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# Quantity-based and toxicity-based evaluation of the U.S. Toxics Release Inventory

## Seong-Rin Lim, Carl W. Lam, Julie M. Schoenung\*

Department of Chemical Engineering and Materials Science, University of California, Davis, CA 95616, USA

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## ABSTRACT

The U.S. EPA Toxics Release Inventory (TRI) represents an extensive, publicly available dataset on toxics and, as such, has contributed to reducing the releases and disposal of toxic chemicals. The TRI, however, reports on a wide range of releases from different sources, some of which are less likely to generate a human or ecological hazard. Furthermore, the TRI is quantity based and does not take into account the relative toxicity of chemicals. In an effort to utilize the TRI more effectively to guide environmental management and policy, this work provides an in-depth analysis of the quantity-based TRI data for year 2007 at industry sector, state, and chemical levels and couples it with toxicity potentials. These toxicity potentials are derived from the U.S. EPA's TRACI (Tool for the Reduction and Assessment of Chemical and other environmental Impacts) characterization factors for cancer, non-cancer and ecotoxicity. The combination of quantity-based and toxicity-based analysis allows a more robust evaluation of toxics use and priorities. Results show, for instance, that none of the highest priority chemicals identified through the toxicity-based evaluation would have been identified if only quantity-based evaluation had been used. As the chemicals are aggregated to the state and industry sector levels, the discrepancies between the evaluation methods are less significant.

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### 1. Introduction

The U.S. EPA Toxics Release Inventory (TRI) has been successfully contributing to reducing the releases and disposal of chemicals in manufacturing industries in the United States [1-3]. The U.S. EPA annually issues the TRI report to facilitate emergency planning, reduce potential toxic chemical accidents, and provide stakeholders with information on releases and disposals of toxic chemicals under the Emergency Planning and Community Right to Know Act (EPCRA) of 1986 [1,4]. The TRI mechanism to reduce environmental impacts is different from command and control regulation practices because the TRI focuses on openly reporting quantity-based data on toxic chemicals to the public [1,4,5]. The TRI induces the active participation of communities near facilities to protect their environment from the harmful effects of toxic chemical releases [1,6], and the voluntary measures of facilities to manage corporate image, liability, and occupational diseases and improve the sustainability of the facilities and companies [1,4]. Furthermore, the TRI information affects consumers and stockholders' decision making as the sensitive reaction of media and stock market to the TRI announcement has effects on sales amount and stock price [2,5].

Within the TRI, reports are provided for the on-site and off-site releases of 498 chemicals (in year 2007) from select industries that fall within designated NAICS (North American Industry Classification System) codes, including manufacturing (NAICS 31), mining (21), utilities (22), wholesale trade (42) and waste management and remediation (562). With the TRI Explorer [7], for instance, the TRI can be searched by: chemical, industry sector, state, county, zip code, facility, federal agency, and over time. The types of releases that are monitored include: (1) on-site: point source air, fugitive air, surface water discharges, other surface impoundments, landfills, other land disposal, and underground injection class I wells; (2) off-site: RCRA (Resource Conservation and Recovery Act, 1976) subtitle C landfills, other landfills, and solidification/stabilization disposal (for metals only); and (3) other on-site and off-site releases.

Clearly, the TRI provides a wealth of information and has had a positive impact on reducing the use of toxics. Several studies have highlighted, however, that the quantity-based TRI does not take into account the relative toxicological properties of chemicals [8-12]. Thus, these previous studies have focused on the need to account for the physical, chemical, and biological characteristics of chemicals in the environment as well as their toxic potency to human health and ecosystems. Horvath et al., for instance, applied toxic emissions indices to TRI analysis to account for the relative toxicity of chemicals on the basis of a threshold limit value [8]. Jia et al., proposed indices to account for the relative toxicity, persistence, and environmental mobility of chemicals to better interpret toxicity potential information from the TRI [9]. Hertwich et al., developed toxicity characterization factors for chemicals by using a generic fate and exposure model to calculate human health toxicity potentials [10]. Chakraborty evaluated environmental risks in the U.S. at the state level from air emission data in the TRI for year

<sup>\*</sup> Corresponding author. Tel.: +1 530 752 5840; fax: +1 530 752 9554. *E-mail address:* jmschoenung@ucdavis.edu (J.M. Schoenung).

