Improved life cycle assessment for desalination : handling the choices and uncertainties

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2014

Zhou, J. (2014). Improved life cycle assessment for desalination : handling the choices and uncertainties. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/55342>

<https://doi.org/10.32657/10356/55342>

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IMPROVED LCA FOR DESALINATION

ZHOU JIN

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HANDLING THE CHOICES AND UNCERTAINTIES**

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School of Civil and Environmental Engineering

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A thesis submitted to the Nanyang Technological University
in fulfilment of the requirements for the degree of
Doctor of Philosophy

2014

ACKNOWLEDGEMENT

The author thanks the Singapore Membrane Technology Center (SMTc) for the funding support of this work. The author also thanks Professor Anthony G. Fane and Professor Victor W.-C. Chang for their continuous guidance of my work.

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SUMMARY

A large number of choices are involved in desalination LCA studies. The aim of this study was to investigate how the choices influence the desalination LCA's outcome, and further explore the approaches in order to capture the technique features and local context to improve the reliability of the results. This work investigated three choices which were considered as high-priority problems in LCA, including the choice of the system boundary, the choice of characterization approach, the choice of in-stock dataset as representative data for background characteristics.

The critical review revealed the lack of consensus on the system boundary definition. Particular attention was given to three phases in foreground system of desalination LCAs, including infrastructure, chemical, and membrane phases. This work proposed to select their system boundaries according to the goal and scope. The advantage of proposed choice was to avoid large uncertainties due to the arbitrary and inconsistent choice. In addition, it also reduced the requirement of on-site primary data by identifying the significant elements in three phases.

To examine the impacts by the choice of predefined life cycle impact assessment method on the result of desalination LCAs, a comparison study was carried out between a generic method and a regional specific method. The results indicated the choice do make a significant difference in the LCA characterization results of desalination. The divergences in the coverage level of different material flows, characterization models, and environmental interventions were identified as the major reasons. This study also provided some suggestions in choosing the appropriate predefined impact assessment method. Both generic method and regional specific method have merits and limitations in desalination applications. The choice should depend on the inventories' availability and also the specific concerns in desalination

technology and local environmental uniqueness. Singapore is still in the early stage of LCA, therefore the generic predefined impact assessment method is recommended for Singapore's desalination LCAs. However, the generic method cannot capture the features of the brine disposal process. Therefore, an improved characterization approach, namely group-by-group approach was developed to estimate the aquatic eco-toxic impact of brine disposal. A comparison study was carried out between the proposed approach and the other two current approaches (chemical-by-chemical approach and whole effluent approach). The results indicated the improved approach reduces the reliance on the comprehensive chemical composition analysis and temporal ecotoxicology test of the complex desalination brine. It also provided a more comprehensive coverage, not only considering the impact of organic chemicals and metals, but also including the contribution of inorganic chemicals.

To investigate the impacts by the choice of in-stock dataset for background system, this thesis compared the environmental burdens of a desalination plant with three different electricity production models in the United States, Singapore, and Spain. One potential problem was that the existing database cannot represent Singapore's local characteristics. This work proposed a cost-effect way to develop the Singapore-specific background data for energy production by taking advantage of in-stock Ecoinvent dataset. The system boundary and characterization approach was selected based on our previous findings. This work provided the environment profile of Singapore's desalinations with improved reliability. The results highlighted Singapore, the country with unique fuel mixes for electricity generation, achieves relatively better environmental savings in most impact categories at the current stage due to engaging a high percentage of natural gas in the fossil fuel matrix.

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LIST OF ACRONYMS

ADP	Abiotic depletion potential
AP	Acidification potential
CDI	Capacitance deionization
CF	Characterization factors
CH	Switzerland
C-HTP	Carcinogenic Human toxicity potential
ED	Electrodialysis
EF	Effect factor
EIO-LCA	Economic-input output life cycle assessment
EP	Eutrophication potential
ES	Spain
ETP	Ecotoxicity potential
ETT	Effluent toxicity test
FEATP	Fresh-water aquatic eco-toxicity potential
FF	Fate factor
FO	Forward osmosis
GH	Gas hydrates
GHG	Greenhouse gas
GLO	Global
GWP	Global warming potential
HDH	Freezing, humidification-dehumidification
HTP	Human toxicity potential
ICE	Integrating controlling of effluents

LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
MAETP	Marine aquatic eco-toxicity potential
MBR	Membrane bioreactor
MED	Multiple-effect distillation
MD	Membrane distillation
MSF	Multi-stage flash
nC-HTP	Non carcinogenic human toxicity potential
ODP	Ozone depletion potential
POCP	Photochemical oxidation potential
RER	Europe
RO	Reverse osmosis
SG	Singapore
TETP	Terrestrial eco-toxicity potential
VC	Vapor compression
WEER	Whole effluent environmental risk
WET	Whole effluent toxicity
XF	Exposure factor

CHAPTER 1 INTRODUCTION

1.1 Desalination and its Environmental Concerns

Desalination technology has been successfully implemented for decades as a supplementary or even the main water source. It is estimated that the capital expenditures for new desalination plants will exceed US\$17 billion by the year 2016 (Subramani, A. *et al.* 2011). The desalination processes can roughly be categorized into two major types: thermal and membrane separation (Van der Bruggen, B. and Vandecasteele, C. 2002; Subramani, A. *et al.* 2011). The thermal distillation process mimics the natural water cycle of evaporation and condensation, and further produces output water with very low salt concentration (Van der Bruggen, B. and Vandecasteele, C. 2002). Multi-stage flash (MSF) and Multiple-effect distillation (MED) are major commercial thermal desalination technologies. The membrane separation process works by prohibiting or permitting the passage of certain salts ions. Reverse osmosis (RO) is the most popular commercial membrane process in the current industry (Malaeb, L. and Ayoub, G.M. 2011). Other than these two types of technologies, there are other emerging technologies that are not widely used at present or are still under development, such as vapor compression (VC), electrodialysis (ED), forward osmosis (FO), membrane distillation (MD), capacitance deionization (CDI), gas hydrates (GH), freezing, humidification-dehumidification (HDH) and solar stills (Mezher, T. *et al.* 2010).

The commercial desalination technologies had attracted increasing concerns, mainly due to the energy requirements, membrane and chemical usage, as well as the concentrate disposal. Both thermal-based and RO technologies are energy-intensive, and the energy is always among the major operating cost component (Avlonitis, S.A. *et al.* 2003; Semiat, R. 2008; Ludwig, H. 2009). Another important factor of RO technology is the membrane cost because they must be replaced regularly to restore the performance (Marwan, M.A. 1993;

Duranceau, S.J. 2000; Avlonitis, S.A. *et al.* 2003; Fernandez-alvarez, G. *et al.* 2010). In addition, chemical usages are inevitable in the pretreatment and post-treatment of desalination plants. Typical chemicals include the acidic solutions used to adjust pH, coagulants/flocculants used to remove the suspended matter, the inhibitors used to prevent scale, fouling, and foam formation, the membrane cleaning solution, *etc.* (Hoepner, T. and Lattemann, S. 2003; Sadhwani, J.J. *et al.* 2005).

The environmental impact of desalination processes is often neglected for various reasons, although it does contribute to the different impact categories at different levels. For example, the concentrated retentate is an unwanted byproduct which is discharged to the environment in the desalination processes. The concentrate disposal is very likely to affect the environmental and the marine life due to the high salinity and the additional chemicals discharged with the brine (Miri, R. and Chouikhi, A. 2005; Sadhwani, J.J. *et al.* 2005; Abdul-Wahab, S.A. 2007). In addition, the intensive energy required for the desalination processes is inevitably associated with the pollutant fluxes in the power generation. Various air pollutants, including sulfur dioxide, nitrogen oxides, hydrocarbon compounds, carbon monoxide, and particulate matters, are among typical concerns. Moreover, Green House Gas (GHG) from fossil fuel burning is a major contributor to global warming (Zhou, J. *et al.* 2011a). Additional atmospheric discharges are also found in the production of membranes and chemicals (Van der Bruggen, B. and Vandecasteele, C. 2002; Sadhwani, J.J. *et al.* 2005). Other than the clean water, the concentrated retentate is also a product of desalination processes.

1.2 Life Cycle Assessment (LCA): Definition, Principles and Advantages

As more and more parties become concerned about the issues of natural resource depletion and environmental degradation caused by the desalination process, the designers, owners, and operators of desalination plants are

investigating ways to minimize their effects. Thus, explore ways of moving beyond compliance using pollution prevention strategies and environmental management systems will be advantageous to improve their environmental performance. One useful tool is Life Cycle Assessment (LCA). There are two primary types of LCA methodologies, including process-based LCA and economic-input output LCA (EIO-LCA). The Process-based LCA is centred on scientifically analysing the actual process (i.e. mass/material balance, scientific characteristics, *etc.*). The ISO Standards, which will be further discussed, are primarily concerned with the process-based methodology. Unlike Process-based LCA tracing out the various resource requirements and environmental emissions associated with a particular process, the EIO-LCA appends the information on the emissions to the environment with the economic transactions between industries (Carnegie Mellon 2010). Given the economic nature of EIO-LCA and its limited applications in desalination processes, this paper will mainly focus on the process-based LCA.

According to ISO standards, a “cradle-to-grave” approach for assessing environmental impacts of products, beginning with the gathering of raw material from earth to create the product and ending at the point when all materials are returned to earth (Pasqualino, J.C. *et al.* 2009). The LCA process is a systematic approach and its framework consists of four principles (ISO 1997; ISO 1998; ISO 2000a; ISO 2000b; ISO 2006).

The ‘**goal and scope definition**’ attempts to set the extent of the inquiry as well as specify the methods used to conduct it in later phases (ISO 1998). It is important to select the functional unit and system boundary during this defining phase. The functional unit describes the primary purpose of a system and enables different systems to be treated as functionally equivalent (Guinee, J.B. *et al.* 2002). The functional unit is often defined as 1 m³ produced water for a desalination system. Boundary selection determines the processes and activities included in a LCA study. Its determination is affected by various

factors such as the purpose of the study, impacted geographic area, relevant time horizon, *etc.* (Reap, J. *et al.* 2008a). Life cycle '**inventory analysis**' is a methodology for estimating the consumption of resources, the quantities of waste flows and emissions caused by, or otherwise attributable to, a product's life cycle (Rebitzer, G. *et al.* 2004). For a desalination plant, the associated material flows, energy flows as well as other environmental exchanges between air, water, and soil are modelled to represent the total inputs/outputs that occur during the life cycle of this plant. Life cycle '**impact assessment**' (LCIA) is to evaluate the product life cycle, on a functional unit basis, in terms of several impact categories (such as climate change, toxicological stress, noise, land use, *etc.*) and, in some cases, in an aggregated way (such as years of human life lost due to climate change, carcinogenic effects, *etc.*) (Rebitzer, G. *et al.* 2004). A few predefined LCIA methods are available in the market, such as Eco-indicator 99, CML, IMPACT2002+, *etc.* In general, the environmental impacts of products may be classified into three different types: the characterization step is usually defined as compulsory in all LCIA methods, while the normalization and weighting are sometimes considered as optional. The '**interpretation**' phase helps make a more informed decision with a cleared understanding of uncertainties and assumptions. ISO 14044 recommend several checks to ensure the conclusion, including contribution analysis, uncertainty analysis, sensitivity analysis, *etc.* The iterations between life cycle interpretation and the other LCA phases often occurs to improve the overall processes (Reap, J. *et al.* 2008b).

One of the biggest advantages for LCA is the holistic evaluation. It enables the estimation of the cumulative environmental impacts resulting from all stages in the product life cycle (desalinated water in this study), often including impacts not considered in more traditional analyses (*e.g.*, the water resource extraction, the production of electricity and materials, brine disposal in desalination system) (Zhou, J. *et al.* 2011a; Zhou, J. *et al.* 2011b). By including the impacts

throughout the product life cycle, LCA provides a comprehensive view of the environmental aspects and a more accurate picture of the true environmental trade-offs in process selection.

Although LCA is a relatively new methodology with a history extending over only three decades, it's getting more and more popular due to the wide application spectrum for various users including industry operators, government authorities, and business stakeholders. LCA has become a core element in assessing environmental impact, shaping environmental policy or in spurring voluntary actions in the European Union, USA, Japan, Korea, Canada, and Australia and is upcoming in booming economies such as India and China (Guinee, J.B. *et al.* 2011). In addition, there has been a remarkable growth in LCA research after the standardization of LCA methodology in 1990s, which is reflected by large number of articles published. SciVerse Scopus mentions over 6000 articles, which is nearly triple the number published before 2000.

1.3 Overview of Prior LCA Studies in Desalination

There had been a number of LCA studies on the major commercial desalination technologies, including Multi-stage flash (MSF), Multiple-effect distillation (MED), and Reverse Osmosis (RO). These LCA studies sometimes were designed to answer different research questions such as to compare different desalination technologies, or to compare the whole water supply or water reuse plans, or to explore different solutions to reduce the environmental burdens. The studies covered are listed in Tables 1-1, 1-2, 1-3, and 1-4.

Since 1990s, life cycle thinking has been used in desalination applications to compare thermal distillation and reverse osmosis. Morton and Callister (1997) qualitatively examined two sea water desalination plants in the Middle East, and identified that membrane process provided advantages over the multi-stage flash (MSF) distillation process, in terms of both marine and

Table 1-1. Chronological review of LCA studies of desalination (a)

Ref	Objective	LCA tool	Background database	Geographical coverage	Scale *	Primary data	LCIA method/ indicator	Uncertainty analysis	Other assessment
(Tarnacki, K. <i>et al.</i> 2012)	Comparing RO with Menstill	NR	Ecoinvent	ES, FR, PT, NL, DE	TS2+TS3	Yes	CML	NA	Nil
(Salcedo, R. <i>et al.</i> 2012)	Evaluating the SWRO+soalr ranking cycles	manual	Ecoinvent	ES	TS3	part	CO ₂	NA	+economic evaluation
(Hancock, N.T. <i>et al.</i> 2012)	Comparing SWRO with a novel hybrid process	Simapro	Ecoinvent	Lab scale	TS2+TS3	Yes	CML	NA	Nil
(Jijakli, K. <i>et al.</i> 2012)	Comparing local BW solar distill, local PV-BWRO, and distant BWRO	Simapro	Ecoinvent	UAE	TS2+TS3	Yes	Eco-indicator99	NA	Rough Economic estimation
(Zhou, J. <i>et al.</i> 2011a)	Comparing BWRO with different LCIA method	Simapro	Ecoinvent	ES	TS3	Yes	CML, TRACI	Monte Carlo	NIL
(Zhou, J. <i>et al.</i> 2011b)	Comparing BWRO with different energy production scenario	Simapro	Ecoinvent	SG, US, ES	TS3	Yes	CML	Monte Carlo	Nil
(Meneses, M. <i>et al.</i> 2010)	Comparing different brine disposal scenarios	SiSOSTA QUA	Ecoinvent	ES	TS1+TS2+TS3+TS4	Yes	CML, FWU, WG, S	NA	Nil
(Beery, M. and Repke, J.U. 2010a; Beery, M. <i>et al.</i> 2010b; Beery, M. <i>et al.</i> 2011)	Comparing MMF+SWRO, UF+SWRO, UF+UV+SWRO	GaBi	PE database	NR	TS2+TS3	NIL	CO ₂	NA	LCC
(Munoz, I. <i>et al.</i> 2010)	Comparing the Ebro river water transfer and AGUA program	Simapro	Ecoinvent	Spain	TS1+TS2+TS3+TS4+TS5	Nil	GWP, HTP, POCP, AP, energy demand	Interval arithmetic	Nil

* TS1 – raw water transport; TS2 – pre-treatment; TS3 – desalting operation; TS4 – post treatment; TS5 – clean water distribution and storage

Table 1-2. Chronological review of LCA studies of desalination (b)

Ref	Objective	LCA tool	Background database	Geographical coverage	Scale	Primary data	LCIA method/ indicators	Uncertainty analysis	Other assessment
(Frutos, A.R. <i>et al.</i> 2009)	Comparing different phase in SWRO	Manual	Not specify	Lab scale	TS2+TS3+TS4	Nil	CO ₂	NA	Nil
(Biswas, W.K. 2009)	Comparing the SWRO with non-renewable energy source and with renewable energy sources	Manual	Local dataset, Ecoinvent	Australia	TS2+TS3+TS4	Yes	CO ₂	NA	Nil
(Vince, F. <i>et al.</i> 2009)	Comparing different phases in SWRO	Eolia Potable Water	Ecoinvent	Australia	TS1+TS2+TS3+TS4+TS5	Part	Impact 2002+	NA	Nil
(Lyons, E. <i>et al.</i> 2009)	Comparing three water scenarios: importation, reclamation, and desalination	Simapro	Ecoinvent	US	TS1+TS2+TS3+TS4+TS5	yes	Eco-indicator99	NA	Single score
(Vince, F. <i>et al.</i> 2008)	Comparing local GW, distant surface water transfer, local SWRO, and Local MED	Not specify	PE database, Ecoinvent	EU	TS1+TS2+TS3+TS4+TS5	Nil	Impact 2002+	NA	NIL
(Munoz, I. and Fernandez-Alba, A.R. 2008)	Comparing BWRO and SWRO	Simapro	Ecoinvent	Spain	TS3	yes	GWP, HTP, POCP, AP, energy demand, TDS	Interval arithmetic	Nil

* TS1 – raw water transport; TS2 – pre-treatment; TS3 – desalting operation; TS4 – post treatment; TS5 – clean water distribution and storage

Table 1-3. Chronological review of LCA studies of desalination (c)

Ref	Objective	LCA tool	Background database	Geographical coverage	Scale	Primary data	LCIA method/ indicator	Uncertainty analysis	Other assessment
(Raluy, R.G. <i>et al.</i> 2006)	Comparing 3 different desalination technologies, RO, MSF, and MED,	Simapro	Ecoinvent	Spain	TS3	Nil	CML Eco-points97 Eco-indicator99	Nil	Single score
(Stokes, J. and Horvath, A. 2006)	Comparing MMWD and OWD water system	WEST	Not specify	US	TS1+TS2+TS3+T S4+TS5	yes	GWP, SO _x , NO _x , PM, VOC, CO	Yes	External cost
(Raluy, R.G. <i>et al.</i> 2005b) 2005.10.4	Comparing SWRO, MED, MSF	Simapro	Ecoinvent	Spain	TS3	Not specify	CML Eco-points97 Eco-indicator99	Nil	Single score
(Tangsubkul, N. <i>et al.</i> 2005)	Compare different water recycling technology (ozone+CMF, MBR+RO, and WSP)	Hybrid tool	MIET + local database	AU	TS2+TS3	Partial	Partial CML + SP	Yes	NO
(Raluy, R.G. <i>et al.</i> 2005c) 2005.10.5	Comparing SWRO with ERWT	Simapro	Ecoinvent	Spain	TS1+TS2+TS3+T S4+TS5	Part	CML Eco-points97 Eco-indicator99	Nil	Single score
(Lundie, S. <i>et al.</i> 2005)	Comparing current metropolitan water service with possible future scenarios	GaBi	Not specify	Australia	TS1+TS2+TS3+T S4+TS5	Nil	Total energy use, water use, GWP, EP, POCP, HTP, FAETP, MAETP, TETP	Nil	Nil

* TS1 – raw water transport; TS2 – pre-treatment; TS3 – desalting operation; TS4 – post treatment; TS5 – clean water distribution and storage

Table 1-4. Chronological review of LCA studies of desalination (d)

Ref	Objective	LCA tool	Background database	Geographical coverage	Scale	Primary data	LCIA method/ indicator	Uncertainty analysis	Other assessment
(Raluy, R.G. <i>et al.</i> 2005a)	Comparing 3 different desalination technologies, RO, MSF, and MED, integrate with renewable energies	Simapro	Ecoinvent	Spain	TS3	Nil	CML Eco-points97 Eco-indicator99	Nil	Single score
(Lundie, S. <i>et al.</i> 2004)	Comparing different metropolitan water service scenarios	GaBi	PE database	Australia	TS1+TS2+TS3+ TS4+TS5	Nil	Total energy use, water use, GWP, EP, POCP, HTP, FAETP, MAETP, TETP	Nil	Nil
(Raluy, R.G. <i>et al.</i> 2004)	Comparing 3 different desalination technologies, RO, MSF, and MED, integrate with different energy production systems	Simapro	Ecoinvent	Spain	TS3	Nil	CML Eco-points97 Eco-indicator99	Nil	Single score

* TS1 – raw water transport; TS2 – pre-treatment; TS3 – desalting operation; TS4 – post treatment; TS5 – clean water distribution and storage

atmospheric discharges. With the standardization of LCA methodology, several attempts had been made to quantitatively estimate the environmental impacts from desalination plants. Raluy *et.al.* (2005b; 2006) compared the environmental loads associated with MSF, MED, and RO by means of LCA methodology. The results showed that the environmental burden associated with RO is one-order of magnitude lower than that with thermal process without taking advantage of the residual heat.

As the RO technology was considered as more environmentally-friendly and commercially-competitive, more research efforts were made to investigate its pre-treatment and energy consumption. Beery *et.al.* (2010a; 2010b; 2011) compared different pre-treatment methods and indicated that the environmental performance of the RO desalination plant was highly dependent on the effectiveness of each pre-treatment method. Raluy and his colleagues (2005b; 2006) confirmed the energy plays a key role in RO desalination as more than 80% of the environmental impact is associated with the electricity consumption. Some other studies on RO desalination were carried out by Abel Rianza Frutos (2009), Biswas (2009), Vince (2009), which lead to similar conclusions on the dominant role of electricity.

Some researchers had used LCA to evaluate different water supply plans. Lundie *et.al.* (2004; 2005), Stokes *et.al.* (2006), Raluy *et.al.*(2005c), Vince (2009), Lyons *et.al.*(2009), and Munoz *et.al.*(2010) compared local desalination with alternative water supply systems (waste water reclamation and surface water transfer). Many had found that the long distance surface water transport requires significant amount of energy, and the associated environmental impact can be comparable with that from the RO desalination. Compared to the waste water reclamation, desalination is suitable to relieve the water stress in potable applications, but might not be appropriate for non-potable purposes due to its high energy consumption.

Other than comparing different desalination technologies and water supply plans, LCA is also used in exploring the solutions to relieve the environmental burdens. Since most environmental impacts are highly

associated with energy demand of desalination, any reduction in energy usage can help lower the environmental impact. According to the LCA results, reducing the salinity of feed water (Munoz, I. and Fernandez-Alba, A.R. 2008), using effective pre-treatment (Beery, M. and Repke, J.U. 2010a; Beery, M. *et al.* 2010b; Beery, M. *et al.* 2011), employing new membrane technology (Hancock, N.T. *et al.* 2012), controlling the impact of concentrate disposal are the promising ways to reduce the overall environmental impact. Another method to improve the environmental performance of desalination is to reduce the heavily reliance on fossil fuel energy. The LCA studies demonstrated moving towards cleaner energy sources, such as natural gas (Zhou, J. *et al.* 2011b), and renewable energies (Biswas, W.K. 2009; Jijakli, K. *et al.* 2012; Salcedo, R. *et al.* 2012) is beneficial.

1.4 Concerns about LCA Reliability

From previous sections, we observed that the environmental impact of desalination is receiving great interests and many LCAs have been published for desalination. However, concerns about the quality of LCA results, not only for desalination LCAs, but for other LCA efforts, have been raised at early stage of LCA development. The decision makers have the impression that the LCAs are of low confidence, owing to their high uncertainty. The reliability of life cycle assessment (LCA) is affected by the data quality as many were not collected for LCA purposes (Rebitzer, G. *et al.* 2004). This may lead to decisions that are unnecessarily costly, or mislead public perception about the environmental profile of a product or process. These are long-since acknowledged problems (Pennington, D.W. *et al.* 2004; Reap, J. *et al.* 2008a; Reap, J. *et al.* 2008b).

Several researchers have put forward different typologies of uncertainty (Van Der Sluijs, J.P. *et al.* 2005; Refsgaard, J.C. *et al.* 2007; Ascough II, J.C. *et al.* 2008). Although a fully satisfying classification may be difficult to agree upon, one should acknowledge that the uncertainties in LCA, and indeed any model, are related to three sources (Björklund, A.E. 2002):

- Data, *e.g.* the energy use and the membrane renewal rate of a desalination plant, the chemical consumption of membrane cleaning process, *etc.*
- Relationship, *e.g.* the linear relationship in concentration-response, the linear dependence of effect factor on 1/ED50, the formula used to derive chronic effect from acute impact, *etc.*
- Choice, *e.g.* the choice of system boundaries, the predefined life cycle impact assessment models, the commercial datasets, *etc.*

If LCA studies address uncertainty, the analysis is typically limited to data uncertainties. The ISO 14044 standard (2006) and other researchers (Huijbregts, M.A.J. 1998a; Huijbregts, M.A.J. 1998b; Björklund, A.E. 2002) have presented uncertainty analysis to quantify the data uncertainties by applying uncertainty ranges and performing a statistical analysis (*e.g.* Monte Carlo simulation, Bayesian analysis, fuzzy set theory, *etc.*). It should be noted that the uncertainty analysis aims to explicitly incorporate the uncertainties. Although it may imply collecting better data is a way to reduce uncertainties, carrying out LCA would become much more time-consuming due to the additional data collection efforts. The urgency of environmental questions often requires swift action and forbids decision makers to wait for the better data for all matters.

In most instances, the relationship uncertainties are usually not considered in LCA studies because of their temporal and spatial complexity (Huijbregts, M.A.J. 1998a). Similar to data uncertainties, doing more research and making models with higher resolution would reduce the uncertainties related to relationship, but same problems arise in the additional long time used to wait for all complete evidence for the improved models. Moreover, it is difficult to incorporate the relationship uncertainties via uncertainty analysis because software platforms do not always support the inclusion of uncertainty distribution for relationships (Finnveden, G. *et al.* 2009).

In contrast to uncertainties related to data and relationship, it is more practical to enhance the confidence of LCA results through managing uncertainties due to choices. Although some choices are mainly derived from lack in knowledge, whereby the subjectivity, without any science being involved, would pose high uncertainties, the credibility and transparency of LCAs would be improved by making rational choices based on technique features or local contextual preference. The ISO standard (2006) presents another technique, namely sensitivity analysis (scenario analysis), to analyse uncertainties, but so far, its application is still restricted to incorporate uncertainties through identification of the most influential LCA inputs or evaluation of possible future situations that reflect different perspectives. Guidance and practice to reduce uncertainties due to choices is still missing.

