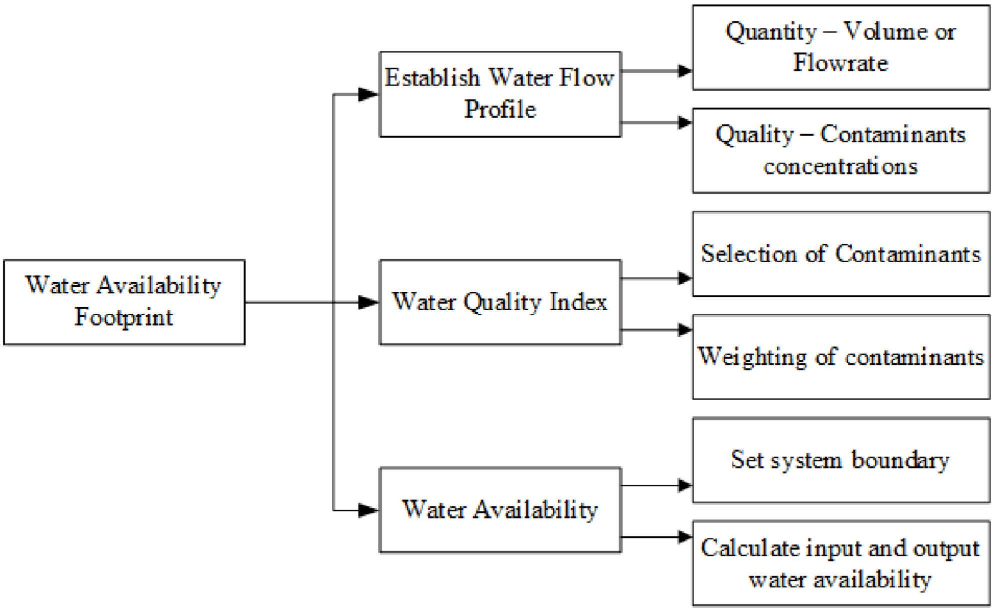

Figure 3-1: Water Availability Footprint Assessment Framework

The first step is to define the system boundary and develop the water flow profile, and list all the quantity and quality of the flows that get in/out of the system. The quantity data are easy to obtain, but the water quality data is usually challenging to collect. In this step, the water quality data is collected in the form of contaminants concentrations. In order to consider the impact of different contaminants, Step 2 develops a water quality index (WQI) as a weighting factor to the water quantity consumption to determine the impact of water quality changes. Based on the water flow profile and water quality index, the EWA can be assessed in Step 3.

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.

3.1.1 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(3-1). 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:

$$\mathrm{WQI}_i = \frac{X_{\max,i} - X_i}{X_{\max,i} - X_{\min,i}} \tag{3-1}$$

where for pollutant i, WQI_i is the water quality index of specific water flow, X_i is the concentration of pollutant i, $X_{\max,i}$ is the upper bound of acceptable the concentration of this pollutant, and $X_{\min,i}$ 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.

Considering the complexity of the water quality assessment, the following assumptions are made to simplify the calculation firstly:

- The number of contaminants (i) can be changed according to the availability and quality of data;
- X_i can be smaller than $X_{\min,i}$, which is the lower bound of the accepted concentration of contaminant i. When the value of $X_{\min,i}$ is selected from local standard, it is possible that the values in the standard are lower than some water bodies because the standard value is set at an average level;
- When X_i is larger than $X_{\max,i}$, then $\mathrm{WQI}_i = 0$.

When i kinds of contaminants are considered, there would be multiple values of WQI for one water flow. Reaching a single value of WQI is necessary to quantify the EWA.

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(3-2), 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:

$$\mathrm{WQI}_{\mathrm{min}} = \min(\mathrm{WQI}_1, \mathrm{WQI}_2, \dots, \mathrm{WQI}_i) \tag{3-2}$$

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(3-3). 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.:

$$\mathrm{WQI}_{\mathrm{avg}} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{WQI}_i \tag{3-3}$$

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.

3.1.2 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(3-4):

$$\mathrm{EWA} = A_{\mathrm{W}} \times \mathrm{WQI} \tag{3-4}$$

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(3-5):

$$\mathrm{WAF} = \mathrm{EWA}_i - \mathrm{EWA}_{\mathrm{o}} \tag{3-5}$$

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 EWA_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. In the provided case study, this is illustrated with a Radar chart.

3.1.3 Case Study

In order to illustrate the application of the proposed framework, a numerical case study is carried out in this section. Let us assume an industrial water use process attached to a primary water treatment unit located in China. The system boundary is shown in Figure 3-2. 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.

In this case study, it is essential to define the upper and lower bounds of the pollutants to calculate the WQI_i. The inflow (F_1 = 2,000 m^3) should meet the requirement of the water use process, and the discharge flow (F_2 = 1,000 m^3) entering the natural water bodies should meet the water discharge standards. The maximum and minimum acceptable concentration of pollutants is set according to the water discharge standard.

The water use requirements are referred from the Environmental Quality Standards for Surface Water (GB3838-2002) (SEPA of China, 2002a). In this standard, the surface water is divided into five categories regarding the purpose of water use, and a range of concentrations of selected contaminants is given for each category. Category I is the water with the best quality and is supposed to be used for water sources for national natural reservation areas. Category II and III can be used as sources of domestic water use, and the aquatic environment for fishes, etc. The water of Category IV is for industrial water use and entertainment water use (indirectly exposed to human bodies). As the case study is for industrial water use process, Category IV is considered as the maximum allowed concentrations of the contaminants ($X_{\max,i}$).

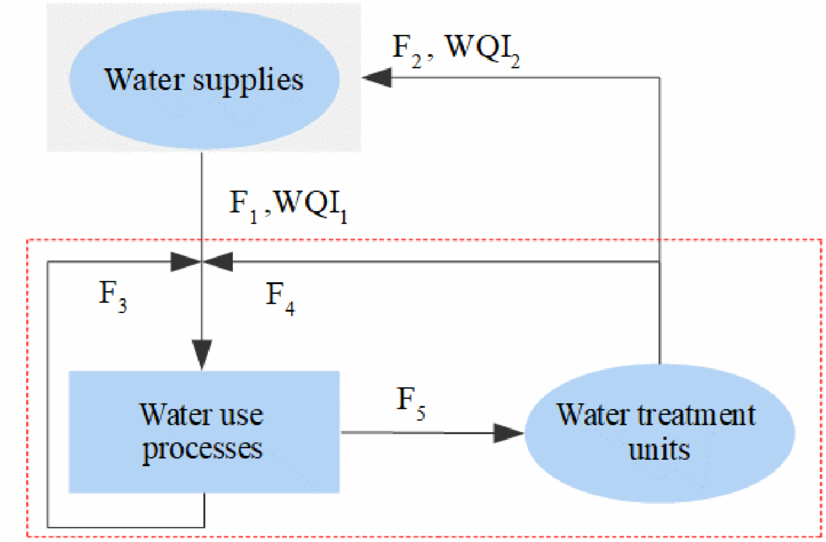

Figure 3-2: Case study: WAF framework and system boundaries

The water discharge requirements are taken from the Discharge Standard of Pollutants for Municipal Wastewater Treatment Plant (GB 18918-2002) (SEPA of China, 2002b). It is required that the discharge water from the water treatment plant should meet the Category B, and the criteria of this category are set as the minimum allowed concentrations ($X_{\min,i}$).

In order to make the inflow and outflow comparable, they are scaled with the same ranges, which means $X_{\min,i}$ and $X_{\max,i}$ are the same for the two flows. Aiming to identify the impact of different water quality on the WAF, we set 3 different water quality profiles for F_2, which are $F_{2\text{-}1}$, $F_{2\text{-}2}$ and $F_{2\text{-}3}$. $X_{\max,i}$ and $X_{\min,i}$ as well as the contaminant concentration of flows are shown in Table 3-1.

Table 3-1: Water quality criteria of boundaries and flows in the system

X_i [mg/m^3]	$X_{max,i}$	$X_{min,i}$	F_1	$F_{2\text{-}1}$	$F_{2\text{-}2}$	$F_{2\text{-}3}$
Chemical Oxygen Demand (COD)	100	20	25	38	80	60
5-day Biochemical Oxygen Demand (BOD_5)	30	4.0	5.0	8.0	26	17
Ammonia Nitrogen (NH_3-N)	20	1.0	1.2	1.8	15	10
Total Phosphorous (TP)	3.0	0.2	0.22	0.35	2.6	1.6
Zinc (Zn)	20	1.0	1.2	1.6	14	10
Fluoride ion (F^-)	1.5	1.0	1.0	1.4	1.3	1.2
Arsenic (As)	0.1	0.05	0.06	0.09	0.08	0.07
Mercury (Hg)	0.001	0.0001	0.0002	0.001	0.0007	0.0005
Chromium (Cd)	0.1	0.005	0.005	0.007	0.07	0.052
Lead (Pb)	0.1	0.05	0.042	0.06	0.08	0.07

Note: $X_{max,i}$ and $X_{min,i}$ are selected from (SEPA of China, 2002a and 2002b)

With Eq(3-1) and the water quality data provided in Table 3-1, the WQI is calculated Figure 3-3.

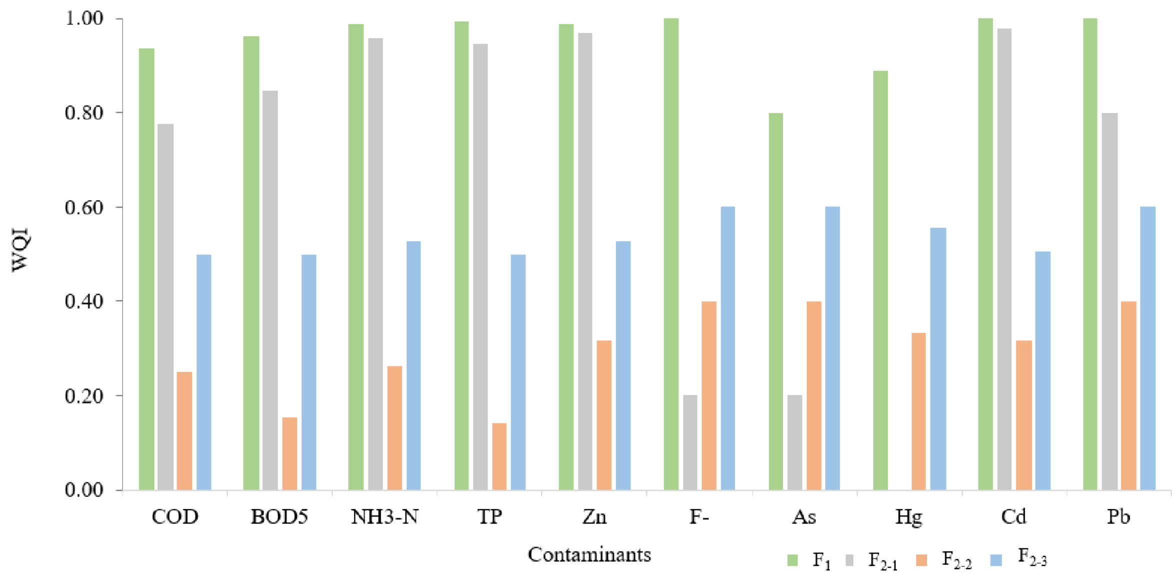

Figure 3-3: WQI of 10 selected contaminants

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_{2-1}, F_{2-2}, and F_{2-3}) 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 3-2.

Table 3-2: 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.

F_1, as the water supply, has the best water profile, with higher WQI_{min} and WQI_{avg}, and therefore has the largest EWA. The WAFs calculated in all situations are higher than the volumetric WF (1,000 m^3), which indicates that considering water quality in WF assessment can yield a more stringent result. The water usability decrease during the water use process is determined more effectively. Only considering the amount of water consumption one can neglect the impact of water quality changes.

For the results of WAF_{min}, it 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. The radar chart was used to find out the critical contaminant of the flow, as is shown in Figure 3-4.

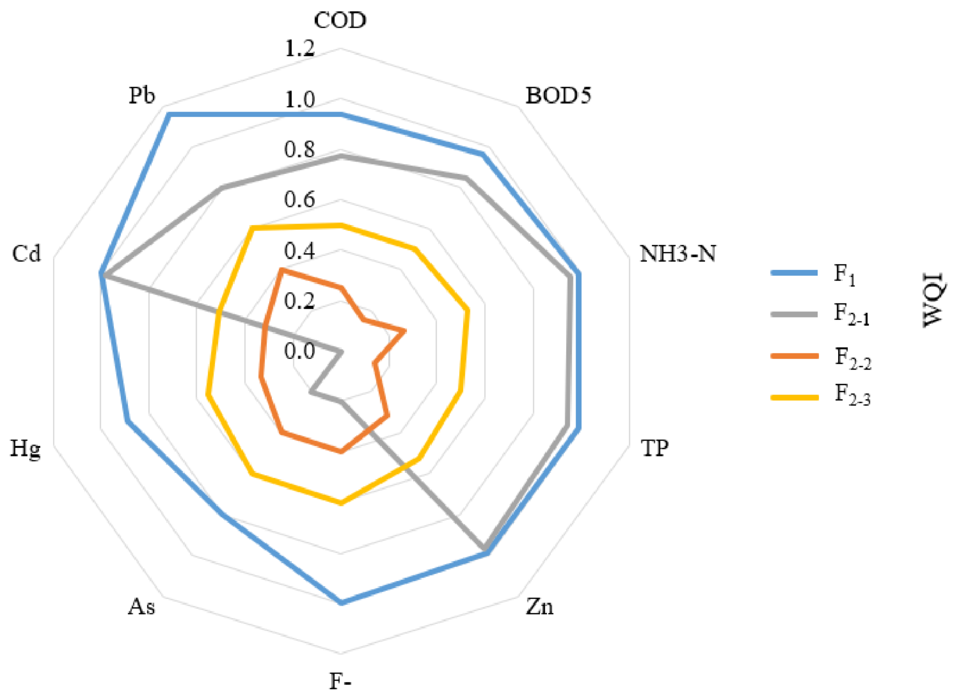

Figure 3-4: Radar chart of WQI of the flows from case studies

The radar chart is able to illustrate the distribution of WQIs of all contaminants, and it also shows the bottleneck of the flow. For example, in Figure 3-4, the pollutants in F_1 are more uniformly distributed, and water quality is more moderate than other flows. While for F_{2-1}, it is obvious that the Mercury (Hg) is the most constraining pollutant (WQI = 0), followed by As and F^- (WQI = 0.20). This can provide useful information for the water users or managers to detect the bottleneck and improve the water flow accordingly to improve water use efficiency.

3.1.4 Discussions

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.

3.1.5 Conclusions

The attempt to optimise industrial processes and other resource-consuming activities has attracted a lot of research efforts. As reviewed recently by (Fan et al., 2018), many new developments have been presented, focusing on energy and materials efficiency improvements. Following this trend, the current paper proposed an extended approach to WAF to quantify water availability. Based on the analysis of WF assessment methods, water quality is integrated into the assessment. EWA has been defined as the quantitative and qualitative extent of a certain body of water which meets the needs of a certain purpose of water use, and a WAF is proposed to determine the human water exploitation of water availability of water quality and quantity. A WQI is proposed to quantify the contribution of water quality on EWA.

The extension to water footprinting approaches has been developed and implemented with a case study. Three outflows are set to discuss the impact of different water quality pattern on the result of WAF. The results showed that for the WAF calculated based on minimum WQI, systems with more average outflows have the lower WAF. The distribution of pollution levels also affects water availability besides the actual pollutant concentration. For the WAF calculated based on average WQI, it indicated that the overall WQI is the only factor for WAF. The case study shows that the WAF calculated based on the concepts of minimum WQI, average WQI, and the blue WF is 1,600 m^3, 1,277 m^3, and 1,000 m^3 (in the case of F2-1). The volumetric footprint is much less than the water footprints considering water quality, which might lead to misleading suggestions.

The WAF considers water quality can reveal many issues neglected by the only-volumetric calculation of blue water footprint. The radar chart of the WAF of multiple contaminants is effective to demonstrate the distribution of the pollutants, which can provide more specific information for water users or managers for minimising water use or improving water quality control.

This study is carried out as the conceptual development of the conventional water footprint methodology. It raised the issue of the contribution of water quality degradation to water scarcity/availability and attempted to integrate the water quality together with the quantity assessment. As the first step, it provides one potential direction of this integration, which is the water quality categorisation. This works as a theoretical basis of the following development of the Qualitative and Quantitative Water Footprint (QQWFP) as well as the Water Scarcity Pinch Analysis (WSPA).

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

3.2.1 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.

This study aims to develop a cost-based assessment tool to evaluate the impact of water use in terms of quantity and quality, which facilitate communication between water users and practical water use management.

3.2.2 Methodology

As discussed previously, water use impacts include quantity consumption and quality degradation, as shown in Figure 3-5. Assessment tools are needed to provide the answer to the question of "How much does it cost to restore the water to its original quantity and quality?" The cost should be determined by adding the cost of water consumption to the cost of removing the contaminants from the polluted water.