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2000 [11]. The current work builds upon a recent study by Zhou and Schoenung [12], in which a variety of environmental impact assessment tools, as well as raw quantity-based TRI statistics, were applied in combination to rate and prioritize the chemicals released within the U.S. chemical manufacturing industry sector. Specifically, the current work aims to expand the scope of this recent study to include all industry sectors that report to TRI. All industry sectors and release categories are considered in detail, then narrowed to focus the study on a comparison of relevant air and water emissions that contribute to human health and ecological toxicity potentials. Both human health and ecological effects are highlighted because humans cannot live separately from ecosystems where particular species in particular places, communities and habitats are vulnerable [13]. Thus, ecotoxicity potentials from the emission of anthropogenic chemicals need to be accounted for, which has not been previously studied for all industries and chemicals in the TRI database. The U.S. EPA's Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) is used to estimate the toxicity potentials [14]. The quantity-based and toxicity-based results are then evaluated together to provide a more robust analysis of key toxic releases in the U.S.

#### 2. Methodology

Basically, there are two aspects to this project: extracting data from the TRI and the application of TRACI. An in-depth analysis of the raw data on releases and disposals from the TRI Explorer for year 2007 (the most recent year for which data is currently available) [7] is used as the basis for the quantity-based characterization of industry sectors, states and chemicals that should be of priority for toxic release management. The data in the TRI Explorer are derived from reports filed by facilities. The TRI analysis considers initially all release and disposal categories, and is then narrowed down to focus on emissions into the air and into the water, since these present the greatest risks for human health and ecological toxicity, as described below. These three sets of quantity-based results (total, air and water) are compared to toxicity-based results to provide a more robust evaluation of priority industry sectors, states and chemicals.

Human health toxicity and ecotoxicity potentials in the U.S. are evaluated from the 2007 TRI data on the basis of the chemicals emitted to the air and water and the respective toxicity potential characterization factors derived from TRACI (specifically, the TRACI 2002 U.S. Average Expanded Format Factors with Fossil Fuels, which is the most recent version available at this time [15]). The air and water emission sources consist of fugitive and point source releases, and surface water discharges in the TRI. The cancer toxicity, non-cancer toxicity (i.e., chronic, subchronic, and developmental health effects [14,16]) and ecotoxicity potentials for water and air are evaluated by multiplying the weight of each chemical by its respective toxicity potential characterization factor from TRACI, which accounts for the fate, exposure, and effects of the chemicals in the U.S. [14]. TRACI is based on the CalTOX model, i.e., a multi-media fate and multiple-exposure pathway model that uses generic parameters for the U.S. assuming steady-state mass balances in a closed system with continuous air and water emissions [14]. The characterization factors for cancer and non-cancer toxicity potentials are determined by using the CalTOX model together with carcinogenic risk potency factors and a reference dose/concentration; for ecotoxicity potentials, the characterization factor is determined by using the concentration-to-source ratio (CSR) from the CalTOX model and the impact-to-concentration ratio (ICR) from the predicted no-effects concentration (PNEC) to estimate potential terrestrial and aquatic impacts. These characterization factors for select chemicals are evaluated relative to reference substances: kilogram benzene-equivalent per kilogram chemical for cancer potential; kilogram toluene-equivalent per kilogram chemical for non-cancer potential; and kilogram 2,4 dichlorophenoxyacetic acid-equivalent per kilogram chemical for ecotoxiticy potential. Chemicals are linked on the basis of the CAS registry number. A key assertion in the current study is that human and ecological health are paramount. Therefore, other potential environmental impacts, such as global warming, acidification and eutrophication are not considered. In order to estimate the toxicity potentials by industry sector and by state, the quantity and type of chemicals emitted into the air and water are first derived from the TRI for a given state or industry sector. The TRACI characterization factors are then applied to each chemical, and a weighted sum of all the chemicals emitted in a given state or industry sector is calculated. All the quantity and toxicity potentials are normalized to obtain their shares and examine their relative significances. It should be noted that toxicity potential evaluation results should be interpreted as relative values because TRACI is used for life cycle impact assessment for a single life cycle stage or the whole life cycle [17].

The issue of metals versus metal compounds is present when using TRACI, because TRACI provides characterization factors for metals only, whereas TRI reports quantities released/disposed for both metals and their compounds, separately. Thus, the toxicity potential of the metal compounds included in the quantity-based TRI data is not accounted for in the toxicity-based assessment. Analysis of the TRI data show, however, that the concentration of metal compounds in air and water emissions are generally fairly low, as described in Section 5; rather, the metal compounds are found primarily in the other release/disposal categories, which are not considered in the toxicity portion of the analysis. It should also be noted that not all TRI chemicals are included in TRACI. Discrepancies are noted in the results below.