1.5 Aim and Scope

As mentioned previously, there are several important factors that can affect LCA outcomes significantly. Some previous studies have made attempts to incorporate the data uncertainties into their frameworks, but none have clearly addressed the issue to handle the uncertainties due to different choices. Therefore, this thesis focuses on the choice-related uncertainties. Other than investigating how the choices affect the LCA result, additional attention is given to provide recommendations to control uncertainty due to choices. As discussed in Section 1.4, the uncertainty reduction can be achieved by formulating “good choices” which can capture the technique features and local contextual preferences. In this thesis, we focus on the desalination technology and Singapore context.

A large number of choices are involved in desalination LCA studies and Tables 1-1, 1-2, 1-3, and 1-4 only listed several of them. This thesis investigates three choices which are considered as high-priority problems in LCA (Reap, J. *et al.* 2008b), including

- the choice of the system boundary

- the choice of characterization approach, including the choice of predefined life cycle impact assessment approach and specific characterization approach for concentrate disposal
- the choice of in-stock dataset as representative data for background characteristics

For each choice listed above, two research scopes are addressed: (1) How the environmental performance of desalination changes due to the choice; (2) How to capture the technique features and local context of desalination to make “good choices”.

1.6 Structure of the Thesis

The structure of the thesis is illustrated in Figure 1-1.

After the introduction (Chapter 1), Chapter 2 presents the comprehensive system boundary for desalination. In practice, the previous studies narrowed the boundary due to the data constraints. Therefore, a review study is carried out to identify inputs, and also assumptions/conditions, which are considered as minor contributors and can be ignored from system boundary. Particular attention is given to infrastructure, chemical, and membrane phases due to the unique characteristics of desalination industry. Recommendations are provided to reduce the uncertainties by outlining the important criteria in drawing the system boundary for desalination.

Chapter 3 and Chapter 4 investigate the influence of the choice in characterization approach. Chapter 3 focuses on the predefined life cycle impact assessment method, which consists of a set of characterization approaches. A comparison study is carried out between a generic method and a regional specific method to verify whether, and to what extent, the choice of predefined method affects the desalination LCA results. Through the discussion on the associated impacts from different choices, this chapter outlines the guidelines to choose the predefined impact assessment method and the processes to develop specialized characterization approach for

desalination applications. Based on the strategy for developing desalination-specialized characterization approach, Chapter 4 makes an attempt to develop an improved approach for assessing aquatic eco-toxic impact of brine disposal. The propose method combines two available approaches to reduce data demand and increase the comprehensiveness. A case study is engaged to illustrate the differences between improved approach and the other two.

Chapter 5 focuses on the choice of in-stock dataset as representative data for background characteristics. This chapter incorporates the findings of last three chapters. The system boundary is defined based on the recommendations provided in Chapter 2. The sensitivity analysis is also engaged to verify the claims. The characterization approach is selected and modified based on Chapters 3 and 4. This chapter does not only carry out scenario analysis to study impacts by the choice of in-stock dataset, but also develop Singapore's inventory using an approach that accounts for the geographical differences by modifying the existing database.

Chapter 6 presents the overall synthesis of the PhD thesis. This chapter outlines the overall consequences of the results within this PhD thesis.

Research scope #1: how the choice affects the result?

Research scope #2: how to reduce uncertainties due to choices?

Figure 1-1. Structure of the thesis

CHAPTER 2 CHOICES OF SYSTEM BOUNDARY

2.1 Introduction

System boundaries can be specified in many dimensions, such as boundaries between different significance levels, the technological systems, geographical areas, time horizon, *etc.*(Finnveden, G. *et al.* 2009). This chapter focuses on the boundary between significant and insignificant processes in desalination domain.

LCA attempts to approximate the comprehensive environmental, health and resource burdens associated with desalination. In theory, this comprehensiveness entails inclusion of all significant burdens from all causally connected processes. The cradle-to-grave system boundary (Figure 2-1) illustrates the causally connected processes in desalination system. All the treatment steps/phases/processes can be categorized into two systems, the foreground and background system.

The foreground system includes the comprehensive treatment steps in desalination. Each treatment step is generally composed of sets of multiple upstream and downstream phases. The upstream phases refer to the required infrastructure, energy, chemical, membrane; while the downstream phases support the end-of-life processing routes relevant to the waste. The input and output flows engaged in foreground system typically include the amount of different construction materials, energy, chemicals, membrane, and waste required/disposed to fulfil the function unit (1 m³ of desalting water in desalination LCAs). The on-site primary data is preferred for the foreground system to better represent the technology and local context uniqueness. In practice, the on-site primary data is usually not available and consequently a number of inputs and outputs might be roughly estimated or even ignored. Ideally, the decisions on inclusion or exclusion would be based on the percentage of an aggregated impact score and/or different impact category indicators of interest. However, in desalination LCAs, the decisions are typically not made on this scientific basis, especially

Figure 2-1. Cradle-to-grave system boundary of desalination LCAs

for the inventory that has never been assessed by the practitioner. Since the negligibility of the excluded inputs/outputs cannot be guaranteed, the subjectivity of system boundary selection may influence the outcomes significantly.

The background system includes the processes that are relatively more remote to the desalination function. In desalination LCAs, the background inventory often includes the extracted natural resources (water, minerals, natural gas, land, *etc.*) and the elementary environment emissions/interventions (CO_2 , VOCs, NO_x , Hg, *etc.*) associated with the production of construction materials, chemicals, and membrane materials, the energy generation, as well as waste management. Overwhelming number of inputs and outputs are usually found in the background inventory. For example, even for a very simple chemical required by the desalination system, *e.g.* H_2SO_4 , there are over 600 natural resource inputs and emission outputs connected with its production. Therefore, it is typical for LCA practitioner to engage the in-stock databases for the background system. As a result, the confidence level the LCA relies heavily on the choice of in-stock database. The impacts are more of concern than the choice of system boundary (see details in Chapter 5).

As sketched above, the focus of this Chapter is the choice of boundary in foreground system of desalination. There are totally five phases engaged in a typical foreground system, including energy, infrastructure, chemical, membrane and waste phases. Almost all of the previous studies reached the consensus on the energy and waste aspects, indicating considerable impacts from both of them. However, the concentrated wastewater from desalination system is usually excluded from system boundary due the limitation of current characterization approach (the details about the limitation can be found in Chapter 4). More importantly, a significant inconsistency can be found in infrastructure, chemical, and membrane phases. The critical review on the previous desalination LCA studies is engaged to investigate the subjective selection with regard to these three

phases. Particular attention is given to the potential risk of the decision on exclusion. The recommended system boundary subjective to the goal and scope are then outlined to reduce the uncertainties due to arbitrary choice of foreground system.

2.2 Critical Review

2.2.1 The Subjective Selection with Regard to Infrastructure Phase

The comprehensive aspects considered in the infrastructure phase are those related to the construction materials and the energy required for building the desalination system. However, due to the difficulties in data procurement, only the production of certain widely used construction materials are included in the infrastructure phase, *e.g.* concrete, cement, steel, PVC, *etc.* Raluy's studies (2004; 2005a; 2005b; 2005c; 2006) have indicated that the infrastructure phase has relatively minor environmental impacts in comparison with the operational phase, with percentage lower than 10%. More LCA studies carried out by Vince *et.al.* (2009), Lyons *et.al.* (2009), Munoz *et.al.* (2008), and Stokes *et.al.* (2006), also lead to similar conclusions on the insignificant role of infrastructure phase.

Some of the studies in this review exercise did not consider the infrastructure phase (Vince, F. *et al.* 2008; Biswas, W.K. 2009; Meneses, M. *et al.* 2010; Beery, M. and Repke, J.U. 2010a; Hancock, N.T. *et al.* 2012; Salcedo, R. *et al.* 2012). The exclusion was made based on two justifications: their minor contribution identified by other previous studies and the small mass of construction materials due to the long time span of infrastructure.

However, the justifications were challenged by three studies. Tangsubkul (2005) assessed the environmental performance of membrane bioreactor (MBR) followed by reverse osmosis (RO) process. The contribution of infrastructure phase is about one third of Global Warming Potential (GWP). Abel Riaza's study (2009) also indicated the high contribution of infrastructure phase in the impact of GWP, with nearly 50%. Jijakli (2012)

compared PV-powered RO unit, the solar still, and water delivery by truck from a central RO plant. The results indicated the steel, stainless steel, PVC and other construction materials are important contributors to the CO₂ emissions. The three higher contributions are probably because that the construction of auxiliary facilities, e.g. the pre-treatment facilities (Frutos, A.R. *et al.* 2009), the renewable energy system (Jijakli, K. *et al.* 2012) *etc.*, are included in the infrastructure phase. The assumption of the small mass due to long time span is usually not applicable when considering the construction materials used in the auxiliary facilities. Furthermore, the production of steel, stainless steel, cement, and PVC, the construction materials widely used in infrastructure facilities, is usually considered as energy-intensive process which lead to significant green house gas (GHG) emissions, especially when coal and heavy fuel oil were used as the energy sources.

2.2.2 The Subjective Selection with Regard to Chemical Phase

Numerous chemicals are used to increase the efficiency and to ensure the life time of desalination plant. They were used to minimize scaling formation, control fouling deposition, reduce membrane degradation/distillate contamination, mitigate the foaming as well as the corrosion problem, *etc.* (Table S-1, S-2, and S-3 in Appendix A). The comprehensive aspects considered in chemical phase should include those related to the production and transportation of the chemicals which are required for operating the desalination system. Similar to the discussion in infrastructure section, most of the previous studies usually considered certain widely used chemicals, mainly due to the data availability (Tables 2-1 and 2-2).

Many studies indicated the overall contribution from the chemical phase was insignificant. However, it will be arbitrary to conclude that the chemical phase could be safely ignored. At different operating conditions, chemical usage and energy consumption change accordingly. These differences can

Table 2-1. System coverage of chemical phase in desalination LCAs (a)

Reference	(Tarnacki, K. <i>et al.</i> 2012)	(Salcedo, R. <i>et al.</i> 2012)	(Hancock, N.T. <i>et al.</i> 2012)	(Jijakli, K. <i>et al.</i> 2012)	(Zhou, J. <i>et al.</i> 2011a) (Zhou, J. <i>et al.</i> 2011b)	(Meneses, M. <i>et al.</i> 2010)	(Beery, M. and Repke, J.U. 2010a)	(Munoz, I. <i>et al.</i> 2010)	(Frutos, A.R. <i>et al.</i> 2009)
Pretreatment									
PH adjustment	H ₂ SO ₄	--	--	--	--	H ₂ SO ₄	--	--	--
Coagulation-flocculation	FeCl ₃	--	FeCl ₃			Coagulant			
Anti-foulant	--	--	--	H ₂ SO ₄	Cl ₂	NaOCl	--	Cl ₂	--
Anti-scalant	Not specify	--	STP	PC	STP	STP	--	STP	--
Dechlorination	NaHSO ₃	--	--	--	--	SMB	--	--	SMB
Membrane cleaning									
	NaOCl/ NaOH+ NaOCl ^a	--	HCl, NaOH, SDBS	--	--	--	--	--	--
Post-treatment									
pH adjustment	--	--	--	--	--	Ca(OH) ₂	--	--	--
remineralisation	--	--	--	--	--	--	--	--	Ca(OH) ₂ CO ₂
disinfection	Cl ₂	--	--	--	--	--	--	--	NaOCl
boron removal	--	--	--	--	--	--	--	--	--

Abbreviation

CA - citric acid; FSA - fluorosilicic acid; PAS - polymer aluminum sulphate; PC – polycarboxylates; SMB - sodium metabisulphite;

STP - sodium tripolyphosphate; SDBS - alkylbenzene sulfonate

^a RO process/Memstill process

Table 2-2. System coverage of chemical phase in desalination LCAs (b)

Reference	(Biswas, W.K. 2009)	(Vince, F. <i>et al.</i> 2009)	(Lyons, E. <i>et al.</i> 2009)	(Vince, F. <i>et al.</i> 2008)	(Raluy, R.G. <i>et al.</i> 2006) (Raluy, R.G. <i>et al.</i> 2005b) (Raluy, R.G. <i>et al.</i> 2005a) (Raluy, R.G. <i>et al.</i> 2004)	(Stokes, J. and Horvath, A. 2006)	(Raluy, R.G. <i>et al.</i> 2005c)	(Lundie, S. <i>et al.</i> 2005)	(Lundie, S. <i>et al.</i> 2004)
Pretreatment									
PH adjustment	H ₂ SO ₄	--	--	--	--	--	--	--	--
Coagulation-flocculation	Polymers	PAS	--	--	--	--	--	--	--
Anti-foulant	NaOCl, DBNPA	Cl ₂	Cl ₂	--	Cl ₂	--	Cl ₂	Cl ₂	Cl ₂
Anti-scalant	Nalco PC1020	PC	--	--	--	--	--	--	--
Dechlorination	SMB	--	--	--	--	--	--	--	--
Membrane cleaning									
	CA Detergent	EDTA, NaOH	H ₂ SO ₄	--	--	--	--	--	--
Post-treatment									
pH adjustment	--	--	--	--	--	--	--	--	--
remineralisation	Ca(OH) ₂ CO ₂ , FSA	CaCl ₂ , Ca(OH) ₂	Ca(OH) ₂	--	--	--	--	Ca(OH) ₂ CO ₂	--
disinfection	Cl ₂	NaOCl	--	--	--	--	--	--	--
boron removal	--	--	--	--	--	--	--	--	--
	--	--	--	--	--	--	--	--	--

Abbreviation

CA - citric acid; FSA - fluorosilicic acid; PAS - polymer aluminum sulphate; PC – polycarboxylates; SMB - sodium metabisulphite;
STP - sodium tripolyphosphate; SDBS - alkylbenzene sulfonate

translate to different levels of environmental impacts. As part of the optimization component, the overall life cycle impact from the chemical usage is an indispensable aspect in trade-off study. The LCA practitioner should take extra cautious when considering excluding the chemical with large dosage to assist the operation. The scale inhibitor used in pre-treatment, the membrane cleaning chemicals, and remineralisation chemicals used in post-treatment are three typical examples. The first had significant contributions to acidification, eutrophication, and photochemical oxidation impacts as indicated in Hancock et.al.'s study (2012), and Zhou's study (2011b), while the second and the last was identified as one of important contributors to global warming impact (Vince, F. *et al.* 2008) and ozone depletion impact (Tarnacki, K. *et al.* 2012), respectively.

2.2.3 The Subjective Selection with Regard to Membrane Phase

The membrane phase represents the activities carried out (*e.g.* extracting the membrane foil) and resources consumed (*e.g.* polymers) during the manufacture of membrane modules. Some desalination LCAs simplified the membrane phase as the production of membrane material, while others modelled the membrane phase with relatively comprehensive inventory, not only including the membrane materials, but also counting in all the materials used to produce spacer, housing, collection tube, and adhesive (Table 2-3 and 2-4).

No matter the membrane phase is simplified or well modelled with comprehensive inventory, its contribution is considered as negligible in all reviewed studies. However, exclusion from system boundary is not recommended because it is membrane phase make the desalination technology distinct from other water and waste water treatment technologies. It is also important to note that all the previous studies didn't count in the impacts from the solvents and coating compounds engaged in the complicated membrane preparation process, whose potential risk to environment have not been identified at the current stage.

Table 2-3. System coverage of membrane phase in desalination LCAs (a)

Reference	(Tarnacki, K. <i>et al.</i> 2012) ^a	(Salcedo, R. <i>et al.</i> 2012)	(Hancock, N.T. <i>et al.</i> 2012)	(Jijakli, K. <i>et al.</i> 2012)	(Zhou, J. <i>et al.</i> 2011a) (Zhou, J. <i>et al.</i> 2011b) (Munoz, I. and Fernandez- Alba, A.R. 2008)	(Beery, M. and Repke, J.U. 2010a)	(Munoz, I. <i>et al.</i> 2010)	(Frutos, A.R. <i>et al.</i> 2009)	(Biswas, W.K. 2009)
Membrane	PA/ PTFE	--	PA	CA	PA	--	PA	--	PA
Spacer	PP/PE	--	PE	cotton fabric, PP	--	--	--	--	--
Membrane Housing	coated steel/ PP+steel	--	glass fibre	--	--	--	--	--	--
Collection tube	PET	--	PVC	--	--	--	--	--	--
Adhesive	--	--	epoxy	ethylene rubber	--	--	--	--	--
Energy	--	--	--	--	extrusion	--	extrusion	--	--

Abbreviation

CA - cellulose acetate; PA – polyamide; PE – polyethylene; PET - Polyethylene terephthalate; PP – polypropylene;

PTFE – Polytetrafluoroethylene; PVC - polyvinylchloride

^a RO process/Memstill process

Table 2-4. System coverage of membrane phase in desalination LCAs (b)

Reference	(Vince, F. <i>et al.</i> 2009)	(Lyons, E. <i>et al.</i> 2009)	(Vince, F. <i>et al.</i> 2008)	(Munoz, I. and Fernandez-Alba, A.R. 2008)	(Raluy, R.G. <i>et al.</i> 2006) (Raluy, R.G. <i>et al.</i> 2005b) (Raluy, R.G. <i>et al.</i> 2005a) (Raluy, R.G. <i>et al.</i> 2004)	(Stokes, J. and Horvath, A. 2006)	(Raluy, R.G. <i>et al.</i> 2005c)	(Lundie, S. <i>et al.</i> 2005)	(Lundie, S. <i>et al.</i> 2004)
<u>Membrane</u>	PA	--	PA	PA	--	--	PA	--	--
<u>Spacer</u>	--	--	--	--	--	--	--	--	--
<u>Membrane Housing</u>	--	--	--	--	--	--	--	--	--
<u>Collection tube</u>	PVC	--	--	--	--	--	--	--	--
<u>Adhesive</u>	epoxy	--	epoxy	--	--	--	epoxy	--	--
<u>Energy</u>	--	--	--	extrusion	--	--	--	--	--

Abbreviation

CA - cellulose acetate; PA – polyamide; PE – polyethylene; PET - Polyethylene terephthalate; PP – polypropylene;
PTFE – Polytetrafluoroethylene; PVC - polyvinylchloride

2.3 Recommendations to Draw System Boundary for Desalination

Although the infrastructure, chemical, and membrane phase have relatively smaller contribution to the environmental burdens as indicated in many previous desalination LCAs, the decision of excluding them from the foreground system should be made with caution. The critical review has indicated that the goal and scope definition is an important consideration in drawing the system boundary of desalination LCAs. As sketched in Section 1.3, the LCA can be used to three applications in desalination, including to compare different desalination technologies, to compare water supply/reuse plans, and to explore the solutions to relieve the environmental burdens. For each defined purpose, the foreground system should be customized accordingly to reduce time and economic burdens on on-site primary data collection. As indicated in Table 2-5, each desalination step includes four phases. The determination of the data source for the processes under each phase is based on the findings from Sections 2.2.1, 2.2.2, and 2.2.3. On-site experiment data (P) is preferable for those processes whose contribution was reported non-negligible by previous studies. The other processes, if identified as minor contributors, can be excluded from system boundary (E) without significantly losing overall accuracy. In practice, the secondary literature data (S) can serve as an alternative for the important processes identified in the background system since their primary data are usually not available in desalination system.

To avoid high uncertainties due to the arbitrary decision of inclusion or exclusion, the boundary selection in infrastructure, chemical, and membrane phases should be determined according to the goal and scope of desalination LCAs. When the LCA is used to compare different desalination technologies, only the core steps, including water desalting, pre-treatment, and post-treatment, are suggested to be included in the system boundary. Among those steps, the CO₂ intensive materials used in infrastructure phase as well as the anti-scalant, membrane cleaning chemicals, and remineralisation additives used in chemical phase should be regarded as

significant elements and to be included in system boundary. As to the membrane phase, a unique phase in desalination, a roughly estimation based on secondary data is suggested because of its minor contributions. When the LCA is used to explore the solutions to relieve the environmental burdens, similar to the comparison of desalination technologies, the LCA study could focus on the core steps. However, the difference is that the on-site primary data is recommended for the mitigation studies in order to better represent different operation conditions. When assessing the water supply/reuse plans, it is better to include additional two steps, the water acquisition and distribution step. Among the two steps, the pipeline materials and CO₂ intensive materials used in their infrastructure phase, are suggested to be considered in system boundary.

2.4 Conclusions

In this chapter, the system boundary of desalination LCA is categorized into two systems: foreground and background system. The foreground system includes the treatment steps of desalination system and each step is generally composed of sets of multiple upstream and downstream phases. The choices of foreground boundary between significant and insignificant phases substantially influence the outcomes.

Most of previous studies indicate the infrastructure, chemical, and membrane phase has insignificant contribution. Through critical review, we find the conclusion of insignificance is subject to the conditions. Excluding the three phases from system boundary, without further investigating the underlying assumptions, would bias the LCA results.

Table 2-5. Recommended system boundaries

Desalination treatment step	Phases		G&S #1	G&S #2	G&S #3
Raw water transport	<i>Infrastructure</i>	•Pipeline material (e.g. PVC)	E	S	S
		•Other construction materials	E	E	E
	<i>Energy</i>		E	P	P
	<i>Chemical</i>	Nil	-	-	-
	<i>Waste</i>		E	E	E
Pre-treatment	<i>Infrastructure</i>	•CO ₂ -intensive material (e.g. steel, cement)	S	S	S
		•Other construction materials	E	E	E
	<i>Energy</i>		P	P	P
	<i>Chemical</i>	•P-based antiscalant	S	S	P
		•Other chemicals	E	E	S
	<i>Waste</i>	•Solid water	E	E	E
		•Effluent waste	P	P	P
Desalting operation	<i>Infrastructure</i>	•CO ₂ -intensive material (e.g. steel, cement)	S	S	S
		•Other construction materials	E	E	E
	<i>Energy</i>		P	P	P
	<i>Chemical</i>	•Membrane cleaning chemicals	S	S	P
		•Other chemicals	E	E	S
	<i>Membrane</i>		S	S	P
	<i>Waste</i>	•Used membrane	S	S	P
		•Solid waste	E	E	E
Post-treatment		•Effluent waste	P	P	P
	<i>Infrastructure</i>	•CO ₂ -intensive material (e.g. steel, cement)	S	S	S
		•Other construction materials	E	E	E
	<i>Energy</i>		P	P	P
	<i>Chemical</i>	•remineralisation chemicals	S	S	P
		•Other chemicals	E	E	S
	<i>Waste</i>	•Solid water	E	E	E
Clean water distribution/Storage		•Effluent waste	P	P	P
	<i>Infrastructure</i>	•Pipeline material (e.g. PVC)	E	S	S
		•Other construction materials	E	E	E
	<i>Energy</i>		E	P	P
	<i>Waste</i>		E	E	E

Abbreviations

G&S #1: Goal and Scope #1 - to compare different desalination technologies

G&S #2: Goal and Scope #2 - to compare water supply/reuse plans,

G&S #3: Goal and Scope #3 - to explore the solutions to relieve the environmental burdens

P – on-site primary data is highly recommended

S – secondary data is acceptable if primary data is not available

E – exclusion from system boundary is acceptable if limited data is available

CHAPTER 3 CHOICE OF PREDEFINED LIFE CYCLE IMPACT ASSESSMENT METHOD

3.1 Introduction

As sketched in Section 1.2, once all the required emission and resource data are collected in an inventory list (LCI-results), an LCIA is performed to translate (characterize) emissions and extractions of life cycle inventories (Jolliet, O. *et al.* 2004). An LCIA methodology is a collection of individual characterization approaches which together address different environmental impacts (defined as impact categories) covered by the methodology. Each characterization method applies its own cause-effect pathway and impact indicator, to produce so called characterization factors (CFs). The CFs are used as weighting factors to aggregate life cycle emissions in midpoint level (such as climate change, toxicological stress, acidification, eutrophication, *etc.*) or endpoint level (such as human health, ecosystem quality, climate change, *etc.*) (ISO 2000a). Since the midpoint methods have often been well-researched and more comprehensive than the endpoint and damage calculations (Bare, J.C. and Gloria, T.P. 2006), this study focuses on the midpoint level approach. The characterization impact score for impact category j is based on Equation (1)

$$\text{Characterization Impact}^j = \sum_i CF_i^j \times m_i \quad \text{Equation (1)}$$

Where CF_i is the characterization factor of substance i , m is the flow of substance i , and j is the impact indicator.

As indicated in Tables 1-1, 1-2, 1-3, and 1-4., only three life cycle impact assessment methods, CML 2, EDIP97, and Eco-indicator 99, have ever been applied in the previous studies (except our own studies), but none had indicated the reasons in choosing a specific LCIA method.

With the improvement in LCA, many impact assessment methodologies had become available to the LCA practitioners (Pennington, D.W. *et al.* 2004; Bare, J.C. and Gloria, T.P. 2006; Reap, J. *et al.* 2008b), and several of them

are implemented in the software commercially available on the market. However, there is no clear information or even guidelines for the general users to choose proper LCIA methods. This chapter aims to examine the three questions: (1) Whether or not, and to what extent, the environmental impacts of the desalination processes vary due to the different LCIA methods? (2) How to choose the appropriate predefined LCIA method for desalination industry? (3) How to develop desalination-specialized characterization approach? The rest of this chapter is organized in line with the framework of LCA, beginning with goal and scope definition, followed by inventory analysis, impact assessment, and interpretation. Finally, the conclusions are presented in last section.

3.2 Model Construction for Comparative LCA Study

3.2.1 Goal and Scope Definition

1) Scenario definition

The present study conducts the environmental LCA of a desalination plant using two common methods in order to investigate the potential advantages and disadvantages as well as the suitability due to the features of different LCIA methods. The subject of this study is a medium-sized RO desalination plant. The plant overview is summarized in Table 3-1. The CML2 (Version 2.05), referred as Scenario 1 in this study, was developed by the Centre for Environmental Studies at University of Leiden. The method of Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI2, V3.03), referred as Scenario 2 hereafter, was developed by US Environment Protection Agency. The CML2 baseline method provides a list of obligatory impact indicators elaborating the problem-oriented (midpoint) approach (Guinee, J.B. *et al.* 2002) and was commonly used as a generic method worldwide. The TRACI was developed specifically for the US using input parameters consistent with US locations and usually considered as a region-specific method.