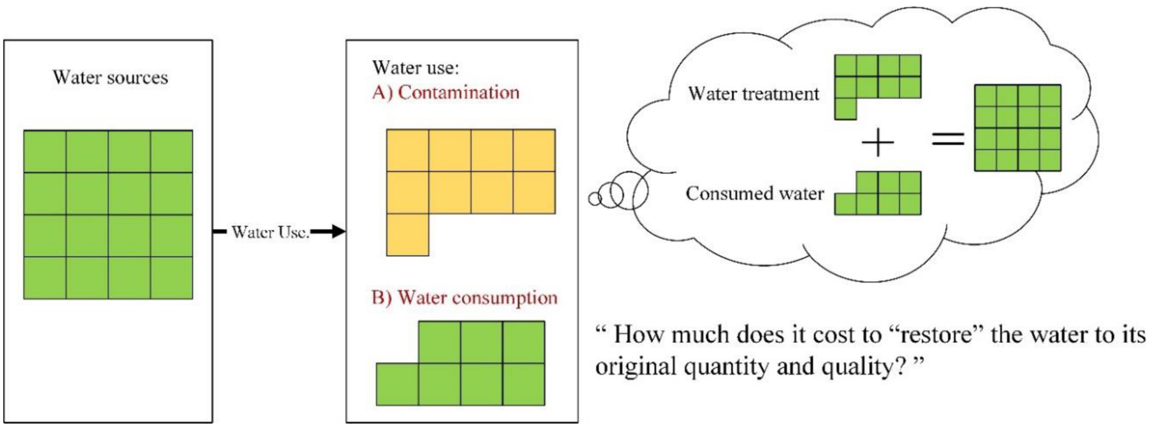

Figure 3-5: Illustration of the research question

Consequently, a Quantitative-Qualitative Water Footprint (QQWFP) is defined in this study as the total cost of net water consumption (Quantitative Water Footprint) and net contamination removal/treatment (Qualitative Water Footprint) and is represented in a cost-oriented criterion with a unit of €/t product. Figure 3-6 presents the framework of the QQWFP.

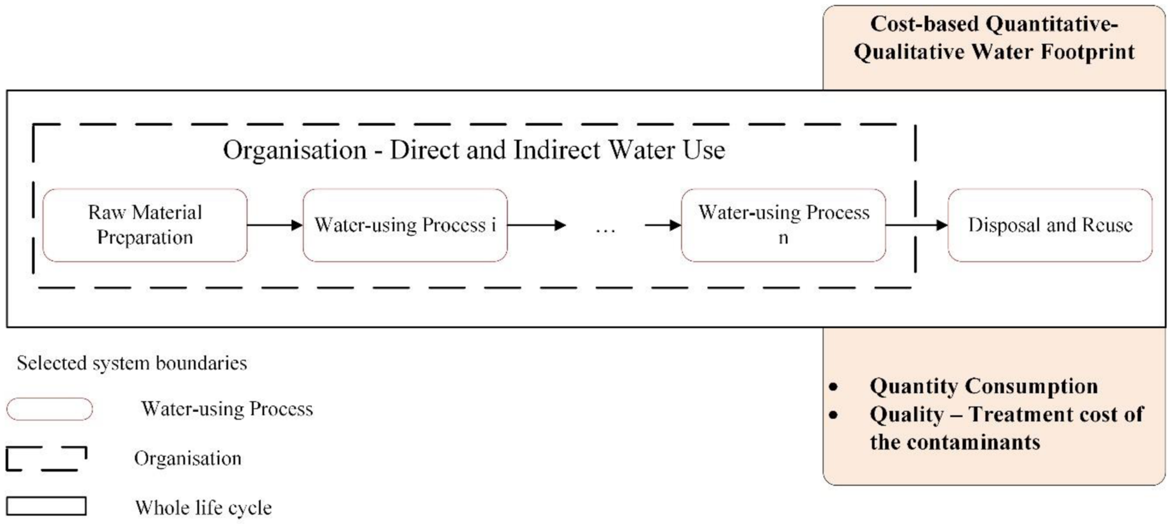

Figure 3-6: Assessment framework of the QQWFP

A cost-based indicator enables the comprehensive assessment covering different water-using units, sectors, plants, and even regions, thanks to its generality. An additional benefit is that a cost-based indicator is an appropriate interface for communicating with water users and managers, and can highly facilitate the systematic management of water and other environmental/economic performances. The QQWFP can be used for the water use assessment of a product, water-using process, as well as an organisation. The system boundary of the QQWFP can be defined based on research objectives and data availability, as shown in Figure 3-6. 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.

3.2.2.1 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 3-7 is an illustration of water use in an industrial plant with n water-using units.

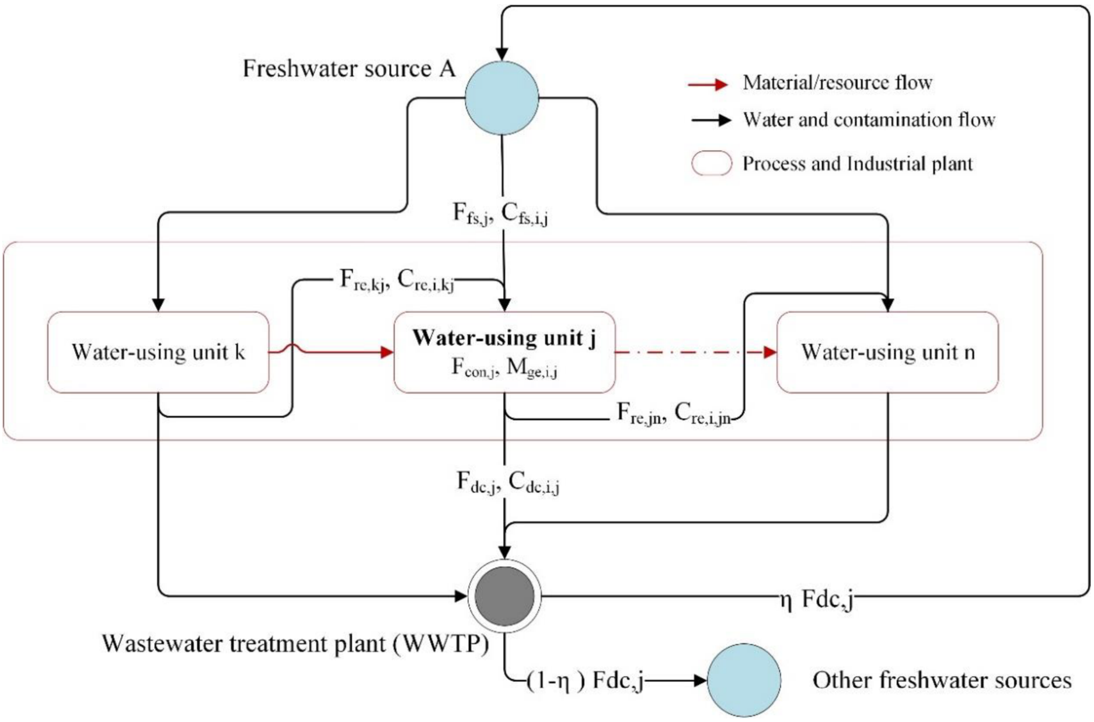

Figure 3-7: Illustration of the industrial water use

Symbols	Explanation
$F_{fs,j}$	The volume of input freshwater to water-using unit *j*, m^3/t product
$C_{fs,i,j}$	The concentration of pollutant *i* in the input freshwater to water-using unit *j*, mg/L
$F_{con,j}$	The water consumption of water-using unit *j*, m^3/t product
$M_{ge,i,j}$	The mass of contamination (*i*) generated in water-using unit *j*, kg/t product.
$F_{re,jn}$	The volume of water reused from water-using unit *j* to *n*, m^3/t product
$C_{re,i,jn}$	The concentration (pollutant *i*) of the reuse flow from water-using unit *j* to *n*, mg/L
$F_{re,kj}$	The volume of reused water input to water-using unit *j*, m^3/t product
$C_{re,i,kj}$	The concentration (pollutant *i*) of the reuse flow to water-using unit *j*, mg/L
$F_{dc,j}$	The volume of water discharged from water-using unit *j*, m^3/t product
$C_{dc,i,j}$	The concentration (pollutant *i*) of the discharge flow from water-using unit *j*, mg/L

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 mass balance of the water flows around the unit j is:

$$F_{fs,j} + F_{re,k,j} = F_{con,j} + F_{re,j,n} + F_{dc,j} \tag{3-6}$$

where, $F_{fs,j}$ and $F_{con,j}$ represent the volume of freshwater input and the internal water consumption (or water loss) of process j, m^3/t product. If the process has a water gain instead of water consumption, it is represented as negative water consumption. $F_{re,kj}$ represents the reused water from process k to process j, m^3. $F_{re,jn}$ and $F_{dc,j}$ represent the volume of water reused to water-using unit n and discharged from process j, m^3/t product.

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:

$$WF_{qt,j} = \mathrm{EC}_{fs} \times \left(F_{fs,j} - \eta F_{dc,j}\right) + \mathrm{EC}_{re} \times (F_{re,kj} - F_{re,jn}) + EC_{dc} \times F_{dc,j} \tag{3-7}$$

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.

3.2.2.2 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 3-8 is an illustration of the mass load of contaminants 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).

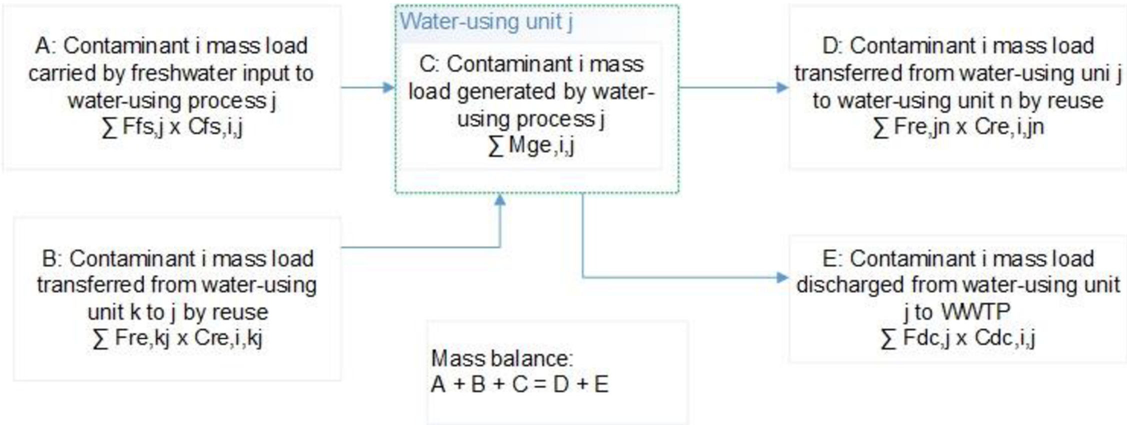

Figure 3-8: Illustration of the contaminants mass balance in water-using unit j

The mass load balance of the contaminations in process j is:

$$\sum_i (F_{fs,j} \times C_{fs,i,j}) + \sum_i (F_{re,kj} \times C_{re,i,kj}) + \sum_i M_{ge,i,j} = \sum_i (F_{re,jn} \times C_{re,i,jn}) + \sum_i (F_{dc,j} \times C_{dc,i,j}) \tag{3-8}$$

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(3-8) it is easy to obtain:

$$\sum_i (F_{dc,j} \times C_{dc,i,j}) - \sum_i \left(F_{fs,j} \times C_{fs,i,j}\right) = \sum_i M_{ge,i,j} + \left[\sum_i (F_{re,kj} \times C_{re,i,kj}) - \sum_i (F_{re,jn} \times C_{re,i,jn})\right] \tag{3-9}$$

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*.

Considering only the cost of treating the contaminants in the discharged water to a specified water quality standard is not accurate, because it is on the assumption to treat the mass contaminant load to 0 from the discharged water, which is not realistic. Besides, it neglects the impact of water reuse on water contamination and the fact that the quality (contamination level) of freshwater from different supplies can vary.

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 3-8) can be calculated by the mass of contaminants multiplying the cost of treating per kg of contaminants:

$$WF_{ql,j} = \sum_i (F_{dc,j} \times C_{dc,i,j} - F_{fs,j} \times C_{fs,i,j}) \times TC_i \tag{3-10}$$

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.

3.2.2.3 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:

$$QQWFP_j = WF_{qt,j} + WF_{ql,j} \tag{3-11}$$

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:

$$QQWFP = \sum_j WF_{q-q,j} \quad (3\text{-}12)$$

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

Figure 3-9 presents the procedure of the QQWFP assessment.

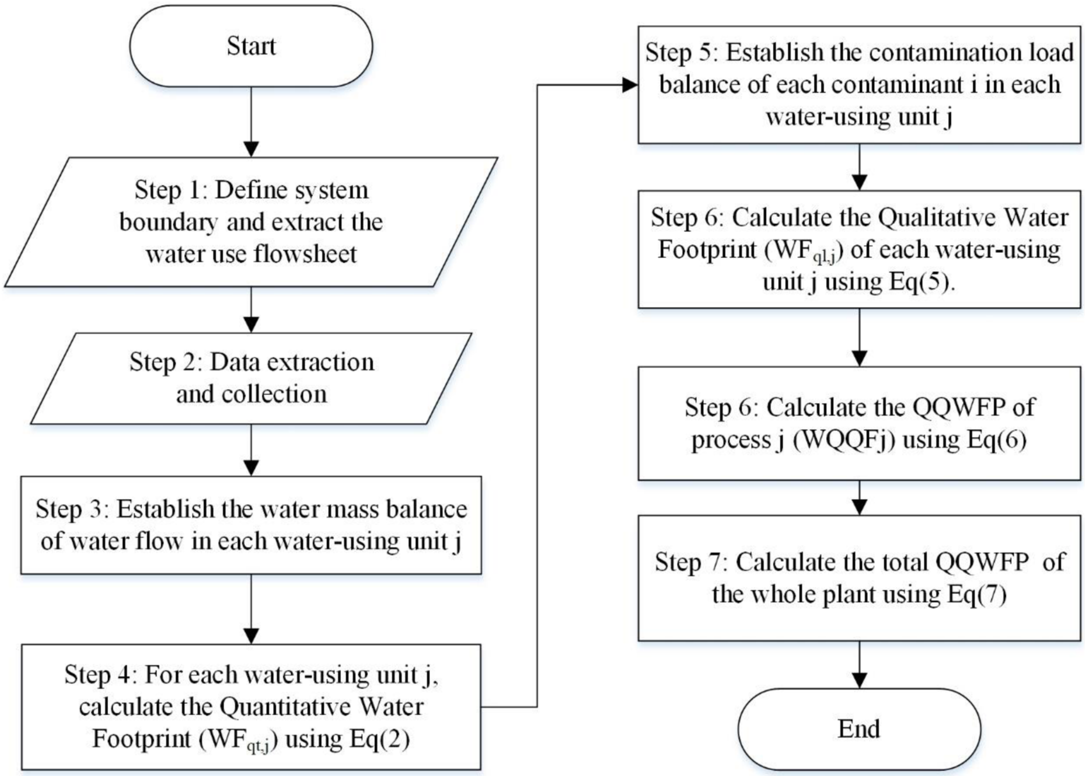

Figure 3-9: Quantitative-Qualitative Water Footprint assessment flowchart

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.

3.2.3 Case Studies – QQWFP of MSG

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 water use data is collected from a monosodium glutamate plant in China. Monosodium Glutamate (MSG) is a commonly used seasoning in food industries and daily lives. The production of MSG consumes lots of raw materials and auxiliary materials and generates wastewater contains high concentrations of COD (30 - 70 g/L), ammonia nitrogen (NH_3-N) (5 - 7 g/L), suspended solids (SS) (12 - 20 g/L), and the very low pH (Jiang et al., 2019).

3.2.3.1 System boundary and data extraction (Step 1)

Figure 3-10 presents the system boundary and water flows in the MSG plant. In the starch production process, maize is used as the main raw materials to produce starch milk after being washed, soaked and separated. The maize starch milk is then transported to the glutamic acid production process, which includes glucose preparation, glutamic acid (GA) fermentation, MSG extraction as well as MSG refining.

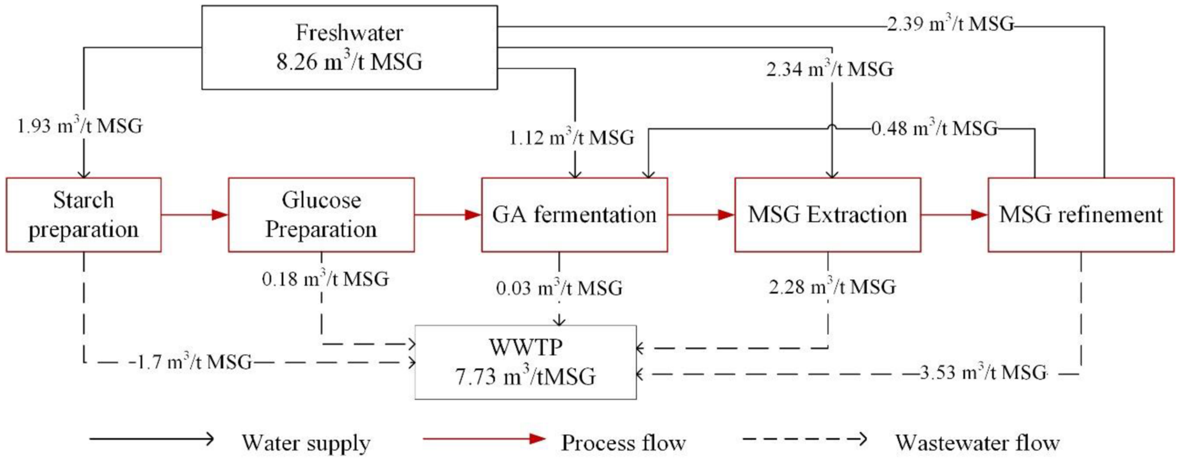

Figure 3-10: The water use flowsheet of the MSG production

In the MSG production processes, the glutamic acid reacts with sodium salt and is converted to monosodium glutamate ($C_5H_8NO_4Na$). Activated carbon is used for decolourisation and purification of sodium glutamate in the MSG refining process, and it is then concentrated, crystallised and dried to produce refined MSG. MSG production consumes a large amount generates high pollution wastewater, especially the mother liquor generated in the MSG extraction with a high concentration of COD, SS, and NH_3-N.