## 3. Priority industry sectors

The industry sectors that represent the largest contributors to toxic releases and disposals are identified as: metal mining (28%), electric utilities (25%), primary materials (12%), chemicals (12%), hazardous waste and solvent recovery (5%), paper (5%), food/beverage/tobacco (4%), petroleum (2%) and fabricated metals (1%). Numeric values for all of the quantity-based and toxicitybased results are provided in Supplementary Materials. In Fig. 1(a), the distribution of these releases/disposals among the various categories is illustrated for the four highest ranked industry sectors, highlighting the wide variation of release type from one industry sector to another. It is important to note that the release and disposal sources for metal mining and primary metals industries consist mainly of surface impoundments, land disposal, and landfill, and the main chemicals from these industries are metal compounds (see Fig. 1(b)). The metal compounds are valueless metal ores with low metals content in the mining industry [18] or wastes such as slag and red mud in the primary metals industry [19], rather than pollutants of concern: the metal ores and wastes, if properly managed, would not have direct or significant toxicity potential in the environment [20–22]. Also, the electric utilities and chemicals industries typically employ proper waste management methods such as landfills and underground injection class I wells [21]. It is important not to include these categories of release and disposal when prioritizing for environmental or human health effects, as they are being managed properly and thus create little potential for risk especially when compared to chemicals directly released into the air and water [21].

In an effort to look at the effect of this distinction more closely, the TRI database was further analyzed to identify industry sectors that are the major contributors to air and water releases. The results of this analysis indicate that the priority industry



Fig. 1. Toxics Release Inventory (TRI) analysis on total release and disposal of chemicals, distributed by: (a) release/disposal category; and (b) chemical, highlighting metal compounds. Source [7].

sectors are now different than they were for all releases/disposals. Now, the priority industry sectors are: (a) for air: electric utilities (49%), chemicals (14%), paper (11%), food/beverage/tobacco (4%), primary metals (3%), and petroleum (3%); and (b) for water: food/beverage/tobacco (35%), primary metals (20%), chemicals (16%), petroleum (10%), paper (8%), and electric utilities (1%). The industry sector of metal mining, which was the first priority on the basis of all releases/disposals, is not on either list.

Moving beyond the quantity-based analysis, the toxicity-based results by industry sector are analyzed for cancer potential, noncancer potential and ecotoxicity potential, through both air and water. The highest priority industry sectors are identified for each toxicity category in Table 1, with those sectors that represent more than 10% of the total toxicity potential in a given category highlighted in gray. The highlighted industry sectors converge into some sectors that were also highlighted in the quantity-based analysis: chemicals, primary metals, petroleum, electric utilities and paper; and some that were not: wood products and cement. The combined results are summarized in Fig. 2 to highlight the differences in prioritization that derive from the nine selected criteria.

#### 4. Priority states

In addition to industry sector, the TRI database can be analyzed by geographic region. The five highest priority states on the basis of all releases/disposals include: Alaska (14%), Ohio (7%), Indiana (6%), Texas (6%) and Nevada (5%). When only air and water-based releases are considered, the five highest priority states change to: (a) for air: Ohio (9%), Georgia (6%), North Carolina (6%), Pennsylvania (6%) and Texas (5%); and (b) for water: Indiana (12%), Virginia

## Table 1

Highest priority industry sectors (greater than 3% of total) and their relative shares from the toxicity-based evaluation. The industry sectors that represent more than 10% of the total toxicity potential in a given category are highlighted in gray.

Rank	Cancer potential (%)		Non-cancer potential (%)				Ecotoxicity potential (%)					
	Air		Water		Air		Water		Air	Water		
1	Chemicals	73	Chemicals	66	Primary metals	45	Chemicals	41	Electric utilities	25	Paper	39
2	Primary metals	8	Wood products	15	Chemicals	11	Primary metals	27	Chemicals	23	Petroleum	23
3	Transportation equipment	3	Petroleum	9	Electric utilities	9	Petroleum	10	Primary metals	17	Primary metals	14
4	Fabricated metals	3	Fabricated metals	5	Cement	6	Paper	5	Cement	14	Chemicals	11
5	Petroleum	3	Primary metals	4	Paper	5	Transportation equipment	4	Petroleum	8	Textiles	3
6	Machinery	2	Paper	1	Petroleum	4	Fabricated metals	3	Electrical equipment	3	Electric utilities	2
7	Paper	2	Plastics and rubber	0.3	Electrical equipment	3	No TRI NAICS Code	3	Food/beverages/tobacco	2	Electrical equipment	2
8	Miscellaneous manufacturing	1	Electric utilities	0.2	Food/beverages/tobacco	3	Electric utilities	3	Stone/clay/glass	2	Plastics and rubber	1