Table 3-1. Plant overview

	Assumptions	Comments
Plant productivity	10,000 m ³ water daily for all scenarios	Since both the relative capital cost and the energy cost of a RO plant decrease as plant size decrease (Greenlee, L.F. <i>et al.</i> 2009), we choose medium-sized desalination plant as study subject to represent average conditions.
Salinity of feed water	around 15,000 mg/L for all scenarios	The salinity of feed water is within reasonable range of brackish water (brackish water in Almeria in southern Spain, TDS is around 15,300 mg/L (Munoz, I. and Fernandez-Alba, A.R. 2008); brackish water in Albuquerque's West Mesa in US, TDS is over 10,000 mg/L (Sandia National Laboratories 2009); although ground water resource is limited in Singapore, one on-going project, called reflux system, taking a portion of the effluent stream on the high pressure side and sending it to the low pressure side of the membrane is used to reduce the input TDS to 10,000 – 20,000 mg/L (Krantz, B. 2009))
Recovery Rate	42.5%	
Quality of produced water	Regard as pure water for all scenarios	
Salinity of concentrate	around 35,000 mg/L	Similar salinity with sea water

The software Simapro 7.1 was used to set up the model structure for both scenarios. Characterization, uncertainty, and contribution analyses were used for result interpretation. The details of the characterization model are summarized in Section 3.2.3. In uncertainty analysis, Monte Carlo simulation is used to evaluate the confidential level of discrepant results cause by the difference in LCIA method used. In contribution analysis, the cut-off criteria are set to neglect the processes whose contribution is less than 1% of the total environmental load.

2) *Function unit, system boundary, and assumptions*

One significant contribution of this study was that this study not only compared the overall impacts between the two scenarios, but also provided

the supporting values to identify the reasons for the discrepant results caused by these LCIA methods. This information, in turn, could guide us to choose or develop proper LCIA method for desalination industry.

The function unit for comparing the alternative systems is chosen as 1 m³ of desalinated water produced. As discussed in Chapter 1, only the desalting operation step is included in system boundary (Table 3-2). The standard deviation used in uncertainty analysis is suggested by either Ecoinvent database or literatures because the primary data is not accessible (Table 3-3). The design and operation of the desalination plant must rely on certain important parameters such as plant size, raw water qualities, product water qualities, and brine disposal, to name a few. The assumptions used in this study are listed in Table 3-1 and 3-2.

3.2.2 Life Cycle Inventories

The input flows of the plant are indicated in Table 3-2. The Ecoinvent database V2.1, considered as one of the most popular life cycle inventory data sources, was used to support the LCA modeling. It is worth to highlight that, while the team tried to engaged US Ecoinvent databases to the greatest extend to better reflect the geological coverage, the material and transportation flows are modeled using Europe (RER), Switzerland (CH) and Global (GLO) scenarios (Table 3-2) mainly because of the incompleteness of the database and the spirit of globalized market - many materials or services are provided by a limited number of famous companies or produced with similar procedure (Rebitzer, G. *et al.* 2004). Although some other processes, such as cement manufacturing, land and marine transportation, show typical continental or national properties, their contribution generally account for less than 1% of the overall impact, which can be considered as negligible.

Table 3-2. System boundary defined to investigate influence of predefined LCIA method

	Assumptions	Comments
Electricity flow in energy phase	2 kWh/m ³ desalted water for all scenarios	Based on plant overview, the average electricity consumption is 2 kWh/m ³ desalted water (Glueckstern, P. <i>et al.</i> 2001; Tsiourtis, N.X. 2001; Munoz, I. and Fernandez-Alba, A.R. 2008)
Material flows in infrastructure phase, chemical phase, and membrane phases	The value of flows are adopted from Munoz's study (2008)	The secondary data is used due to comparative nature of this study and unavailability of primary data.
Transportation of construction material, membranes, chemicals and waste materials	Excluded from system boundary	
Concentrate disposal	Excluded from system boundary	At present, this is a matter of active research and some studies already qualitatively discussed the environmental issues of the concentrate disposal (Glueckstern, P. <i>et al.</i> 2001; Tsiourtis, N.X. 2001; Al-Agha, M.R. and Mortaja, R.S. 2005). However, reliable quantitative study with regard to environmental impacts of concentrate disposal is not available. Therefore, we assume it is coastal BWRO plant for all scenarios and the concentrate is piping to the discharge point under the seawater. The concentrate is diluted into large seawater body without influencing the feed water composition. The only indicator used to characterize concentrate is TDS (35,000 mg/L).
Pre-treatment and post-treatment	Excluded from system boundary	Given similar feed water and effluent, we assume the pre-treatment and post-treatment are similar for all scenarios. They are excluded from boundary due to the comparative nature of this study.
Raw water transport and clean water storage/distribution	Excluded from system boundary	Raw water transport and clean water storage/distribution steps are excluded from the study because it is a site-specific rather than a process-specific aspect.

Table 3-3. Square of geometric standard deviations for uncertainty analysis and supporting databases for modeling

	(Geometric SD) ²	Database
For electricity flows^a		
Electricity distribution	2 ^a	Modeled with US Ecoinvent database
Transmission, medium voltage	2 ^a	
Electricity, medium voltage	1.5 ^a	
Transmission, high voltage	2 ^a	
Electricity, high voltage	1.5 ^a	
Electricity, production mix	1.5 ^a	
electricity from coal	1.05 ^a	
electricity from natural gas	1.05 ^a	
electricity from heavy fuel oil	1.3 ^a	
electricity from nuclear	1.05 ^a	
electricity from industrial gas	1.3 ^a	
electricity from waste incineration	1.3 ^a	
electricity from clean energy (photovoltaic, hydropower, wind)	1.3 ^a	
electricity from other sources	1.3 ^a	
For material flows^b		
Concrete, brick, bitumen, steel	1.2	Modeled with RER, CH, GLO Ecoinvent database
Soil excavation, gravel, PVC pipe, rubber, PE liner, Iron, chlorine	1.3	
PE pipe, GRP	1.6	
Membranes, anti-scalant	2	
Stainless steel, sand, rock, geotextile	2.1	
For waste flows^b		
Landfill of membranes, concrete, PVC, GRP, PE	3.1	Modeled with CH Ecoinvent database
Landfill of sand	3.3	
Landfill of geotetile	3.7	

^a Data is available from Ecoinvent database for US

^b Data from Munoz's work (Munoz, I. and Fernandez-Alba, A.R. 2008)

3.2.3 Life Cycle Impact Assessment Methodology

LCIA methodology elaborates how to simplify the complexity of hundreds of flows involved in the system boundary into a few environmental areas of interest for systematic evaluation of the impacts. One of the challenges in conducting meaning comparisons between the two methodologies is the selection of impact indicators. Both CML2 and TRACI methods include

similar five impact categories, but the categories were indicated by different indicators. For example, human health was represented by Human Toxicity Potential (HTP) in CML2, while TRACI further divides it into three subcategories including carcinogenic, non-carcinogenic, and respiratory impact potentials to better reflect the local health concerns and regulatory focus. The comparison of impact categories, indicators, and characterization models of two methods were summarized in Table 3-4.

Another important concern for a meaningful comparison is the characterization factor used to convert various compounds into a reference compound equivalent. Both CML2 and TRACI provide a set of science-based characterization conversion factors in terms of mid-point or end-point categories. In this study, we focus on the mid-point characterization step.

3.3 Results Interpretation and Discussion

Table 3-4 listed the results from two scenarios with characterizations for different indicators from CML2 and TRACI methods. Both methods have common indicators in five categories including global warming, ozone depletion, acidification, eutrophication, and photochemical oxidation. However, human health impacts are represented by a single indicator as human toxicity potential in CML2, while TRACI further separates it into three subcategories. This is a good example of regional method incorporating special indicators to address the specific concerns in the region. It is also worth noted that CML2 engages three subcategories for ecotoxicity while TRACI only uses one indicator to simplify the inventory and associated data collections. This again highlights another difference between the region-specific (TRACI) and generic global (CML2) methods. The generic global method can afford to engage a comprehensive database with the contributions from various sources, while the regional specific method might want to limited the coverage level due to the data maintenance and compilation requirement.

Table 3-4. The characterization results of desalination using two predefined LCIA method

impact categories	CML2 Indicators	Characterization model	Value	Unit	TRACI Indicators	Characterization model	Value	Unit
Global warming	Global warming potential ($GW P_{CML}$)	(Houghton, J.T. <i>et al.</i> 1997)	1.58E+00	kg CO ₂ eq	Global warming potential ($GW P_{TRACI}$)	(Houghton, J.T. <i>et al.</i> 1997)	1.58E+00	kg CO ₂ eq
Ozone depletion	Ozone depletion potential (ODP_{CML})	(WMO 1999)	4.30E-08	kg CFC-11 eq	Ozone depletion potential (ODP_{TRACI})	(WMO 1999)	4.34E-08	kg CFC-11 eq
Acidification	Acidification potential (AP_{CML})	(Huijbregts, M.A.J. 1999b)	1.16E-02	kg SO ₂ eq	Acidification potential (AP_{TRACI})	(Bare, J.C. <i>et al.</i> 2003)	5.64E-01	kg H ⁺ eq
Eutrophication	Eutrophication potential (EP_{CML})	(Heijungs, R. <i>et al.</i> 1992)	6.27E-04	kg PO ₄ ³⁻ eq	Eutrophication potential (EP_{TRACI})	(Bare, J.C. <i>et al.</i> 2003)	7.66E-04	kg N eq
Photochemical oxidation	Photochemical oxidation potential ($POCP_{CML}$)	(Jenkin, M.E. and Hayman, G.D. 1999)	4.55E-04	kg C ₂ H ₄ eq	Photochemical oxidation potential/smog formation ($POCP_{TRACI}$)	(Bare, J.C. <i>et al.</i> 2003)	3.04E-03	kg NO _x eq
Human health	Human toxicity potential (HTP_{CML})	(Huijbregts, M.A.J. 1999a)	5.62E-01	kg 1,4-DB eq				
			--	--	Carcinogenic human toxicity potential ($C - HTP_{TRACI}$)	(McKone, T.E. 1993)	3.39E-03	kg benzene eq
			--	--	Non carcinogenic human toxicity potential ($nC - HTP_{TRACI}$)	(McKone, T.E. 1993)	2.44E+01	kg toluene eq
			--	--	Respiratory effects/ Criteria air pollutants (REP_{TRACI})	(Bare, J.C. <i>et al.</i> 2003)	3.02E-03	kg PM2.5 eq
Ecotoxicity					Ecotoxicity potential (ETP_{TRACI})	(McKone, T.E. 1993)	3.48E+00	kg 2,4-DCB eq
	Fresh water aquatic ecotoxicity ($FAETP_{CML}$)	(Huijbregts, M.A.J. 1999a)	1.42E-01	kg 1,4-DB eq				
	Marine aquatic ecotoxicity ($MAETP_{CML}$)	(Huijbregts, M.A.J. 1999a)	3.21E+02	kg 1,4-DB eq				
	Terrestrial ecotoxicity ($TETP_{CML}$)	(Huijbregts, M.A.J. 1999a)	4.64E-03	kg 1,4-DB eq				

Different units were found in the categories of acidification, eutrophication, photochemical oxidation, human health, and ecotoxicity. In order to facilitate meaningful comparison, unit conversion was carried out according to the general conversion guideline. For human health impact category in TRACI, Carcinogenic Human Toxicity Potential (C-HTP) and Non Carcinogenic Human Toxicity Potential (nC-HTP) were aggregated to represent Total Human Toxicity Potential (THTP), then compared with corresponded indicator (HTP) used in CML2. Respiratory effect indicator from TRACI is not included in the discussion as it is a special addition to further evaluate the impacts from the air-born pollutants which is not covered in CML2. The abiotic resource depletion in CML2 was also excluded from this study due to lack of comparable indicator in TRACI and the same was fossil fuel use. The scenario with higher impacts in each category was normalized as 100% for easy comparison. As indicated in Figure 3-1, small or even negligible differences were observed in global warming (GWP), ozone depletion (ODP), and acidification (AP), but remarkable disagreements were found in eutrophication (EP), photochemical oxidation (POCP), human health (HTP), and ecotoxicity (ETP).

Figure 3-1. Comparison between Scenario 1 (CML2) and Scenario 2 (TRACI).

After running the Monte-Carlo simulation 100 times, and setting a confidence interval of 95%, the result for uncertainty analysis is also displayed in Figure 3-1. The variability of the results, meaning 95% of the results lie within the range indicated by the vertical line. On the one hand, it can be seen that LCIA scores have a significant variability, especially for POCP, HTP, and ETP in TRACI scenario, the maximum value being threefold to dozens of times of minimum value. If the two scenarios are compared based on these data, the overlapping of their distributions cannot be observed in EP, POCP, HTP, and ETP, indicating significant discrepancy is caused by the different LCIA method used. Compared to CML2 scenario, the TRACI scenario is $4.29\text{E-}04 \sim 1.20\text{E-}03$ kg N eq. smaller for EP, $1.03\text{E-}02 \sim 1.60\text{E-}02$ kg NO_x eq. smaller for POCP, $2.78\text{E+}02 \sim 4.46\text{E+}02$ kg 1, 4-DCB eq. smaller for ETP, but $6.77\text{E+}00 \sim 1.73\text{E+}01$ kg 1, 4-DCB eq. higher for HTP.

To understand the differences between CML2 and TRACI, and further identify the related major contributors, between the results from these two methods, this study conducted a detailed contribution analysis and discovered the results discussed below.

3.3.1 The Relative Scale of the Impact Category

As indicated in Figure 3-1, almost identical results were found in global warm and ozone depletion potential, which generally represented in a larger geographic scale in terms of the sources and impacts. Both methods engaged the midpoint metric proposed by the International Panel on Climate Change (IPCC) for calculating the global warming potentials, and another metric proposed by the World Meteorological Organization for ozone depletion potentials. To further investigate the consistency of these two methods, Table S-4 (see Appendix A) compared the global warming characterization factor in TRACI and CML2, represented as $CF^{GWP}(TRACI)$ and $CF^{GWP}(CML)$, embedded in each method. There are three interesting findings from this comparison: (1) Both $CF^{GWP}(TRACI)$ and $CF^{GWP}(CML)$ are similar for most of the compounds, with the differences within 2%; (2) There

are big gaps between $CF^{GWP}(TRACI)$ and $CF^{GWP}(CML)$ for some halogenated organic emissions (e.g. Chloromethane, HFE 7100, Tetrafluoromethane) and Nitrogen trifluoride, and (3) The list of environmental interventions is not identical between TRACI and CML2 methods. For example, TRACI didn't list Dichloromethane as an elementary flow. As a result, the global warming impact of Dichloromethane was not included in TRACI method, while the CML2 method assigned a separate CF^{GWP} as 8.7 kg CO₂ eq. / kg Dichloromethane. The associated impacts on the global warming potentials from the last two points, however, are relatively small due to two major reasons. The first is the identical CF^{GWP} for the carbon dioxide, which is the dominant contributor in this category accounting for nearly 95% of the total global warming impact for the desalination plant (Table 3-5). Secondly, the elementary mass flows for those with different CF^{GWP} are relatively small, resulting the negligible global warming impact falling under the 1% cut-off criteria.

Table 3-5. Contribution analysis of global warming potential

	Scenario 1		Scenario 2	
LCIA method	CML2		TRACI	
Total (kg CO ₂ eq.)	1.58E+00		1.58E+00	
Contribution breakdown	kg CO ₂ eq	% of total	kg CO ₂ eq	% of total
<i>Carbon dioxide</i>	1.49E+00	94.5	1.49E+00	94.5
<i>Methane</i>	6.41E-02	4.1	6.41E-02	4.1
<i>Remaining</i>	2.28E-02	1.4	2.31E-02	1.4

Similar trends were found in the estimating process for ozone depletion potential. The CFC-114 and Halon 1301 combined accounts for more than 80% of the total ozone depletion potentials (Table 3-6) and both CML2 and TRACI have very similar ozone depletion characterization factors for these two key substances, leading to the similar ozone depletion potential results from these two scenarios. Based on the comparisons above, one can see that, both region-specific (TRACI) and generic global (CML2) methods will

lead to very similar results for the environmental concerns related to larger spatial or time scales.

Table 3-6. Contribution analysis of ozone depletion potential

	Scenario 1		Scenario 2	
LCIA method	CML2		TRACI	
unit	kg CFC-11 eq	% of total	kg CFC-11 eq	% of total
Total	4.29E-08	100	4.34E-08	100
Contribution breakdown				
<i>HCFC-140</i>	4.91E-10	1.1	5.36E-10	1.2
<i>CFC-114</i>	2.51E-08	58.4	2.77E-08	63.9
<i>Halon 1211</i>	1.42E-09	3.3	1.67E-09	3.8
<i>Halon 1301</i>	1.27E-08	29.5	1.27E-08	29.2
<i>R-40</i>	2.36E-09	5.5	Excl ^a	
<i>CFC-10</i>	6.15E-10	1.4	Excl	
<i>Remaining</i>	3.08E-10	0.7	7.64E-10	1.8

^a the substance is not considered as environmental interventions in TRACI

3.3.2 The Effect of LCIA Coverage

Apart from the global warming and ozone depletion potentials discussed above, both scenarios also reported similar impacts in acidification potential with only 4% difference. However, a detailed contribution analysis revealed that the key substance coverage levels varied quite significantly and the small difference of 4%, is actually the result of two contradicting factors compensating each other's.

As indicated in Table S-5 (see Appendix A), hydrogen chloride (HCl), hydrogen fluoride (HF), nitrogen oxides (NO₂, NO, and NO_x), and sulphur dioxide (SO₂) emissions to the air were the only environmental interventions to acidification in TRACI, while the CML2 included 31 types of emissions to air, soil and water compartment. In addition, the contribution analysis (Table 3-7) also identified that most significant acidification impacts were from the NO_x and SO₂. Comparing to the contribution break down in Scenario 1, the acidification potential caused by NO_x in Scenario 2 was

increased by more than 57%, while the acidification by SO₂ was reduced by nearly 17%. The reason for increasing acidification impact from NO_x will be discussed in Section 3.3.3 (higher CF^{AP} for NO_x). The reduction of the acidification potential associated with SO₂ in TRACI is mainly because of the fact that acidification emissions to water are not considered in TRACI method. The combinations of two compensating contributions lead to a small difference in the estimated results of acidification potential.

Table 3-7. Contribution analysis of acidification potential

Scenario 1			Scenario 2			Scenario 2/ Scenario 1
LCIA method	CML2		TRACI			0.96
Unit	kg SO2 eq	% of total	H ⁺ moles eq	kg SO2 eq ^a	% of total	
Total	1.16E-02	100	5.64E-01	1.11E-02	100	
Contribution breakdown						
<i>Ammonia</i>	Negligible	<1	5.98E-03	1.18E-04	1.1	1.57
<i>Hydrogen chloride</i>	Negligible	<1	1.24E-02	2.45E-04	2.2	
<i>Nitrogen oxides</i>	1.50E-03	12.9	1.20E-01	2.36E-03	21.3	
<i>Sulfur dioxide</i>	9.99E-03	86.2	4.23E-01	8.32E-03	74.9	
<i>Remaining</i>	1.00E-04	0.9	2.88E-03	5.68E-05	0.5	

^a The unit conversion is based on 1 kg SO₂ = 5.08 H⁺ moles (see Table S-5 in Appendix A)

As similar in acidification potential evaluation, the differences in coverage level also affected the photochemical oxidation and ecotoxicity potentials, but resulted in much larger discrepancies in the estimated impacts. As indicated in Table 3-8, SO₂ was identified as the major contributor to the photochemical oxidation potential in Scenario 1, while the NO_x was the one in Scenario 2. Further investigation revealed that the TRACI method didn't include the potential influence of SO₂, the dominant stressor in CML2, as the environmental interventions (Table S-6 in Appendix A). This exclusion leads to a much lower photochemical oxidation potential estimated by TRACI method. From a fundamental photochemical reaction point of view, the role of SO₂ varies significantly depending on the associated environmental conditions. One should evaluate the local circumstances to

select the proper modules for impact estimations. Since coal remains as one of the major energy sources in the US, it is logical to recommend TRACI to incorporate SO₂ module in the acidification potential estimation.

Table 3-8. Contribution analysis of photochemical oxidation potential

Scenario 1				Scenario 2		Scenario 2/ scenario 1
LCIA method	CML2	kg NO _x eq ^a		TRACI		
Unit	kg C ₂ H ₄ eq		% of total	kg NO _x eq	% of total	
Total	4.55E-04	1.62E-02	100	3.04E-03	100	0.19
Contribution breakdown						
<i>Nitrogen oxides</i>	Negligible ^b	Negligible	<1	3.00E-03	98.7	-
<i>Sulfur dioxide</i>	4.00E-04	1.43E-02	87.9	Excl ^c	0	--
<i>Carbon monoxide</i>	1.77E-05	6.32E-04	3.9	Excl	0	--
<i>Methane</i>	1.67E-05	5.97E-04	3.7	Excl	0	--
<i>Toluene</i>	7.85E-06	2.80E-04	1.7	Negligible	<1	--
<i>Remaining</i>	1.27E-05	4.54E-04	2.8	4.02E-05	1.3	--

^a the unit conversion is calculated on 1 kg NO_x = 0.028 kg C₂H₄ (see Table S-6 in Appendix A)

^b the contribution is below 1% cut-off

^c the emission is not considered as environmental interventions in TRACI.

In addition, the TRACI method engaged only one characterization value for ecotoxicity impact (ETP), while the CML2 has three subcategories including freshwater aquatic (FAETP), marine aquatic (MAETP), and terrestrial (TETP). As the subcategories used in CML2 is difficult to replicate in TRACI, this study separated both TRACI and CML2 results according to the emission compartments as airborne, waterborne, and soil to facilitate proper comparisons. As indicated in Table 3-9 and Table 3-10, the ecotoxicity impacts from the desalination plant by emissions to soil is negligible comparing to those from airborne and waterborne emissions in both cases. Scenario 1 (CML2) indicated the water is the dominating emission compartment with Vanadium, Barium, and Beryllium as the important contributors. However, TRACI did not have these compounds in the methodology, thus aluminum emissions to air was listed as the major contributor. To further investigate the sources of Vanadium, Barium, and

Table 3-9. Contribution analysis of ecotoxicity potential - scenario 1

Scenario 1								
LCIA method	CML2 FAETP		MAETP		TETP		FAETP+MAETP+TETP	
	kg 1,4-DCB eq	% of total	kg 1,4-DCB eq	% of total	kg 1,4-DCB eq	% of total	Kg 1,4-DCB eq	% of total
Total of all compartments	1.59E-01	100	3.64E+02	100	4.78E-03		3.64E+02	100
Contribution analysis								
Total of airborne emission	2.60E-03	1.6	4.21E+01	11.6	2.30E-03	48.1	4.21E+01	11.6
<i>Vanadium</i>	1.64E-03	1.0	1.16E+01	3.2	6.31E-04	13.2		
<i>Hydrogen fluoride</i>	0	0	1.85E+01	5.1	0	0		
<i>Chromium VI</i>	0	0	0	0	9.44E-05	2.0		
<i>Selenium</i>	0	0	6.63E+00	1.8	0	0		
<i>Nickel</i>	0	0	0	0	5.05E-05	1.1		
<i>Mercury</i>	0	0	0	0	1.14E-03	23.9		
<i>Arsenic</i>	0	0	0	0	3.23E-04	6.8		
<i>Remaining</i>	9.60E-04	0.6	5.44E+00	1.5	5.74E-05	1.2		
Total of waterborne emission	1.56E-01	98.2	3.22E+02	88.4	1.02E-05	0.2	3.22E+02	88.4
<i>Vanadium, ion</i>	8.55E-02	53.6	8.17E+01	22.5	0	0		
<i>Barium</i>	2.38E-02	14.9	8.76E+01	24.1	0	0		
<i>Beryllium</i>	1.88E-02	11.8	1.11E+02	30.5	0	0		
<i>Nickel, ion</i>	1.44E-02	9.0	1.06E+01	2.9	0	0		
<i>Cobalt</i>	4.94E-03	3.1	6.35E+00	1.7	0	0		
<i>Copper, ion</i>	3.84E-03	2.4	1.29E+01	3.5	0	0		
<i>Remaining</i>	5.20E-03	3.3	6.61E+00	1.8	1.02E-05	0.2		
Total of emission to soil	2.99E-04	0.2	2.24E-01	0.1	2.47E-03	51.7	2.27E-01	0.1

Table 3-10. Contribution analysis of ecotoxicity potential - scenario 2

	Scenario 1	Scenario 2			Scenario 2/Scenario 1
LCIA method	CML2 ^a	TRACI			
unit	kg 1,4-DCB eq	kg 2,4-DCB eq	kg 1,4-DCB eq ^b	% of total	
Total of all compartments	3.64E+02	3.48E+00	2.03E+00	100	56/10000
Contribution analysis					
Total of airborne emission	4.21E+01	1.02E+00	1.85E+00	91.0%	439/10000
<i>Aluminum</i>	--	1.01E+00	1.82E+00	89.7%	
<i>Remaining airborne emission</i>	--	1.44E-02	2.60E-02	1.3%	
Total of waterborne emission	3.22E+02	2.44E+00	1.14E-01	5.6%	4/10000
<i>Aluminum</i>	--	2.35E+00	1.10E-01	5.4%	
<i>Copper, ion</i>	--	3.84E-02	1.79E-03	0.1%	
<i>Remaining waterborne emission</i>	--	4.91E-02	2.29E-03	0.1%	
Total of emission to soil	2.27E-01	1.40E-02	6.81E-02	3.4%	3002/10000

^a data are from Table 3-9

^b the unit conversion is based on 1 kg 2,4-DCB = 0.55 kg 1,4-DCB for airborne emissions, 1 kg 2,4-DCB = 21.4 kg 1,4-DB for waterborne emissions, 1 kg 2,4-DCB = 0.20 kg 1,4-DCB for emissions to soil

Beryllium in the CML2, bottom ash disposal from coal burning (energy/power generation) showed significant contribution. This implied that TRACI might need to include these considerations into the future revision as coal-fired power plants remain as the major power supply sources in the region.

3.3.3 The Effect of Model Differences

In addition to the coverage level of associated compounds in the method, the model engaged for impact assessment also contribute significantly in the estimation results. As discussed previously, CML2 used a single indicator (1, 4-DCB equivalent) in human toxicity potential while TRACI engaged non-carcinogenic (toluene equivalent), carcinogenic (benzene equivalent), and respiratory (PM_{2.5} equivalent) subcategories for human health related evaluation. As shown in the database, the $CF^{nC-HTP}(TRACI)$ and $CF^{C-HTP}(TRACI)$ are derived using a closed -system, steady-state version of CalTOX (Version 2.2), which is a multimedia fate and multiple-exposure pathway model with fixed generic parameters for the United States. The closed system is used to provide a scenario in which a chemical can only be moved from the environment by transformation, not by relocation, to other locations (Bare, J.C. *et al.* 2003). Therefore, the human toxicity characterization factors provided by TRACI differed widely from the factors used in the CML2 model, which is developed in the absence of site-specific emissions inventory and chemical property data.

