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An improved life cycle impact assessment (LCIA) approach for assessing aquatic eco-toxic impact of brine disposal from seawater desalination plants

Jin Zhou, Victor W.-C. Chang *, Anthony G. Fane

Singapore Membrane Technology Centre, School of Civil and Environmental Engineering, Nanyang Technological University, 639798, Singapore

HIGHLIGHTS

► An improved LCIA approach to estimate the aquatic eco-toxicity of brine disposal
► Hybridization of two common approaches to form the group-by-group approach
► New approach to reduce the data requirement and broaden the coverage

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ABSTRACT

Most Life Cycle Assessment (LCA) studies did not quantify the aquatic eco-toxic potential (aquatic ETP) of the brine disposal mainly due to the limitation of current life cycle impact assessment (LCIA) approaches. The purpose of this study is to develop an improved approach for assessing the aquatic ETP of brine disposal from seawater desalination plants. The proposed approach, named group-by-group approach, calculates the average aquatic ETP as the sum of the impacts generated by acknowledged groups of influential chemicals. This approach firstly identifies the influential chemicals. According to the chemical property and the impact pathway to the aquatic ecosystem, the important chemicals are then categorized into groups under three categories. Depending on the characteristics of the defined groups, different strategies are applied to determine the impact of each group. The group-by-group approach takes the merits of two most commonly-used approaches, chemical specific approach and whole effluent approach. The results from the case study indicated that this 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.

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1. Introduction

Over the past several decades, the rapid growth in human populations and industrial activities continued to place ever-increasing pressure upon the demand for clean water. As a result, many nations are turning to seawater desalination to complement other sources of water supply.

Although desalination is a relatively mature technology positively contributing to relieve the water shortage, several environmental issues are associated with the desalination plant. Life Cycle Assessment (LCA) is a useful tool to quantify and compare the environmental impacts of providing fresh water from desalination system to our societies. LCA is a comprehensive assessment tool and considers all potential environmental burdens throughout the life cycle, from raw material acquisition, via production and usage phases, to waste management [1]. The framework for LCA includes goal and scope definition, life cycle inventory (LCI) analysis, life cycle impact assessment (LCIA), and life cycle interpretation [1]. LCA has been applied to desalination since the 1990s. One of the most importation applications of LCA was to examine and compare different desalination technologies [2–6]. Most of the previous study highlighted the dominant role of energy demand. LCA was also used to evaluate different water supply plans [7–9]. The results indicated that in potable applications, local desalination was preferable in terms of environmental performance because of high energy consumption in long distance surface water transfer. In addition, LCA was used to explore the solutions to relieve the environmental burdens by reducing the salinity of feed water [10], by employing effective pretreatment [11,12], or by engaging cleaner energy sources, such as natural gas [13], renewable energies [3,14], and waste heat [15].

Other than the energy issues of desalination, there is a growing interest in understanding the aquatic eco-toxic impact of brine disposal. Many laboratory research [16–18], field-based experiments [17–19], and ecological monitoring studies [18,20–22] suggested that high salinity might cause reduced growth or even increased mortality of flora and fauna. Concern also exists regarding the release of metals

* Corresponding author. Tel.: +65 67904773.
E-mail addresses: zhou0141@ntu.edu.sg (J. Zhou), wcchang@ntu.edu.sg (V.W.-C. Chang), agfane@ntu.edu.sg (A.G. Fane).

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coming from corrosion and the use of certain additives. Some studies found that the desalination brine with high chemical contaminant level has the potential to impair biological communities [19,23,24] and even cause accumulation of toxic chemicals in macroalgae, mussels, etc. [25–27].