3.2.3.2 Data extraction and collection (Step 2)

The water use quantity and quality data are extracted and presented in Table 3-3.

The assessment only covers the MSG production process, namely from "gate to gate" due to the limit of data availability. In the current stage, the cost of virtual water is not yet considered in this determination and should be covered in future studies. In terms of water quality, Chemical oxygen demand (COD), Biochemical oxygen demand (BOD), Ammonia

(NH_3-N) and suspended solids (SS) are selected in the assessment in this study based on the features of the MSG wastewater. BOD is the amount of oxygen required by micro-organisms to degrade the organic matter and can be calculated as BOD of diluted and undiluted samples. The BOD values depend on the dissolved organic matter in the wastewater samples. The test of COD with the use of strong chemical agent (such as potassium dichromate), is done to degrade both the organic as well as inorganic matter present in the wastewater samples. COD includes both biodegradable and non-biodegradable substances, and BOD contains only bio-degradable organic matters.

Table 3-3: Input and output data of water quality and quantity in the MSG production plant

Input	**Volume (m^3/t MSG)**	**Contaminants (mg/L)**				Remarks
		COD	**BOD**	**NH_3-N**	**SS**	**Source**
Starch Preparation (Maize)	1.93					Municipal water
Glucose Preparation	0.00					
GA Fermentation	1.12	30	6	1.5	100	Municipal water
	0.48					Recycle from MSG refining
MSG Extraction	2.34					Municipal water
MSG Refining	2.39					Municipal water
Output		**COD**	**BOD**	**NH_3-N**	**SS**	**Use**
Starch Preparation (Maize)	1.70	3,940	2,660	50.2	1,020	Low density wastewater
Glucose Preparation	0.18	1,500	900	1.5	300	Washing
GA Fermentation	0.03	1,500	900	1.5	300	Washing
MSG Extraction	2.26	50,000	12,000	6,000	16,000	Mother liquor
	0.02	1,200	500	25	300	Washing
MSG Refining	2.21	500	2,000	1,500	200	Washing
	1.80	30	6	1.5	100	Cooling water

Table 3-4 lists the cost of water consumption and contaminants treatment.

Table 3-4: Cost of water withdraw, discharge, and contaminants treatment

Item	**Cost**	**Reference**
Water supply	€/m^3	
Freshwater	0.6	Jinan Water Group (2020)
Reused water	0.2	
Wastewater discharge	0.2	
Contaminant treatment	€/kg	
CODcr	0.6	Dong et al. (2018)
BOD_5	1.4	
NH_3N	7.7	
SS	1.3	

The cost of contaminants treatment is retrieved from the study of Long et al. (2018), in which the cost of contaminant treatment in two wastewater treatment plants are analysed. When calculating the WFqt, the proportional coefficient of treated water returned to the environment (η) is set as 75 %, which means 75 % of the treated water is returned to the original water source as water withdrawn for MSG production. The rest of the water is allocated to other sources. Note that when applied to other cases, the unit cost of water consumption and contaminants treatment, as well as the return rate of treated water should be selected based on the local practical condition. The water supply and discharge cost, which is originally in Chinese Yuan (CNY) is converted with a rate of 0.12 to Euro (€).

3.2.3.3 QQWFP results of MSG production (Result from Step 3-7)

Following the proposed method, the cost-based Quantitative-Qualitative Water Footprint assessment (QQWFP) of the MSG production is determined. Figure 3-11a illustrates the breakdown of quantity and quality footprints and the detailed breakdown of different contaminants in the Qualitative Water Footprint. The total QQWDP of producing 1 t MSG in the studied plant is 302.1 €. 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.

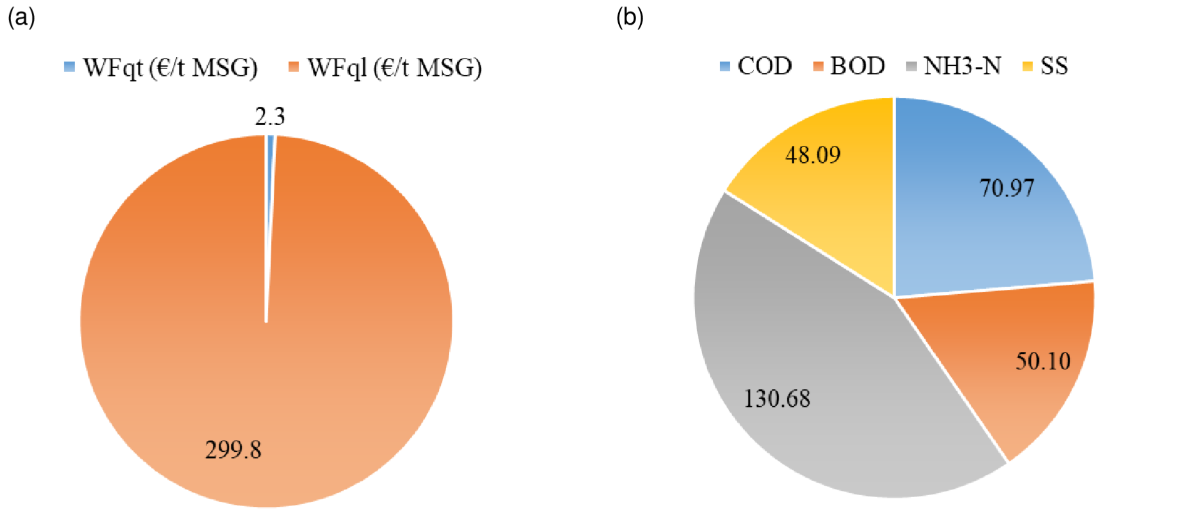

Figure 3-11: a) Breakdown of the QQWFP, and b) Detailed breakdown of the Qualitative Water Footprint (WFql) [€/t MSG]

Figure 3-11b 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 3-12a 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 3-12 b-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. This process is the only process that "cleans" the water.

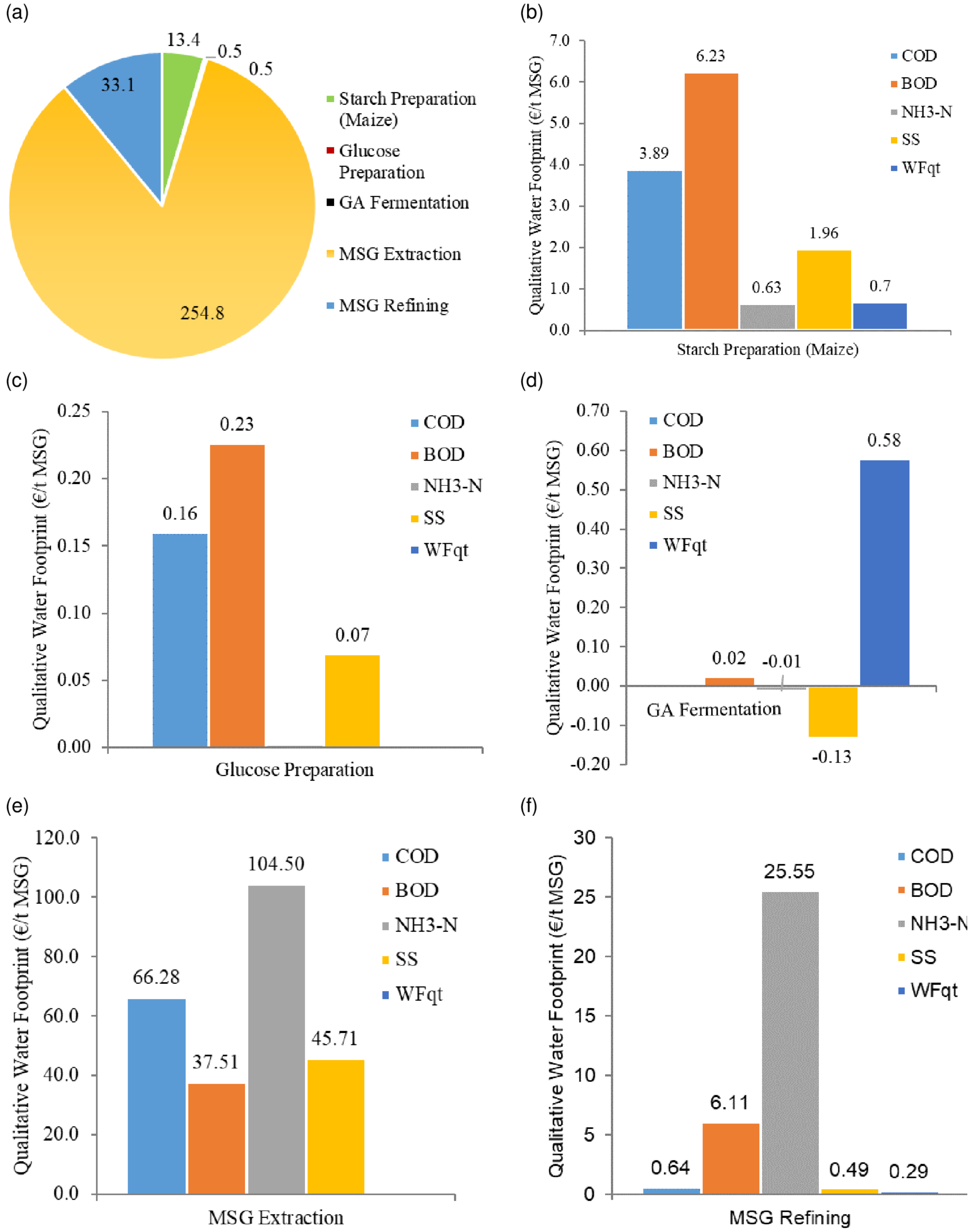

Figure 3-12: QQWFP breakdown of different processes

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.

3.2.4 Discussions

- **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 3-5).

Table 3-5: 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 €
Remarks	a) Difficult for the users and policymakers to understand and hard to guide water use management b) Not able to aggregate between water quality and quantity footprints, neither among the water quality footprint c) Describing the impact done by human water-use activities on the environment	a) Intuitive for users to monitor and manage water use b) Calculated with the current cash flow, provide more accurate information to guide water use c) Describing the impact of human activity on the water itself

The QQWFP uses cost to determine the impact of water-use activities on the water quantity and quality, which is easily understandable. Both qualitative and quantitative water use are covered, and the results of the two aspects are comparable, which enables the identification of critical water use impacts. For example, 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. The quantification of using contaminant equivalents in the ISO water footprint decides that the method is designed for scientific benchmarking of the environmental impact of water use, but it is hardly feasible for users and managers to apply in practical cases. The QQWFP, which uses cost as the quantification, can be easily understood and applied by both water users (individual, process, organisation, as well as region) and water managers (e.g. the government). The results can provide the users with insights of alternative water supplies selection, adjust water use strategies (e.g. to use cleaner water or to improve the process to reduce contaminants generation).

- **Implications based on the proposed method**

The proposed method is designed to encourage users to reduce the negative quantitative and qualitative water use and presented in the form of cost, which enables easy communication for all stakeholders. The Quantitative Water Footprint (WFqt) covers all freshwater input, reuse water, and water returned to the same water source. This encourages the reuse and prior selection of local water sources instead of transported water sources from distant spots. Comparing with existing water footprint assessment methods, the calculation of Qualitative Water Footprint (WFqt) determines the net contaminants generation instead of only counting the contamination level in the discharged water. This allows the user to improve the water footprint by using less clean (but still usable) water or improve water discharge quality.

- **Directions for future development**

At this stage, some issues are worth further investigation. First is the consideration and selection of indirect contaminants such as BOD and COD. As it is difficult to determine the generation and treatment of organic matters, BOD and COD are used to indicate biodegradable and non-biodegradable organic substances in practical water quality monitoring. Both BOD and COD are accounted in this case study considering both indicators are used as criteria for treated water discharge from WWTP. The results of WFql, in this case, would be slightly larger than the cost of treating all organic matters as part of the cost are double-counted in BOD and COD. The selection of these indicative metrics should be made based on the specific case and features of contaminants generation and treatment. Second is that indirect water use (quantity and quality) from material and energy utilisation have not still been covered in the determination stage. It is significant to establish corresponding co-efficient database of indirect water use in order to enable the wider implementation of the QQWFP.

3.2.5 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 4 WATER PINCH ANALYSIS IN SCARCITY ASSESSMENT

This chapter presents an extended methodology based on the Water Pinch Analysis method (Jia et al., 2020). Different from the extended water footprint assessment methods proposed in the previous chapters, the proposed Water Scarcity Pinch Analysis (WSPA) work as an assessment tool and optimisation tool at the same time. The research gap and literature review of this chapter is supported by the author's work published in the journal of Renewable and Sustainable Energy Reviews, with the title of New Directions in the Implementation of Pinch Methodology (PM). In that paper, the author dedicated her major contribution in Section 3 – Significant PM developments in energy and water systems. The major research part of this chapter is supported by the author's work published in the journal of Resources, Conservation and Recycling, with the title Regional Water Resources Assessment using Water Scarcity Pinch Analysis.

4.1 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.

4.2 Methodology – Water Scarcity Pinch Analysis

Water quality problems contribute significantly to water scarcity in addition to the shortage of water quantity. The increase of water degradation raises the economic cost of water treatment and transportation, as well as its environmental impacts. Regional water scarcity has been investigated in terms of volumetric comparison of demand and supply with minimal regards for quality. But a region with enough quantity of water may also face water scarcity due to low water quality, which will cause an increased cost for water treatment processes and energy consumption. Overlooking the water scarcity caused by low quality can lead to ineffective water allocation between various water supplies and demands. There is an urgent need to strengthen fundamental research and enable more efficient water resources management.

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.

4.2.1 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.

4.2.2 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 4-1: 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 4-1.

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.

4.2.3 Water Profile Table

T Water Profile Table presents the water quality categories and water supply and demand data for the Water Scarcity Pinch Analysis (Table 4-2).

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 4-2: 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).

4.2.4 Water Scarcity Pinch Analysis (WSPA)

The Composite Demand-Supply Curve is constructed based on the water profile, as illustrated in Figure 4-1. Regional data are used and the water categories 1-5 are used to represent I – V in Table 4-2.

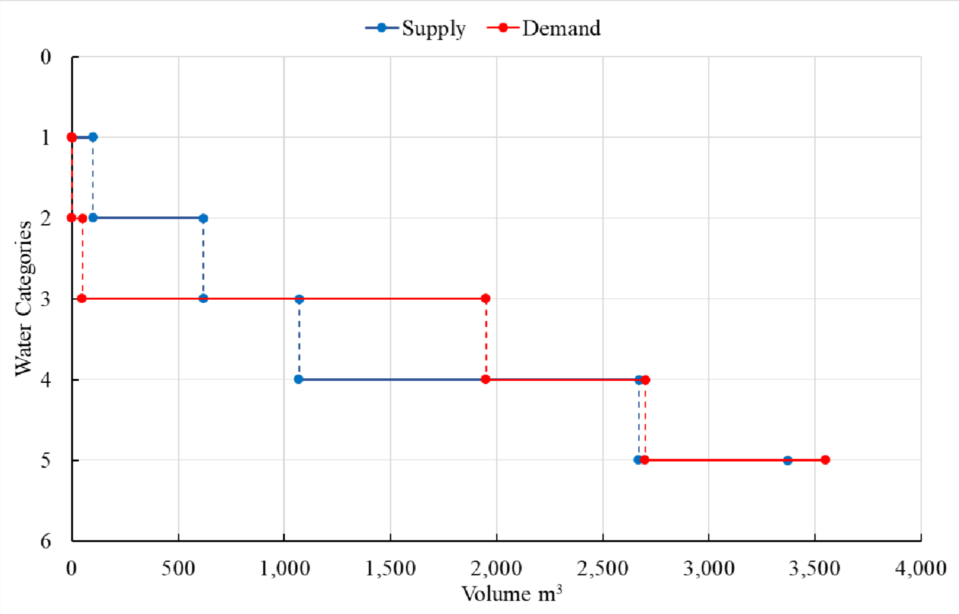

Figure 4-1: Illustration of the Composite Water Supply-Demand Curve

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 4-2).