	3% ≤ Share < 10%			10% ≤ Share < 30% Share ≥ 30%								
	C	uantity-base	ed	Toxicity-based								
Industry	Total Releases and Disposals	Air Emission	Water Emission	Cancer Potential for Air	Cancer Potential for Water	Non-cancer Potential for Air	Non-cancer Potential for Water	Ecotoxicity Potential for Air	Ecotoxicity Potential for Water			
Cement												
Chemicals												
Electric Utilities												
Electrical Equipment												
Fabricated Metals												
Food/Beverages/Tobacco												
Hazardous Waste/Solvent Recovery												
Metal Mining												
Paper												
Petroleum												
Plastics and Rubber												
Primary Metals												
Textiles												
Transportation Equipment												
Wood Products												
No TRI NAICS Code												

Fig. 2. Industry sector analysis comparing quantity-based results with toxicity-based results.

(8%), Nebraska (7%), Texas (6%) and Louisiana (5%). There is limited overlap of priority states among these three lists, with only Texas on all three, making it difficult to generalize from the quantity-based TRI data the states that might need the most intervention.

For comparison, toxicity-based results for the six impact categories were generated, identifying the highest priority states for each category (see Table 2). The quantity-based results are compared with the toxicity-based results in Fig. 3. From the toxicity-based results, the states with the highest priority become Louisiana, Ohio and Texas. Additional high priority states include West Virginia and Illinois. It is interesting to note that California, Iowa, Kansas, New York, and Oregon, all of which are on the toxicity-based lists, are not on any of the quantity-based lists, and that Alaska, Florida, Maryland, Mississippi, Nevada, and Utah, although on the quantity-based lists, are not on any of the toxicitybased lists.

#### Table 2

Highest priority states (greater than 3% of total) and their relative shares from the toxicity-based evaluation. The states that represent more than 10% of the total toxicity potential in a given category are highlighted in gray.

Rank	Cancer potentia	al (%)			Non-cancer pote		Ecotoxicity potential (%)					
	Air		Water		Air		Water		Air		Water	
1	Texas	32	Louisiana	50	Illinois	17	Louisiana	20	Ohio	10	Texas	12
2	Louisiana	24	Illinois	14	Ohio	7	Ohio	16	Alabama	8	Ohio	11
3	Kansas	7	Texas	10	Louisiana	7	Texas	12	Louisiana	6	South Carolina	9
4	Kentucky	5	Georgia	7	Texas	6	West Virginia	10	Indiana	6	Louisiana	9
5	Ohio	4	Indiana	7	Alabama	6	Georgia	6	Iowa	5	Alabama	6
6	Arkansas	3	New Jersey	4	Pennsylvania	5	Alabama	5	Texas	5	North Carolina	5
7	Tennessee	3	Alabama	3	Indiana	5	Tennessee	4	Tennessee	4	New York	4
8	Pennsylvania	3	Kansas	1	Tennessee	4	Illinois	4	California	4	Georgia	4
9	Illinois	2	Tennessee	1	Michigan	3	Pennsylvania	3	Pennsylvania	4	Virginia	4
10	California	2	West Virginia	1	North Carolina	3	Washington	2	Nebraska	4	Illinois	4

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Fig. 3. State-level analysis comparing quantity-based results with toxicity-based results.

#### 5. Priority chemicals

Also of great interest is the prioritization of the actual chemicals that are released and/or disposed of. The ten highest priority chemicals on the basis of all releases/disposals include: zinc compounds (18%), hydrochloric acid (12%), lead compounds (12%), nitrate compounds (7%), barium compounds (6%), manganese compounds (5%), copper compounds (4%), ammonia (4%), methanol (4%) and sulfuric acid (3%). The ten highest priority chemicals for air emissions are (see Fig. 4): hydrochloric acid (38%), sulfuric acid (10%), methanol (10%), ammonia (9%), hydrogen fluoride (5%), toluene (3%), styrene (3%), n-hexane (3%), xylene (2%) and carbonyl sulfide (1%). For water emissions, the priority chemicals are: nitrate compounds (90%), manganese compounds (2%), methanol (2%), ammonia (2%), and sodium nitrite (1%). Again, there is significant variation depending on the release category used for the basis of prioritization. It is also noted that metal compounds occur in the ten highest priority chemicals only when all releases/disposals are considered. When

only air and water are considered, only manganese compounds are found on the highest ten lists.