Altogether, we observed that the LCA is a useful tool to assess the potential impacts of desalination system, and the role of concentrate disposal as an important source of aquatic eco-toxic impact is well established. However, most of the 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 [28] 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, but the result was restricted by the site specific conditions with limited reference value to other studies [29]. Many LCA studies assumed that the brine was fully diluted before discharge and posed minor impacts on the aquatic eco-system [2,4,5,8,30]. 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 research fall far behind the growing concern of brine disposal. First is 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. Second, the misconception of taking the available LCIA 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 study is to develop a low-data-demand and more comprehensive LCIA approach for assessing the aquatic eco-toxic potential (aquatic ETP) of brine disposal from seawater desalination plants. The rest of this paper is organized as follows. The next section reviews the LCIA approaches to quantify the aquatic eco-toxic impact of brine disposal, and then proposes an improved approach named group-by-group approach. A case study is also engaged to illustrate the implementation and the advantages of the improved approach. Finally, the conclusions are presented in the last section.

2. Improving LCIA approach to quantify aquatic ETP of brine disposal

2.1. Critical review of available approaches

The overall framework for LCA consists of four important aspects including (1) goal and scope definition; (2) life cycle inventory (LCI) analysis; (3) life cycle impact assessment (LCIA); and (4) life cycle interpretation [1].

Life cycle impact assessment (LCIA) approaches aim to translate (characterize) emissions and extractions of life cycle inventories (LCI-results), on the basis of impact pathways, to their potential environmental damages [31]. The result of the LCIA is an evaluation of a product life cycle, on a functional unit basis, in terms of several impact categories in midpoint level (such as climate change, toxicological stress, acidification, eutrophication, etc.) and, in some cases, in an aggregated way (such as skin cancer, crop impacts, impacts on animals in endpoint level, or human health, ecosystem quality, climate change, and resources in damage level) [32]. As discussed in the Introduction, the aquatic ETP of brine disposed from the desalination plant is the impact indicator of interest. Since the midpoint methods have often been well-researched and more comprehensive than the endpoint and damage calculations [33], this study 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 Eq. (1).

$$Aquatic\,ETP\,of\,brine\,disposal = \sum_i m(i) \times CF^{aquatic\,ETP}(i) \tag{1}$$

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, i is defined as an individual chemical in the desalination brine, while i stands for the entire effluent in the whole effluent approach.

2.1.1. 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 [29]. 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 the United Nations Environmental Programme (UNEP) and the Society for Environmental Toxicology and Chemistry (SETAC) [34]. This model covers the chemical fate, exposure, and effect and can be expressed as Eq. (2).

$$CF^{aquatic\,ETP}(i) = FF_i \times XF_i \times EF_i \tag{2}$$

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 as seen in Eq. (3). 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].

$$EF = 0.5/\mathrm{HC50} \tag{3}$$

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.