Using similar approaches as in ecotoxicity impact comparisons, this study further broke up the human toxicity impacts into air, water, and soil compartments as shown in Table 3-11 and Table 3-12. Lead discharged into water was identified as the dominant contributor in the non-carcinogenic human toxicity potential as well as the total human toxicity potential in TRACI. Although both LCIA methods had included lead in the characterization factor lists, the CML doesn't differentiate the pure Lead metal and its ions. The value in $CF^{nC-HTP}(TRACI)$ for lead ion is more than 2 million times of that in $CF^{nC-HTP}(CML)$ (Table S-7 in Appendix A). The

significantly higher value of TRACI characterization factor for lead, the dominant substance, posed a two-orders-of-magnitude jump in human toxicity potential from waterborne emissions and increased by four times in the total HTP, comparing to CML2.

Table 3-11. Contribution analysis of human toxicity potential - scenario 1

Scenario 1			Scenario 2		Scenario 2/ Scenario 1
LCIA method	CML		TRACI ^a		
unit	kg 1,4-DCB eq	% of total	kg 1,4-DCB eq	% of total	
Total	5.62E-01	100	1.26E+01 ^a	100	22.4
Contribution breakdown					
Total impact of airborne emissions	3.96E-01	70.5	8.09E-01	6.4	2.04
<i>PAH</i>	1.41E-01	25.1			
<i>Chromium VI</i>	1.07E-01	19.0			
<i>Arsenic</i>	6.97E-02	12.4			
<i>Benzene</i>	1.78E-02	3.2			
<i>Nickel</i>	1.52E-02	2.7			
<i>Selenium</i>	1.49E-02	2.7			
<i>Vanadium</i>	5.92E-03	1.1			
<i>Remaining substances</i>	2.44E-02	4.3			
Total impact of waterborne emissions	1.65E-01	29.4	1.15E+01	91.3	70
<i>Barium</i>	6.62E-02	11.8			
<i>Vanadium, ion</i>	3.01E-02	5.4			
<i>Selenium</i>	2.85E-02	5.1			
<i>Thallium</i>	1.44E-02	2.6			
<i>Molybdenum</i>	8.82E-03	1.6			
<i>Remaining</i>	1.70E-02	3.0			
Total impact by emissions to soil	4.23E-04	0.1	Negligible ^b	2.3	--

^a. The data are from Table 3-12

^b. The contribution is below 1% cut-off

Table 3-12. Contribution analysis of human toxicity potential - scenario 2

Scenario 2								
LCIA method	TRACI							
indicator	C-HTP ^a			nC-HTP ^b			C-HTP+ nC-HTP	
Unit	kg benzen eq	kg 1,4- DCB eq	% of total	kg toluene eq	kg 1,4-DCB eq	% of total	kg 1,4- DCB eq	% of total
Total	3.39E-03	3.03E-03	100	2.44E+01	1.26E+01	100	1.26E+01	100
Contribution analysis								
Total impact of airborne emissions	2.04E-03	1.64E-03^c		3.11E+00	8.08E-01^f	6.4	8.09E-01	6.4
Arsenic	1.70E-03	1.37E-03	45.3	Excluded	Excluded	0		
Dioxins	2.76E-04	2.23E-04	7.4	Excluded	Excluded	0		
Aluminum	Excluded	Excluded	0	1.61E+00	4.17E-01	3.3		
Lead	Excluded	Excluded	0	8.14E-01	2.11E-01	1.7		
Dioxins	Excluded	Excluded	0	3.06E-01	7.94E-02	0.6		
Total impact of waterborne emissions	1.34E-03	1.38E-03^d	45.5	2.12E+01	1.15E+01^g	91.3	1.15E+01	91.3
Arsenic, ion	7.07E-04	7.27E-04	24.0	Excluded	Excluded	0		
Lead	6.32E-04	6.50E-04	21.5	2.04E+01	1.11E+01	88.0		
Cadmium, ion	Negligible	Negligible	<1	6.66E-01	3.61E-01	2.9		
Remaining	5.75E-07	5.91E-07	0.0	9.80E-02	5.32E-02	0.4		
Total impact by emissions to soil	5.17E-06	6.38E-06^e	0.2	7.63E-02	2.94E-01^h	2.3		2.3

^a C-HTP: carcinogenic human health impact^b nC-HTP non-carcinogenic human health impact^c The unit conversion of C-HTP by airborne emission is based on 1 kg benzene = 1.24 kg 1,4-DCB^d The unit conversion of C-HTP by waterborne emission is based on 1 kg benzene = 0.97 kg 1,4-DCB^e The unit conversion of C-HTP by emissions to soil is based on 1 kg benzene = 0.81 kg 1,4-DCB^f The unit conversion of nC-HTP by airborne emission is based on 1 kg toluene = 3.85 kg toluene^g The unit conversion of nC-HTP by waterborne emission is based on 1 kg toluene = 1.84 kg toluene^h The unit conversion of nC-HTP by emissions to soil is based on 1 kg toluene = 0.26 kg toluene

As two models sometimes assigned different characterization factor values to the same compounds, the resulting effects were observed in other impact categories as well. The development of $CF^{AP}(TRACI)$, $CF^{EP}(TRACI)$, $CF^{POCP}(TRACI)$, and $CF^{ETP}(TRACI)$ in TRACI were also based on the United State localized model. The differences arisen highly depended on

the impact category, the substance type, and the emission compartment of the associated compounds. For example, the localized model used in TRACI resulted in around 10% increase in acidification characterization factors in acidification potentials (Table S-5 in Appendix A), but usually four to five-orders-of-magnitude changes in characterization factors for photochemical oxidation smog formation (Table S-6 in Appendix A) and human toxicity (Table S-7 in Appendix A) when comparing to CML2. This highlights the importance assigning/computing values for the characterization factors. In addition, substance type is also critical in CF evaluations. Among the environmental interventions, the $CF^{EP}(TRACI)$ s for NO_x , NO_2 , and NO are 10% higher than the factors used in CML2, but acidification characterization factors for ammonia (NH_3) and hydrogen chloride (HCl) were almost identical between two LCIA methods (Table S-8 in Appendix A).

Furthermore, the emissions compartment is also important, it was found that the $CF^{EP}(TRACI)$ s for the emissions to air were only one tenth (10%) of the factors used in CML2, but eutrophication characterization factors for water borne emissions were identical between two LCIA methods (Table S-8 in Appendix A), which combined led to more than half reduction in eutrophication potential relative to the estimation from CML2 method (Table 3-13).

3.3.4 The Effect of Substances Aggregation

Other than the characterization models, the processes of aggregating similar compounds also affect the characterization factors. For example, unlike CML2 provided a comprehensive CF list for various volatile organic compounds (VOCs) and Dioxins, TRACI only assigned the generic factors to represent the overall impacts. Therefore, the generic $CF^{POCP}(TRACI)$ was used to calculate the photochemical oxidation potential induced by all VOCs, and generic $CF^{C-HTP}(TRACI)$ to estimate the human toxicity potential. The advantage for this aggregating approach is clear as it can greatly simplify the burden of database maintenance and lower the

Table 3-13. Contribution analysis of eutrophication potential

	Scenario 1			Scenario 2		Scenario 2/ Scenario 1
LCIA method	CML2			TRACI		
Unit	Total kg PO ₄ ³⁻ eq	kg N eq ^a	% of total	Total kg N eq	% of total	
Total	6.65E-04	1.58E-03	100	7.66E-04	100	0.48
contribution breakdown						
Total of airborne emission	4.12E-04	9.81E-04	61.9	1.40E-04	18.3	0.14
<i>Nitrogen oxides</i>	3.90E-04	9.28E-04	58.6	1.33E-04	17.3	0.14
<i>Ammonia</i>	2.19E-05	5.22E-05	3.3	Negligible ^b	<1	--
<i>Remaining airborne emission</i>	2.79E-07	6.65E-07	0.0	7.53E-06	1.0	--
Total of waterborne emission	2.52E-04	6.01E-04	37.9	6.26E-04	81.7	1.04
<i>Phosphate</i>	2.23E-04	5.32E-04	33.6	5.32E-04	69.5	1.00
<i>COD, Chemical Oxygen Demand</i>	1.73E-05	4.11E-05	2.6	3.93E-05	5.1	0.95
<i>BOD5, Biological Oxygen Demand</i>	Negligible	Negligible	<1	2.74E-05	3.6	--
<i>Nitrate</i>	Negligible	Negligible	<1	9.21E-06	1.2	--
<i>Remaining waterborne emission</i>	1.15E-05	2.73E-05	1.7	1.79E-05	2.3	--

^a The unit conversion is based on : 1 kg N = 1 0.42 kg PO₄³⁻

^b the contribution is below 1% cut-off

challenges in data collections. However, the disadvantage for this approach is also obvious as it might lose the sensitivity from the individual compound. In general, the substance aggregation is only applied to those with small or even negligible mass flows, so that the corresponded impacts are relatively minor in most cases. There is also one point that attracted our attentions during the comparison process in this study. As TRACI did not separate NO₂ and NO in its photochemical smog formation, an identical $CF^{POCP}(TRACI)$ for NO_x was assigned to both. This can lead to a considerable bias because the mass flow for NO is relatively large comparing to other trace gases. More importantly, NO can be oxidized to NO₂ and further trigger associated propagation cycles under photochemical

reactions. In CML2 database, the characterization factor for NO in photochemical oxidation is listed as $CF^{POCP} = -0.427 \text{ kg C}_2\text{H}_4 \text{ eq /kg NO}$ and all other nitro-oxides share a generic $CF^{POCP} = 0.028 \text{ kg C}_2\text{H}_4 \text{ eq./kg substance}$. Comparing these two approaches, CML2 provides a better justification by separating NO and other nitro-oxides as their impacts vary significantly. Based on the discussions above, one should review the simplification and aggregation processes carefully to avoid the potential bias, especially for those industries which might engage high mass flow of NO.

3.4 Recommendations to Choose and Develop LCIA Method for Desalination

From the discussions above, one can see that CML2 method has the advantages of more comprehensive coverage on the associated elements with generic approaches for common applications. However, the disadvantage of CML2 is also obvious as the implementation the comprehensive LCA was obstructed by overwhelming data requirement. TRACI is designed specifically to reflect the US context and reduce the effort in data collection and compilation, but this approach also restricted its application because of the narrow coverage of environmental interventions, customized characterization models, and aggregation of substances. As the inventory database (LCI) is usually the main concern in many LCA practices, one might want to choose the proper LCIA method depending on the feature of the inventory. Regional specific method, *e.g.* TRACI for the US, is a good choice if the local inventory is readily available or if some specific concerns are to be addressed in the local context. The CML2 is often used in comprehensive assessment by using the generic average inventories because it provides a general reference for most applications.

When evaluating the environmental impacts from an RO desalination plant, one should note that the RO processes highly depend on the feed water quality, local power supply model, and also the brine disposal approaches. These factors make it difficult to choose between CML2 and TRACI as

neither of them provides a good match. CML2 is very generic without considering the local context, which might lead to significant bias in the characteristic factors; while TRACI might over-simplify the database and overlook some important impacts from certain compounds that had been used quite heavily in the desalination industry. To better develop a customized LCIA method for desalination LCA, this study endeavor to propose some suggestions for researchers, especially those who are outside of Europe or America, where the CML2 and TRACI were developed.

(1) A group of specific impact categories can be developed to focus on the features of desalination process. Other than the traditional pollution categories for global warming, ozone depletion, smog formation, acidification, and eutrophication, it might be beneficial to form a new category for brine disposal, because the current aquatic eco-toxic characterization approach is not applicable due to the complexity of brine mixture as well as the limited coverage of the characterization approach.

(2) The ideal LCIA method should have a good balance between the sufficient coverage of environmental interventions and the minimal efforts to collect and compile the data. The development of a customized LCIA method can follow an iterated process as shown in Figure 3-2. Prior to developing a specific LCIA method, a comprehensive LCA study using generic LCIA method (e.g. CML2) is conducted to identify a small number of key substances responsible for the vast majority of the environmental impacts in the categories of interest. This list of the key substances could be used to prioritize the efforts to construct the interventions coverage for this customized LCIA method. The new LCIA method is then applied to other desalination study. Comparing the estimated results from this new LCIA with the generic LCIA methods, one can further modified the prioritized coverage list to ensure the concise integrity of the database without significantly losing the accuracy. An optimal balance might be reached after several iteration processes.

Figure 3-2. Iterated steps for developing customized LCIA method.

(3) The selection or development of characterization model should be consistent with the scopes and goals of the desalination project. Since ocean and inland disposals have disparate transport routes, the customized characterization model has certain fundamental differences in the fate and exposure modeling. However, it is difficult to develop a model as the stressor-effect chains behind the model are usually not clear and the characterization models are generally affected by a large amount of variables, such as local hydrodynamic conditions, the sensitivity of local species, and the brine characterization. In most situations, the generic model may be the only choice. Instead of developing a specific model, one might want to consider engaging the local context in the weighting step as the optional add-on in the LCIA processes.

3.5 Conclusions

Many researchers conducted the LCA on desalination without elaborating the reasons for choosing a specific LCIA method in their studies. This might lead to a significant bias if they overlooked this important factor. This study provides a good comparison to highlight the associated impacts from different LCIA methods in different impact categories. Generally speaking, choosing an inappropriate LCIA method might only have minimal impacts in the large-scale issues such as global warming potential and ozone depletion potential. The impacts, however, might be quite considerable in the categories for acidification, eutrophication, photochemical oxidation, human health, and ecotoxicity. These differences were mainly caused by the unequal coverage of the LCIA method, diversity of the characterization models, and differentiation of environmental interventions.

This study also proposes some suggestions in choosing the appropriate LCIA method for the desalination industry. Both LCIA methods evaluated in this study demonstrated specific advantages and limitations. The choice of the LCIA method should depend on the feature of the inventories available and also the specific concerns in the region if any:

(1) For those studies carried in the region without specific LCIA method, one might want to consider using a generic LCIA method, *e.g.* CML2, in the initial assessments. However, lots of efforts are required to deal with the difficulties in data gathering and compilation. Therefore, it is necessary to develop a feasible regional specific LCIA method to save time and money used in future studies. The initial studies with CML2 method can provide a general reference for developing the specific method: the selection of the right categories and indicators, determination of the coverage, and availability of characterization model are essential to a customized LCIA method.

(2) Engaging a regional specific method whenever available, *e.g.* TRACI for the US, might be beneficial as it requires less data and accounts in the local

context with certain specific concerns with local interests. However, to ensure reliability of the result, it is important to double check if all important emissions are all covered by the specific method.

Neither the CML2 nor TRACI method is the perfect choice for LCA of desalination. This study suggests improving the current TRACI method by complementing the missed important emissions to achieve the advantage of less data requirement without sacrificing the reliability of result significantly.

CHAPTER 4 CHOICE OF AQUATIC ECO-TOXIC CHARACTERIZATION APPROACH FOR BRINE DISPOSAL

4.1 Introduction

There is a growing interest in understanding the aquatic eco-toxic impact of brine disposal. Many laboratory researches (Latorre, M. 2005; Sanchez-Lizaso, J.L. *et al.* 2008; Dupavillon, J.L. and Gillanders, B.M. 2009), field-based experiments (Latorre, M. 2005; Sanchez-Lizaso, J.L. *et al.* 2008), and ecological monitoring studies (Fernandez-Torquemada, Y. *et al.* 2005; Gacia, E. *et al.* 2007; Ruso, Y.D.P. *et al.* 2007; Sanchez-Lizaso, J.L. *et al.* 2008) suggested that high salinity might cause reduced growth or even increased mortality of flora and fauna. Concern also exists regarding the release of metals coming from corrosion and the use of certain additives. Some studies found that the desalination brine with high chemical contaminant level have the potential to impair biological communities (Paquin, P.R. *et al.* 2000; Hoepner, T. and Lattemann, S. 2003) and even cause accumulation of toxic chemicals in macroalgae, mussels, *etc.* (Romeril, M.G. 1977; Sadiq, M. 2002; Liu, C. *et al.* 2012).

Although the role of concentrate disposal as an important source of aquatic eco-toxic impact is well established, most of previous studies only focused on the planning and operational phases mainly to address the energy shortage concern. Only limited efforts were made on quantifying the aquatic eco-toxic impact of brine disposal. Meneses (2010) compared the brine final disposal alternatives by means of LCA methodology, but the impact of salinity is not considered because the current Life Cycle Impact Assessment (LCIA) approach cannot translate the salt ions into aquatic eco-toxic impact. The liquid discharge potential impact was incorporated in Vince's study (2009), but the result was restricted by the site specific conditions with limited reference value to other studies. Many LCA studies assumed that the brine was fully diluted before discharge and posed minor impacts on the aquatic eco-system (Raluy, R.G. *et al.* 2004; Raluy, R.G. *et al.* 2005b; Raluy, R.G. *et al.* 2005c; Raluy, R.G. *et al.* 2006; Zhou, J. *et al.* 2011a). The

exclusion of brine disposal process might lead to the biased results and actually contradicts to the 'cradle-to-grave' nature of LCA – LCA should not only consider the emissions from operation and transportation phase, but also include the pollutants in concentrate disposal process.

There are two reasons contributing to the fact that the current LCA researches fall far behind the growing concern of brine disposal. (1) The intensive data requirement. It takes substantial efforts to carry out the comprehensive composition analysis and on-site ecotoxicology test, mainly due to the complexity and high variation of brine composition. (2) The misconception of taking the available aquatic eco-toxic characterization approaches as universally accepted 'standardized approaches' without further considering the suitability and the applicability of those approaches. The coverage of current approaches might not be able to satisfy the assessment requirement when it comes to the desalination brine.

Therefore, the focus of this chapter is to develop a low-data-demand and more comprehensive characterization approach for assessing the aquatic eco-toxic potential (aquatic ETP) of brine disposal from seawater desalination plants. A comparison study is engaged to illustrate the implementation and the advantages of the improved approach. In order to be consistent with Chapter 3, the rest of this chapter is also organized in line with the framework of LCA.

4.2 Model Construction for Comparative LCA Study

4.2.1 Goal and Scope Definition

1) Scenario definition

The purpose of this study is to develop an improved characterization approach to characterize the aquatic eco-toxic impact of brine disposal. A comparison study with six different scenarios was engaged to illustrate the improvement. Two current available approaches (the chemical specific approach and the whole effluent approach) and the approach proposed by

this study (group-by-group approach), were used to investigate the aquatic eco-toxic impacts of two different concentrates from sea water reverse osmosis desalination plant (SWRO) and multistage flash plant (MSF). Six scenarios were defined in Table 4-1. The details about the three aquatic eco-toxic characterization approaches are presented in Section 4.2.3.

Table 4-1. Scenario definition used to investigate the influence of aquatic eco-toxic impact of brine disposal

Scenario #	Desalination type	LCIA approach for aqua-ETP
1	SWRO	Chemical specific
2	SWRO	Whole effluent
3	SWRO	Group-by-group
4	MSF	Chemical specific
5	MSF	Whole effluent
6	MSF	Group-by-group

2) Function unit, system boundary, and assumptions

The function unit for scenario comparison was chosen as 1 m³ of brine. As a general illustration, this case study would focus on the impact of effluent at outfall point, therefore the disturbing and dilution effects in mixing zone were not considered as those are specific to the local conditions.

Characterization, uncertainty, contribution, and sensitivity analyses were used for results interpretation. The characterization analysis was used to quantify the aquatic eco-toxic impact of different scenarios. The characterization factors were derived in Section 4.2.3. In the uncertainty analysis, Monte Carlo simulation was used to evaluate the influence of variations in brine composition and the uncertainty of characterization approaches. The contribution analysis and sensitivity analysis were used to identify the most problematic chemicals and to investigate the possible ways to lower the aquatic eco-toxic impact of brine disposal.

4.2.2 Life Cycle Inventory

The brine composition was indicated in Table 4-2.

It was assumed that the concentration of each chemical fluctuated within a range of ± 20 percentage points of average. It is important to note that, compared to the other LCA studies which did not consider the uncertainty of the characterization factors; this study intentionally included this variable in order to ensure the scenario comparison result remains valid under different conditions. A large uncertainty ($\pm 50\%$) was assigned to $CF^{aquatic\ ETP}(\text{eff})$ because the $CF^{aquatic\ ETP}(\text{eff})$ used in this case study was derived from EoliaTM Potable Water (Vince, F. *et al.* 2009) instead of the local on-site monitoring data. Since the chemical grouping activity might introduce extra variations, the aquatic eco-toxic characterization factor for each group was assumed to have a higher uncertainty value ($\pm 30\%$) than USEtox chemical-specific characterization factor ($\pm 20\%$).

4.2.3 Aquatic Eco-toxic Characterization Approach

1) Critical review of available approaches

As sketched in Section 4.1, this section focuses on the midpoint level approach. Given the function unit is defined as 1 m^3 of brine, the aquatic eco-toxic impact of brine disposal is commonly estimated based on the Equation (2):

$$\text{Aquatic ETP of brine disposal} = \sum_i m(i) \times CF^{aquatic\ ETP}(i) \quad \text{Equation (2)}$$

Where $m(i)$ is the mass of i in 1 m^3 of brine and $CF^{aquatic\ ETP}(i)$ is the aquatic eco-toxic characterization factor for i . Two different approaches are available to identify the aquatic eco-toxic characterization factor: the chemical specific approach and the whole effluent approach. In the chemical specific approach, the i is defined as individual chemical in the desalination brine, while the i stands for the entire effluent in the whole effluent approach.

Table 4-2. Brine composition and its correspondence CF from USEtox database^a

Chemicals	SWRO brine Composition ⁱ (ave, mg.L ⁻¹ / uncertainty)	MSF brine Composition ^j (ave,mg.L ⁻¹ / uncertainty)	CF provided by USEtox database ^k (ave, PAF m ³ .d.kg ⁻¹ / uncertainty)
TDS	80028.4/±20%	50300/±20%	-- ^b
pH	Neutralized	Neutralized	--
T	34°C	34.5°C	--
Turbidity	Neutralized	Neutralized	--
Salt ions			
Ca ²⁺	891.2/±20%	N.R. ^c	--
Mg ²⁺	2877.7/±20%	N.R.	--
Na ⁺	24649.2/±20%	N.R.	--
K ⁺	888/±20%	N.R.	--
Sr ²⁺	N.D. ^d	N.D.	--
Cl ⁻	43,661.5/±20%	N.R.	--
SO ₄ ²⁻	6,745.1/±20%	N.R.	--
HCO ₃ ⁻	315.3/±20%	N.R.	--
Br ⁻	N.D.	N.D.	--
BO ₃ ³⁻	N.D.	N.D.	--
Residuals of Chemical additives			
Free chlorine	Neutralized	0.5	--
Chloramine	N.D.	N.D.	3.2E+03/±10%
Antifoaming agent	N.A. ^e	0.05 polyethylene glycol	--
Corrosion inhibitor	N.A.	N.R.	--
Coagulants	0.02 FeO(OH) /±20%	N.R.	--
	0.04 polyelectrolyte/±20%		
Scale control chemical	0.04 SHMP/±20%	0.671 polymer	--
	0.04 polymer/±20%		
By-products of chemical additives			
Tribromomethane	N.D.	0.085	1.9E+02/±10%
Dibromochloromethane	N.D.	N.D.	1.1E+02/±10%
Bromodichloromethane	N.D.	N.D.	2.1E+01/±10%
Chloroform	N.D.	N.D.	4.1E+01/±10%
Chlorophenol	N.D.	N.D.	1.0E+03/±10%
Chlorobenzenes	N.D.	N.D.	3.9E+02/±10%
Membrane cleaning chemicals			
HCl	Neutralized	Neutralized	--
C ₆ H ₈ O ₇	Neutralized	Neutralized	--
H ₃ PO ₄	Neutralized	Neutralized	3.0E+02/±10%
NaOH	Neutralized	Neutralized	--
SHMP, formaldehyde, Isothiazole, benzotriazole, etc,	N.D.	N.D.	1.3E+03/±10%
Metal and ion			
Copper	0.015/±20%	0.1	5.5E+04/±10%
Nickel ^f	0.003/±20%	0.02	1.5E+04/±10%
Iron	0.00013/±20%	N.D.	--
Chromium	0.0035/±20%	N.D.	1.0E+05/±10%
Molybdenum	0.0004/±20%	N.D.	--
Other trace chemicals	N.D.	N.D.	--

^a the reported pH and turbidity of the brine is neutralized before disposal ^b --: the chemical is not covered by USEtox database. The CF is defined as 0 in the chemical-specific approach. ^c N.R.: not reported ^d N.D.: not detected because of low concentration ^e N.A.: not applicable ^f the Ni concentration is assumed as 20% of Cu concentration (Lattemann, S. and Hopner, T. 2003). ⁱ ref: (Baig, M.B. and Al Kutbi, A.A. 1998; Lattemann, S. and Hopner, T. 2003; Fritzmann, C. *et al.* 2007) ^j ref: (Abdel-Jawad, M. and Al-Tabtabaei, M. 1999; Lattemann, S. and Hopner, T. 2003) ^k ref: (Henderson, A.D. *et al.* 2011)

a. The chemical specific approach

The chemical specific approach, which is traditionally employed by LCA, calculates the average effluent impacts as the sum of the impacts generated by all acknowledged chemicals within the effluent based on the aquatic ETP of each elementary chemical (Vince, F. *et al.* 2009). A number of different characterization models have been developed for calculating $CF^{aquatic\ ETP}(i)$ over 15 years. These models vary in their scopes and modeling principles due to specific concerns and applications. Recently, a more transparent and consensus characterization model, USEtox, was developed by life cycle initiative under United Nations Environmental Programme (UNEP) and the Society for Environmental Toxicology and Chemistry (SETAC) (Henderson, A.D. *et al.* 2011). This model covers the chemical fate, exposure, and effect and can be expressed as Equation (3):

$$CF^{aquatic\ ETP}(i) = FF_i \times XF_i \times EF_i \quad \text{Equation (3)}$$

Where $CF^{aquatic\ ETP}(i)$ is the aquatic eco-toxic characterization factor, representing aquatic ecotoxicological impact of individual chemical i , where the impact is quantified as the potentially affected fraction (PAF) of species [$PAF.m^3.day/kg$]. FF_i is the fate factor, calculated as persistence time of chemical i staying in the aqueous phase [day]. XF_i is the exposure factor, representing the bioavailability of the chemical i to aquatic organisms [*non-dimensional*]. For aquatic systems, the XF_i is calculated as the dissolved fraction of a chemical i . EF_i is the effect factor, expressing the ability of a chemical i to cause toxic effects to the exposed aquatic ecosystems [$PAF.m^3/kg$]. It is calculated by determining the linear slope along the concentration-response relationship up to the point where the fraction of effect species is 0.5 (Equation 4). The $HC50$, the geometric means of laboratory-derived single species $EC50$ data, is defined as hazardous concentration of representative chemical at which 50% of a population displays an effect (e.g. mortality) [$PAF.m^3/kg$].

$$EF = 0.5/HC50 \quad \text{Equation (4)}$$

The chemical specific approach is a high quality analytical method suitable for assessing effluents containing relatively few contaminants which themselves have well-defined ecotoxicological properties. However, applying this chemical specific approach to brine disposal is not easy because it contains tens of thousands of chemicals, by-products and transformation products, many of which are presented at extremely low concentrations. It requires a great amount of time and resources to analyze the ecotoxicological property for all these compounds. In addition, this approach has limited coverage of the aquatic ETP pollutants. It usually does not account for the impact of the chemicals which haven't been reported in USEtox.

b. The whole effluent approach

There is increasing recognition regarding the limitations to the chemical specific approach. Consequently, many researchers are exploring more holistic techniques such as whole effluent assessment. There are a number of different terminologies for approaches involving whole effluent assessment, such as Whole Effluent Toxicity (WET) used by USA (and some European Countries), Effluent Toxicity Test (ETT) used by Canada, Integrating Controlling of Effluents (ICE) used by Germany, Whole Effluent Environmental Risk (WEER) used by the Netherlands, *etc.* (Hardisty, P.E. 2010). Compared to the chemical specific approach, the whole effluent approach does not need to characterize the composition of the effluent, but provides a measure of the combined effects of all the components in a complex effluent, such as synergistic, additive or antagonistic effects (Gotvajn, A.Z. and Zagorc-Koncan, J. 1998). Therefore, given the function unit is defined as 1 m³ of brine, the equation *Aquatic ETP of brine disposal* = $\sum_i m(i) \times CF^{aquatic\ ETP}(i)$ can be rephrased as Equation (5):

$$Aquatic\ ETP\ of\ brine\ disposal = \sum m(eff) \times CF^{aquatic\ ETP}(eff) \quad \text{Equation (5)}$$

Where $m(eff)$ is the mass of entire effluent, and $CF^{aquatic\ ETP}(eff)$ represents the aquatic eco-toxic characterization factor for the complex mixture.