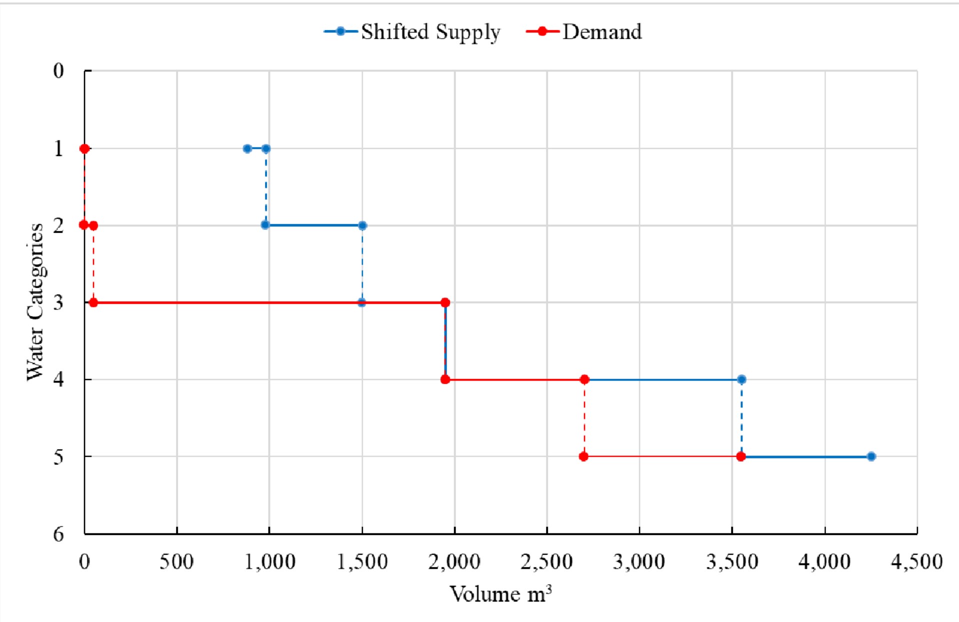

Figure 4-2: Illustration of the Pinched Composite Water Supply-Demand Curve

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 4-3.

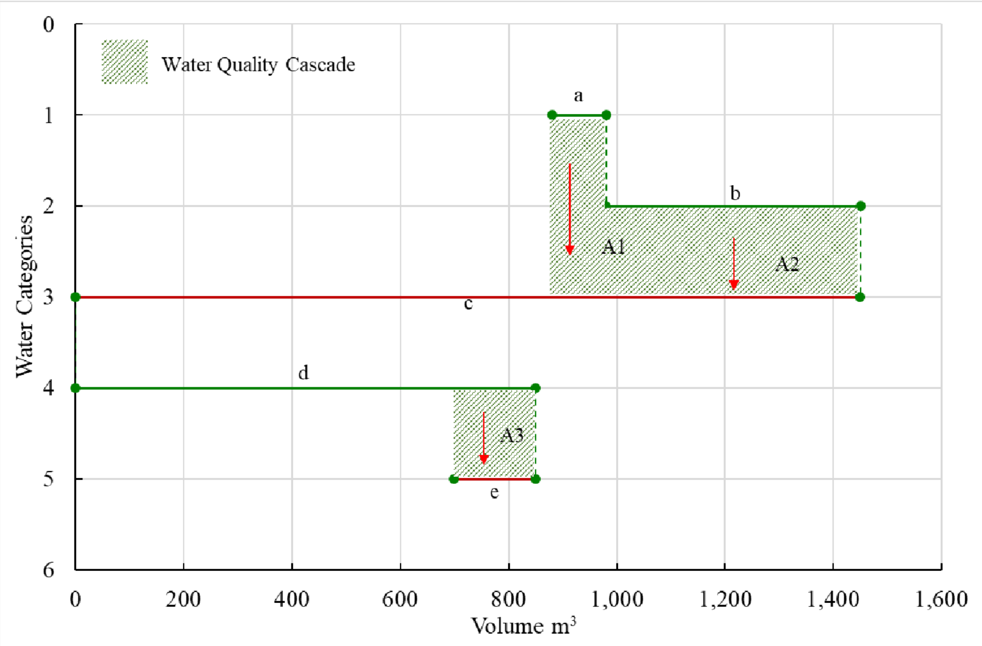

Figure 4-3: Water Scarcity GCC

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 4-3, 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 4-3 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.

4.2.5 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 (4-1), (4-2) and (4-3).

$$V_{Xi} \times C_{Xi} + V_{Yi} \times C_{Yi} = (V_{Xi} + V_{Yi}) \times C_{Zi} \quad (4\text{-}1)$$

$$V_{Xi} = V_{Yi} \times \frac{(C_{Yi} - C_{Zi})}{(C_{Zi} - C_{Xi})} \quad (4\text{-}2)$$

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.

$$V_X = Max(\, V_{Xi}) \quad (4\text{-}3)$$

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

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).

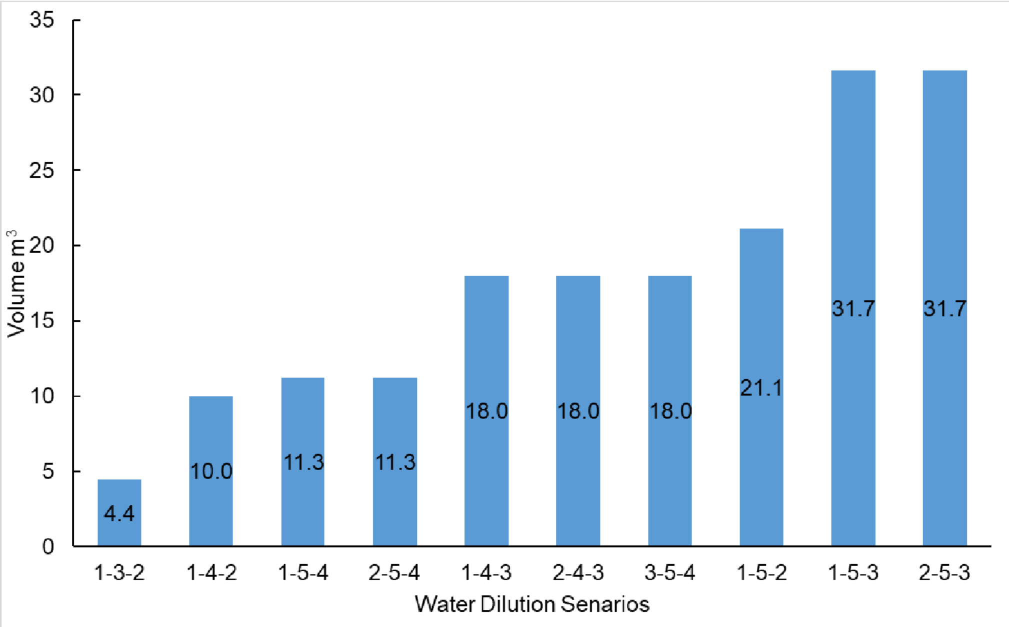

Figure 4-4: Water dilution factors of selected scenarios

The dilution factors in Figure 4-4 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.

4.3 Case Studies

4.3.1 Case Study 1

The proposed method is implemented in detail in this case. The water quality categorisation adopts the results from the example presented in Section 2.1 based on the data provided by the Chinese surface water standard (Ministry of Ecology and Environment of the People's Republic of China, 2002).

Water profile table

For region A, the water supply and demand profile table of Case 1 is presented in Table 4-3 and Table 4-4.

The supply and demand data are considered as the average data of a specific time (e.g. annual or monthly), which describes the current water scarcity condition. The water quality categories and contamination data is presented in Table S1.

Table 4-3: Water Supply Profile Table: Case 1 (m^3)

Sub-Regions	Category I	Category II	Category III	Category IV	CategoryV	Total
SubR 1	200			500		700
SubR 2		150	280			430
SubR 3	150					150
SubR 4		220				220
SubR 5		200	200	200		600
SubR 6	100		250			350
SubR 7				500	200	700
SubR 8				400	300	700
SubR 9		100		500	200	800
Regional Total	450	670	730	2,100	700	4,650

Table 4-4: Water Demand Profile Table: Case 1 (m^3)

Sub-Regions	Backup	Environmental	Residential	Industrial	Agricultural	Total
Requirement	I	I, II	I, II, III	I, II, III, IV	I, II, III, IV, V	
SubR 1		100				100
SubR 2		100	100			200
SubR 3		120	100		200	420
SubR 4			200	50	150	400
SubR 5		50	400		200	650
SubR 6			300	100		400
SubR 7			300	200		500
SubR 8			450	250	300	1,000
SubR 9			250	150	200	600
Regional Total	0	370	2,100	750	1,050	4,270

Water Scarcity Pinch Analysis

As explained in the methodology section, the regional total supplies and demands of different water quality categories can be plotted in a stack form, which is the Water Supply and Demand Composite Curve (Figure 4-5).

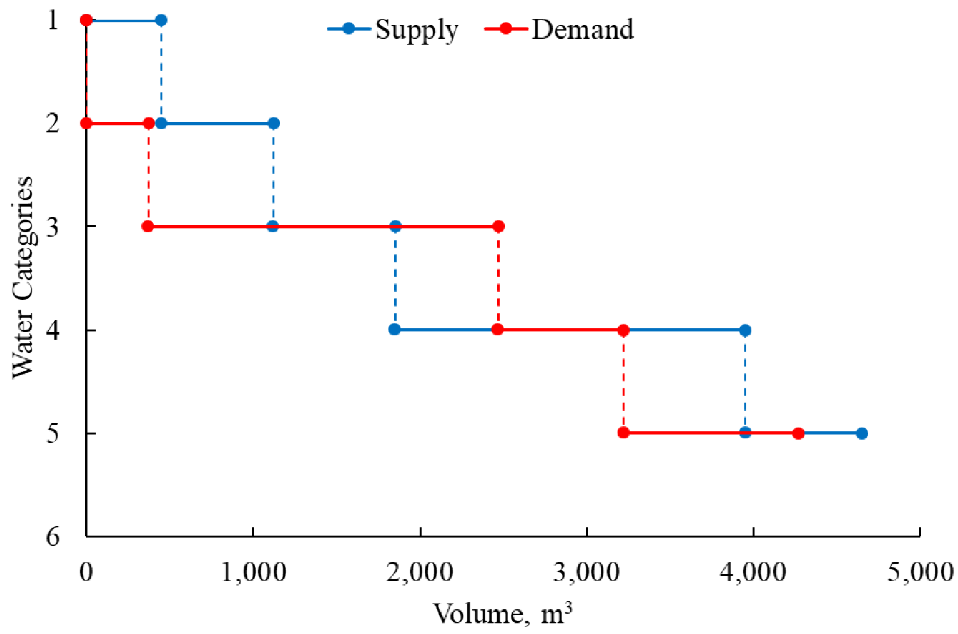

Figure 4-5: Supply-Demand Composite Curve – Case 1.

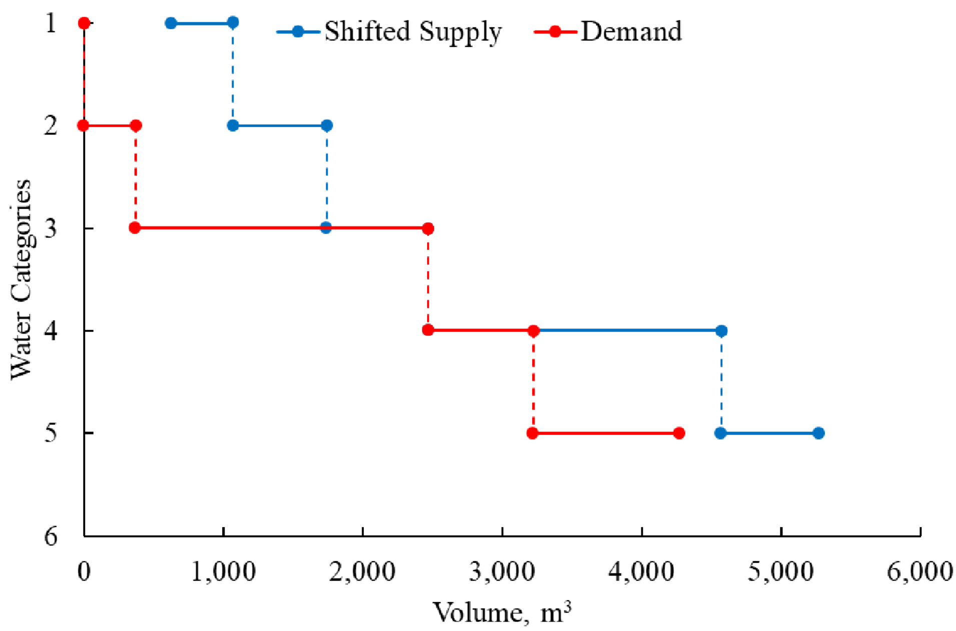

Figure 4-6: Shifted Supply-Demand Composite Curve – Case 1.

The water supply composite curve is then shifted to the right until the two curves are overlapped just to avoid a crossover (Figure 4-6). The "Pinch Point" occurred between Category III and IV when the supply curve is shifted to the right for a volume of 620 m^3, which means region A has a water scarcity of 620 m^3 water with quality Category III.

The Water Scarcity GCC (WS GCC) is then constructed based on the net differences between supplies and demands, as shown in Figure 4-7. 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 segment a (+450 m^3, Category I) and b (+300 m^3, Category II) and d (+1,350 m^3, Category IV) present the net surplus volume of water. Segment c (-1370 m^3, Category III) and e (-350 m^3, Category V) represent the net deficit. The WS GCC also indicate the possibility of water quality cascade, as shown in the "Pinch Pockets" (green shades A1, A2, and A3) in Figure 4-7. When the cleaner categories (I and II, and IV) have a surplus, they can be directly used to offset the deficit of less clean categories (III and V). 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.

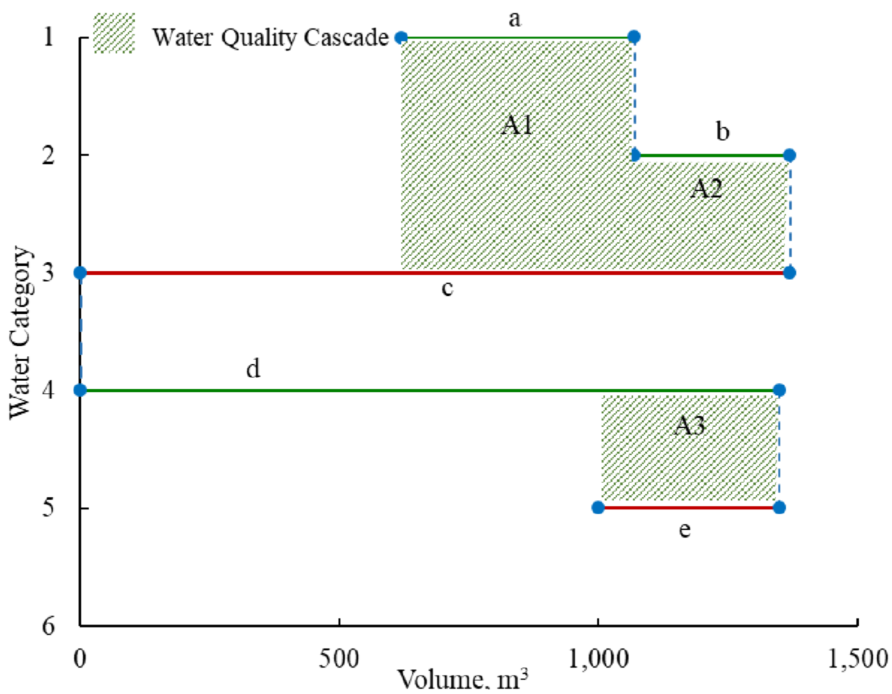

Figure 4-7: Water Scarcity GCC – Case 1

Water quality upgrading

The WS GCC in Figure 4-7 also indicates the possibility of using higher quality categories to upgrade the lower categories to reach minimal water scarcity. As shown in Figure 4-7, 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 4.2.5, the water scarcity of applying Water Dilution is calculated and compared with the result of applying Water

Quality Cascade (Figure 4-8).

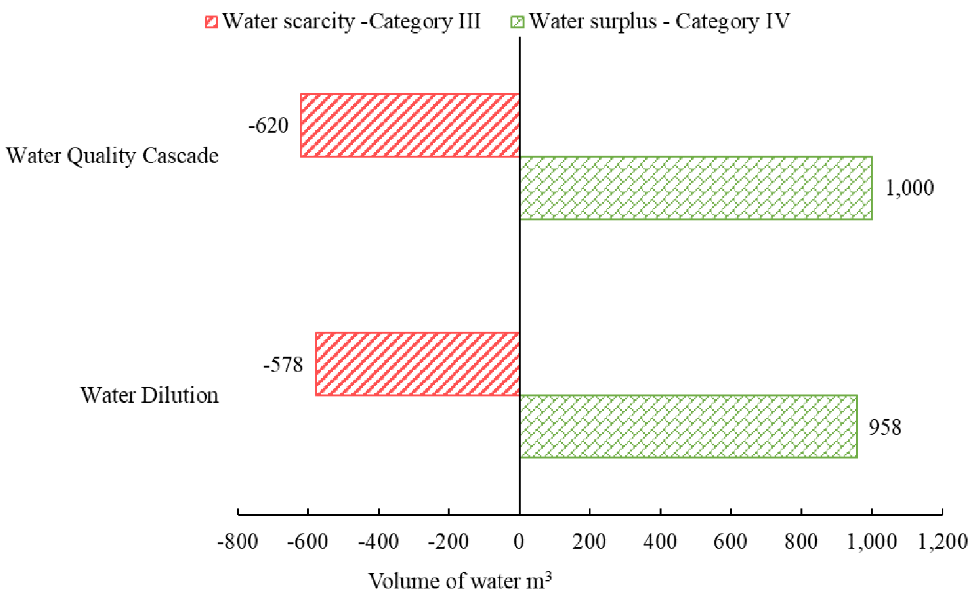

Figure 4-8: Water scarcity of Water Quality Cascade and Water Dilution - Case 1

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 minimise the water scarcity to 578 m^3 water (Category III) with a surplus of Category IV (958 m^3).