2.1.2. 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

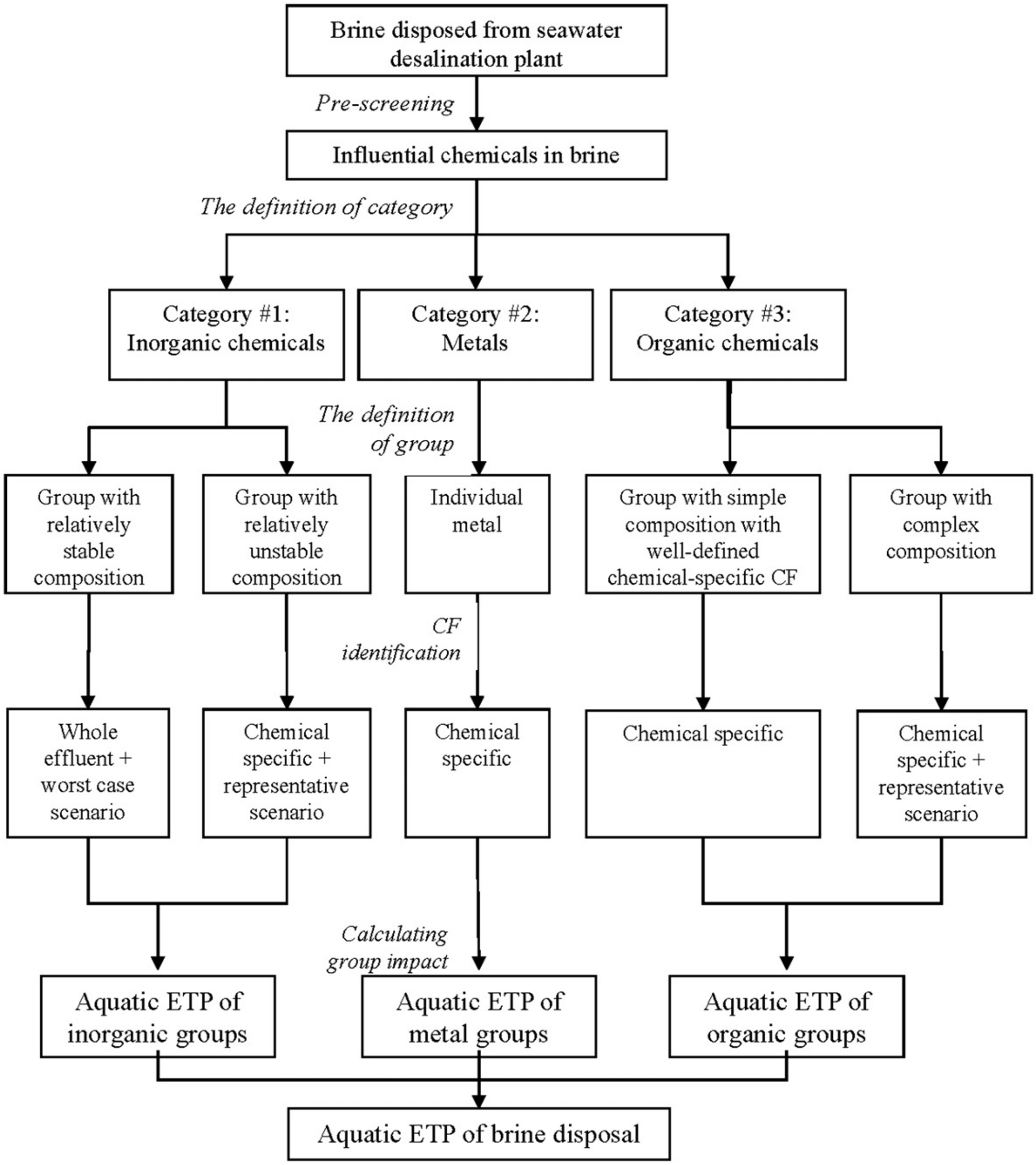

Fig. 1. The procedure for the group-by-group approach.

whole effluent assessment, such as Whole Effluent Toxicity (WET) used by the 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. [35]. 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 [36]. Therefore, Eq. (1) can be rephrased as Eq. (4), given the function unit is defined as 1 m^3 of brine.

$$Aquatic\,ETP\,of\,brine\,disposal = \sum m(eff) \times CF^{aquatic\,ETP}(eff) \tag{4}$$

Where $m(eff)$ is the mass of the 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 [37]. 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

Table 1
Scenario definition.

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

worst case scenario. The fate factor for the entire effluent is defined as the residence time of the most persistent 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 Eq. (5)

$$CF^{aquatic\,ETP}(eff) = MAX(FF_i) \times 1 \times EF_{eff}. \quad (5)$$

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.

2.2. Development of an improved approach

As mentioned in Section 2.1, 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 makes 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 is illustrated in

Table 2
Brine composition and its correspondence CF from USEtox database.[a]

Chemicals	SWRO brine composition [43–45] (average, mg.L^{-1}/uncertainty)	MSF brine composition [44,46] (average, mg.L^{-1}/uncertainty)	CF provided by USEtox database [34] (average, PAF.m^3.day/kg/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%		
0.04 polyelectrolyte/±20%	N.R.	–	
Scale control chemical	0.04 SHMP/±20% 0.04 polymer/±20%	0.671 polymer	–
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	–
$C_6H_8O_7$	Neutralized	Neutralized	–
H_3PO_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 are 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 [44].

Table 3
Identification of influential chemicals in desalination brine.