The typical whole effluent assessment schemes only assess the toxicity to aquatic organisms (EF_{eff}) because the currently available persistence tests and biodegradation tests are designed to measure the transport and exposure of individual chemical, not mixtures (ECETOC 2004). In order to implement the whole effluent approach in LCA, the fate factor and exposure factor for the mixture can be estimated based on the worst case scenario. The fate factor for the entire effluent is defined as the residence time of the most persistence chemical in the mixture [$FF_{eff} = MAX(FF_i)$]. In brine disposal applications, all the chemicals are assumed to be in the totally dissolved form [$XF_{eff} = MAX(XF_i) = 1$]. Then the aquatic eco-toxic characterization factor for the entire effluent can be expressed by Equation (6).

$$CF^{aquatic ETP}(eff) = MAX(FF_i) \times 1 \times EF_{eff} \quad \text{Equation (6)}$$

The principal advantage of the whole effluent approach is to provide a better assessment on the ecotoxicological property of those poorly characterized and complex effluents (i.e. those containing unknown mixtures of chemicals), and hence improve their impact quantification in LCA. However, since the whole effluent approach only provides a temporal estimation of EF_{eff} , the variation of brine composition and intrinsic water quality (e.g. salinity, pH, hardness) might lead to a large uncertainty.

2) *Development of an improved approach*

As discussed above, both the chemical specific approach and the whole effluent approach have its own merits and disadvantages. In order to properly assess the complex and unstable desalination effluents, this study make an attempt to integrate the advantages from both approaches. The improved approach, called the group-by-group approach, calculates the average aquatic ETP impact as the sum of the impacts generated by acknowledged groups of influential chemicals. The overall procedure of the group-by-group approach (Figure 4-1) is derived from the process shown in

Figure 3-2. Given the function unit is defined as 1 m³ of the desalination brine, this approach can be expressed by Equation (7).

$$\text{Aquatic ETP of brine disposal} = \sum_j m(\text{group } j) \times CF^{\text{aquatic ETP}}(\text{group } j)$$

Equation (7)

Where $m(\text{group } j)$ is the mass of the acknowledged group j , and $CF^{\text{aquatic ETP}}(\text{group } j)$ represents the aquatic eco-toxic characterization factor for group j .

Figure 4-1. The procedure for the group-by-group approach

As discussed above, the total aquatic eco-toxic impact of brine disposal depends on the definition of Group j and the estimation of $CF^{aquatic ETP}(group\ j)$.

a. The definition of Group j

The plume of brine typically contains all or some of the following constituents:

- Concentrated major constituents in seawater, including Cl^- , Na^+ , SO_4^{2-} , Mg^{2+} , Ca^{2+} , K^+ , HCO_3^- , Br^- , BO_3^{3-} , and Sr^{2+} .
- Other concentrated miscellaneous elements in seawater, such as F^- , Li^+ , SiO_3^{2-} , Zn^{2+} , Ar, Fe, *etc.*
- Residuals of antifouling additives. Chlorine, in gas or liquid forms, or hypochlorite and its derivatives, is commonly used as biocides to reverse fouling.
- Residuals of antiscaling additives. The organophosphonate-, polyphosphate- or polymer-type compounds are usually added to prevent precipitation (Greenlee, L.F. *et al.* 2009).
- Other residuals of chemical additives, such as ferric chloride used as coagulant, various anti-foaming agents and corrosion control chemicals used in thermal desalination, *etc.*
- Metals and their ions. The corrosion process from the effect of water flow, dissolved gases and treatment chemicals on the alloys utilized in the construction of desalination pipes and equipment may cause the increase in metal concentrations in the brine (Lattemann, S. *et al.* 2008).
- The untreated backwash water and membrane cleaning solutions which typically contains high load of suspended solids and can be either quite acid or alkaline.

- Other contaminants originally in feed, such as boron, the pharmaceuticals and personal care products (PPCPs), various industrial additives, *etc.*
- By-products of chemical additives, such as halogenated hydrocarbons and chloramine from chlorination, derivatives of corrosion inhibitors like benzotriazole, *etc.*

The first step to define the Group *j* is to identify the influential chemicals to the aquatic eco-toxic impact of brine disposal. Two principles are applied to the pre-screening stage.

- Chemicals with concentrations higher than the regulated level if the regulation is available; or with concentrations much higher than the other constituents in the desalination brine if the regulation is not available. Taking copper as an example, the U.S. EPA recommends a maximum concentration of 4.8 µg/L for brief exposure and 3.1 µg/L for long-term exposure (Ortiz, O. *et al.* 2010). Values at the same order of magnitude were also found in European saltwater environments (Batlles, F.J. *et al.* 2010). Copper should be included in the influential chemical list because its concentration is usually high in brine discharge. Similarly, chemicals with significantly high concentrations should be included in the influential list even if they are not regulated. A typical example is the salt ions in the desalination brine. The concentrations of salt ions are typically four orders of magnitude higher than the other constituents.
- Chemicals with characterization factors much higher than other constituents in the desalination brine. This principle is used to avoid the truncation error caused by the assumption made in previous principle. Even with expected low concentrations, chemicals with high impact characterization factor are suggested to be considered as influential chemicals. For example, nickel is a typical corrosion product from heat exchanger surfaces in MSF system. The high

impact characterization factor makes it important as an influential chemical although its concentration is usually low.

The chemicals that meet either of the principles are regarded as influential, while the other chemicals are assumed to pose negligible or minor contribution to the overall impact. However, it should be noted that the list of influential chemicals/parameters should be revised along with the improvement of scientific knowledge and the local conditions. In this study, we assume the pH value of the brine is neutralized before discharge. The pH neutralization can be achieved by mixing with the desalination brine, followed by seawater dilution or chemical adjustment. Although the neutralized pH value is not considered as an influential factor in this study, more efforts might be needed to evaluate the impacts when significant pH alternation is presented. Based on the industrial practice, significant lower/high pH values may occur during acid/alkaline cleaning rather than during normal operation of MSF and RO plants. For example, a pH of 2 is often needed to clean MSF distiller (El Din et al. 1994), while a pH range of 2.3-4 for RO membrane cleaning (DuPont 1994). From the ecology point of view, the acidic/alkali blow-down might carry significant impacts to the local marine biota, especially the starfish and other less mobile organisms. Due to the limitation of current LCIA methods, this study also assumed the temperature the brine is adjusted to that of the surrounding seawater before discharge. In actual practice, MSF effluent temperature is generally elevated due to the processes. Reported seasonal temperature differences varied between 5-6 °C (Abdel-Jawad, M. and Al-Tabtabaei, M. 1999), 6-9 °C (Mickley, M. 1995) and 10-15 °C (Altayaran, A.M. and Madany, I.M. 1992) above the naturally occurring seawater temperature. The potential effects of elevated temperatures include insufficient dissolved oxygen, failures in process integration, desiccation (inter-tidal organisms), enzyme inactivation, change in lipid state, increase in protoplasmic viscosity, increase in cell membrane permeability, protein denaturation, and release of toxic substances from damaged cells (CCME 1999). Other than the pH value and temperature, the impact from the turbidity, pharmaceuticals, and other

micro pollutants of are not included in this study, because their associated eco-toxicity impacts are not well-characterized based on current scientific understandings, thus the associated impacts are not included in this study. There are more and more research efforts focusing on the eco-toxicity field. These impact parameters should be incorporated into LCIA methods when enough knowledge is obtained.

The next step is to group the influential chemicals. Generally, these chemicals can be divided into three categories according to the chemical property: the metals, organic chemicals and inorganic chemicals. Each category can be further divided into several groups according to the impact pathway (cause-effect train). For example, in the inorganic category, the salt ions can be defined as one group. The organisms suffer from the osmotic stress when they exposed to elevated concentration of salt ions due to more dissolved ions in ambient water compared to their body liquids (Einav, R. *et al.* 2003).

There is no universally agreeable grouping method in the current LCA community. This study provides two suggestions in grouping stage. Firstly, the number of category/group depends on the data availability and the expected confidence level of the study. Increasing the category/grouping number can reduce the uncertainty of the results, but the information required also increase accordingly. Secondly, the grouping of important chemicals should base on the goal and scope of the project. In brine disposal applications, it is advisable to put the chemicals with similar characteristics, such as chemical property, impact pathway, or local concerns, *etc.* into same group. The salt ions, for example, are all inorganic ions and affect organisms via similar pathway (osmotic stress). They also contribute to significant high salinity, which is always a concern for local environment. Therefore, rather than following substance-by-substance approach, which needs to identify the concentration of each salt ion, this work suggests categorizing all the salt ions into one group, and the salinity can be used to properly characterize this group.

b. Identification of group-specific characterization factors

As discussed previously, it might be useful to categorize the chemicals into at least three categories in the common practice, namely the metal category, organic category, and inorganic category. Each category can be further divided into groups depending on the chemical composition and the availability of characterization factors. Given the significant difference among these groups, it is better to employ different strategy to determine the group-specific characterization factor.

In metal category, the number of influential metals in brine is usually manageable. In addition, the characterization factors for these metals have been well documented in the USEtox database. Therefore, every single influential metal can be regarded as a group and the chemical specific approach can be applied to assess the impact of the metal category.

On the contrary, the organic group is probably still complex mixture. It is a challenge to go for the pure chemical specific approach due to the intensive data requirement. It might be more appropriate to further prioritize the influential organic chemicals in each group. The chemicals with either high characterization factors or high concentrations can be considered as representative organic chemicals for this group. With this practice, one can only focus on the representative chemicals without sacrificing the reliability of the results significantly. The USEtox database has included the characterization factors for nearly 3000 organic chemicals which might cover most of representative organic chemicals in the brine. If a specific organic chemical is not on the list, the fate, exposure, and effect model mentioned in the chemical specific approach can be used to derive the characterization factor.

Due to the large uncertainties in the fate and exposure models for the inorganic chemicals, the whole effluent approach is a better choice to estimate the characterization factor for the inorganic group. As mentioned in whole effluent approach, instead of USEtox fate model and exposure

model, it is more appropriate to estimate both two factors based on worst case scenario: the fate factor is calculated as the residence time of most persistent chemical in the inorganic group, while the exposure factor is usually defined as 1. It is important to note that the whole effluent approach is more preferable when evaluating the impact from the inorganic group with relatively stable composition. For the group with high variation in composition, or in a situation of limited resources for carrying out ecotoxicological test, the representation strategy discussed in organic category is a possible alternative.

3) *Deriving characterization factors for scenarios*

USEtox database was used to support the chemical specific approach. The USEtox database have documented eco-toxic characterization factors for over 3000 organic chemicals and 21 metals, however, only part of brine constituents was covered (the last column of Table 4-2). The impacts of the chemicals which were not reported in USEtox were not counted in the chemical specific approaches (Scenarios 1 and 4).

As mentioned in whole effluent approach, the characterization factor for the entire effluent was calculated based on Equation $CF^{aquatic\ ETP}(eff) = MAX(FFi) \times 1 \times EF_{eff}$. The Eolia™ Potable Water have defined the EF_{eff} as $5.8E-04\ PAF\ m^3/kg$ (Vince, F. *et al.* 2009). The most persistence chemical in brine was the salt ions (thousands of years), but the FF_{eff} was calculated as the residence time of Cu (37 days based on USEtox fate model), which was the second most persistence chemical in the mixture. This was because that the persistence time of salt ions was far beyond the range of midpoint level (acute aquatic eco-toxic potential). The XF_{eff} was defined as 1 because all the chemicals were assumed to be in the totally dissolved form in term of aquatic eco-toxic impact. The Eolia™ Potable Water did not differentiate between SWRO and MSF plants, therefore, scenario 2 and 5 employed same characterization factor as $2.15E-02\ PAF\ m^3\ day/kg$.

The procedure described in Figure 4-1 was used to establish the group-by-group approach. The influential chemicals were identified based on the concentrations and characterization factors (Table 4-3). The influential chemicals were then classified into several groups under three categories: salt ions group and free chlorine group in inorganic category, halogenated hydrocarbons group in organic category, as well as Copper, Nickel, and Chromium in metal category. The characterization factor for each group was calculated in Table 4-4.

4.3 Results Interpretation and Discussion

Figure 4-2 showed the results from the characterization analysis. The black dot with horizontal line through the center of the circle indicated the average aquatic ETP for each scenario. The Monte Carlo simulation for 100 runs with a confidence interval of 95% was carried out in uncertainty analysis. The range of the result was illustrated as vertical bar in Figure 4-2. It can be seen that the chemical specific approach (Scenarios 1 and 4) reported lowest aquatic eco-toxic impact of brine disposal. This result was expected as it did not count the impact of salt ions, free chlorines and other chemicals which were not reported in USEtox. As mentioned in the critical review of approaches, the chemical specific approach is a high quality analytical method suitable for assessing effluents with limited numbers of contaminants which themselves have well-defined fate, exposure, and effect factors. The reliability of this approach highly depends on if the attached ecotoxicological database could provide sufficient coverage over the complex chemical composition. The users should always pay attention to this coverage issue to avoid under-estimation as seen in this case.

Table 4-3. Identification of influential chemicals in desalination brine

Pre-screen criteria	Influential chemical		Comments
	Brine from RO plant	Brine from MSF plant	
<u>High concentration</u>			
> regulation level			
		Free chlorine (500 µg/L)	regulation level of free chlorine <ul style="list-style-type: none">• 7.5 µg/L (US EPA long-term),• 13 µg/L (US EPA, short-term)• 0.06 µg/L (The European PNEC)
		Tribromomethane Bromodichloromethane Dibromochloromethane Chloroform (THMs, 85 ug/L)	regulation level of CBPs <ul style="list-style-type: none">• $\text{total THMs} = C_{\text{Chloroform}} / 300 \mu\text{g.L}^{-1} + C_{\text{BDCM}} / 21 \mu\text{g.L}^{-1} + C_{\text{DBCM}} / 100 \mu\text{g.L}^{-1} + C_{\text{Bromoform}} / 100 \mu\text{g.L}^{-1} \leq 1$ (WHO)• total THM's < 80 µg.L⁻¹ (US EPA)
	Cu (15 ug/L)	Cu (100 ug/L)	regulation level of Cu <ul style="list-style-type: none">• 4.8 µg/L (US EPA short-term)• 3.1 µg/L (US EPA long-term)• 5.6 µg/L (European PNEC)• 8 µg/L (Mediterranean)
> other constituents			
	Cl ⁻ , Na ⁺ , SO ₄ ²⁻ , Mg ²⁺ , Ca ²⁺ , K ⁺ , HCO ₃ ⁻	Cl ⁻ , Na ⁺ , SO ₄ ²⁻ , Mg ²⁺ , Ca ²⁺ , K ⁺ , HCO ₃ ⁻	Concentration is 4 orders of magnitude higher than others
<u>High characterization factor</u>			
		Chlorophenol Chlorobenzenes	CF>1E+2 PAF m ³ .d.kg ⁻¹
	Nickel, Chromium	Nickel, Chromium	CF>1E+4 PAF m ³ .d.kg ⁻¹

Table 4-4. Identification of group and derivation of group-specific CF

Category	Factors	Value	Comments
inorganic category			
Salinity Group, including Cl^-, Na^+, SO_4^{2-}, Mg^{2+}, Ca^{2+}, K^+, HCO_3^-			
	FF(d)	37	The FF model mentioned in chemical specific approach is not applicable to inorganic salts. Therefore, The FF for salinity is estimated for the worst case scenario. The most persistence chemical in this group is Na^+ , with residence time of 210million yrs, which exceeds the range the acute test (100yr). Therefore, the residence time of Cu^{2+} , a major composition, was employed here.
	XF (-)	1	The salts are 100% dissolved in water.
	EF (PAF m^3/kg)	1.25E-02	The derivation is available from Table 4-5
	CF (PAF $m^3 d/kg$)	4.62E-01	CF = FF*XF*EF
Free chlorine Group, including $HClO$, $NaOCl$, $Ca(OCl)_2$, etc			
	CF (PAF $m^3 d/kg$)	3.20E+03	The EF for free chlorine is not available. The major composition of free chlorine is $HClO$, therefore it is selected as the representative chemical for this group. The multimedia model mentioned in chemical specific approach is not applicable. The CF for a similar disinfectant, chloramine-T ^a is used here. CF for chloramine-T ^b is available from USEtox database.
organic category			
Halogenated hydrocarbons Group, including Tribromomethane, Bromodichloromethane, Dibromochloromethane, Chloroform, Chlorophenol, Chlorobenzenes, etc			
	CF (PAF $m^3 d/kg$)	1.90E+02	$CHBr_3$ is selected as the representative chemical because it is dominant composition in this group and has relatively high CF. Its CF is available from USEtox database.
metal category			
Cu			
	CF (PAF $m^3 d/kg$)	5.50E+04	CF is available from USEtox database.
Ni			
	CF (PAF $m^3 d/kg$)	1.5E+04	CF is available from USEtox database
Cr			
	CF (PAF $m^3 d/kg$)	1.0E+05	CF is available from USEtox database

^a chloramine-T breaks down to the hypochlorite ($HClO$) in water. Chloramine-T is an N-chlorinated and N-deprotonated sulfonamide.

Table 4-5. The derivation of effect factor of salinity on marine community ^{a, b, c}

Species	acute-EC50 (g/l)	chronic-EC50 = acute-EC50/2 (g/l) ^d	Log (chronic-EC50) ^d	GEOMEAN of Log(chronic-EC50)	log(HC50)	HC50	EF (PAF m3/kg)
phytoplankton species							
S. costatum	53.76	26.88	1.43	1.41	1.37	23.36	2.14E-02
C. vulgaris	60.20	30.10	1.48				
T. suecica	55.51	27.76	1.44				
I. galbana	41.17	20.59	1.31				
macroalgae							
U. pertusa	52.00	26.00	1.41	1.41			
zooplankton species							
Brachinonus plicatilis	53.66	26.83	1.43	1.36			
Tigriopus japonicus	39.02	19.51	1.29				
demersal fish							
Paralichthys olivaceus	39.02	19.51	1.29	1.29			

^a the derivation of EF is based on USEtox principles (<http://www.usetox.org/>)

^b the acute EC50 data is available from (Yoon, S.J. and Park, G.S. 2011)

^c the density of sea water is 1.025 g/l

^d the derived chronic-EC50 is far below the salinity of seawater. This means the acute-to-chronic factor of 2 defined in USEtox is not applicable to this calculation. Therefore, the threshold concentration for acute toxicity of salinity (40g/l) is used to derive the EF. This assumption underestimates the aquatic eco-toxic impact

The results reported from the whole effluent approach (scenario 2 and 5) and from the group-by-group approach (scenario 3 and 6) were on the same order of magnitude, with the later estimated a slightly higher impact. The whole effluent approach regarded all the chemicals in brine as one group to estimate the aquatic eco-toxic impact, while the group-by-group approaches only introduce this whole effluent concept to salinity group. Compared to the whole effluent approach, the group-by-group approach showed two important advantages.

Figure 4-2. Characterization and uncertainty analysis results

- Reducing reliance on temporal ecotoxicology properties of the desalination brine. As mentioned previously, the whole effluent approach depended on the on-site ecotoxicology test instead of USEtox database. The EF_{eff} defined in Eiolia™ Potable Water is specific to the particular brine sample used in the ecotoxicological test. High uncertainty probably occurs when applying this sample-specific EF_{eff} to the brines discharged from other seawater desalination plants or even same plant but with different operation conditions. In the group-by-group approach, the whole effluent concept was only used to estimate the impact of salinity group, while different strategies as illustrated in Figure 4-1 were applied to the other chemical groups. The salinity of SWRO/MSF brine has a small variation because the salinity of sea water is relatively stable and recovery rate of SWRO/MSF plants are usually well controlled in a narrow range. Therefore, the effect factor determined by the ecotoxicology test is considered as a relatively stable intrinsic property of the salinity group and can be applied to all salinity groups across different brines.
- Facilitating interpretation of characterization result. The whole effluent approach does not distinguish the contribution of individual chemical or group. Therefore, it is of limited help to recommend the potential solutions if one wants to reduce the total aquatic eco-toxic impact. On the contrary, characterization results from the group-by-group approach can be further interpreted by contribution analysis and sensitivity analysis. The contribution analysis results (Figure 4-3) indicated that the group-by-group approach (scenario 3 and 6) provided a broader coverage of metals, organic chemicals, as well as salt ions and free chlorine in inorganic category. Sensitivity analysis was used to investigate the possible ways to lower the aquatic eco-toxic impact of brine disposal. Table 4-6 showed the results for the comparison of “what if” scenarios against the “baseline” scenario.

The results suggested salinity control as an effective way to reduce the impact of brine disposal.

It is also worth to note that the chemical specific approach also provides the information on the contribution analysis and sensitivity analysis. Due to the limited chemical coverage in the current USEtox database, the chemical specific approach suggested a different solution by reducing copper emission.

Scenario 1: SWRO brine + chemical specific

□ Cu ■ Ni ▨ Cr

Scenario 3: SWRO brine + group-by-group

■ salinity group □ metal group

Scenario 4: MSF brine + chemical specific

□ Cu ■ Ni □ CHBr3

Scenario 6: MSF brine + group-by-group

■ salinity group ▨ free chlorine group
▨ halogenated hydrocarbons group □ metal group

Figure 4-3. Contribution analysis results

Table 4-6. Sensitivity analysis results

		chemical specific approach	group-by-group approach
<i>Eco-toxic impact of discharging 1 m³ of brine from RO plant</i>			
"Baseline" scenario	Ave (PAF m ³ day/m ³ effluent)	1.22	37.8
		100%	100%
"What if" scenarios	reduce Cu by 10%	-7%	negligible
	reduce Ni by 10%	Negligible ^a	negligible
	reduce Cr by 10%	-3%	negligible
	reduce salinity by 10%	0 ^b	-10%
	reduce all metals by 10%	-10%	negligible
<i>Eco-toxic impact of discharging 1 m³ of brine from MSF plant</i>			
"Baseline" scenario	Ave (PAF m ³ day/m ³ effluent)	5.75	30.4
		100%	100%
"What if" scenarios	reduce Cu by 10%	-10%	-2%
	reduce Ni by 10%	negligible	negligible
	reduce CHBr ₃ by 10%	negligible	negligible
	reduce salinity by 10%	0	-8%
	reduce free chlorine by 10%	0	-1%
	reduce halogenated hydrocarbons by 10%	negligible	negligible
	reduce all metals by 10%	-10%	-2%

^a. "negligible" means this "what if" scenario has **minor** effect on the final result

^b. "0" means this "what if" scenario has **no** effect on the final result

4.4 Recommendations and Conclusions

Many researchers conducted the LCA on desalination without considering the aquatic eco-toxic impact of brine disposal in their studies mainly due to the limitation of current LCIA approaches (Lundie, S. *et al.* 2004; Raluy, R.G. *et al.* 2004; Lundie, S. *et al.* 2005; Raluy, R.G. *et al.* 2005a; Raluy, R.G. *et al.* 2005b; Raluy, R.G. *et al.* 2005c; Raluy, R.G. *et al.* 2006; Munoz, I. and Fernandez-Alba, A.R. 2008; Frutos, A.R. *et al.* 2009). This study provides a good critical review of two approaches that are commonly used in the LCA practice for assessing aquatic eco-toxic impact of brine disposal, namely the chemical specific approach and the whole effluent approach. The chemical specific approach has limited application because it is not practical to carry out comprehensive composition analysis of the complex desalination effluent. The whole effluent approach does not need to characterize the effluent, but it only provides a temporal estimation. Significant uncertainty probably occurs due to the variation of brine composition and intrinsic water quality.

This study developed an improved approach, named the group-by-group approach, to quantify the impact of complex and variable seawater desalination concentrates. This approach takes the merits of the two common approaches discussed above. It calculates the average aquatic eco-toxic impact as the sum of the impacts generated by acknowledged groups of influential chemicals within the desalination concentrate based on the impact of each group. Two important characteristics make this approach ideal for quantifying the aquatic eco-toxic impact of brine disposal. The first virtue of the group-by-group approach is that it requires less data to estimate the associated impact without sacrificing the reliability significantly. A pre-screening practice is engaged to identify a limited number of chemicals as important contributors based on their concentration and characterization factor. These important chemicals are then classified into several groups under three categories. The aquatic eco-toxic potential of each group can be calculated by the chemical specific approach or the

whole effluent approach based on the characteristic of the group and availability of characterization factors. For the groups remain highly complicated in chemicals, representative chemicals can be defined via the activity similar to the pre-screening practice to further reduce the data requirement. The second advantage is to provide a more comprehensive coverage for the complex brine. The group-by-group approach not only considers the impact of organic chemicals and metals, but also includes the contribution of inorganic chemicals, which are considered problematic in the impact assessment due to the lack of associated characterization factors.