4.3.2 Case Study 2

Case Study 2 is set to investigate the performance of the proposed method with identifying regional water scarcity and potential in implicating suggestions for water scarcity minimisation.

Table 4-5 and Table 4-6 list the water supply and demand of Region B. All items have the same meaning as in Case Study 1 and are explained previously in section 3.1.1.

Table 4-5: Water Profile Table: Case 2 – Water Supply (m^3)

Sub-Regions	**Category I**	**Category II**	**Category III**	**Category IV**	**Category V**	**Total**

SubR 1	200			500		700
SubR 2		150	280			430
SubR 3	150					150
SubR 4		220				220
SubR 5		200	200	200		600
SubR 6	100		250			350
SubR 7				500	200	700
SubR 8				400	300	700
SubR 9		100		500	200	800
Total	**450**	**670**	**730**	**2,100**	**700**	**4,650**

Region B has the same total water supply and demand as Region A in Case Study 1 (4,650 m^3), but the distribution of water quantity in different water quality categories are different. There are more sources of medium quality water, e.g. Category IV (2,100 m^3), Category III (730 m^3), and Category V (700 m^3), and demands for lower categories, e.g. Category IV (1,500 m^3), Category III (1,250 m^3), and Category V (1,150 m^3).

Table 4-6: Water profile of Case 2 – Water Demand (m^3)

Sub-Regions	Backup	Environmental	Residential	Industrial	Agricultural	Total
Requirement	**I**	I, **II**	I, II, **III**	I, II, III, **IV**	I, II, III, IV, **V**	
SubR 1		100				100
SubR 2		100		100	100	300
SubR 3		120		100	200	420
SubR 4			200	50	150	400
SubR 5		50	300		200	550
SubR 6			200	200		400
SubR 7			300	200		500
SubR 8			250	450	300	1,000
SubR 9			250	150	200	600
Total	**0**	**370**	**1,500**	**1,250**	**1,150**	**4,270**

Following the method illustrated in the Methodology Section and in Case 1, the water scarcity of Region B is assessed using WSPA. The water Supply-Demand composite curve and shifted curves are shown in Figure 4-9 and Figure 4-10.

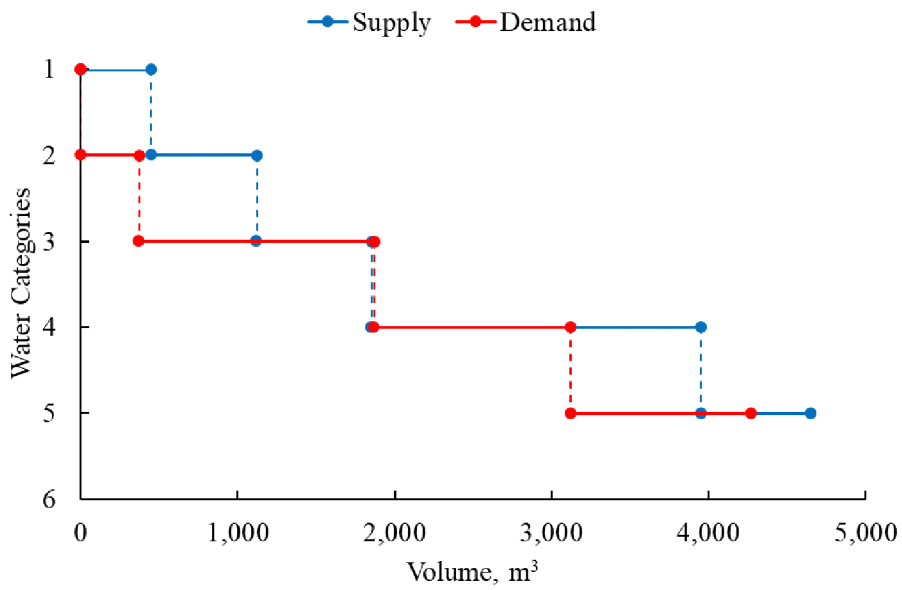

Figure 4-9: Supply-Demand Composite Curve – Case 2

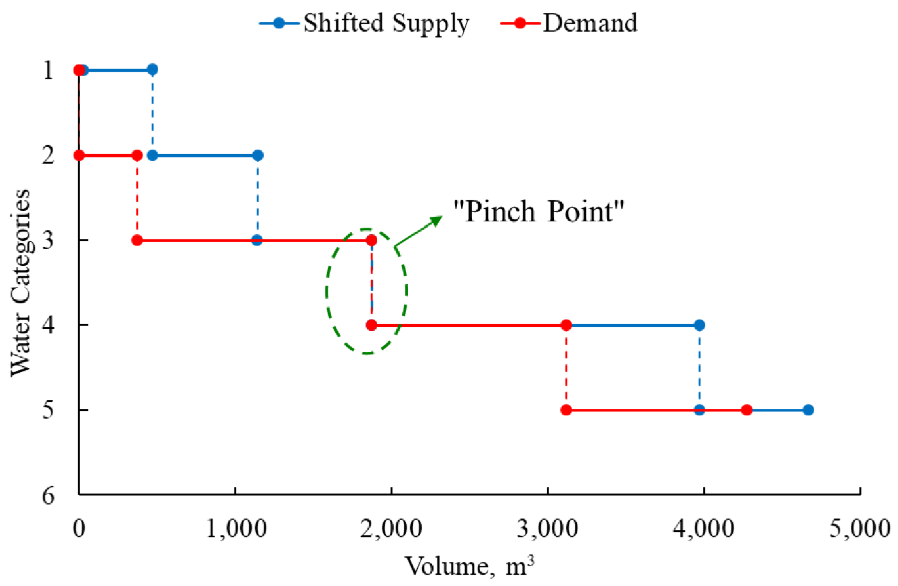

Figure 4-10: Shifted Supply-Demand Composite Curve – Case 2

The water supply curve is then shifted to right 20 m^3 until the "Pinch Point" occurred when the volume of Category III is 750 m^3. Based on the supply and demand composite curves, the Water Scarcity GCC can be constructed in Figure 4-11, 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.

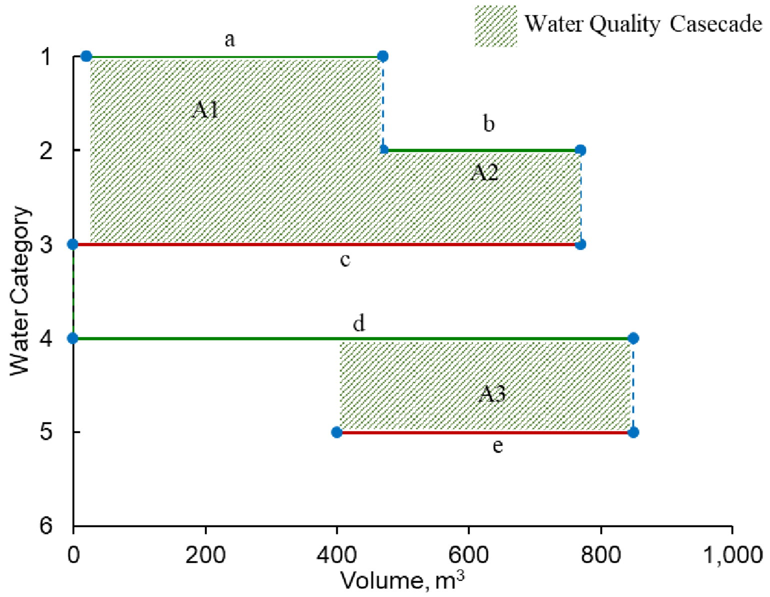

Figure 4-11: Water Scarcity GCC – Case 2

The water scarcity of applying WQC and WD are presented in Figure 4-12, 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).

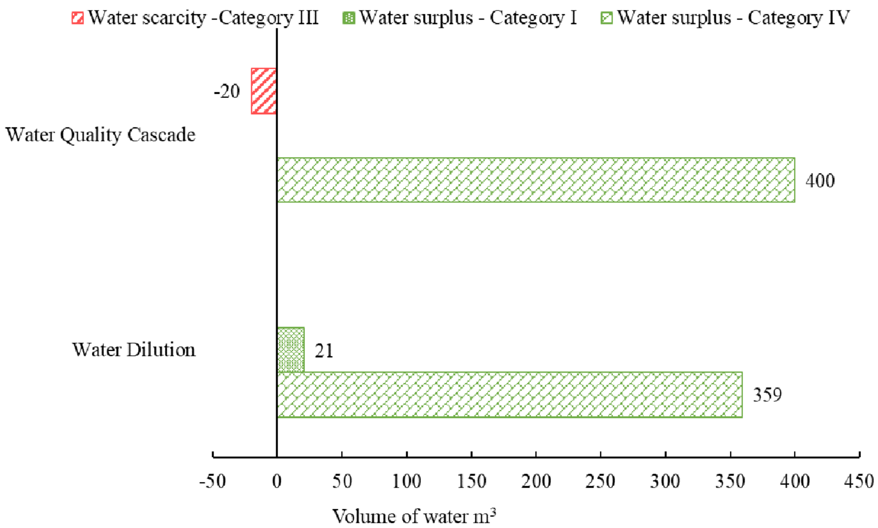

Figure 4-12: Water scarcity of Water Quality Cascade and Water Dilution - Case 2

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.

4.3.3 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. Similar to Case 2, the assessment process is introduced in brief. The water quantity and quality data of the supplies and demands in Regions C are presented in Table 4-7 and Table 4-8.

Table 4-7: Water Profile Table: Case 3 – Water Supply (m^3)

Sub-Regions	**Category I**	**Category II**	**Category III**	**Category IV**	**Category V**	**Total**
SubR 1	200			500		700
SubR 2		150	280			430
SubR 3	150					150
SubR 4		220				220
SubR 5		200	200	200		600
SubR 6	100		250			350
SubR 7				300	200	500
SubR 8				250	300	550
SubR 9		100		300	200	600
Total	450	670	730	1,550	700	4,100

Table 4-8: Water profile of Case 3 – Water Demand (m^3)

Sub-Regions	**Backup**	**Environmental**	**Residential**	**Industrial**	**Agricultural**	**Total**
Requirement	**I**	I, **II**	I, II, **III**	I, II, III, **IV**	I, II, III, IV, **V**	
SubR 1		100				100
SubR 2		100		100	100	300
SubR 3		120		100	200	420
SubR 4			200	50	150	400
SubR 5		50	300		200	550
SubR 6			200	200		400
SubR 7			300	200		500
SubR 8			250	450	300	1,000
SubR 9			250	150	200	600
Total	0	370	1,500	1,250	1,150	4,270

Based on the supply and demand data, the Supply-Demand Composite Curve are constructed in Figure 4-13 and Figure 4-14.

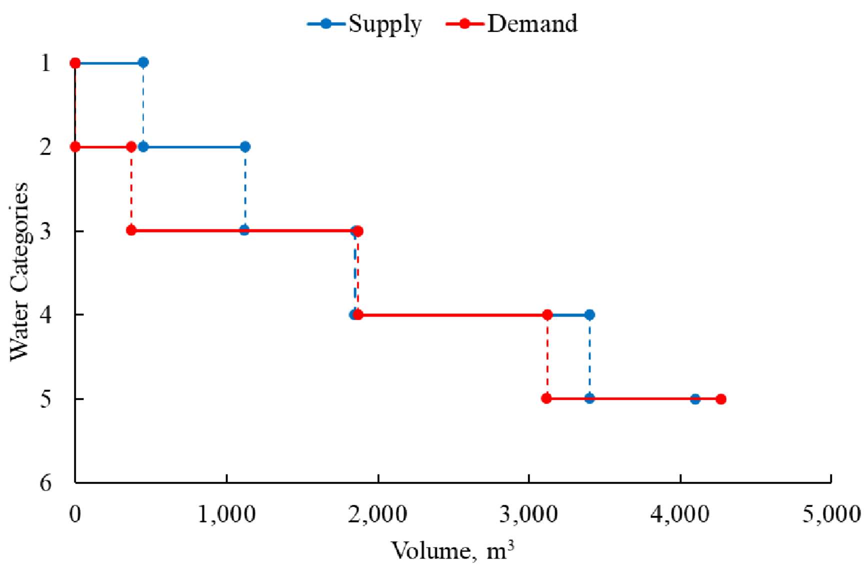

Figure 4-13: Demand-Supply Composite Curve– Case 3

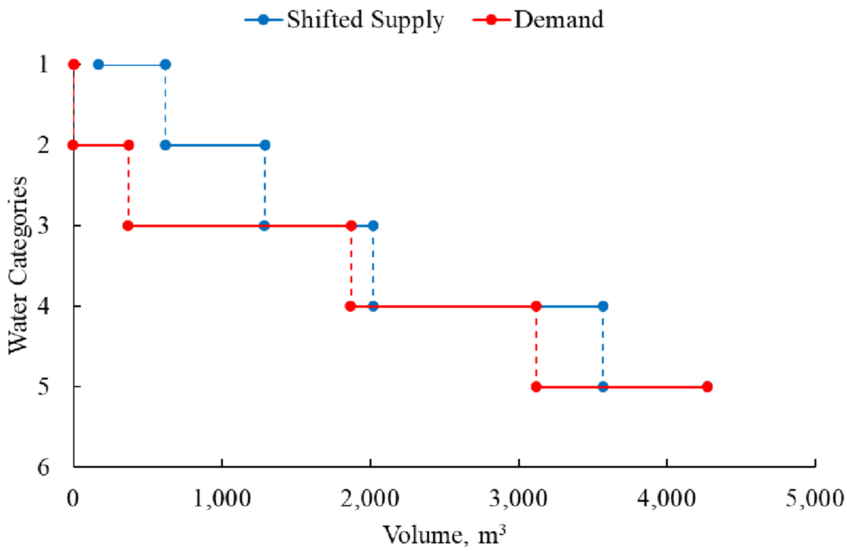

Figure 4-14: Shifted Demand-Supply Composite Curve– Case 3

The Water Supply Curve is shifted to right 170 m^3 until the Pinch Point occurred with the volume of Category III of 750 m^3. The GCC is constructed in Figure 4-15. 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.

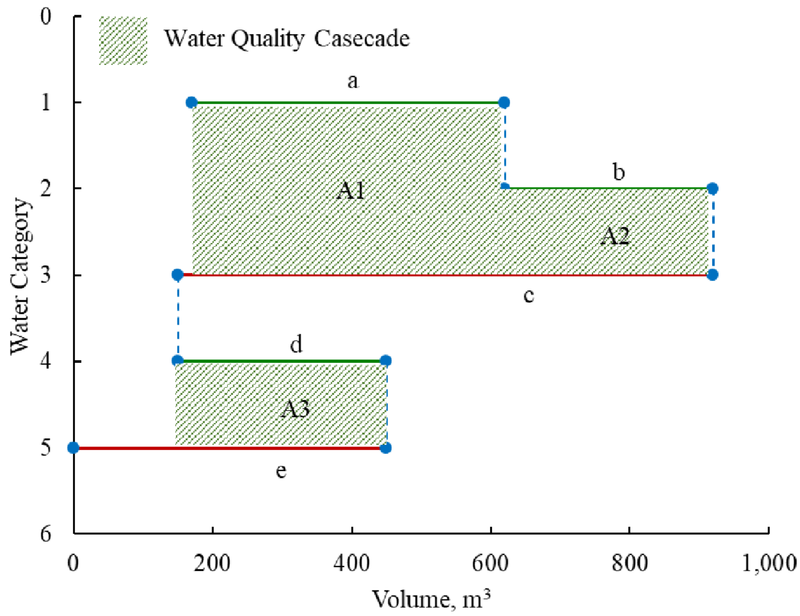

Figure 4-15: Water Scarcity GCC – Case 3

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 4-16.

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 reduced the water scarcity and shifted the scarcity from higher to lower quality water.

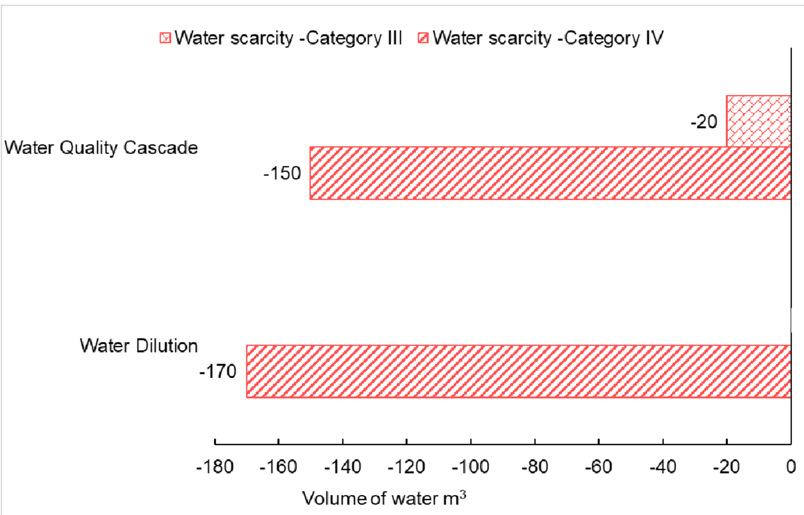

Figure 4-16: Water scarcity of Water Quality Cascade and Water Dilution - Case 3

4.4 Discussion and Directions for Future Work

The three case studies illustrate the application and the performance of the proposed Water Scarcity Pinch Analysis (WSPA), as summarised in Table 4-9.