Pre-screen criteria	Influential chemical		Comments
	Brine from RO plant	Brine from MSF plant	
High concentration > regulation level			
		Free chlorine (500 μg/L)	Regulation level of free chlorine • 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 μg/L)	Regulation level of CBPs • Total THMs $= C_{Chloroform}/300\ \mu g.L^{-1} + C_{BDCM}/21\ \mu g.L^{-1} + C_{DBCM}/100\ \mu g.L^{-1} + C_{Bromoform}/100\ \mu g.L^{-1} \leq 1$ (WHO) • Total THMs $< 80\ \mu g.L^{-1}$ (US EPA)
	Cu (15 μg/L)	Cu (100 μg/L)	Regulation level of Cu • 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
High characterization factor			
		Chlorophenol Chlorobenzenes	CF > 1E + 2 PAF.m^3.day/kg
	Nickel, chromium	Nickel, chromium	CF > 1E + 4 PAF.m^3.day/kg

Fig. 1. Given the function unit is defined as 1 m^3 of the desalination brine, this approach can be expressed by Eq. (6).

$$Aquatic\,ETP\,of\,brine\,disposal = \sum_j m(group\,j) \times CF^{aquatic\,ETP}(group\,j) \quad (6)$$

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

According to Eq. (6), the total aquatic eco-toxic impact of brine disposal depends on the definition of group j and the estimation of $CF^{aquatic\ ETP}(group\ j)$.

(1) 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 [38].
- 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 equipments may cause the increase in metal concentrations in the brine [39].
- 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, derivates of corrosion inhibitors like benzotriazole, etc.

The first step to define 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 [40]. Values at the same order of magnitude were also found in European saltwater environments [41]. 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 the 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 should be revised along with the improvement of scientific knowledge and the local conditions. In this study, we assume the pH value and turbidity of the brine are neutralized before discharge. Therefore, they are not considered as influential substances. In addition, the eco-toxicity impacts from the temperature, pharmaceuticals, and other micro pollutants are not well-characterized based on current scientific understanding, 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 are exposed to elevated concentration of salt ions due to more dissolved ions in ambient water compared to their body liquids [42].

There is no universally agreeable grouping method in the current LCA community. This study provides two suggestions in the 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 increases accordingly. Secondly, the grouping of important chemicals should be based 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 the same group.

(2) 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 strategies 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 a 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 scarifying 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 Section 2.1.1 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 Section 2.1.2, instead of USEtox fate model and exposure model, it is more appropriate to estimate both 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 to the inorganic group with relatively stable composition unless high uncertainty probably occurs. 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. Case study using different approaches

3.1. Scenario identification and assumptions

A comparison study with six different scenarios was engaged to illustrate the improvement of the group-by-group approach. Three different approaches including the chemical specific approach, the whole effluent approach, and the group-by-group approach proposed by this study, were used to investigate the aquatic eco-toxic impacts of two different concentrates from seawater reverse osmosis desalination plant (SWRO) and multistage flash plant (MSF). Six scenarios were defined in Table 1.

The function unit for scenario comparison was chosen as 1 m^3 of brine. The brine composition was indicated in Table 2. As a general illustration, this case study would focus on the impact of effluent at outfall point, therefore the disturbing and dilution effects in the mixing zone were not considered as those 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 the next section. In the uncertainty analysis, Monte Carlo simulation was used to evaluate the influence of variations in brine composition and the uncertainty of characterization approaches. It was assumed that the concentration of each chemical fluctuated within a range of 20 percentage points of average. Because the $CF^{aquatic\ ETP}(eff)$ used in this case study was derived from Eolia™ Potable Water [29] instead of the local on-site monitoring data, a large uncertainty (±50%) was assigned to $CF^{aquatic\ ETP}(eff)$. 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 (±30%) than USEtox chemical-specific characterization factor (±20%). 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. 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.

3.2. Deriving characterization factors for different approaches

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 the brine constituents was covered (the last column of Table 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 Section 2.1.2, the characterization factor for the entire effluent was calculated based on Eq. (5). The Eolia™ Potable Water has defined the EF_{eff} as 5.8E−04 PAF.m^3/kg [29]. The most persistent chemical in the 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 persistent chemical in the mixture. This was because 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 terms of aquatic eco-toxic impact. The Eolia™ Potable Water did not differentiate between SWRO and MSF plants, therefore, scenarios 2 and 5 employed the same characterization factor as 2.15E−02 PAF.m^3.day/kg.