CHAPTER 5 CHOICE OF IN-STOCK DATASET AS REPRESENTATIVE DATA FOR BACKGROUND CHARACTERISTICS

5.1 Introduction

As indicated in Section 1.2, a life-cycle assessment of a product or process aims at capturing a range of environmental liabilities or impacts that accumulate over the entire cradle-to-grave period. Generally speaking, in desalination, these impacts can occur directly during the treatment step, and/or during the process. They can also occur indirectly during the provision of energy, infrastructure, chemicals, membranes, waste management services into the treatment. The direct impacts are generally based on the generic characteristics of the desalination foreground system which might be more consistent throughout different locations, while the indirect impacts can vary widely with the structure and performance of the supplying background systems.

Therefore, quantifying the environmental performance of a desalination plant requires amassing geographical-specific background data regarding the whole life cycle. As indicated in Table 1-1, 1-2, 1-3, and 1-4, most of desalination LCAs are carried out in European background. This is because the most commonly used database is Ecoinvent followed by the PE data, both of which mainly rely on the data collected in Europe. This is even truer for Ecoinvent database as most of the information is based on the Switzerland industry.

The LCA practitioners, especially those in Asia, are struggling to find proper databases corresponding to the specific geographical characteristics. The in-stock database (Ecoinvent, PE databases, *etc.*) supplies a wide range of data sets. Taking advantage of the in-stock datasets might be a cost-effective way to support the very specific data needs for different locations. Especially for the South East Asia countries which are lack of national-

specific inventories, it is important to explore the possibility to modify the existing datasets to better represent background characteristics.

Since energy consumption is an indispensable background system for desalination LCA studies, the purpose of this study is to examine whether the choice of the national-specific inventory for power generation can lead to significant differences in overall impact. In addition, in order to extend the desalination LCA studies to the locations other than European countries, the Singapore-specific inventory for power generation is developed based on the in-stock Ecoinvent database. The rest of this chapter is organized in line with the framework of LCA.

5.2 Model Construction for Comparative LCA study

5.2.1 Goal and Scope Definition

a. Scenario identification

The present study includes three scenarios; each conducts environmental LCA with the United States (US), Singapore (SG), and Spain (ES) electricity models. Comparing these three electricity profiles, two major differences attracted our attention. Firstly, coal is currently used as the major energy source in ES and the US, while a unique fuel mix with nearly 80% of natural gas is used in Singapore (Table 5-1). This study has made an attempt to identify the associated differences in the environmental impacts due to the energy profiles. It is also the first study to consider the environmental impact of desalination in a city which relies almost entirely on natural gas for electricity generation. Secondly, although the ratios of electricity generated from coal in ES and the US are quite similar, and so are the ratios of electricity from heavy fuel oil in ES and SG (see Table 5-1), the actual electricity production profiles differ widely in certain aspects, such as power plant efficiencies, fuel exploration methods, and fuel production technologies. This study made an effort to illustrate the resulting environmental impacts due to these varieties.

The software Simapro 7.1 with Ecoinvent database V2.1 was used to set up the model structure for all scenarios. Prior to scenario comparison, Singapore LCI for electricity production mix was developed for the first time. Characterization, contribution, uncertainty, and sensitivity analyses were used for result interpretations. One significant contribution of this study was that most previous studies only derived the contributors from the phase and sub-phase levels, while this study further extended it to the process, sub-process and even substance levels. This information can be used to identify possible options to improve the design and operation of the desalination plants with different energy supply based on the availability and limitations of local resources.

Table 5-1. Fuel mixes for US, SG, and ES

Fuel mixes (%)	US ^a	SG ^b	ES ^a
electricity from coal	49.7	--	47.1
electricity from natural gas	17.4	78.7	11.6
electricity from heavy fuel oil	3.3	17.8	19.6
electricity from nuclear	19.7	--	1.5
electricity from industrial gas	0.1	<0.1	8.4
electricity from waste incineration	<0.1	0.9	<0.1
electricity from clean energy(photovoltaic, hydropower, wind)	8.1	2.4	11.2
electricity from other sources	<1.6	<0.1	<0.5

^a data are from Ecoinvent V2.1; ^b data are based on Singapore statistics 2007.

b. Function unit, system boundary, and assumptions

The function unit for comparing the alternative systems is chosen to be 1 m³ of desalinated water produced. As addressed in Section 5.1, this chapter focuses on the influence of national-specific inventory for power generation. Therefore, only the desalting operation step is covered in system boundary considering its energy-intensive nature (Table 5-2). This chapter uses same plant with Chapter 3 (Table 3-1). To make these three scenarios comparable, relevant assumptions are listed in Table 5-2.

Table 5-2. System boundary defined to investigate the influence of in-stock dataset

	Assumptions	Comments
Electricity flow in energy phase	2 kWh/m ³ desalted water for all scenarios	Based on plant overview, the average electricity consumption is 2 kWh/m ³ desalted water (Glueckstern, P. <i>et al.</i> 2001; Tsiourtis, N.X. 2001; Munoz, I. and Fernandez-Alba, A.R. 2008)
Material flows in infrastructure phase, chemical phase, and membrane phases	The value of flows are adopted from Munoz's study (2008)	The secondary data is used due to comparative nature of this study and unavailability of primary data.
Transportation of construction material, membranes, chemicals and waste materials	Excluded from system boundary	
Concentrate disposal	Included system boundary	The concentrate is discharged to rivers for US and ES scenario, but ocean disposal is used for SG scenario, considering its local context. The aquatic eco-toxic impact of brine disposal is evaluated with the characterization method proposed in Chapter 4. The potential influence of brine disposal on the feed water composition is not considered in this study.
Pre-treatment and post-treatment	Excluded from system boundary	Given similar feed water and effluent, we assume the pre-treatment and post-treatment are similar for all scenarios. They are excluded from boundary due to the comparative nature of this study.
Raw water transport and clean water storage/distribution	Excluded from system boundary	Raw water transport and clean water storage/distribution steps are excluded from the study because it is a site-specific rather than a process-specific aspect.

Characterization, contribution, uncertainty, and sensitivity analysis are used to facilitate the interpretation of the result. The characterization analysis, the characterization approach for freshwater aquatic ecotoxicity and marine aquatic eco-toxicity are modified, while the rest eight indicators employ the CML characterization system. In contribution analysis, the cut-off criteria are set to neglect the processes whose contribution is less than 1% of the total environmental load. In uncertainty analysis, Monte Carlo simulation is used to assess the influence of variations in process data, model choices and other variables, on the results. In addition, Table 5-3 summarizes the comparison of “baseline” and “what if” scenarios used in sensitivity analysis to investigate the possible ways to lower the environmental burdens of desalination.

5.2.2 Life Cycle Inventories

a. Data for desalination plant

The input flows of the plant are indicated in Table 3-1. To study the associated environmental impacts from different electricity models, it is recommended to use the proper inventory specific to the geographic location. It is worth to highlight that, while the team tried to engaged the local databases to the greatest extend, the material flows are modelled with Europe (RER), Switzerland (CH) and Global (GLO) scenarios (Table 5-4 and Table 5-5) mainly because of the incompleteness of the database and the spirit of globalized market - many materials or services are provided by a limited number of famous companies or produced with similar procedure (Rebitzer, G. *et al.* 2004). The standard deviations for material flows, energy flows, disposal flows and transportation flows are summarized in Table 5-4 and 5-5. Although some other processes such as cement manufacturing, land and marine transportation show typical continental or national properties, their contribution generally account for less than 1% of overall impacts which can be considered as negligible.

Table 5-3. Scenarios assessed in sensitivity analysis

Scenario	Description
Baseline scenario	Plant description and assumptions as Table 3 listed ^a ; Desalination powered by Singapore electricity generation models (Table 2)
(1) the influence of different mitigation strategies	
<u>Changing energy scheme of desalination</u>	
Scenario 1	Identical plant description and assumptions with baseline scenario, but the share of electricity from heavy fuel oil burning is reduced by 5% using natural gas as replacement
Scenario 2	Identical plant description and assumptions with baseline scenario, but the share of electricity from heavy fuel oil burning is reduced by 5% using PV energy as replacement
Scenario 3	Identical plant description and assumptions with baseline scenario, but the share of electricity from heavy fuel oil burning is reduced by 5% using wind energy as replacement
Scenario 4	Identical plant description and assumptions with baseline scenario, but the share of electricity from heavy fuel oil burning is reduced by 5% using nuclear energy as replacement
<u>Changing feed water salinity, energy conservation, and process design</u>	
Scenario 5	Increasing feed water salinity to 40,000 mg/L, 50% recovery, using Pelton Turbine as energy recovery system and high energy consuming pre-treatment (MF/UF pre-treatment) ^b
Scenario 6	Identical feed water salinity and recovery with scenario 5, but using work exchanger as energy recovery system and low energy consuming pre-treatment (conventional pre-treatment) ^c
(2) the influence of system boundary selection	
Scenario 7	Identical plant description and assumptions with baseline scenario, but the simplified construction phase is replaced by more comprehensive one. The inventory of additional construction materials is available from (Munoz, I. and Fernandez-Alba, A.R. 2008)
Scenario 8	Identical plant description and assumptions with baseline scenario, but the simplified chemical phase is replaced by more comprehensive one. The inventory of additional chemicals is available from (Tarnacki, K. <i>et al.</i> 2012)
Scenario 9	Identical plant description and assumptions with baseline scenario, but the simplified membrane phase is replaced by more comprehensive one. The inventory of additional construction materials is available from from (Tarnacki, Meneses <i>et al.</i> 2012)
^a To produce 1 m ³ of fresh water from salted water, it needs 0.44 g of polyamide membrane, and it consumes 2 kWh of electricity, 4.5 g of Sodium tripolyphosphate, and other chemicals with trace amount (Munoz, I. and Fernandez-Alba, A.R. 2008).	
^b To produce 1 m ³ of fresh water from salted water, it consumes 4.9 kWh of electricity (Ludwig, H. 2009), 0.37 g of polyamide membrane, 3 g of Sodium tripolyphosphate, and 0.65 g of citric acid, 0.04 g of caustic soda and other chemicals with trace amount (Biswas, W.K. 2009).	
^c To produce 1 m ³ of fresh water from salted water, it consumes 3.9 kWh of electricity (Ludwig, H. 2009). Considering the conventional pre-treatment is less efficient than membrane pre-treatment (Beery, M. and Repke, J.U. 2010a), the consumption of membranes and chemicals is assumed to be increased by 20%.	

Table 5-4. Square of geometric standard deviations for uncertainty analysis and supporting databases for modelling (a)

(Geometric SD) ²	US	SG	ES	Database
<i>For material flows^a</i>				Modeled with RER, CH, GLO Ecoinvent database
Concrete, brick, bitumen, steel	1.2	1.2	1.2	
Soil excavation, gravel, PVC pipe, rubber, PE liner, Iron, chlorine	1.3	1.3	1.3	
PE pipe, GRP	1.6	1.6	1.6	
Membranes, anti-scalant	2	2	2	
Stainless steel, sand, rock, geotextile	2.1	2.1	2.1	
<i>For transportation flows^a</i>				Modeled with RER Ecoinvent database
<i>For disposal flows^a</i>				Modeled with CH Ecoinvent database
Landfill of membranes, concrete, PVC, GRP, PE	3.1	3.1	3.1	
Landfill of sand	3.3			
Landfill of geotextile	3.7	3.7	3.7	
Brine disposal	1.2	1.2	1.2	Chapter 4

^a Data from Munoz's work (Munoz, I. and Fernandez-Alba, A.R. 2008)

Table 5-5. Square of geometric standard deviations for uncertainty analysis and supporting databases for modelling (b)

(Geometric SD) ²	US	SG	ES	Database
For electricity flows				ES scenario: modeled with ES Ecoinvent database SG scenario: modeled with self-developed SG database US scenario: modeled with US Ecoinvent database
Electricity distribution	2 ^a	3.1724 ^c	3.1614 ^a	
Transmission, medium voltage	2 ^a	3.1819 ^c	3.1614 ^a	
Electricity, medium voltage	1.5 ^a	1.13 ^c	1.1 ^a	
Transmission, high voltage	2 ^a	3.1775 ^c	3.1614 ^a	
Electricity, high voltage	1.5 ^a	1.1527 ^c	1.2355 ^a	
Electricity, production mix	1.5 ^a	1.1030 ^b	1.2355 ^a	
electricity from coal	1.05 ^a	--	1.05 ^a	
electricity from natural gas	1.05 ^a	1.39 ^b	1.05 ^a	
electricity from heavy fuel oil	1.3 ^a	2.07 ^b	1.05 ^a	
electricity from nuclear	1.05 ^a	--	1.0511 ^a	
electricity from industrial gas	1.3 ^a	2.43 ^b	1.05 ^a	
electricity from waste incineration	1.3 ^a	2.43 ^b	1.208 ^a	
electricity from clean energy (photovoltaic, hydropower, wind)	1.3 ^a	2.43 ^b	1.208 ^a	
electricity from other sources	1.3 ^a	2.43 ^b	1.208 ^a	

^a Data is available from Ecoinvent database for US & ES

^b Data is calculated based on Singapore statistics. The calculation of geometric SD refers to (Wikipedia 2010)

^c Data is calculated based on equation $CV = \frac{SD_{SG}}{Mean_{SG}} = \frac{SD_{proxy}}{Mean_{proxy}}$

CV : Coefficient of variance;

SD_{SG} , $Mean_{SG}$: the standard deviation and mean value of the flow in Singapore inventory;

SD_{proxy} , $Mean_{proxy}$: the standard deviation and mean value of the flow in proxy inventory

This approach is mainly relying on the concept of coefficient of variance (CV): a normalized measure of dispersion of a probability distribution. The first step is to identify a proper proxy inventory according to the criteria discussed below. The standard deviations can be calculated by assuming that two datasets with identical process should have the same measure of dispersion of a probability distribution (CV).

b. Development of life cycle inventory for Singapore's electricity production mix based on Ecoinvent database

A good LCA relies on a robust LCI, the quantification database of material and energy (resources and wastes) flows associated with a product system. No matter how well a specific impact measure is crafted, nor how well a

software tool is designed, the quality of results can never exceed the quality of the underlying LCI data (Torcellini, P. *et al.* 2004). Life cycle inventory for ES and US electricity production models can be obtained from the Ecoinvent database (see details in www.ecoinvent.org). However, since the LCI for SG electricity production model is not available, it is necessary to establish the datasets specific to SG for further meaningful comparisons. The developing processes of the LCI for Singapore followed the same procedure used in the Ecoinvent database for the US and ES (Figure 5-1).

Figure 5-1. Procedure for establishing SG LCI for electricity production

The primary sources include Singapore government reports, published papers, and mass media. For those data could not be obtained from these primary sources, information from reputable private companies was used.

There has been growing interest in conducting LCA research in Southeast Asia, but the availability and credibility of datasets is always the major limiting factor. This study proposes the use of two different approaches, namely technique-defined and material- defined approaches, to select

appropriate substitutions from other existing datasets when the local data are not available or incomplete. The technique-defined approach is recommended when the environmental impact is highly associated with the technology used in the process, while the material-defined approach is applied when environmental performance is more sensitive to the chemical composition of a product. For example, when developing LCI for electricity generated from natural gas, certain datasets are substituted by the available datasets using similar technology because the environmental impacts from different natural gas sources are similar, thus the exploration technology or efficiency of a power plant becomes the dominant factor. However, since the chemical constituents of crude oil contribute significantly in the impact assessment, it is recommended to choose proper substitutions with similar compositions (i.e. oil source country) in this regard. The details about the establishment of Singapore LCI for electricity generation are summarized in Tables 5-6, 5-7, and 5-8.

5.2.3 Life Cycle Impact Assessment Methodology

a. Predefined life cycle impact assessment method.

This chapter selects the generic CML2 method to translate the emissions and extractions of life cycle inventories. As discussed in Chapter 3, compared to the regional methods in the market, the CML2 method has the advantages of more comprehensive coverage on the associated elements with generic approaches for common applications. In addition, the data requirement doesn't limit CML2 applications in this study, because a relative comprehensive Ecoinvent database is used to support background system. Singapore is still on its early stage of LCA. The emission and resource extraction statistics are far beyond the identification of the acknowledged environmental stressors. Therefore, the development of a new regional life cycle impact assessment method specific to Singapore context is not covered in this study.

Table 5-6. Establishing SG LCI for electricity production

Processes	Comments
Singapore electricity production mix	<p>(1) The assumptions for developing datasets of electricity from heavy fuel oil are summarized in Table 4-14</p> <p>(2) The assumptions for developing datasets of electricity from natural gas are summarized in Table 4-15. The Wobbe Index of natural gas is assumed to be 45.2 MJ/m³ (EMA 2005). The natural gas composition is assumed to be the same with Chan's study (2000) .</p> <p>(3) The overall performance of Orimulsion is about 9% lower than heavy fuel oil (Hägglund, T. 2002). Therefore, the data used to represent electricity from Orimulsion is modified from the heavy fuel oil dataset in French scenario.</p> <p>(4) The photovoltaic electricity generation in Singapore is modelled as German scenario</p> <p>(5) The datasets of electricity from waste incineration and diesel combustion are modelled as Switzerland scenario, which is the only available data in Ecoinvent database.</p>
<p>↑</p> <p>Electricity transmission and distribution</p>	<p>(1) ABB is a major contractor for the management and operation of Singapore's electricity transmission and distribution network (Business & Technology News 2008). Therefore, all the construction of transmission and distribution network in Singapore is assumed to use the same technology as Switzerland. However, some changes were made to simulate local context. Firstly, wood poles and wood preservative process are removed because the transmission and distribution network in Singapore are all underground cables; secondly, extra excavation process was added for digging trenches for cables.</p> <p>(2) The overall electricity power transmission and distribution loss in Singapore is about 5% (World Bank 2006). Since the transmission distance in Singapore is limited, the loss of transmitting electricity at high voltage is assumed as 2%, while the electricity loss during medium-voltage is 3%</p>

Table 5-7. Establishing SG LCI for electricity from heavy fuel oil

Processes	Comments
Electricity, oil, at power plant ↑	It is calculated based on power plant efficiency (33%) (Kannan, R. <i>et al.</i> 2004)
Heavy fuel oil, burned in power plant ↑	Senoko Power, the largest oil-fired power generation company in SG, employs the technology of Hitachi steam (Power Seraya 2007). It is appropriate to use Japanese (JP) dataset as a proxy for SG. In addition, the dataset for JP oil-fired power plant is the same as that in French (FR) scenario in Ecoinvent database. The FR dataset is modified to fit SG context. The release of NO _x and SO _x is reduced to 30% with the help of retaining technology
Heavy fuel oil, at regional storage ↑	This process mainly accounts for the impacts imposed by transporting heavy fuel oil from refinery to end user. Ecoinvent provide datasets for Europe (RER) and Switzerland (CH) scenario. Since the impacts of transportation is proportional to distance, the CH scenario is used as the proxy for SG scenario
Heavy fuel oil, at refinery ↑	The technology used in SG is assumed the same with FR. Therefore, this datasets is established based on the modification of RER scenario.
Crude oil production ↑	Share of oil imported in Singapore: Middle East (RME) - 88%, Malaysia (MY) – 5%, Indonesia (ID) – 2%, China(CN) – 1%, Vietnam (VN) – 1%, Russia (RU) – 1%, others – 2% (STDB 2008). The transportation of crude oil from exploration site to refinery is modelled as Europe scenario.

Table 5-8. Establishing SG LCI for electricity from natural gas

Process	Comments
Electricity, natural gas, at power plant	It is calculated based on power plant efficiency (50%) (Kannan, R. <i>et al.</i> 2005).
↑	
Natural gas, burning in power plant	Singapore's gas-fired power plant is modelled as German (DE) scenario since two of largest power generation company in Singapore, Senoko Power (2008) and Power Seraya (2007), are identified as using Siemens Combined-Cycle Plants.
↑	
Natural gas, high pressure, at consumer	Both SG and JP are the Asian countries with highest population density (UN 2001), so the SG dataset of natural gas distribution network is calculated based on that in JP scenario, assuming the length of pipelines is proportional to the territorial area.
↑	
Natural gas, production MY and ID, at long-distance pipeline	About 75% of natural gas is imported from ID, while 25% is from MY (Wong, K. and Reinbott, D. 2009). It is assumed that half of the natural gas pipelines transported from Malaysia /Indonesia to Singapore are onshore pipeline, while another half are offshore pipelines. The leakage of Singapore's natural gas transportation is assume to be similar to reference (Prabhu, A. <i>et al.</i> 2009).
↑	
Natural gas, at production MY and ID	The composition of natural gas is relatively constant and carries similar impacts, so the developed datasets using the similar technology is adopted to mimic the upstream process of natural gas in SG scenario. it was Royal Dutch Shell that began the gas exploration and production there (Wikipedia 2009), the production of natural gas in MY and ID is modelled as Netherlands (NL) scenario.
↑	
Natural gas, production NL	It is assumed that 70% of natural gas is produced offshore, while another 30% is onshore.

The CML2 impact assessment method includes a list of obligatory impact indicators at mid-point level: Abiotic Depletion Potential (ADP), Acidification Potential (AP), Eutrophication Potential (EP), Global Warming Potential in 100 years (GWP100), Ozone Depletion Potential (ODP), Human Toxicity Potential (HTP), Fresh-water Aquatic Eco-Toxicity Potential (FEATP), Marine Aquatic Eco-Toxicity Potential (MAETP), Terrestrial Eco-Toxicity Potential (TETP), and Photochemical Ozone Creation Potential (POCP). The details of the characterization model are summarized in Table 5-9.

b. Improvement of CML aquatic eco-toxic characterization approach for brine disposal

As indicated in Table 5-2, US and ES scenario discharge the contrite to freshwater rivers, while SG scenario uses ocean disposal. To incorporate brine disposal, the characterization approaches for aquatic eco-toxic potential (FAETP and MAETP) presented by CML impact assessment method are modified. The improved approach combines: (1) the CML-FAETP, CML-MAETP characterization approach focusing on the energy and material required by the desalination plant; and (2) the group-by-group characterization approach (Chapter 4) for brine disposal. It is important to note that the brine disposal affect the freshwater aquatic system for US and ES scenario due to inland disposal to rivers. The effect factor of salinity derived for marine system (Section 4.2.3) is not applicable. Therefore, a freshwater-specific effect factor of salt group is developed in Tables 5-10 and 5-11.

Table 5-9. Characterization models used in Life cycle impact assessment

Impact category	Indicator	Characterization model
Abiotic depletion	Abiotic Depletion Potential (ADP)	(Guinee, J.B. and Heijungs, R. 1995)
Acidification	Acidification Potential (AP)	(Huijbregts, M.A.J. 1999b)
Eutrophication	Eutrophication Potential (EP)	(Heijungs, R. <i>et al.</i> 1992)
Global warming	Global Warming Potential (GWP100)	(Houghton, J.T. <i>et al.</i> 1994; Houghton, J.T. <i>et al.</i> 1997)
Ozone layer depletion)	Ozone layer Depletion Potential (ODP)	(WMO 1992; WMO 1994; WMO 1999)
Human Toxicity	Human Toxicity Potential (HTP)	(Huijbregts, M.A.J. 1999a)
Fresh water aquatic ecotoxicity	Fresh water Aquatic EcoToxicity Potential (FAETP)	(Huijbregts, M.A.J. 1999a)
Marine Aquatic ecotoxicity	Marine Aquatic EcoToxicity Potential (MAETP)	(Huijbregts, M.A.J. 1999a)
Terrestrial ecotoxicity	Terrestrial EcoToxicity Potential (TETP)	(Huijbregts, M.A.J. 1999a)
Photochemical oxidation	Photochemical Ozone Creation Potential (POCP)	(Derwent, R.G. <i>et al.</i> 1996; Derwent, R.G. <i>et al.</i> 1998) (Jenkin, M.E. and Hayman, G.D. 1999)

Table 5-10. The derivation of effect factor of salinity on freshwater community (a) ^{a, b, c}

Species	acute-EC50 (g/l)	chronic-EC50 = acute-EC50/2 (g/l)	Log (chronic-EC50)	GEOMEAN of Log(chronic-EC50)	log(HC50)	HC50	EF (PAF m ³ /kg)
Cladoceran (Gonçalves, A.M.M. <i>et al.</i> 2007)							
<i>Daphnia magna</i>		50.00	1.70	1.51			
<i>Daphnia longispina</i>		22.00	1.34				
Fish (Myers, J.J. and Kohler, C.C. 2000)							
<i>Morone chrysops</i> x <i>Morone saxatilis</i>	27.9	13.95	1.14	1.15			
<i>Morone saxatilis</i>	28.0	14.00	1.15				
Scallop (Rupp, G.S. and Parsons, G.J. 2004)					0.61	4.09	1.22E-01
adults <i>Nodipecten nodosus</i>	23.2	11.60	1.06	1.05			
juveniles <i>Nodipecten nodosus</i>	23.6	11.80	1.07				
spat <i>Nodipecten nodosus</i>	20.1	10.05	1.00				
planktonic larvae (Bochert, R. <i>et al.</i> 1996)							
adult <i>Marenzelleria viridis</i>	0.03	0.015	-1.82	0.90			
Juvenile <i>Marenzelleria viridis</i>	0.05	0.025	-1.60				
Larvae <i>Marenzelleria viridis</i> 4-16 set	0.57	0.285	-0.55				
Larvae <i>Marenzelleria viridis</i> 1-3 set	0.77	0.385	-0.41				

^a the derivation of EF is based on USEtox principles (<http://www.usetox.org/>)

^b mS/cm x 0.5 = g/l of TDS

^c The density of freshwater is assumed to be 1g/l

Table 5-11. The derivation of effect factor of salinity on freshwater community (b) ^{a, b, c}

Species	acute-EC50 (g/l)	chronic-EC50 = acute-EC50/2 (g/l)	Log (chronic-EC50)	GEOMEAN of Log(chronic-EC50)	log(HC50)	HC50	EF (PAF m ³ /kg)
Oligochaete (Chapman, P.M. <i>et al.</i> 1982)							
<i>Limnodrilus hoffmeisteri</i>	10.0	5.00	0.70				
<i>Branchiura sowerbyi</i>	7.5	3.75	0.57				
<i>Tubifex blanchardi</i>	9.0	4.50	0.65				
<i>Quistadrilus multisetosus</i>	7.5	3.75	0.57	0.60			
<i>Spirosperma nikolskyi</i>	7.5	3.75	0.57				
<i>Spirosperma ferox</i>	7.5	3.75	0.57				
<i>Stylodrilus montana</i>	7.5	3.75	0.57				
<i>Veriechaeta pacifica</i>	7.5	3.75	0.57				
Baetid mayfly(Hassell, K.L. <i>et al.</i> 2006)					0.61	4.09	1.22E-01
<i>Cloeon dipterum</i>		1.05	0.02	0.05			
<i>Centroptilum luteolum</i>		1.35	0.13				
Macroinvertebrate (Kefford, B.J. <i>et al.</i> 2012)							
<i>Coleoptera and Odonata</i>	14.8	7.42	0.87				
<i>Crustaceans</i>	13.6	6.78	0.83				
<i>Diptera and Hemiptera</i>	15.2	7.60	0.88				
<i>Ephemeroptera</i>	3.6	1.82	0.26	0.63			
<i>Hydracarina subcohort</i>	9.6	4.82	0.68				
<i>Lithobius forficatus</i>	6.9	3.48	0.54				
<i>Hydropsyche pellucidula</i>	8.3	4.15	0.62				

^a the derivation of EF is based on USEtox principles (<http://www.usetox.org/>)

^b mS/cm x 0.5 = g/l of TDS

^c The density of freshwater is assumed to be 1g/l

5.3 Results Interpretation and Discussion

5.3.1 Characterization Analysis Results

Figure 5-2 shows the results from the life cycle impact assessment characterization for different categories. The scenario with highest environmental impact in each category was normalized as 100%. The results indicated that operating a desalination plant in the US carried the highest environmental loadings in most impact categories, especially for ADP, GWP100, HTP, FEATP, MAETP, and POCP. By operating the same plant in SG, we expected the least burdens in six out of total ten categories, including ADP, AP, EP, FAETP, TETP, and POCP. However, it is worth noting that the SG scenario produced nearly 40% more than two others in ODP. In addition, the environment impact of the ES scenario was the highest in EP and TETP, while the lowest in GWP100, HTP, and MAETP.