Table 4-9: Comparisons of the outcomes of the three case studies

	Supply Minus Demand	Demand-to-Supply	Water scarcity by WSPA	Minimal Water scarcity
Case Study 1	380 m^3	0.92	620 m^3, Category III	578 m^3 Category III
Case Study 2	380 m^3	0.92	20 m^3, Category III	No water scarcity
Case Study 3	-170 m^3	1.04	20 m^3, Category III and 150 m^3, Category V	170 m^3 Category V

It showed that the proposed WSPA identifies the water scarcity in terms of water quality together with quality, and provides guidance information for regional water scarcity minimisation. In Case 1 and 2, WSPA identifies the water quality caused scarcity, which is overlooked by the conventional ratio-based. Case 3 showed that the WSPA covers both water quality and quantity scarcity, and results in minimal water scarcity. Water quality cascade can reduce water scarcity, and water quality upgrading by water dilution can minimise (in Case 1 and 3) and even eliminate the regional water scarcity (in Case 2). The overall results indicate that the proposed method has a high potential for water scarcity minimization in regional water resources management.

The novel contributions of the work include: 1) Account water quality together with quantity in water scarcity assessment. Water scarcity has been redefined in this study, which is the net deficit of water supply with certain water quality category and has been illustrated by the Grand Composite Curve. 2) Applying water quality categorisation in the WSPA is a critical improvement of the conventional WPA. This modified the conventional Water Supply and Demand Composite Curve from a linear form to a staircase form. The Water Scarcity Pinch is no longer a single point but a 2-dimension vector of value with a descriptive water quality category. 3) Applying the graphical Pinch Analysis to a macro level, which is more direct and evident than the conventional ratio-based methods. 4) WSPA provides implications for water scarcity minimisation through maximising water use efficiency.

This study aims to redefine the water scarcity and propose a WSPA to determine the water scarcity. At the design stage, there are still some limitations of the proposed methods. First, is the water quality of the output side has not been considered directly. It is assumed that all the discharged water from wastewater treatment plants meets the discharge standards and have the same quality as the water sinks. With this assumption, the assessment results would be smaller than the real value. Second, at this stage, practical factors such as the cost and energy consumption of water transportation are not considered in the analysis of water quality cascade and water dilution. In addition, sensitivity analysis is not carried out as the numerical case studies are just set to illustrate the implementation of the method. Overall, this study serves as the initial step of redefining the water quality-quantity scarcity and proposing the WSPA for water scarcity quantification. Future works should tackle the above-mentioned limitations and further develop the WSPA for regional water use optimisation and scarcity minimisation.

4.5 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 constructed with the water quality categories and water volume 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 of the three case studies 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.

4.6 Other Water Pinch Analysis works

In addition to the comprehensive literature review of the Water Pinch Analysis and the proposed Water Scarcity Pinch Analysis method, the author also participated in and contributed to other water integration network design and total site environmental assessment (list as follows) work which have been published in international journals, including (Jia et al., 2018), (Fan et al., 2019), and (Zhang et al.., 2020). These publications can be found in the reference list, and more detailed information can be found from the full published article.

CHAPTER 5 WATER-ENERGY NEXUS: AN ILLUSTRATION OF SEAWATER DESALINATION

Improving water use efficiency and reduce water wasting are solutions from the perspective of reducing expenditure, it is also important to "increase the sources" to provide more alternative water supplies. Desalted seawater has been one of the major alternative water supplies for many countries, especially in the Gulf region. Seawater desalination is a process of "energy to water", means it consumes available resources (e.g. energy) and "produce" freshwater from salty seawater. As energy is also one of the major critical resources for human lives and economic development together as water resources, it is important to investigate how the water and energy are interconnected in the seawater desalination processes.

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.

5.1 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 minimization 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. A report from the Water Desalination

Report by the International Desalination Association presented the current installed capacities of the world desalination by countries (International Desalination Association, 2017). Figure 5-1 shows the water desalination capacities of the world by countries from 2010 to 2016 (International Desalination Association, 2017). In the last six years, the world total water desalination capacity, including brackish water and seawater desalination, increased steadily with an annual rate of about 9%. A large proportion came from the Gulf region, and not surprisingly, the Kingdom of Saudi Arabia (KSA) and the United Arab Emirates (UAE), which take a proportion of 15% and 11% of the world's total desalination capacities in 2016. Next is the USA, which takes 10% of the world total installed desalination capacity. China has the fourth-largest water desalination capacity, with a share of 5% of the world total installed capacity.

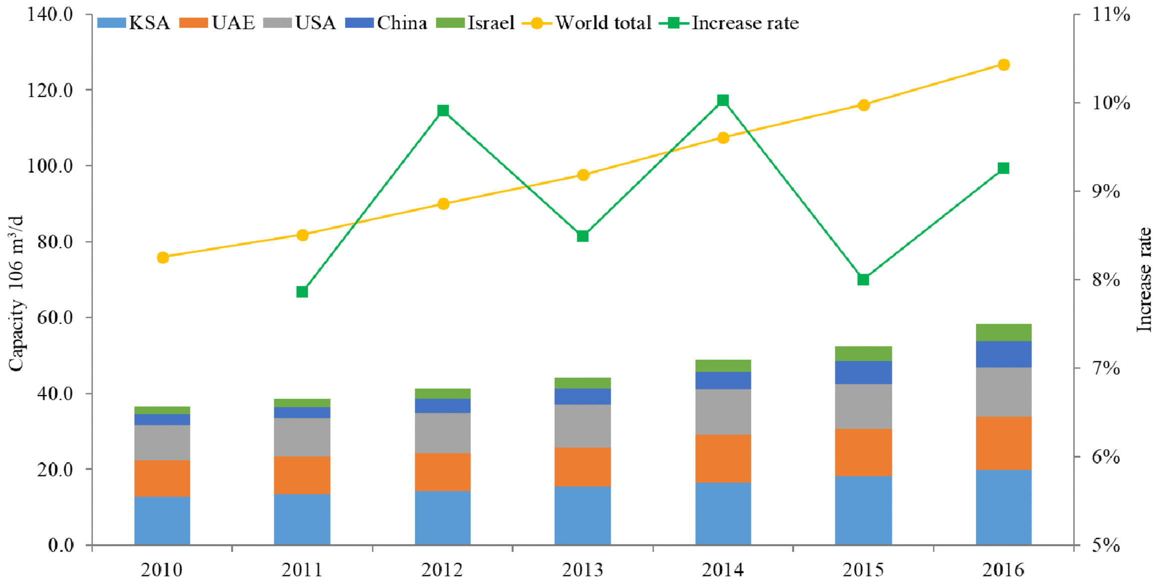

Figure 5-1: Water desalination capacities of the world and selected countries from 2010 to 2016 (derived from (International Desalination Association, 2017)). KSA: Kingdom of Saudi Arabia; UAE: United Arab Emirates.

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 5-2.

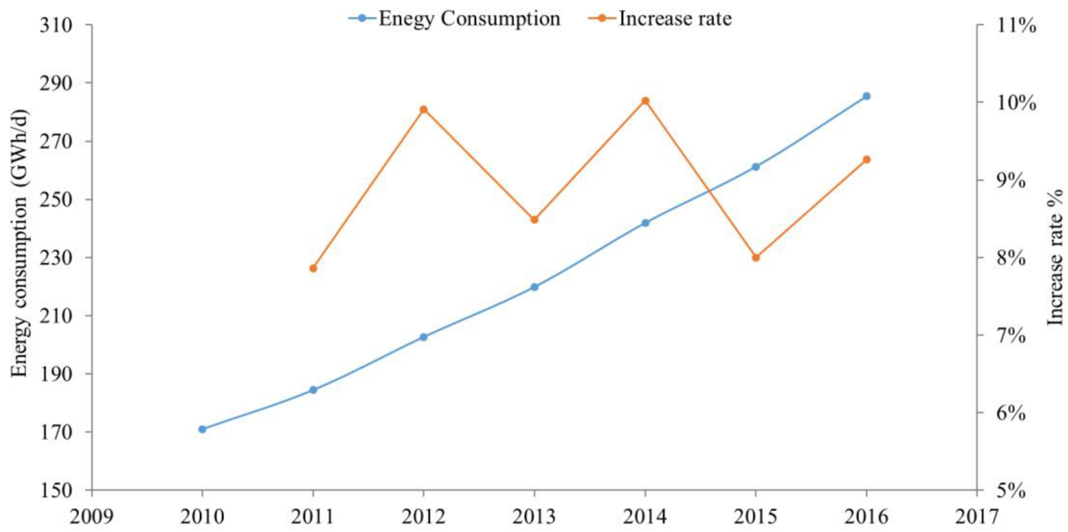

Figure 5-2: Water desalination energy consumption (electricity) from 2010 to 2016

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.

For producing freshwater, seawater desalination has been actively implemented in the Gulf region and is emerging in East Asia, where are facing severe water stress issues. China has the fourth-largest capacity of seawater desalination in the world, and water desalination is still an emerging industry. The major driving force is increasing water shortage. China is becoming one of the countries with a severe water shortage, especially in the most developed northeast region (Li et al., 2017). For example, in 2016, the average water resource per capita was 2,355 m^3 (National Data, 2019a), which is about 40 % of the average world value (The World Bank, 2014). For the capital city of China, Beijing, the amount is 162 m^3 (National Data, 2019b), which is less than 3 % of the average world value. The increasing population and urban land in these water stress areas are still increasing (Li et al., 2017), which indicates an increasing freshwater demand. One fact is that about 71% of the Earth's surface is covered by water, and the oceans hold approximately 96.5% of all Earth's water (USGS, 2020). However, there is still is a shortage of clean freshwater, which will lead to an increase in cost and resource consumption and potential environmental impacts.

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 techniques and projects. From 2006 to 2016, the installed seawater desalination has increased from 20×10^6 m^3/y to 390×10^6 m^3/y (Ministry of Natural Resources of the People's Republic of China, 2018). Until 2016, there have been 15 newly released standards by the government to facilitate the promotion and management of water desalination projects (Ministry of Natural Resources of the People's Republic of China, 2018). Seawater desalination has been considered as one of the most promising techniques due to the abundance of seawater and improving operating efficiency (Hua et al., 2014). The resources consumption and environmental impacts of seawater desalination are also concerned with its increasing capacity.

The majority of studies have focused on either the advancement of the desalination process or specific case plants. Sores (2018) proposed and tested a novel supercharger which can be applied to a seawater desalination RO system and found that the efficiency of the tidal supercharger is currently lower than 20%, although the efficiency increased from 12% to 14%, with the seawater flow rate increasing from 290 m^3/h to 440 m^3/h. The application of renewable energies is also discussed in current studies. For instance, Zuo et al. (2018) proposed a model of a wind supercharged solar chimney power plant combined with seawater desalination and claimed that the utilization of solar energy could be raised by 70% with integration. Li et al. (2018) developed a high-efficiency membrane for seawater desalination using solar energy, and the results showed a 90% efficiency of converting solar energy. Desalination plants in China have seldom been discussed. Liu et al. (2018) carried out the systems process analysis of the freshwater cost of seawater desalination, with a case study of a 25,000 m^3/d seawater desalination plant in Huanghua Port, Hebei Province, China. The study determined that the freshwater consumption of the plant is 4.5×10^5 m^3/y, which is 5% of the annual freshwater production (9.2×10^6 m^3/y). The World Resources

Institute (Hua et al., 2014) investigated the carbon emissions footprint of different scenarios in Qingdao. It showed that in 2020 with a water desalination capacity of 400×10^3 m^3/d, the carbon footprint of the water desalination will be 541.31 kt CO_{2eq}/y (with a cost of 8 CNY/m^3), which is 1.81 times more expensive than water supplies from surface and groundwater (with a cost of 1.17 CNY/m^3). Other studies also reported that water desalination with various techniques has other atmospheric emissions, e.g. dust, NOx, and SO_x (Raluy et al., 2006).

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.

5.2 Seawater Desalination in China

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, which can be seen from Figure 5-3 (Ministry of Natural Resources of the People's Republic of China, 2018).

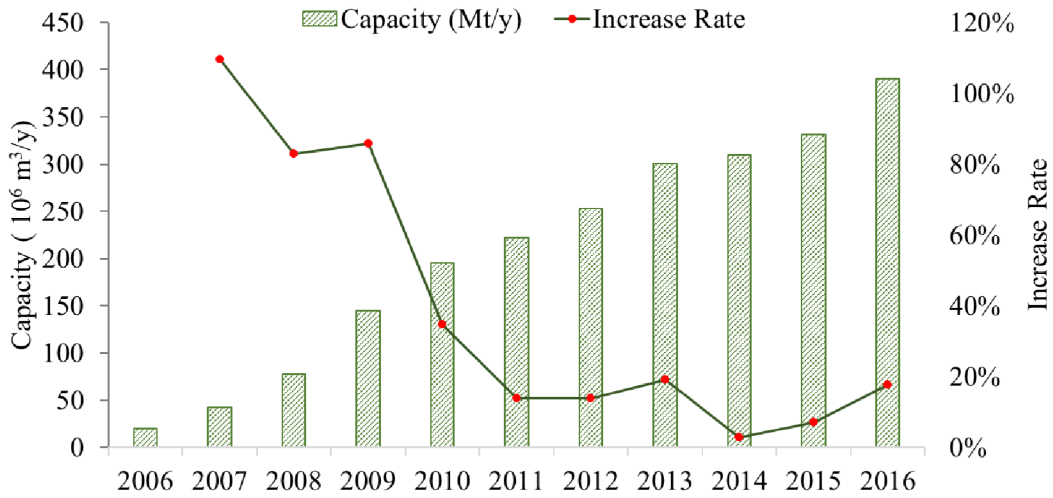

Figure 5-3: Total seawater desalination plant capacities in China from 2006 to 2016, derived from (Ministry of Natural Resources of the People's Republic of China, 2018)

Due to the introduction of relevant policies and standards by the government, seawater desalination has been one of the promising solutions to the water shortage in China. According to the State Oceanic Administration of China Ministry of Natural Resources of the People's Republic of China, 2018), there have been 131 seawater desalination plants/projects up until 2016 in mainly coastal cities in China, and the total capacity has reached to 1.19×10^6 m^3/d. The plants with different capacities are evenly distributed.

Table 5-1: Water desalination projects development in China until 2016. Derived from (Ministry of Natural Resources of the People's Republic of China, 2018)

Item	Description	Value
Quantity	Number of plants	131
	Total Project capacity	1.19×10^6 m^3/d
Capacity	Plants capacity > 10^4 m^3/d	Number of plants: 36, Total capacity 10^6 m^3/d
	Plants capacity ($1–10^4$ m^3)	Number of plants: 38, Total capacity 118×10^3 m^3/d
	Plants capacity < 10^6 m^3	Number of plants: 57, Total capacity 11×10^3 m^3/d
Benefits	The added value of seawater desalination plants	1.5×10^9 CNY/y

As shown in Table 5-1, there are 36 plants/projects with a capacity larger than 10 km^3/d, with a total capacity of 10^6 m^3/d. 38 plants have a capacity of 10^3 m^3/d to 10^4 m^3/d, with a total capacity of 1.2×10^5 m^3/d. Another 57 smaller plants/projects have a total capacity of 1.1×10^4 m^3/d. The largest water desalination plant in China is in Tianjin, with a total capacity of 2×10^5 m^3/d.

Regionally, large-scale seawater desalination plants are located on the northeastern coast of China with relatively severe water scarcity issues, e.g. Tianjin, Shandong, and Hebei. Figure 5-4 shows the seawater desalination capacities of the plants by desalination process, as well as the estimated water stress index of the provinces with seawater desalination plants. Tianjin, as a coastal city next to Beijing (the capital of China), has the largest total capacity of 317×10^3 m^3/d, with RO and multiple-effect distillation (MED) being the main processes, multi-stage flash (MSF) and electrodialysis (ED) are less applied in China. The Tianjin Beijing seawater desalination plant, with a capacity of 200×10^3 m^3/d, is the largest seawater desalination plant in China. Tianjin also has the largest installed seawater desalination plants with the MED process. Shandong has the second-largest seawater desalination capacity (282 × 10^3 m^3/d). The largest water desalination plant in Shandong is located in Qingdao, an international city facing severe water shortage issues, with a capacity of 10^5 m^3/d. The total capacity of water desalination plants in Qingdao reached 235× 10^3 m^3/d in 2016, which takes 83% of the total capacity of Shandong province (Karabelas et al., 2018). One large-scale plant in southern China is in Zhejiang Province, with a capacity of 228 × 10^3 m^3/d. Other seawater desalination plants in southern China (e.g. Guangdong, Fujian, Jiangsu, and Hainan) are mainly small plants. Most of the plants are built after 2009, and the main processes applied are reverse osmosis (RO, with a proportion of 86%) and MED (with a proportion of 12%). Other technologies such as MSF and ED are also applied in a few plants, with a total ratio of 2%.