The procedure described in Section 2.2 was used to establish the group-by-group approach. The influential chemicals were identified based on the concentrations and characterization factors (Table 3).

The influential chemicals were then classified into several groups under 3 categories: salt ion group and free chlorine group in inorganic category, halogenated hydrocarbon 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.

3.3. Results and discussion

Fig. 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 Fig. 2. It can be seen that the chemical specific approach (scenarios 1 and 4) reported the 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 Section 2.1.1, 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 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
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 Section 2.1.1 is not applicable to inorganic salts [47]. Therefore, The FF for salinity is estimated for the worst case scenario. The most persistent chemical in this group is Na^+, with residence time of 210 million years, which exceeds the range of the acute test (100 years). 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	EF = 0.5/EC50. EC50(salinity) = 40,000 mg/L [39]
	CF (PAF.m^3.day/kg)	4.62E−01	CF = FF∗XF∗EF
Free chlorine group, *including HClO, NaOCl,* $Ca(OCl)_2$, *etc.*			
	CF (PAF.m^3.day/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 Section 2.1.1 is not applicable. The CF for a similar disinfectant, chloramine-T[a] is used here. CF for chloramine-T is available from USEtox database.
Organic category			
Halogenated hydrocarbon group, *including tribromomethane, bromodichloromethane, dibromochloromethane, chloroform, chlorophenol, chlorobenzenes, etc.*			
	CF (PAF.m^3.day/kg)	1.90E+02	$CHBr_3$ is selected as the representative chemical because of its dominant composition in this group and has relatively high CF. Its CF is available from USEtox database.
Metal category			
Cu			
	CF (PAF.m^3.day/kg)	5.50E+04	CF is available from USEtox database.
Ni			
	CF (PAF.m^3.day/kg)	1.5E+04	CF is available from USEtox database.
Cr			
	CF (PAF.m^3.day/kg)	1.0E+05	CF is available from USEtox database.

[a] Chloramine-T breaks down to the hypochlorite (HClO) in water.

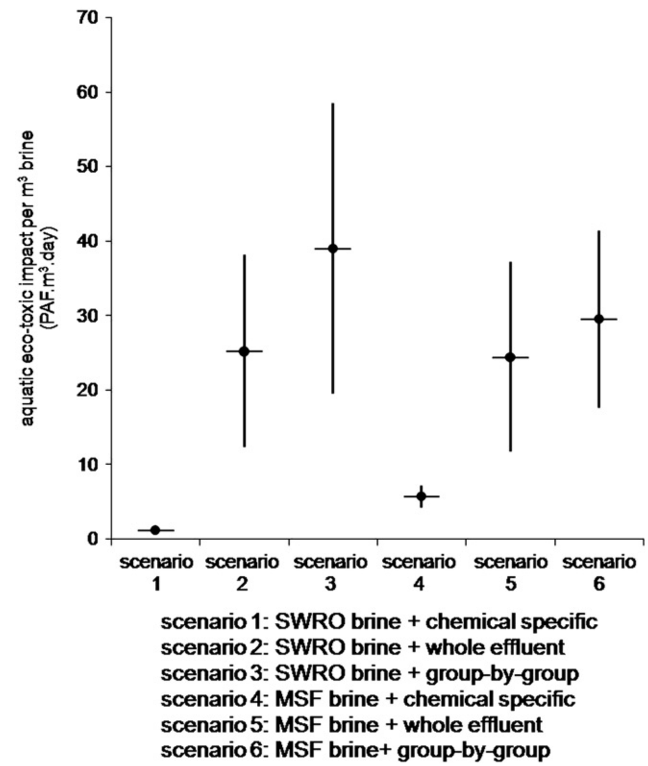

Fig. 2. Characterization and uncertainty analysis results.