5.3.2 Contribution Analysis Results

The results of contribution analysis are summarized in Tables 5-12 and 5-13. As discussed in Chapter 2, the desalting operational phase includes five tree flows - energy, chemicals, membranes, infrastructure, and waste management. The first two combined are responsible for more than 95% of the contribution in all impact categories, except FEATP. This indicates that the contribution of infrastructure and membranes is relatively insignificant and can be safely treated as identical for all scenarios without sacrificing accuracy significantly. Furthermore, electricity demand itself accounts for more than 80% of the overall contribution, except in EP, FEATP. This finding, once again, highlights that the variation of environmental impacts in all scenarios can be largely represented by the differences in electricity production models. The importance of electricity consumption can also be seen in the desalination of feed water with a wide range of salinity, from 1500 to 35 000 mg/L (see Figure S-1 in Appendix A).

Figure 5-2. Characterization result for comparison of US, SG and ES scenario

Table 5-12. Contribution analysis of US, SG, and ES scenarios ^{a,b} (a)

Process contribution (%)	ADP			AP			EP			GWP100			ODP			HTP			FAETP ^c			MAETP ^d			TETP			POCP		
country code	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES
ELECTRICITY	98	97	97	96	84	96	72	61	74	97	96	96	94	97	96	94	91	87	5	41	3	91	89	85	92	92	93	96	83	95
<u>Electricity from coal</u>																														
Hard coal																														
mining	70		53							2		2																2		2
burning				59		52	37		35	68		45	4			43		16				6		6	18		18	53		47
ash disposal							5		2							10		12	3		2	41		40						
Lignite																														
mining	4		7																											
burning				1		26			4	2		7						1								2	1			27
ash disposal																		4			0.5	5		16						
<u>Electricity from heavy fuel oil</u>																														
extraction	2	29	14																											
production							1	1	2				26	84	38															
transportation					9	3		4	4			1					1	3										7		2
refinery					2																								11	1
burning				3	52	9	3	36	14	2	29	14				2	33	12		24		2	27	8	11	84	17	3	33	7
Wastewater discharge																	3	2		4			1							
<u>Electricity from natural gas</u>																														
well for exploration and production					2			3										31	4				1	56	7				1	
extraction	18	64	21							1						13			1			26						1		
transportation				2						1				11	41	3												4		
production				20	2	1																						20	2	1
burning					9		2	12	3	12	60	16				4	15	6										2	17	1

Table 5-13. Contribution analysis of US, SG, and ES scenarios ^{a,b} (b)

Process contribution (%)	ADP			AP			EP			GWP100			ODP			HTP			FAETP ^c			MAETP ^d			TETP			POCP		
country code	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES	US	SG	ES
ELECTRICITY	98	97	97	96	84	96	72	61	74	97	96	96	94	97	96	94	91	87	5	41	3	91	89	85	92	92	93	96	83	95
<u>Electricity from nuclear</u>																														
blasting				2			9		2																					
enrichment													58		14															
<u>Electricity from wood</u>																														
wood burning												5					2													
wood												-5																		
<u>Transmission network</u>																														
wood preservatives																	2								52		48			
<u>Other processes</u>	4	4	2	9	8	5	15	5	8	9	7	11	6	2	3	19	8	23	1	13	0.5	10	5	8	11	8	8	10	12	7
ANTISCALING	1	2	2	3	14	4	26	36	24	2	2	2	3	2	3	4	5	8	1	44	1	7	9	11	3	3	3	3	14	4
INFRASTRUCTURE PRODUCTION	1	1	1	0	1	0	1	1	1	1	1	1	2	1	1	2	3	4		8		1	1	2	5	5	5	0	2	0
MEMBRANE PRODUCTION					1		1	1					1																1	
INFRASTRUCTURE DISMANTLING								1												5		1	1	1						
OTHER PROCESSES																			94	96										
REMAINING PROCESSES				1				1		1	1					1	1		2			1					1		1	

^a abbreviations: ADP, Abiotic Depletion Potential; AP, Acidification Potential; EP, Eutrophication Potential; GWP100, Global Warming Potential in 100 years; ODP, Ozone Depletion Potential; HTP, Human Toxicity Potential; FAETP, Fresh-water Aquatic Eco-Toxicity Potential; MAETP Marine Aquatic Eco-Toxicity Potential; TETP, Terrestrial Eco-Toxicity Potential; POCP, Photochemical Ozone Creation Potential

^b the blank cells stand for contribution is less than 1%

^c FAETP(CML+aqua ETP) for US and ES scenario. The other process for US and ES scenario is the brine disposal process.

^d MAETP(CML+aqua ETP) for SG scenario. The other process for SG scenario is the brine disposal process.

To further identify the key process and substances for each individual category, a detailed contribution analysis was conducted with the results discussed below.

For the **Abiotic Depletion Potential**, the US scenario consumes the highest amount of abiotic resources, and 70% of its ADP is associated with coal burning activity (Table 5-12 and 5-13). This is reasonable due to the fact that nearly half of US electricity is fuelled by coal, which has the lowest heating value and efficiency compared with heavy fuel oil and natural gas, as supported by Table 5-14. Although coal electricity generation in ES is similar to the US, the ADP in ES is 30% lower than the US scenario because the average efficiency (36%) of coal-fired power plant in ES is higher than that (31%) in the US (Ecoinvent 2009). It requires less coal for ES to produce the same amount of electricity, thus reducing environmental impact in ES scenario.

Table 5-14. Heating value, power plant efficiency, and emission factor for fuels

Fuel	Heating value (MJ/kg)	Efficiency (%)	Emission factor from power plant ^h	
			SO ₂ (mg/kg fuel)	NO _x (mg/kg fuel)
Coal	15-27 ^a	30 - 40 ^b	22 - 40	11 - 20
Natural gas	60.9 – 86.7 ^c	50 - 60 ^d	<0.2	1.2 - 1.6
Oil	44.8 – 47.3 ^e	30 - 40 ^f	21-22	2.1 - 2.2

^a Refer to (NIST 2008)

^b Refer to (Boshu, H. and Changhe, C. 2002; Chikkatur, A.P. *et al.* 2007; Odeh, N.A. and Cockerill, T.T. 2008; DOE 2009)

^c Assuming the density of natural gas is 0.58 kg/m³ (Union Gas Limited 2009) with heating value of 35.3 – 50.3 MJ/m³ (EMA 2005) under normal temperature and pressure

^d Refer to (Kannan, R. *et al.* 2005)

^e Refer to (NIST 2008)

^f Refer to (Kannan, R. *et al.* 2004)

^h Derived from (Hasanen, E. *et al.* 1986)

The SG scenario contributes the lowest burden in **Acidification Potential** and **Eutrophication Potential**, which are mainly linked with the combustion by-products such as SO₂ and NO_x. As coal-firing power plants remain the main method of electricity generation in the US and ES, it is not surprising to see higher impacts in these categories for these two regions. Other than

electricity generation, phosphoric acid used in antiscalant production is another source contributing to EP, accounting for 20%–40% in the category.

The CO₂ and other greenhouse gases emitted from combustion are the major contributors for the **Global Warming Potential**. The use of coal contributes 30% more in GWP100 in the US scenario which is directly linked to the fact that coal has higher carbon dioxide emission factor (97 – 180 g CO₂/10⁶ BTU of coal input to industrial boiler) than natural gas and heavy fuel oil, 59 922– 69 924 g CO₂/10⁶ BTU of natural gas input to combined-cycle gas turbine and 82 675 g CO₂/10⁶ BTU of fuel oil input to industrial boiler, respectively (Wang, M.Q. 1999). It is worth noting that, even with coal-firing electricity generation, the ES scenario produces similar impacts to SG which is mainly using heavy fuel oil. The main reason is that nearly 12% of ES electricity is fuelled by clean energy sources such as photovoltaic, hydropower, and wind power indicated in Table 5-1. This implies the importance of clean energy alternatives in the future.

For the **Ozone Depletion Potential**, the major corresponding processes in each scenario are uranium enrichment (58% of total ODP) for the US, crude oil production (84% of total ODP) for SG, and the leakage of natural gas during transportation (41%) along with crude oil production (38%) for ES. One thing to be noted is that, although both SG and ES produce nearly 20% of their total electricity from heavy fuel oil with similar efficiencies in the power plants (33–34%), the ODP for SG is more than double that of ES. This big difference is mainly caused by the exploration sites of crude oil. About 90% of crude oil imported by Singapore is produced in Middle East, while ES has a relatively balanced share of oil imports. Halon 1301 and equivalents, which have higher ODP emission factors, are the main contributors to ODP in the process of crude oil production. As shown in Table 5-15, the SG scenario predicted more Halon1301 generation from crude oil production processes, which leads to the higher ODP.

Table 5-15. The impacts break down of crude oil production in ODP

Countries	Crude oil exploration site	Shares of oil imported	Major ODP substances	Amount (kg / kg crude oil produced)	ODP emission factor (in kg CFC-11 eq./kg)
SG	RME onshore	88%	Halon 1301	5.82E-8	12
	Others	12%			
ES	RME onshore	24%	Halon 1301	5.82E-8	12
	NO offshore	22%	Halon 1211	7.30E-10	5.1
	RU onshore	18%	Halon 1301	5.82E-8	12
	GB offshore	17%	Halon 1301	4.68E-10	12
	RAF onshore	10%	Halon 1301	5.82E-8	12
	Others	9%			

The emissions of PAH, barite, and chromium VI from fuel combustion are the major contributors to the **Human Toxicity Potential**. Coal burning accounts for 43% of HTP in the US scenario, which makes its impact the highest among the three. Well drilling in natural gas exploration and production is also an important source of HTP, only second to fuel combustion, in the SG scenario. There are three possible reasons for the ES scenario achieving the lowest impacts in the HTP category. Firstly, coal-fired power plants in ES have higher efficiency, resulting in 60% lower impacts in HTP than that in US; secondly, HTP from oil combustion in the ES scenario is only half of that in SG, mainly due to the lower nickel and vanadium contents in the oil compositions; finally, much less barite is released in the ES scenario because there is less drilling work required (nearly 70% of its natural gas is produced onshore) compared to SG scenario (about 70% of its natural gas is from offshore).

In scenarios with inland river disposal (US and ES scenario), brine is the major contributor in the **Fresh-water Aquatic Eco-Toxicity Potential**. SG scenario employs ocean disposal. Given the condition of the chemicals are produced locally, the disposal of phosphorous acid used in anti-scalant production becomes an important factor in FAETP.

Different from the FAETP, the ocean brine disposal in SG scenario doesn't affect the **Marine Aquatic Eco-Toxicity Potential** significantly, under the

assumption of the salinity of concentrate is close to seawater. In countries with high dependency on coal-burning, ash disposal is the major contributor to MAETP, while in countries with low or no coal burning activities, the well drilling process plays the key role.

All scenarios perform similarly in the overall impacts for **Terrestrial Eco-Toxicity**. However, the contribution analysis indicates different key processes for each scenario. The TETP of the US and ES are dominated by the wood preservative used for the wooden poles in the electricity transmission network. As SG uses underground cables to transmit electricity, vanadium emitted from drilling offshore wells for natural gas exploration and production becomes the dominate factor in SG context.

Derwent (1996) has identified that certain types of hydrocarbons play important roles in the **Photochemical Ozone Creation Potential**. The associated nitrogen oxides and photochemical reactions are also important in ambient ozone formation. A contribution analysis in this study does not specifically identify the contribution from hydrocarbons and nitrogen oxides as they perform similarly in all the scenarios, but the sulfur dioxide released from coal and heavy fuel oil combustion becomes the key factor when evaluating POCP, even though it contributes a much lower percentage. This unusual result implies that the current model, relying on sulfur dioxide emission for POCP impact estimation, might lead to bias in the real world practices. Further verification is needed to make sure all the important hydrocarbon emissions are reasonably covered in outflows of the model.

5.3.3 Uncertainty Analysis Results

Figure 5-3 shows the results from a Monte-Carlo simulation for 1000 runs with a 95% confidence level. The percentage indicates the probability for a specific scenario achieving lower impacts compared to another one. Comparing the US, SG, and ES scenarios, the environmental savings in SG are significant in AP, EP, FAETP, TETP, and POCP, all with possibilities higher than 70%. The SG scenario, on the other hand, tends to cause more

impact in ODP, with possibilities higher than 75% (Figure 5-3a and 5-3c). The US scenario estimates higher environmental loads than the SG scenario in most impact categories, all with a likelihood of more than 70%, except for ADP, ODP, and MAETP (Figure 5-3a). However, the disadvantage of the US scenario is less significant when compared with the ES scenario (Figure 5-3b).

Figure 5-3. Results of the uncertainty analysis with Monte Carlo simulation with a 95% confidence interval and 1000-times simulation

5.3.4 Sensitivity Analysis Results

Table 5-16 shows the results for the comparison of “what if” scenarios against the “baseline” scenario for each environmental indicator. The descriptions of “baseline” and “what if” scenarios are listed in Table 5-3.

a. The influence of mitigation strategies

The total energy demand and chemical consumption of the first four scenarios were kept identical, but the share of electricity from heavy fuel oil burning was reduced by 5%, using natural gas, PV, wind, and nuclear energy as the replacement. All four scenarios predicted lower environmental burdens across all impact categories. Scenario 1 achieves a relatively smaller improvement in ADP and GWP mainly because the others use naturally replenished sunlight, wind or a small amount of uranium resources, which are non-carbon-based energy sources. Compared to Scenario 3, Scenario 2 causes 4–6% less reductions in HTP, FAETP, and MAETP because of heavy metals released from the production process of photovoltaic (PV) panels. Scenario 4 indicates little improvement in ODP due to the CFC-114 emissions from uranium enrichment process. However, one should be cautious in directly applying LCA for cases engaging the newest green technologies because the inventory might not be up-to-date due to the rapid development of those technologies.

Compared to the baseline scenario, the Scenario 5 and 6 have a much higher salinity of feed water. It is obvious that increasing feed salinity causes elevated environmental burdens since more energy is required to overcome the osmotic pressure. Scenario 6 has a better environmental performance than Scenario 5 due to a higher efficiency of the energy recovery system and lower energy consumption for the pre-treatment. Scenario 6, however, consumes more chemicals relative to Scenario 5. Therefore, the increasing in EP and FAETP are not as significant as the improvements in other categories. Table 5-16 investigates some important factors such as the share of clean energy in the energy scheme of

Table 5-16. Comparison of scenarios against the baseline case for each environmental indicator ^a

Indicators	ADP	AP	EP	GWP	ODP	HTP	FAETP	MAETP	TETP	POCP
Baseline Scenario	7.83×10^{-3} kg Sb eq. 100%	2.54×10^{-3} kg SO ₂ eq. 100%	4.81×10^{-4} kg PO ₄ ³⁻ eq. 100%	1.15 kg CO ₂ eq. 100%	8.91×10^{-8} kg CFC-11 eq. 100%	3.71×10^{-1} kg 1,4-DCB eq. 100%	5.69×10^{-2} kg 1,4-DCB eq. 100%	2.88×10^2 kg 1,4-DCB eq. 100%	4.34×10^{-3} kg 1,4-DCB eq. 100%	1.08×10^{-4} kg C ₂ H ₄ eq. 100%
Scenario 1	-5%	-18%	-11%	-5%	-22%	-8%	-9%	-5%	-24%	-15%
Scenario 2	-8%	-17%	-8%	-8%	-21%	-5%	0%	-4%	-23%	-14%
Scenario 3	-9%	-19%	-11%	-9%	-23%	-9%	-6%	-8%	-24%	-16%
Scenario 4	-9%	-19%	-12%	-9%	-19%	-7%	-5%	-7%	-23%	-16%
Scenario 5	140%	117%	79%	139%	140%	130%	54%	137%	133%	117%
Scenario 6	92%	76%	50%	91%	92%	85%	33%	103%	87%	76%
Scenario 7	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Scenario 8	0%	5%	0%	1%	0%	0%	1%	0%	0%	0%
Scenario 9	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%

^a the descriptions of “baseline” scenario and “what if” scenarios are listed in Table 5-3

desalination, the salinity of feed water, the efficiency of energy recovery devices, and the design of the pre-treatment process. The plant capacity, although not included in the table, might also affect the environmental burdens. For example, a larger pump can usually provide a higher pressure which increases efficiency of the energy recovery devices, thus helping to reduce environmental impacts indirectly.

b. The influence of boundary selection

In the baseline scenario, the system boundary is defined based on the recommendations made in Chapter 2. The simplified infrastructure phase includes the steel and concrete, the antiscalant for chemical phase, and the polymers for membrane phase. However, the last three scenarios indicated in Table 5-3 expand the system coverage to include the auxiliary materials. The result indicates only little increase in last three scenarios compared to baseline (Table 5-16). This finding further validates our recommendation made in system selection (Chapter 2).

5.4 Recommendations and Limitations

To make desalination plants more energy efficient and environmentally friendly, Tables 5-17, 5-18, and 5-19 show an attempt to identify the key processes/substances that caused significant environmental burdens. Several potential strategies can be derived based on information provided by the sensitivity analysis and three tables below.

Table 5-17. Summary of life cycle analysis results (a)

Impact categories		Low impact	→	High impact
ADP	country	SG	ES	US
	Likelihood ^a	-	-	-
	key substances ^b	natural gas, crude oil	hard coal, natural gas	hard coal
AP	country	SG	ES	US
	likelihood	+++	+	+
	key process ^c	heavy fuel oil burning	hard coal burning	hard coal burning , natural gas production
	key substances	SO ₂	SO ₂ , NO _x	SO ₂
EP	country	SG	US	ES
	likelihood	++	-	-
	key process	heavy fuel oil burning, antiscaling	hard coal burning , antiscaling	hard coal burning, antiscaling
	key substances	NO _x , PO ₄ ³⁻	NO _x , PO ₄ ³⁻	NO _x , PO ₄ ³⁻

^a +++ likelihood>90%; ++ likelihood 80%-90%; + likelihood 70%-80%; - likelihood<70%

^b Contribution>20%

^c Contribution >20%

Table 5-18. Summary of life cycle analysis results (b)

Impact categories		Low impact	→	High impact
GWP	country	ES	SG	US
	likelihood	-	-	++
	key process	hard coal burning	natural gas burning, heavy fuel oil burning	hard coal burning
	key substances	CO ₂	CO ₂	CO ₂
ODP	country	US	ES	SG
	likelihood	++	+	+
	key process	Uranium enrichment, crude oil production	natural gas transportation, crude oil production	crude oil production
	key substances	CFC-114, Halon 1301	Halon 1211, Halon 1301	Halon 1301
HTP	country	ES	SG	US
	likelihood	+	+	+
	key process	hard coal burning and ash disposal	heavy fuel oil burning, wells for natural gas exploration and production	hard coal burning and ash disposal
	key substances (>15%)	PAH	Barite, PAH, Nickel	PAH, Chromium IV

Table 5-19. Summary of life cycle analysis results (c)

Impact categories		Low impact	→	High impact
FAETP	country	SG	ES	US
	likelihood	+++	+	+
	key process	Antiscaling, heavy fuel oil burning	Brine disposal to inland river	Brine disposal to inland river
	key substances	phosphorous acid during chemical production, Vanadium and its ion	Salinity, metals in brine	Salinity, metals in brine
MAETP	country	ES	SG	US
	likelihood	-	-	-
	key process	hard coal ash disposal	wells for natural gas exploration and production, heavy fuel oil burning	hard coal ash disposal
	key substances	Beryllium, Vanadium ion	Barite, Vanadium	Barium, Beryllium, Vanadium ion
TETP	country	SG	US	ES
	likelihood	+	-	-
	key process	heavy fuel oil burning	wood preservative	wood preservative
	key substances	Vanadium	chromium IV, Mercury	chromium IV, Mercury
POCP	country	SG	ES	US
	likelihood	+++	-	-
	key process	heavy fuel oil burning	hard coal burning	hard coal burning
	key substances	SO _x	SO _x	SO _x

(1) Whenever and wherever possible, engaging low salinity water resources is the most beneficial approach. If the resources are not available, it is important to explore the possibilities of reducing the electricity demand of RO desalination by improving energy recovery devices, optimizing RO process layout and operation conditions, as well as enhancing the efficiency of unitary equipment (*i.e.* pre-treatment, pumps, high permeability membranes). In addition, antiscalant used in the RO processes is another important contributor to environmental loads, particularly for EP and FAETP. As phosphorus related products are generally associated with greater environmental impacts, choosing antiscalants with lower phosphorus contents can significantly relieve the environmental burdens in EP and FAETP. For example, 2-phosphonobutane-1,2,4-tricarboxylic acid (PBTCA), Vitec SR, INDION 8111, and AQUAFEED 600 are potential candidates featuring low-phosphorus content chemicals with excellent scale inhibition properties. Furthermore, discovering new membrane materials to provide higher resistance to scaling and fouling is another feasible way to reduce chemical consumption, which would then lead to a lower environmental impact of desalination. If inland river disposal is employed, then the high salinity of the concentrate is the most concern of the FEATP. Pre-treatment and management before disposal is the effect way to reduce the impact on the freshwater ecosystem.

(2) Most environmental impacts are highly associated with electricity. Any improvement in electricity generation can help lower the environmental impact. It is a common practice to connect a desalination system to the local electricity network. This means that the environmental impacts of desalination plants are linked to the impact of the national power grid. Moving towards cleaner energy sources such as natural gas or renewable energies can be beneficial. In addition, engaging generators with higher efficiency in the power plant is another possible approach which is good for both new and retrofit plants.

(3) Changing the national electricity production scheme might not be feasible in a short period of time as it is associated with many factors such as national policy, diplomatic relations, and national development plans. It is another option for many desalination plants, especially for those located in the grid-limited villages or isolated islands, to incorporate stand-alone **renewable** or **nuclear energy** systems on top of the traditional power grid. The most common **renewable energies** used in the current practices include wind and photovoltaic (PV). As three quarter of wind energy harvesting facilities were installed in Europe and another one fifth in North America (Ackermann, T. and Soder, L. 2002), wind turbine assisted RO membrane processes currently see wider applications in US and ES, while a great potential is observed in Asia with significant research efforts involved. In addition, the coupling of small-scale desalination with solar energy is another promising method for places with intense solar radiation, such as Denver, Mesquite, the Virgin Islands in the US (Ghermandi, A. and Messalem, R. 2009) and Pozo Izquierdo, and Gran Canaria in Spain (Tzen, E. 2009). **Nuclear power** might also be equally viable as an energy source for desalination. The utilization of nuclear energy for desalination is technically feasible and economically competitive with fossil and renewable energy if, and only if, the other social, safety, and engineering concerns can be properly taken care of. Although coupling renewable energy or nuclear power with desalination technology could relieve the substantial adverse environmental burdens from the fossil fuels, an accelerated switch to clean energy sources might lead to other new challenges:

- The health of the general public may be affected by chronic exposure to heavy metal compounds released into the environment as a by-product of different manufacturing steps, or as waste from the uncontrolled disposal of spent photovoltaic modules in PV-RO systems. Similarly, for a wind turbine-RO system, the environmental cost may migrate to noise concerns and construction of wind turbines because large amount of stainless steel, aluminium, copper, cast iron, plastic, and associated building work is required by the wind farm. In

addition, for both PV-RO and wind-turbine system, another important concern is the heavy metals released from manufacturing, disposing of and recycling the storage batteries.

- Coupling a nuclear reactor with a desalination processes also involves a number of potential issues including safety concerns from the nuclear power plant operation, nuclear waste disposal, radioactive contamination of product water, and ecosystem alteration from the warm cooling water.

For Singapore, a small island state with limited indigenous resources in fresh water and fossil fuels, clean energy adaptation is even more crucial. Singapore does not have sizable hydro, geothermal, or wind energy resources due to geographical restrictions. Furthermore, much of its sea space is used for ports, anchorage, and shipping lines which limit the application of ocean energy technology. Although Singapore is a tropical country, PV-driven RO desalination is limited by the cloudy and humid weather, the high cost of PV cells, and the unsatisfactory efficiency of PV systems. Nuclear energy is also restricted in Singapore because of the lack of minimum safety distances (Strait Times 2008). Due to the lack of renewable energy and security issues of nuclear power, Singapore does not show environmental competitiveness to the US and ES in the long term, based on the current evaluation. But as technology evolves, there are still possible ways for Singapore to utilize cleaner energy for seawater desalination. For example, a better management for traditional and new energy sources might help to reduce environmental burdens. The rapid development of solar energy also seems to offer potentials that allow financially-attractive solar assisted RO desalination in the short to medium term. On top of photovoltaics, it might be worthwhile exploring the solar thermal alternative, which collects solar radiation and transfers thermal energy into electrical or mechanical power required by medium- and large-scale RO desalination, *e.g.* a concentrating solar power (CSP)-RO desalination system. The combination of more than one clean energy

source may also be favourable in RO desalination. The nuclear energy hybrid with solar power can achieve steady-state operation under varying solar irradiation levels. Offshore wind turbines may combine favourably with a nuclear plant built on a floating platform out at sea due to safety and resource concerns.