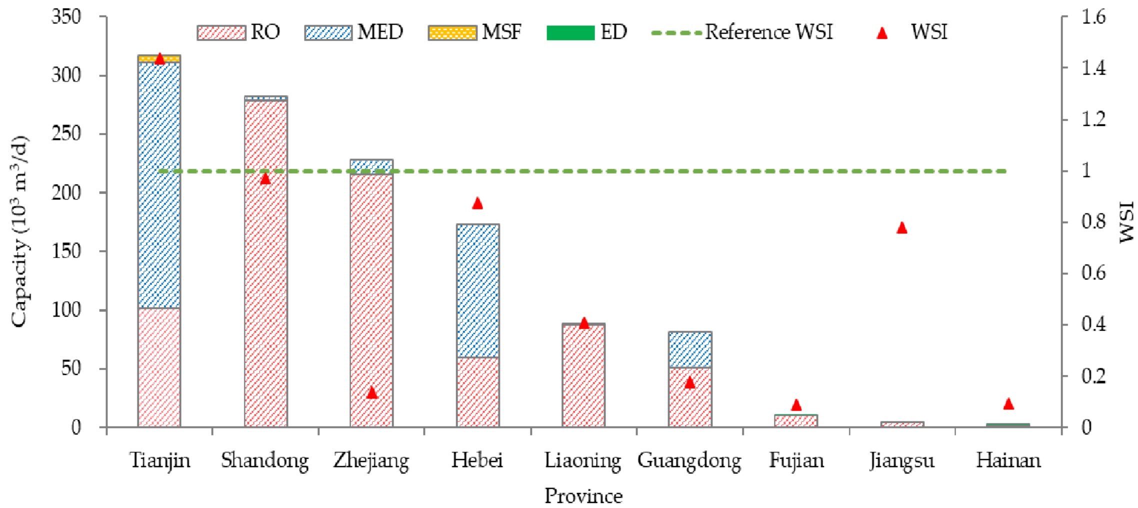

Figure 5-4: Water desalination capacity by provinces. WSI: water stress index, RO: reverse osmosis; MED: multiple-effect distillation; MSF: multi-stage flash; ED: electrodialysis. Derived from (Ministry of Natural Resources of the People's Republic of China, 2018)

Figure 5-4 also indicates that the provinces/cities with large seawater desalination plants also have a higher water stress index (WSI), which is the ratio of the annual water consumption and the available natural water resources (Pfister et al., 2009). A higher WSI indicates that consumption is closer to the available water resources and, higher water stress. When the value is higher than 1, it means the water consumption of the region has exceeded the available freshwater resources, and the region has a high water stress level. The WSI of the selected provinces is estimated with the method of (Pfister et al., 2009), based on the data from (National Data, 2019a), as shown in Figure 5-4. The green dash line is the reference WSI with a value of 1. For most of the selected provinces, provinces with higher water stress have higher seawater desalination capacity, which indicates the driving factors of the development of seawater desalination. Two exceptions are Zhejiang and Jiangsu. Zhejiang has the third-largest seawater desalination capacity, but the water stress is rather small. Jiangsu has a very small seawater desalination capacity but with relatively high water stress.

In terms of water use, as shown in Figure 5-5, a major proportion (66.6%) of desalted water is used in industry, and followed by domestic use with a ratio of 33.1%, and a small fraction (0.3%) is used for other purposes, e.g. watering in parks and greenbelts. Within the industry, main users of desalinated water are fossil fuel power plants (31.6% of total), steel making industries (13.1%), and petrol chemical industries (12.3% of total). The major use in industries indicates that the quality of the desalted seawater needs to meet the quality requirement for industrial use.

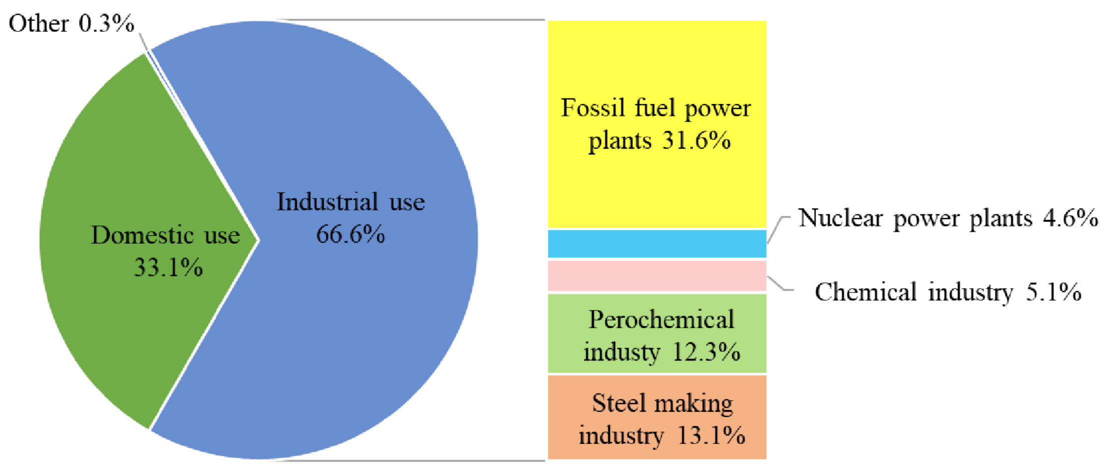

Figure 5-5: Distribution of desalinated water use in 2016, Derived from (Ministry of Natural Resources of the People's Republic of China, 2018)

Water treatment, seawater desalination, and water resource transfer are the main solutions for the freshwater shortage in China. Wastewater treatment, as the most conventional approach, has been well developed and implemented. The wastewater treatment approach can only offset part of the consumed water by removing the contaminants from the polluted water and return the treated water to the available natural resource, but usually, the water quality of the discharged water is not as high as previous. When there is not enough available natural water resource, the cycle of supply- use-treatment-return cycle would be difficult to maintain. Water transfer is usually a huge project that has a considerable economic and ecological cost, with large-scale changes to the inhabitants along the channel. Due to this reason, the existing water transfer projects in China are still under controversial discussion (Wilson et al., 2017). Seawater desalination is considered as one of the most promising approaches to produce freshwater.

Although seawater desalination is a reliable water supply and is not vulnerable to climate change, it consumes a lot of energy, and it requires a lot of investment and public acceptance. The increasing capacity and wide distribution in different regions also result in the issue of increasing energy consumption, GHG emissions, as well as the economic cost. It is vital to analyze and benchmark the environmental and financial performance, in order to provide insightful data for the further planning and optimization of energy use and emission reduction in seawater desalination.

5.3 Methodology: Determination of Energy Consumption and GHG emissions

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.

5.3.1 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).

$$EC_a = \sum SEC_i \times C_i \times 365 \times P_a \tag{5-1}$$

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 5-2.

Table 5-2: 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

5.3.2 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:

$$G_e = EM_e + EM_{in} + EM_{waste} \qquad (5\text{-}2)$$

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.

$$EM_e = EC_a \times E_f \qquad (5\text{-}3)$$

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).

5.3.3 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:

$$UPC = \frac{{CC}/{Pl} + OP_a}{Ca \times Pa} \tag{5-4}$$

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:

$$^{CC_x}/_{CC_{rf}} = [^{Ca_x}/_{Ca_{rf}}]^m \tag{5-5}$$

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:

$$CC_x = e^{m \times ln(Ca_x) - m \times ln(Ca_{rf}) + ln(CC_{rf})} \tag{5-6}$$

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 5-3).

Table 5-3: 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.

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 5-4).

Table 5-4: 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 %

The operating cost can be calculated with energy cost and the energy/operating cost ratio as in Eq(5-7):

$$OP_a = Eco/EOP \quad (5\text{-}7)$$

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 5-4.

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(5-8):

$$Eco = SEC_i \times C_i \times P_e \quad (5\text{-}8)$$

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. The water conveyance and distribution, as well as the brine disposal, are yet considered.

5.4 Results and Discussions

5.4.1 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 5-6). 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.

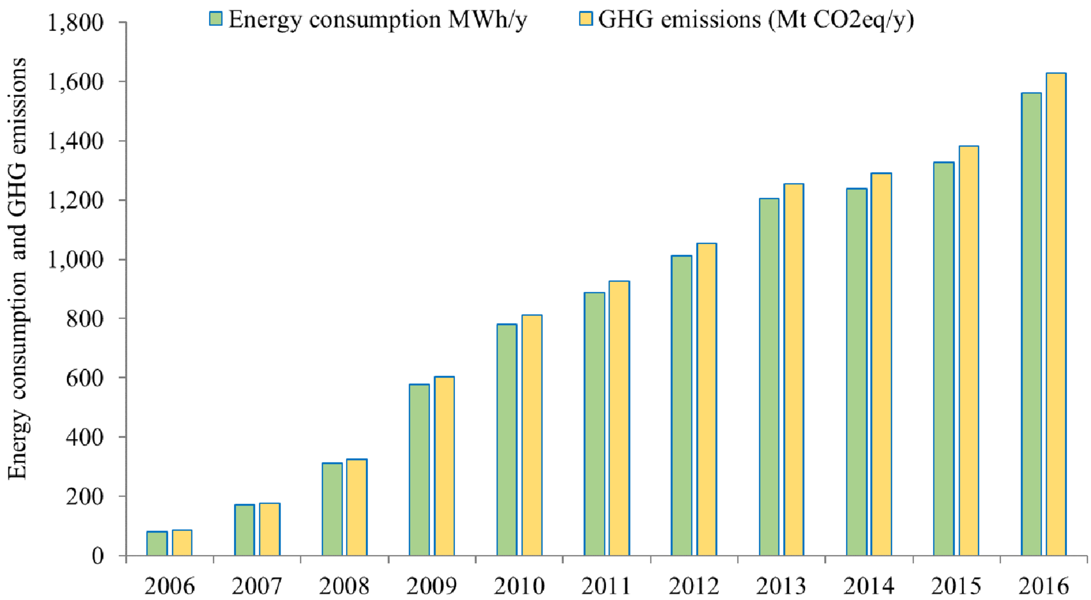

Figure 5-6: Overall seawater desalination energy consumption and GHG emissions from 2006–2016.

The breakdowns of GHG emissions by province and desalination processes are estimated for the year 2016, as shown in Figure 5-7.

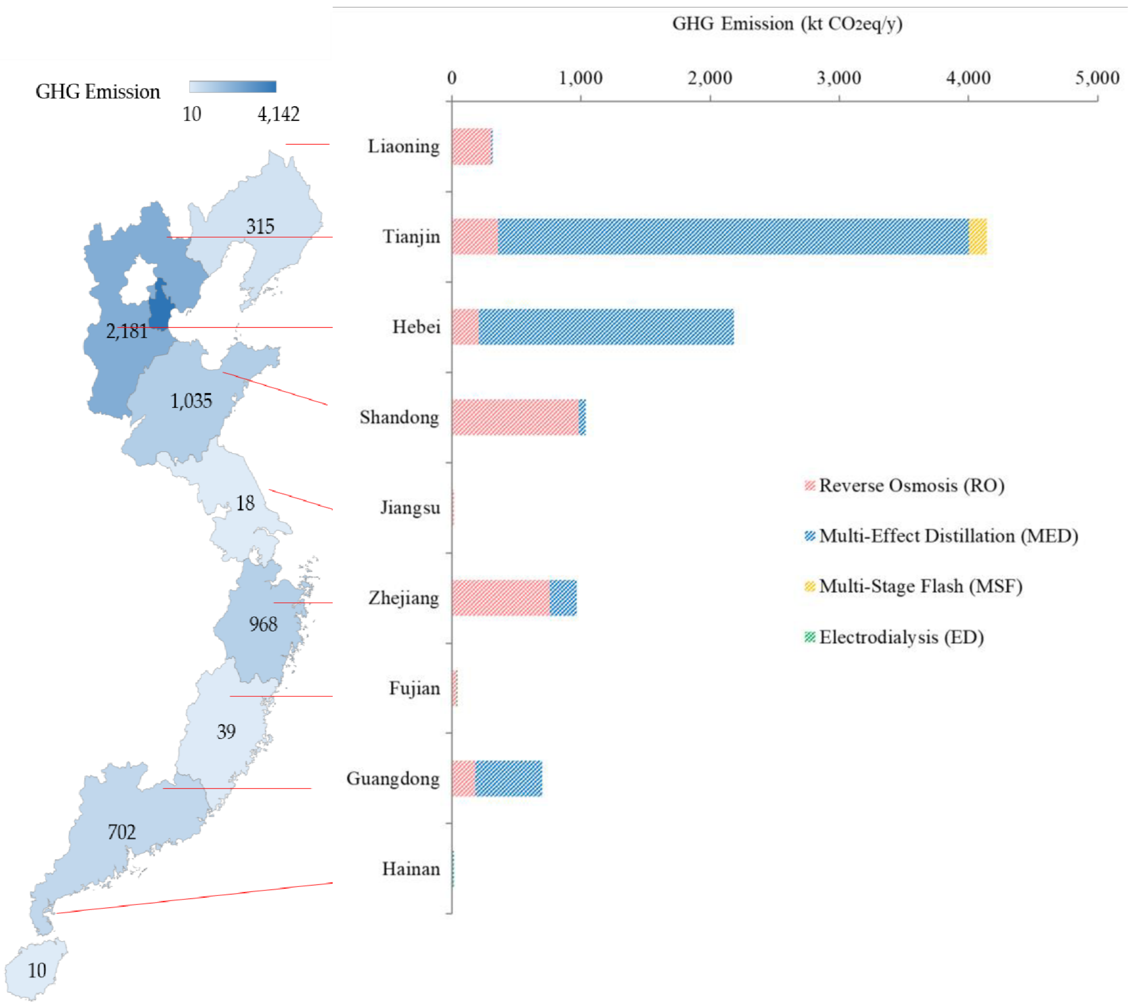

Figure 5-7: GHG emissions of seawater desalination: Regional distribution and breakdowns by processes.

The map in Figure 5-7 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. 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. Shandong Province has the second-largest seawater desalination capacity, but the GHG emissions are much lower (1,035 Mt CO_{2eq}) compared to Hebei, which has larger emissions (2,183 Mt CO_{2eq}) with smaller desalination capacity. The main reason is that the seawater desalination plants in Shandong are all RO plants. For Hebei Province, about 65% of the total desalination capacity is MED, which is more energy and GHG emission-intensive. On the other hand, the south part of China has relatively lower GHG emissions, due to a smaller capacity and less energy-intensive processes.

5.4.2 Unit Product Cost

The Unit Product Cost (UPC) is correlated with the desalination processes and the capacity of the plant, 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 5-8, and the desalination process is specified.

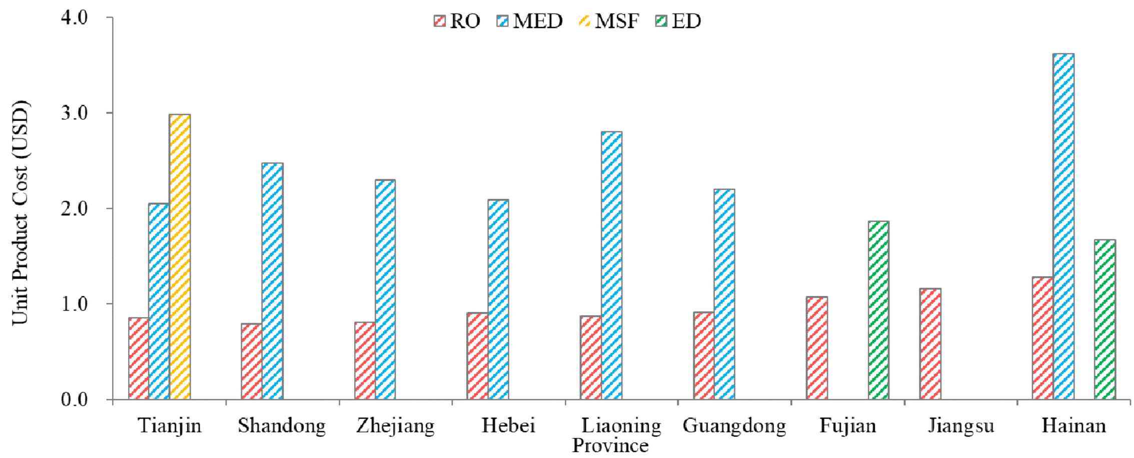

Figure 5-8: Unit product cost of water desalination by provinces in 2016.

The UPC of RO desalination plants shows a slight difference (Figure 5-8). Firstly, 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. 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. The UPC for ED process desalination of Fujian and Hainan are 1.9 and 1.7 USD. It can be seen that for different processes, the UPC in increasing order is RO < MED < ED < MSF, with RO as the cheapest and most applied desalination process. 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.

5.4.3 Discussion and Future Directions

Seawater desalination has high water supply potential, but high energy consumption, GHG emissions, and cost. Water desalination has a considerable water supply potential due to the abundance of its water source, and the desalination technology is improving. On the other hand, this type of water supply is still supported by higher cost and intensive energy consumption and GHG emission. Even though the cost and energy use are decreasing (Shrestha et al., 2011), seawater desalination is still an energy-intensive and costly approach compared to other freshwater alternatives. The World Resources Institute investigated the energy consumption of water desalination plants in Qingdao, Shandong province in China. The results showed that electricity is the main energy used for water desalination (Hua et al., 2014), and the SEC of different water supplies are shown in Table 5-5.

Table 5-5: Energy demand and water supply potentials of water supply alternatives (from (Hua et al., 2014)

Water Supplies	Energy Demand (kWh/m^3)	Water Supply Potential (Mm^3)
Surface water	0.43	980
Water transfer from Yellow River	0.70	1,090
Groundwater	0.78	1,700
Reclaimed water	0.82	2,100
Water transfer from Yangtze river	1.14	2,410
Brackish water desalination	1.40	2,470
Seawater desalination (RO) (Caldera et al., 2016)	4.34	2,650

It showed that for the various water supply alternatives, surface water has the lowest energy demand for per unit water (about 10 % of seawater desalination), and at the same time with the lowest water supply potential (37 % of seawater desalination). On the other hand, seawater desalination (RO process) has the highest energy demand with the highest water supply potential. For other desalination processes, the energy demand is even higher.