The results reported from the whole effluent approach (scenarios 2 and 5) and from the group-by-group approach (scenarios 3 and 6) were on the same order of magnitude, with the latter estimated at 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.

(1) 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 Eolia™ 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 the 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 Fig. 1 were applied to the other chemical groups. The salinity of SWRO/MSF brine has a small variation because the salinity of seawater is relatively stable and recovery rate of SWRO/MSF plants is usually well controlled in a narrow range. Therefore, the effect factor determined by the ecotoxicology text is considered as a relatively stable intrinsic property of the salinity group and can be applied to all salinity groups across different brines.

(2) 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

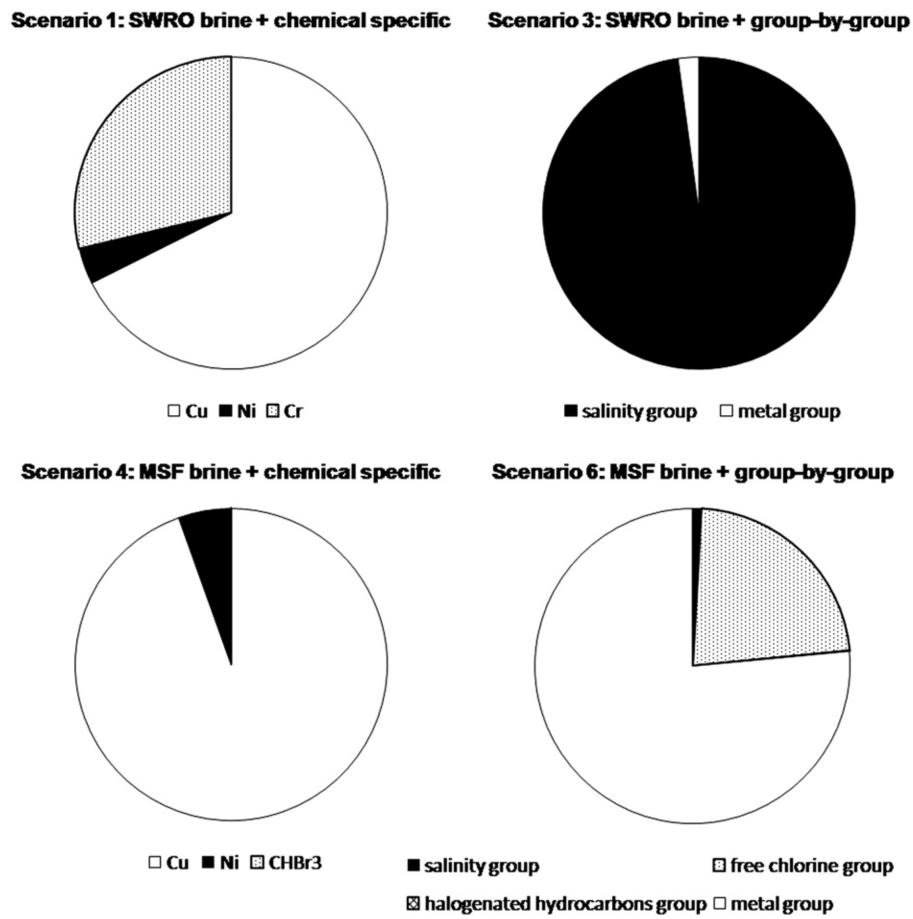

Fig. 3. Contribution analysis results.

the group-by-group approach can be further interpreted by contribution analysis and sensitivity analysis. The contribution analysis results (Fig. 3) indicated that the group-by-group approach (scenarios 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 5 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.

4. 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. This study provides a good critic 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

Table 5
Sensitivity analysis results.

		Chemical specific approach	Group-by-group approach
Eco-toxic impact of discharging 1 m^3 of brine from RO plant			
"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 by10%	−10%	Negligible
Eco-toxic impact of discharging 1 m^3 of brine from MSF plant			
"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 the "what if" scenario has minor effect on the final result.
[b] "0" means the "what if" scenario has no effect on the final result.

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 that 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.

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