To further extend the applications and findings, it will be beneficial to note the limitations of this study:

(1) The current steady-state LCI for electricity generation only represented temporal information on the pollutants emitted from the specific energy systems. However, pollutants released from the current electricity production profile generally do not carry the same impacts after a few decades of progress in the background system. For example, the fuel profile in electricity generation, and the engaging technologies (processing and generator efficiencies), are progressing dynamically. This highlights the needs to introduce the concept of dynamic LCA which incorporates the environmental characteristic features of future energy systems.

(2) Note that the conclusions in the next section were based on the assumptions made in Section 5.2.1. In reality, RO plants located in different countries probably have site-specific conditions in terms of water resource quality (salinity), end user applications (irrigation, industry or domestic), and plant design (pre-treatment and post-treatment process). The electricity and materials associated with long-distance water pumping in the water acquisition and distribution systems might be included in the system boundary if needed. The effect of concentrate disposal, particularly for those inland plants discharging their concentrate to local rivers or lakes, is essential to the overall environmental burden of RO plants. Moreover, additional considerations related with economic costs and social impacts could also be formulated in future work.

5.5 Conclusions

It is of interest to note that Singapore, a country with a unique fuel profile for electricity generation, shows significant differences in environmental impact from the desalination plant. Results indicated lower impacts in almost all environment related categories due to choosing natural gas as the major fuel source instead of the coal used in other countries. This also made heavy fuel oil burning become the dominant contributor in the SG scenario. In addition, the importance of chemical in SG scenario is promoted in the EP and FAETP categories due to the diminished overall environment burdens compared to alternative scenarios. Other than fuel combustion and antiscalant usage, fuel exploration and production showed significant contributions in ODP and HTP evaluation in the SG scenario. The ocean brine disposal has considerable contribution to MAETP, if the impact from fuel resources acquisition is excluded. It is worth pre-treating and managing the concentrate before discharge to ocean.

The share of coal in the fuel profile for electricity generation is similar for both the US and ES. Operating RO plants in ES, however, resulted in much lower impact in ADP, GWP, and HTP, mainly due to higher efficiencies in power plant operations. In addition, although ES and SG have similar heavy fuel oil usage, with comparable power plant efficiencies, the ES scenario caused a lower impact in the ODP category due to the different oil exploration and production processes. The inland oil wells resulted in a lower environmental burden compared to the offshore sites.

It is also important to note that despite nearly 20% of electricity coming from nuclear power in the US scenario, its contribution to the environmental burden was relatively negligible, with only the ODP emissions from the nuclear enrichment process. It does not mean that nuclear power carries no environmental burdens. It actually highlighted the fact that the current LCA processes can be further improved to fully capture the associated impacts. For example, the LCI database was not complete for nuclear power generation; the nuclear waste disposal was not included because of the

system boundary; the selected ten impact categories might not be enough to fully describe the overall environmental burdens. All the possibilities mentioned above suggested the areas that researchers might be able to work on in the future.

This study also made an attempt to explore the possibilities of reducing the environmental cost of RO plants, either by decreasing the amount of energy consumption and chemical usage in desalination, or by reducing the emissions associated with unit energy and chemical production. The selection of feasible solutions highly depends on site-specific conditions.

As addressed in Section 5.3.2, most of the environmental impacts of RO plants, regardless of using feed water with low salinity or the seawater with high TDS, are associated with energy consumption and brine disposal. Thus the conclusions derived from this study could be further extended to other medium-salinity or high-salinity plants as long as it is an energy-dominated process.

The environmental and economic costs of desalination are usually higher than conventional water treatment techniques. However, there has also been a significant amount of effort in certain directions, such as the reduction of energy consumption in the desalination processes, the coupling of clean energy sources, the improvement of fossil fuels, and other cleaner energy production. With the predicted growing water scarcity problem globally, desalination should always be regarded as an alternative source of fresh water.

CHAPTER 6 SYNTHESIS AND CONCLUSIONS

6.1 Summary and Contributions

As discussed in the previous chapters, one has to decide on a large number of choices when trying to perform desalination LCA. Making decisions without careful selection criteria and background knowledge might sacrifice the confidence level of the study, and even lead to biased conclusion.

This thesis focuses on three choices which are considered as high-priority issues in LCA, namely the choice of the system boundary, the choice of characterization approach (including predefined LCIA method and specific characterization approach for brine disposal), and the choice of in-stock dataset as representative data for background characteristics. The aim of this thesis is to investigate how the choices influence the LCA results and further explore the approaches to capture the technique features and local context to improve the credibility of the results. The contribution of this work includes of four “good choices” in determination of system boundary, characterization approach, and supporting dataset.

(1) This work recommends to select system boundary for infrastructure, chemical, and membrane phases in foreground system according to the goal and scope of desalination LCAs.

In the LCA practice, it is sometimes necessary to ignore a number of inputs and outputs in order to lower the burdens of collecting on-site primary data. Most of previous studies had reported that the infrastructure, chemical, and membrane phases in foreground system have minor contribution. However, their justification is subject to certain underlying assumptions. To avoid high uncertainties due to the arbitrary decision of inclusion or exclusion, the boundary selection in infrastructure, chemical, and membrane phases should be determined according to the goal and scope of desalination LCAs. When the LCA is used to compare different desalination technologies, only the core steps, including water desalting, pre-treatment, and post-treatment, are suggested to be included in the system boundary. Among those steps,

the CO₂ intensive materials used in infrastructure phase as well as the anti-scalant, membrane cleaning chemicals, and remineralisation additives used in chemical phase should be regarded as significant elements and to be included in system boundary. As to the membrane phase, a unique phase in desalination, a rough estimation based on secondary data is suggested because of its minor contributions. When the LCA is used to explore the solutions to relieve the environmental burdens, similar to the comparison of desalination technologies, the LCA study could focus on the core steps. However, the difference is that the on-site primary data is recommended for the mitigation studies in order to better represent different operation conditions. When assessing the water supply/reuse plans, it is better to include additional two steps, the water acquisition and distribution step. Among the two steps, the pipeline materials and CO₂ intensive materials used in their infrastructure phase, are suggested to be considered in system boundary.

(2) This work recommends to choose predefined life cycle impact assessment method for desalination industry depending on the feature of the inventories availability and the specific concerns of the technology.

The desalination LCAs usually use a predefined life cycle impact assessment method, which is a collection of individual characterization approaches which together address different environmental impacts covered by the methodology. However, the reasons for choosing a specific predefined life cycle impact assessment method in their studies have never been elaborated. This thesis provides a good comparison between generic LCIA method and regional specific LCIA method in different impact categories. Generally speaking, the choice of predefined LCIA method might only have minimal influence in the large-scale issues such as global warming potential and ozone depletion potential. The influence, however, might be quite considerable in the categories for acidification, eutrophication, photochemical oxidation, human health, and ecotoxicity. These differences were mainly caused by the unequal coverage of the LCIA method, diversity

of the characterization approaches, and differentiation of environmental interventions. This thesis proposes some suggestions in choosing the appropriate predefined method for the desalination industry. Both generic and regional specific method demonstrated advantages and limitations. The choice of the LCIA method should depend on the feature of the inventories available and also the specific concerns of the technology if any. Given Singapore is still on its early stage of LCA studies, the generic LCIA method is recommended to provide the baselines. However, other than the traditional pollution categories included in generic LICA method (e.g. global warming, ozone depletion, smog formation, acidification, and eutrophication, etc.), it might be beneficial to form a new category for brine disposal.

(3) This work develops an improved characterization approach to estimate the aquatic eco-toxic impact of desalination concentrate disposal.

The choice of aquatic eco-toxic characterization approach for brine disposal is a specific concern for desalination technology. Many researchers conducted the LCA on desalination without considering the aquatic eco-toxic impact of brine disposal in their studies mainly due to the limitation of current characterization approaches. This thesis provides a good critical review of two approaches that are commonly used in the LCA practice for assessing aquatic eco-toxic impact of brine disposal, namely the chemical specific approach and the whole effluent approach. The chemical specific approach has limited application because it is not practical to carry out comprehensive composition analysis of the complex desalination effluent. The whole effluent approach does not need to characterize the effluent, but it only provides a temporal estimation. Significant uncertainty probably occurs due to the variation of brine composition and intrinsic water quality. To capture the technique features of desalination, this thesis developed an improved approach, named the group-by-group approach, to quantify the impact of complex and variable seawater desalination concentrates. This approach takes the merits of the two common approaches discussed above. It calculates the average aquatic eco-toxic impact as the sum of the impacts

generated by acknowledged groups of influential chemicals within the desalination concentrate based on the impact of each group. The improved approach reduces the reliance on the comprehensive chemical composition analysis and temporal ecotoxicology test of the complex desalination brine. It also provides a more comprehensive coverage, not only considering the impact of organic chemicals and metals, but also including the contribution of inorganic chemicals.

(4) This work provides the environment profile of Singapore's desalinations with geographical-specific background data.

The choice of in-stock dataset for energy production process included in the background system can lead to significant differences if not choosing properly. We compare the environmental burdens of a desalination plant with three different electricity production models in the United States, Singapore, and Spain. One potential problem is that the existing Ecoinvent database cannot represent Singapore's local characteristics. Therefore the geographical-specific background data for Singapore's power production is developed by modifying the in-stock datasets in Ecoinvent. The system boundary and characterization approach is selected based on our precious findings. The results highlight Singapore, the country with unique fuel mixes for electricity generation, achieves relatively better environmental savings in most impact categories at the current stage due to a high percentage of natural gas in the fossil fuel matrix. Results from uncertainty analysis further recognize the significance of this advantage. Furthermore, the results indicate the antiscalant application, power plant efficiency, and fuel exploration and production are also highly associated with the environmental performance of desalination plant in certain categories. This work provides the environment profile of Singapore's desalinations for the first time. It also provides a good reference for potential strategies to relieve their environmental burdens.

6.2 Recommendations and Future Work

The “good choice” concept developed by this research suggests interesting avenue to improve the credibility of LCA results. There are important issues worthwhile to further investigate in order to better capture the technique features and local contextual preferences of desalination. Relevant questions to be answered are:

- How sensitive is the desalination LCAs’ outcome to different levels of data quality? Although the on-site primary data is recommended to model the significant elements defined in the system boundary, we sometimes have to turn to secondary data if the primary data is not available. Their impacts on the variability of LCA result should be more thoroughly investigated. It could be useful to better evaluate what level of performance to expect, given the available data and information resources.
- To what extent can the generic characterization approach affect the acidification, eutrophication, and photochemical oxidation impacts of Singapore’s desalination? The characterization factors used in baseline impact assessment method is derived under generic environmental conditions. An important further investigation is to improve the generic approach to satisfy the Singapore’s environmental uniqueness.
- How the hydrodynamic conditions influence the impact of brine disposal? This work only focuses on the impact of effluent at outfall point. To explore the control strategies, it is necessary to consider the disturbing and dilution effects in mixing zone. It would be useful to design the discharge point and diffusers.
- How to improve the application of LCA in decision-making in Singapore’s water industry? Singapore has limited access to the water and land resources; therefore, the issue of water and land use requires additional attention in desalination appraisals. It would be

useful to develop Singapore-specific characterization approach to estimate the water and land impacts. In addition, although the use of desalination LCAs in decision making has benefited from developments of environmental economics, life cycle sustainability assessment, and multi-criteria decision analysis, it would be necessary to develop a new weighting method to satisfy Singapore local conditions.

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APPENDIX A Supplementary Tables and Figures

Table S-1. Chemicals used in the pre-treatment step of desalination

<u>Pre-treatment</u>	Purpose	Chemical added	comments
PH adjustment	To lower carbonate concentration and protect membrane from hydrolysis	Sulfuric Acid	The pH of raw water and target pH determines the dosage. It is often to reduce the pH of the feed water to 5–7. The study (ref LCA of AUS) used 0.69 mg/L to adjust pH. The sulfate will stay in concentrate.
Coagulation-flocculation	To coagulate and flocculate colloidal particles and dissolved organics	Inorganic coagulant (<i>e.g.</i> ferric chloride, aluminum sulfate) Organic coagulant (<i>e.g.</i> dimethyldiallylammonium chloride, polyamines)	Typical dosage is 5–30 mg/L (Dmuh, Y. and Umair, S. 2006; Greenlee, L.F. <i>et al.</i> 2009). The flocs will be settled, removed by filtration and become sludge. Typical dosage is 0.2–1.0 mg/L (Dmuh, Y. and Umair, S. 2006; Greenlee, L.F. <i>et al.</i> 2009). The flocs will be settled, removed by filtration and become sludge.
Anti-foulant	To prevent membrane from fouling	Sodium hypochlorite (NaOCl), Cl ₂ , KMnO ₄ , or O ₃	The dosage is depended on the fouling potential of feed water and the type of antifouling chemicals. It is likely to form by-products.
Anti-scalant	To prevent membrane from scaling	Polyphosphates: Sodium hexametaphosphate (NaPO ₃) ₆ , Pentasodiumtriphosphate (Na ₅ P ₃ O ₁₀); Phosphonates: Bayhibit, Etidron Polycarboxylic acids: Polyacrylic acid, Polymaleic acid	The dosage is depended on the scaling potential of feed water and the type of antiscaling chemicals. Complexes formed will stay in concentrate.
Dechlorination	To neutralize the residual active chlorine, especially for a polyamide-type RO Membrane.	Sodium metabisulfite (Na ₂ S ₂ O ₅), Sodium metabisulfite (NaHSO ₃)	Sulphate and chloride generated will stay in concentrate.

Table S-2. Chemicals used in the membrane cleaning

<u>Membrane cleaning</u>	purpose	Chemical added	comments
	To remove NOM acids	alkaline (NaOH)	The type of cleaning agent and its concentration determines the cleaning efficiency and dosage. The membrane cleaning solutions will stay in concentrate.
	To remove inorganic scales	Acid (citric acid or H ₃ PO ₄),	The type of cleaning agent and its concentration determines the cleaning efficiency and dosage. The membrane cleaning solutions will stay in concentrate.
	To remove scalants (e.g., CaSO ₄),	ethylene diamine tetraacetate (EDTA),	The type of cleaning agent and its concentration determines the cleaning efficiency and dosage. The membrane cleaning solutions will stay in concentrate.
	To remove bio-fouling (biofilm)	chlorine (Cl ₂),	The type of cleaning agent and its concentration determines the cleaning efficiency and dosage. The membrane cleaning solutions will stay in concentrate.
	To remove colloids	surfactants/ detergents	The type of cleaning agent and its concentration determines the cleaning efficiency and dosage. The membrane cleaning solutions will stay in concentrate.

Table S-3. Chemicals used in the post-treatment step of desalination

<u>Post-treatment</u>	purpose	Chemical added	comments
pH adjustment	To prevent pipelines from corrosion, protect aquatic life at discharge point, and meet potable water specifications	NaOH, soda ash, lime	pH is adjusted to a range of 6.8 to 8.1 to meet potable water specifications.
remineralisation	To re-harden to prevent pipelines from corrosion and meet potable water specifications	Liming materials followed by carbon dioxide (CO ₂)	The LSI is adjusted to above 0.
disinfection	To prevent bacteria growth in distribution network	chlorine, ozone, sodium hypochlorite, chloramines, and UV radiation	The disinfection by-products formed will stay in permeate.
boron removal	To elevate boron removal rate To regenerated resin	NaOH HCl or sulphuric acid + caustic	

Table S-4. Comparison between $CF^{GWP}(CML)$ & $CF^{GWP}(TRACI)$ ^{a,b}

	$CF^{GWP}(CML)$	$CF^{GWP}(TRACI)$	$\frac{CF^{GWP}(TRACI)}{CF^{GWP}(CML)}$
Unit	(kg CO ₂ eq / kg substance)	(kg CO ₂ eq / kg substance)	
1,1,1-Trichloroethane [Halogenated organic emissions to air]	146	144	0.99
2,2,2-Trifluoroethanol [Halogenated organic emissions to air]		57	
Carbon dioxide [Inorganic emissions to air]	1	1	1.00
Carbon dioxide [Renewable resources]	1	1	1.00
Carbon dioxide (biotic) [Inorganic emissions to air]	1	1	1.00
Carbon dioxide, land transformation [Inorganic emissions to air]	1		
Carbon tetrachloride (tetrachloromethane) [Halogenated organic emissions to air]	1400	1380	0.99
Chloromethane (methyl chloride) [Halogenated organic emissions to air]	13	16	1.23
Dichloromethane (methylene chloride) [Halogenated organic emissions to air]	8.7		
HFE 7100 [Halogenated organic emissions to air]	297	397	1.34
Methane [Organic emissions to air (group VOC)]	25	23	0.92
Methane (biotic) [Organic emissions to air (group VOC)]	25	23	0.92
Methyl bromide [Halogenated organic emissions to air]	5	5	1.00
Nitrogen trifluoride [Inorganic emissions to air]	17200	10970	0.64
Tetrafluoromethane [Halogenated organic emissions to air]	7390	5820	0.79

^a. The blank cell stands for the LCIA method doesn't take into account of the impact by this substances

^b. Only part of environmental interventions are listed in this table

Table S-5. Comparison between $CF^{AP}(CML)$ & $CF^{AP}(TRACI)^{a\ b}$

	$CF^{AP}(CML)$	$CF^{AP}(TRACI)$	$CF^{AP}(TRACI)$	$\frac{CF^{AP}(TRACI)}{CF^{AP}(CML)}$
Unit	(1kg SO ₂ eq/ kg substance)	1 mol H ⁺ eq/ kg substance)	(1kg SO ₂ eq/ kg substance)	
Ammonia				
[Inorganic emissions to air]	1.88E+00	9.55E+01	1.88E+00	1.0
Hydrogen chloride [Inorganic emissions to air]	8.80E-01	4.47E+01	8.80E-01	1.0
Hydrogen fluoride [Inorganic emissions to air]	1.60E+00	8.13E+01	1.60E+00	1.0
Nitrogen dioxide [Inorganic emissions to air]	7.00E-01	4.00E+01	7.88E-01	1.1
Nitrogen monoxide [Inorganic emissions to air]	1.07E+00	6.13E+01	1.21E+00	1.1
Nitrogen oxides [Inorganic emissions to air]	7.00E-01	4.00E+01	7.88E-01	1.1
Sulfur dioxide [Inorganic emissions to air]	1.00E+00	5.08E+01	1.00E+00	1.0
Ammonium [Inorganic emissions to air]	3.76E+00			
Ammonium nitrate [Inorganic emissions to air]	8.46E-01			
Hydrogen bromine (hydrobromic acid)				
[Inorganic emissions to air]	3.95E-01			
Hydrogen chloride [Inorganic emissions to soil, water]	8.80E-01			
Hydrogen fluoride (hydrofluoric acid) [Inorganic emissions to soil, water]	1.60E+00			
Hydrogen sulphide [Inorganic emissions to air, soil, water]	1.88E+00			
Nitric acid [Inorganic emissions to air, soil, water]	5.10E-01			
Phosphoric acid [Inorganic emissions to air, soil, water]	9.80E-01			
Sulphur trioxid [Inorganic emissions to air]	8.00E-01			
Sulphuric acid [Inorganic emissions to air, soil, water]	6.50E-01			
Sulphuric acid aerosol [Inorganic emissions to air]	6.50E-01			
The unit conversion is based on 1 kg SO ₂ = 5.08H ⁺ moles				

^a. The blank cell stands for the LCIA method doesn't take into account of the impact by this substance

^b. The unit conversion is based on 1 kg SO₂ = 5.08 H⁺ moles

Table S-6. Comparison between $CF^{POCP}(CML)$ & $CF^{POCP}(TRACI)^{a,b,c}$

	$CF^{POCP}(CML)$	$CF^{POCP}(CML)$	$CF^{POCP}(TRACI)$	$\frac{CF^{EP}(TRACI)}{CF^{EP}(CML)}$
Unit	kg C ₂ H ₄ / kg substance	kg NO _x / kg substance	kg NO _x / kg substance	
Carbon monoxide	2.70E-02	9.64E-01	1.34E-05	1.39E-05
Methane	6.00E-03	2.14E-01	2.96E-06	1.38E-05
Nitrogen dioxide	2.80E-02	1.00E+00		
Nitrogen monoxide	-4.27E-01	-1.53E+01		
Nitrogen oxides	2.80E-02	1.00E+00	1	1
Sulphur dioxide	4.80E-02	1.71E+00		
Toluene (methyl benzene)	6.37E-01	2.28E+01	8.32E-04	3.66E-05

^a The unit conversion is calculated based on 1 kg NO_x = 0.028 kg C₂H₄

^b The blank cell stands for the LCIA method doesn't take into account of the impact by this substance.

^c This table only lists the interventions whose contribution is above 1%

Table S-7. Comparison between $CF^{HTP}(CML)$ & $CF^{nC-HTP}(TRACI)^{a,b,c,d,e}$

	$CF^{nC-HTP}(CML)$	$CF^{nC-HTP}(TRACI)$	$CF^{nC-HTP}(TRACI)$	$\frac{CF^{nC-HTP}(TRACI)}{CF^{nC-HTP}(CML)}$
Unit	kg 1,4-DB/ kg substance	kg toluene/ kg substance	kg 1,4-DB/ kg substance	
emissions to air				
Aluminum oxide (dust)	8.20E-01	1.12E+04	2.90E+03	3536
Dioxins (unspec.)	1.93E+09	1.44E+07	3.74E+06	0.002
Lead (+II)	4.67E+02	2.17E+06	5.65E+05	1209
emissions to water				
Cadmium (+II) [Fresh water]	2.29E+01	2.01E+06	5.23E+05	22838
Cadmium (+II) [Heavy metals to fresh water]	2.29E+01	2.01E+06	5.23E+05	22838
Cadmium (+II) [Heavy metals to sea water]	1.04E+02	2.01E+06	5.23E+05	5029
Lead (+II) [Fresh water]	1.23E+01	1.13E+07	2.94E+06	2390024
Lead (+II) [Heavy metals to fresh water]	1.23E+01	1.13E+07	2.94E+06	2390024
Lead (+II) [Heavy metals to sea water]	7.88E+01	1.13E+07	2.94E+06	37310

^a Abbreviation: nC-HTP non-carcinogenic human health impact

^b This table only lists the interventions whose contribution is above 1%

^c The unit conversion of nC-HTP by airborne emission is based on 1 kg toluene = 3.85 kg toluene

^d The unit conversion of nC-HTP by waterborne emission is based on 1 kg toluene = 1.84 kg toluene

^e The unit conversion of nC-HTP by emissions to soil is based on 1 kg toluene = 0.26 kg toluene

Table S-8. Comparison between $CF^{EP}(CML)$ & $CF^{EP}(TRACI)^{a,b}$

	$CF^{EP}(CML)$	$CF^{EP}(CML)$	$CF^{EP}(TRACI)$	$\frac{CF^{EP}(TRACI)}{CF^{EP}(CML)}$
Unit	kg PO_4^{3-} /kg substance	kg N/kg substance	kg N/kg substance	
eutrophication emissions to air				
Ammonia	3.50E-01	8.33E-01	1.19E-01	0.1
Nitrogen dioxide	1.30E-01	3.10E-01	4.43E-02	0.1
Nitrogen monoxide	2.00E-01	4.76E-01	6.86E-02	0.1
Nitrogen oxides	1.30E-01	3.10E-01	4.43E-02	0.1
Phosphorus	3.06E+00	7.29E+00	1.12E+00	0.2
eutrophication emissions to water				
Ammonium / ammonia	3.30E-01	7.86E-01	7.79E-01	1.0
Biological oxygen demand (BOD)	2.20E-02	5.24E-02	5.00E-02	1.0
Chemical oxygen demand (COD)	2.20E-02	5.24E-02	5.00E-02	1.0
Nitrate	1.00E-01	2.38E-01	2.37E-01	1.0
Nitrogen	4.20E-01	1.00E+00	9.86E-01	1.0
Phosphate	1.00E+00	2.38E+00	2.38E+00	1.0
Phosphorus	3.06E+00	7.29E+00	7.29E+00	1.0

^a The unit conversion is based on : 1 kg N = 1 0.42 kg PO_4^{3-}

^b The table only lists the interventions whose contribution is above 1%

(a) The energy demand of desalination has dominant contribution to environmental impacts (feed water is low-salinity brackish water with TDS of 1500 mg/L; it consumes 1 kWh of electricity to produce 1 m³ of fresh water from feed water(Park, G.L. *et al.* 2011))

(b) Typical energy consumption is 4KWh/m³ for sea water

■ infrastructure Production □ antiscaling ■ electricity ■ membranes ■ infrastructure dismantling ■ others

(b) The energy demand of desalination has dominant contribution to environmental impacts (feed water is sea water with TDS of 35000 mg/L; it consumes 4 kWh of electricity to produce 1 m³ of fresh water from feed water(Raluy, R.G. *et al.* 2006))

Figure S-1. The contribution of individual processes under different salinity levels

APPENDIX B PUBLICATION LIST

Jin Zhou, Victor W.C. Chang, Anthony G. Fane (2011a). "Environmental Life Cycle Assessment of Reverse Osmosis Desalination: The Influence of Different Life Cycle Impact Assessment Methods on the Characterization Results", *Desalination*, Vol. 283, pp. 227-236.

Jin Zhou, Victor W.C. Chang, Anthony G. Fane (2011b). "Environmental Life Cycle Assessment of Brackish Water Reverse Osmosis Desalination for Different Electricity Production Models", *Energy and Environmental Science*, Vol. 4, No. 6, pp. 2267-2278.

Jin Zhou, Victor W.C. Chang, Anthony G. Fane (2013). "An Improved Life Cycle Impact Assessment (LCIA) Approach for Assessing Aquatic Eco-toxic Impact of Brine Disposal from Seawater Desalination Plants", *Desalination*, Vol. 308, pp. 233-241.

Jin Zhou, Victor W.C. Chang, Anthony G. Fane (2013). "Issues of Applying Life Cycle Assessment to Desalination: Feasibility, Reliability, and the Potential to Use LCA for Decision Making", submitted to *Water Research*

Bernard J.H. Ng, Jin Zhou, Apostolos Giannis, Victor W.C. Chang, Jing-Yuan Wang (2013). "Environmental Life Cycle Assessment of Different Domestic Wastewater Streams: Policy Effectiveness in a Tropical Urban Environment", submitted to *Journal of Environmental Management*.

Jin Zhou, Victor W.-C. Chang, Christian Zwiener, Christina Schmalz, Anthony G. Fane (2013). "Health Risk Evaluation of Disinfection By-Products (DBPs) for Indoor Swimming Pool Users via Life Cycle Impact Assessment Approach", in preparation.

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