This indicates that with the current situation of techniques, a water desalination is still an option with higher cost. Considering the continuously increasing population and the demand for freshwater, seawater desalination has the potential of providing a stable amount of freshwater and should be viewed as a crucial component in the future development of non-conventional water supplies (Zarzo and Prats, 2018). The energy demand and thus GHG emissions are highly related to the capacity and techniques applied in the plant (Pinto and Marques, 2017). The study of Al-Karaghouli and Kazmerski (2013) showed that for a water desalination plant with capacity from 5 to 15 m^3/d, the total electricity consumption would vary from 14.45 to 21.35 kWh/m^3, and the MED process has the highest energy demand, which is inconsistent with the results of this study (Figure 5-8). This indicates the potential for energy consumption and GHG emission reduction can be optimized with improving the combination of capacities and processes. According to the results of (Hua et al., 2014), a case study of Qingdao, the overall cost of different water supplies from the lowest to the highest are local surface water < groundwater < reclaimed water < brackish water desalination < seawater desalination. Seawater desalination is still currently a more expensive approach for producing freshwater compared to other water supply alternatives.

Determining the energy consumption, GHG emissions, as well as the cost of seawater desalination would be helpful to identify the potential of improving the energy efficiency and productivity of seawater desalination. New and advanced technologies, e.g. low energy reverse osmosis membranes, improved energy recovery devices, highly energy-efficient pumps, and optimized pre-treatment systems, can enhance the energy efficiency of seawater desalination. The application of energy recovery units in the desalination processes can also highly increase the energy use efficiency (Attarde et al., 2017). Increasing the efficiency of the process and the application of the energy recovery system will reduce its energy consumption and thereby its CO_2 emissions.

The energy consumption, GHG emissions, and the cost of seawater desalination in China are higher than the average values of the major desalination contributors in East Asia, e.g. Singapore. Singapore has the second-largest seawater desalination capacity of 0.45×10^6

m^3/d (Water Technology, 2018), which is 36% of the seawater desalination capacity of China. The average UPC of the two large scale RO seawater desalination plants is 3.5 $kWh/m^{3,}$ and the cost is estimated as 0.75 USD/m^3 (Grubert et al., 2014), and the price is estimated to increase due to the higher price of energy. The energy consumption and cost per m^3 desalinated water in Singapore are lower than in China. However, as these indicators are affected by the specific process, type, quality, and price of the energy, as well as the location of the plants, etc. The comparison between different countries would be limited to provide insightful information, but a comprehensive analysis of different water supply alternatives, or different desalination processes in the same region would facilitate regional water use management.

The correlation between the UPC and the capacity needs further investigation. In this study, the UPC and capacity of seawater desalination plants showed a very obvious correlation. Identifying this correlation would be helpful for the optimization of seawater desalination. Figure 5-9 showed the trend line of the UPC-availability plots. As MSF and ED are rarely applied, there is not enough sample data, and only RO and MED are discussed. For RO plants, the correlation between the UPC and the capacity fits the logarithmic correlation with a R^2 of 0.9847 and 0.9359 for MED plants.

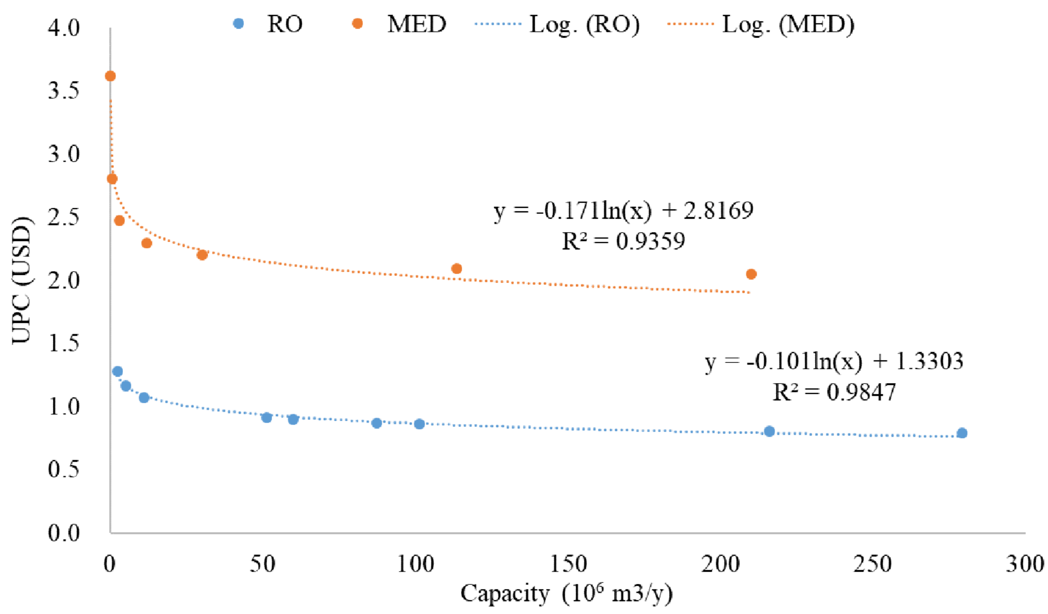

Figure 5-9: The correlation between unit product cost (UPC) and the seawater desalination capacity.

The figure showed a decreasing UPC with the capacity increasing. According to a statistic of China seawater desalination (Hua et al., 2014), in 2016, large plants (capacity > 10^4 m^3/d), the average cost is 6.22 CNY/m^3 (0.90 USD), and the average of desalination cost in medium plants (10^4 < capacity < 10^3) is 7.20 CNY/ m^3 (1.05 USD). In this study, Shandong has the lowest UPC (0.8 USD) with the highest RO capacity of 0.28 × 10^6 m^3/d. Following is Zhejiang, with the same UPC and a RO capacity of 0.22 × 10^6 m^3/d Tianjin. For MED the trend is not clear. The correlation analysis between the capacity and the UPC should be further investigated with more sufficient data.

In addition to energy consumption and GHG emission, there are other potential environmental issues of seawater desalination. Along with the desalted seawater, a remarkable amount of brine is also produced from the process. A common approach is currently to dispose of the brine back to the sea, which might cause harm to the regional aquatic life due to high salinity. The utilization and treatment technologies of the brine are still. Similarly, chemical and thermal pollutions in the near-plant area should be further investigated in future works.

A limitation of this work, which should form the potential future works, is less investigation of the energy consumption by different forms of energy, e.g. heat and electricity in different processes. In this study, the energy used in different processes is converted into electricity due to the limit of data. But it is necessary to investigate different energy forms for a more detailed analysis, and the cost analysis would be more accurate. The usage of renewable energies should also be further reviewed. To cover the whole life cycle, the waste generated during the desalination process, including brine, wastewater, and waste heat should be investigated. Another limit is that the capital cost of the plants should be calculated based on the type of process. Alternatives for process integration should be investigated—e.g. efficiency of using the energy, heat integration, and renewables in water desalination, as well as the utilization of total site heat integration.

5.5 Conclusions

This study analysed the water-related energy consumption and GHG emissions of the seawater desalination industries in China. Seawater desalination is one of the typical examples of water-energy nexus. As the major principle of the process is to use energy to purify the seawater to freshwater, which is an exact illustration of consuming energy to solve the water issue. This study identifies the huge energy consumption and GHG emissions of the whole industry and pointed out the potential direction of expanding the single assessment to a more comprehensive emulation in regional water resource assessment. Seawater desalination is an emerging approach for producing freshwater in China, and the number of plants, as well as the installed capacity, are increasing. Simultaneously, energy consumption and environmental impacts are also increasing. This study initially investigated the energy consumption, GHG emission of the seawater desalination in China from 2006 to 2016, and the unit product cost in 2016. The key findings 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 now being highly encouraged and developed in China and 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 6 CONCLUSIONS AND PROPOSED FUTURE DEVELOPMENT

6.1 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 has been carried out 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 study 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 method is demonstrated with a case study of monosodium glutamate (MSG) plant in China. Results show that to produce 1 t MSG, the QQWFP is 302.1 €, among which the Quantitative Water Footprint is only 2.3 €, and Qualitative Water Footprint is 299.8 €, taking more than 99 % of the total QQWFP. The results 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.

6.2 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. 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 3.2). 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 4). 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 5).

6.3 Future Development

As a scientific research work aiming to seek solutions and inspire new studies, this thesis also identifies the following aspects worth further investigation. The first point is the lack of a water-use database with water quality parameters. Currently, most of the statistical data specify the volume of water use but not the contaminant generation of water use. It is difficult to assess and monitor regional water use (in terms of quality) without a robust database. The second aspect that needs to be further discussed is the consideration of multiple contaminants. The methods proposed in this method (QQWFP and WSPA) accounts the impact of water quality in a very different way. QQWFP determines the cost of treating each kind of contaminants (e.g. COD, BOD, N-NH_3, etc.), which might double counts the cost of treating organic matters and lead to a larger value of contaminant treatment cost. The WSPA did not directly account the absolute value of contaminants (mass/concentration/cost), but uses a relative indicator – Water Quality Index – to quantify the impact of water use on water quality. In this way, detail information such as the contribution of the critical contaminants is lost. In other words, different water using system might have specific requirements for different types of contaminants and generates different contaminants. But when these water flows fall into the same water quality category, these differences are ignored. Further efforts are needed to investigate the quantification of the impact of different contaminants. The third aspect, which has been common in existing assessment/optimisation tools, is to improve the feasibility in practical implementation.

Many indicators widely used in academic research are still rarely used in practice, mainly because the results are difficult to understand or lack of physical meanings. The last point worth further investigation is that in water-related energy consumption assessment, the energy sources (e.g. hydropower, solar power, coal-fired power) should be specified as it is critical in environmental assessment (especially GHG emissions).

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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

APPENDIX

A – Publication List

1. **Jia X.,** Klemeš J.J., Wan Alwi S.R., Varbanov P.S., 2020. Cost-based Quantitative-Qualitative water footprint Considering Multiple Contaminants, RCR. **[IF = 8.086, CiteScore = 10.7]** (Under Review)
2. Yang F., Fan X.Y., **Jia X.X,** Klemeš J.J., Liu Z.Y., 2020. An Iterative Design Approach for Water Networks with Multiple Regeneration Units. Journal of Cleaner Production, p.122483. **[IF = 7.246, CiteScore = 10.9]**
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]**
4. Yang D., **Jia X.,** Dang, M., Han, F., Shi, F., Tanikawa, H., Klemeš, J.J., 2020. Life cycle assessment of cleaner production measures in monosodium glutamate production: A case study in China. Journal of Cleaner Production, p.122126. **[IF = 7.246, CiteScore = 10.9]**
5. Zhang, L., Li, A.H., **Jia, X.,** Klemeš, J.J., Liu, Z.Y., 2020. Design of Total Water Networks of Multiple Properties based on Operator Potential Concepts and an Iterative Procedure. Energy & Environment, p.122483. **[IF = 1.775].**
6. **Jia, X**., Varbanov, P.S., Wan Alwi, S.R., Klemeš, J.J., 2020. Total Site Water Main Concentration Selection: A Case Study, Chemical Engineering Transactions, 81, 259-264. DOI: 10.3303/CET2081044. **[CiteScore = 1.3]**
7. **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]**
8. **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]**
9. **Jia, X**., Klemeš, J.J., Wan Alwi, S.R., Varbanov, P.S., 2019. Blue Water Footprint of the Czech Republic. Chemical Engineering Transactions, 76, DOI: 10.3303/CET1976178. **[CiteScore = 1.3]**
10. Makarova, A.S., **Jia, X.,** Kruchina, E.B., Kudryavtseva, E.I. and Kukushsin, I.G., 2019. Environmental Performance Assessment of the Chemical Industries Involved in the Responsible Care® Program: Case Study of the Russian Federation. Journal of Cleaner Production, 222, 971-985. **[IF = 7.246, CiteScore = 10.9]**
11. Fan, X.Y., Klemeš, J.J., **Jia, X.,** Liu, Z.Y., 2019. An iterative method for design of total water networks with multiple contaminants. Journal of Cleaner Production, 240, p.118098. **[IF = 7.246, CiteScore = 10.9]**
12. Klemeš, J.J., Varbanov, P.V., Walmsley, T.G., **Jia, X.,** 2018. New directions in the implementation of Pinch Methodology (PM). Renewable and Sustainable Energy Reviews, 98, 439-468. **[IF = 10.556, CiteScore = 25.5]**

13. Varbanov P.S., **Jia X.**, Kukulka D.J., Liu X., Klemeš J.J., 2018. Emission Minimisation by Improving Heat Transfer, Energy Conversion, CO_2 Integration and Effective Training, Applied Thermal Engineering, 131, 531-539. **[IF = 4.026, CiteScore = 8.8]**
14. **Jia X.,** Klemeš J.J.; Varbanov P.S.; Wan Alwi S.R., Energy-emission-waste nexus of food deliveries in China, Chemical Engineering Transactions, 70, 661-666, DOI: 10.3303/CET1870111. **[CiteScore = 1.3]**
15. Varbanov P.S., Walmsley T.G., Klemeš J.J., Wang, Y., **Jia, X.**, 2018. Footprint Reduction Strategy for Industrial Site Operation. Chemical Engineering Transactions, 67, 607-612. DOI: 10.3303/CET1867102. **[CiteScore = 1.3]**
16. Walmsley T.G., **Jia X.,** M., Nemet A., Liew P.Y., Klemeš J.J., Varbanov P.S., 2018. Total Site Utility System Structural Design Using P-graph, Chemical Engineering Transactions, 63, 31-35. DOI: 10.3303/CET1863006. **[CiteScore = 1.3]**
17. Ren X.Y., **Jia X.,** Varbanov P.S., Klemeš J.J., Liu Z.Y., 2018. Targeting the cogeneration potential for Total Site utility systems, Journal of Cleaner Production, 170, 625-635. **[IF = 7.246, CiteScore = 10.9]**
18. **Jia, X.,** Varbanov, P.S., Walmsley, T.G., Klemeš, J.J., Ren, X.Y., Liu, Z.Y., 2018. Extended Indicators for Total Site Targeting. Chemical Engineering Transactions, 63, 211-216. DOI: 10.3303/CET1863036. **[CiteScore = 1.3]**
19. Walmsley, T.G., **Jia, X.,** Varbanov, P.S., Klemeš, J.J., Wang, Y., 2018. Total Site Utility Systems Structural Design Considering Environmental Impacts. In Computer Aided Chemical Engineering, 43, 1305-1310, Elsevier.
20. **Jia X.,** Varbanov P.S., Walmsley T.G., Yan Y., 2017, Water Pollution Impact Assessment of Beijing from 2011 to 2015: Implication for Degradation Reduction, Chemical Engineering Transactions 61, 1525-1531. DOI: 10.3303/CET1761252. **[CiteScore = 1.3]**
21. Ren X.Y., **Jia X.,** Varbanov P.S., Klemeš J.J., Liu Z.-Y, 2017, Calculation of Cogeneration Potential of Total Site Utility Systems with Commercial Simulator, Chemical Engineering Transactions 61, DOI: 10.3303/CET1761203. **[CiteScore = 1.3]**

B – List of Presentations at International Conferences

1. **Jia X**., Klemeš, J.J., Wan Alwi, S.R., Varbanov, P.S. A Modified Water Scarcity Pinch for Regional Water Use Assessment and Optimisation, 4^{th} SEE SDEWES Conference 2020, Online
2. Jia X., Varbanov, P.S., Wan Alwi, S.R., Klemeš, J.J. Total Site Water Main Concentration Selection, 23^{rd} PRES Conference 2020. Online
3. Jia X., Klemeš, J.J., Varbanov, P.S., Wan Alwi, S.R. Blue Water Footprint of the Czech Republic, 22th PRES 2019, Crete, Greece
4. Jia X., Klemeš, J.J., Varbanov, P.S., Wan Alwi, S.R. Water-Energy Nexus in Seawater

Desalination, 14th SDEWES 2019, Dubrovnik, Croatia

5. Jia X., Klemeš, J.J., Varbanov, P.S., Wan Alwi, S.R. Overview of the Water Desalination in China: Development, Energy Demand and Emissions. 13th SDEWES 2018, Palermo, Italy
6. Jia X. X., Klemeš, J. J., Varbanov, P. S., Wan Alwi, S. R. Energy-emission-waste nexus of food deliveries in China. 21st PRES 2018, Prague, Czech Republic
7. Jia X., Klemeš, J.J., Varbanov, P.V., Alwi, S.R.W. Impact of Water Scarcity and Degradation on Urban Ecosystem Services. 3rd SEE SDEWES 2018, Novi Sad, Serbia
8. Jia X., Klemeš, J.J., Varbanov, P.V., Alwi, S.R.W. Water Desalination: Development and Energy Demand, ICCHMT 2018, Krakow, Poland
9. Jia X., Varbanov, P.V., Klemeš, J.J. Overview and Perspectives of Water Availability Footprint, 12th SDEWES 2017, Dubrovnik, Croatia
10. Jia X., Varbanov, P.V., Walmsley, T.G., Yan Y. Water Degradation Potential: Case study of Beijing, 20th PRES Conference 2017, Tianjin, China