The toxicity-based analysis was again conducted for the six impact categories, identifying the highest priority chemicals for each category (see Table 3). The results are compared to the quantity-based results in Fig. 5. From the toxicity-based analysis, arsenic, benzo(g,h,i)perylene, carbon tetrachloride, chromium, formaldehyde, hexachlorobenzene, mercury, lead (Pb), and vanadium are of greatest concern. None of these chemicals, it is noted, are on the quantity-based lists. On the other hand, hydrochloric acid, which is not on any of the toxicity-based lists, is identified as a substance of concern on the quantity-based lists.

It is important to recall that not all chemicals in TRI have characterization factors in TRACI. For instance, those among the quantity-based high priority chemicals emitted to air or water that do not have characterization factors in TRACI have been so indicated (see Figs. 4 and 5). As a consequence, these chemicals cannot appear on any of the toxicity-based lists. This is of greatest concern

#### Table 3

Highest priority chemicals (greater than 3% of total) and their relative shares from the toxicity-based evaluation. The chemicals that represent more than 10% of the total toxicity potential in a given category are highlighted in gray.

Rank	Cancer potential	Non-cancer potential				Ecotoxicity potential						
	Air		Water		Air		Water		Air		Water	
1	Carbon Tetrachloride	62	Arsenic	59	Lead	51	Mercury	51	Mercury	85	Formaldehyde	37
2	Chromium	12	Hexachloro-benzene	21	Mercury	30	Lead	33	Benzo(g,h,i)Perylene	6	Benzo(g,h,i)Perylene	34
3	Ethylene Oxide	4	Carbon Tetrachloride	8	Aluminum	7	Copper	10	Copper	3	Vanadium	14
4	Lead	4	Ethylene Oxide	2	Hydrogen Cyanide	3	Arsenic	2	Thiram	1	Naphthalene	9
5	Chloromethane	3	1,2,3-Trichloropropane	2	Copper	2	Vanadium	1	Nickel	1	Copper	5
6	Benzene	3	Lead	1	Phosgene	2	Cadmium	1	Zinc	1	Carbon Disulfide	0.3



**Fig. 4.** TRI analysis on chemicals emitted on-site to: (a) air, and (b) water. Source [7].

for nitrate compounds in water emissions, since they dominate the quantity-based evaluation. Thus it is noted that high concentrations of nitrate in drinking water can induce infant methemoglobinemia [23] and impair aquatic life [24]. Nitrate compounds are emitted primarily by the food/beverages/tobacco, primary metals, chemicals, and petroleum industry sectors, with the largest quantity of emissions coming from the state of Indiana. The only other chemical contributing more than 10% to the air or water emissions, that does not have a TRACI characterization factor, is sulfuric acid. Sulfuric acid can impact human respiratory organs and increase morbidity and mortality among people with respiratory and cardiopulmonary diseases [25]. Sulfuric acid is emitted primarily by the electric utilities industry sector, with the largest quantities of emissions coming from the states of Kentucky, Indiana, and Ohio.

## 6. Discussion

The differences in prioritization between the quantity-based and toxicity-based approaches, especially for the chemicals themselves, highlight the need to consider both evaluation methods when setting goals for environmental management and policy. Furthermore, the results by chemical further highlight the severe toxicity potential associated with select chemicals used in fairly small quantities. These chemicals and their potential to impact the environment merit a bit more discussion. The links between these chemicals and the industry sectors and states of priority are discussed. Subsequently, the reasons why TRACI was used in this study are discussed by briefly describing the limitations of alternative impact assessment methods. Arsenic, emitted primarily by the chemical (65%) and wood products (25%) industry sectors, is a significant contributor to the cancer potential for water, especially in Louisiana and Illinois. Although wood products are regarded as environmentally friendly in terms of being a renewable material, this industry has significant cancer potential for water because chromated copper arsenate (CCA) is still the most common preservative used in the U.S. to treat wood for non-residential applications, even though arsenic-free preservatives are available on the market [26]. Exposure to arsenic can cause lung cancer [27].

Benzo(g,h,i)perylene, a mutagenic polycyclic aromatic hydrocarbon (PAH) [28], which is emitted primarily by the petroleum (55%) and paper (22%) industry sectors, is a significant contributor to ecotoxicity in water, especially in Ohio, and less-so in air.

Carbon tetrachloride is a significant contributor to the cancer potential for air, especially in Louisiana and Texas. Ninety-seven percent of the carbon tetrachloride is emitted by the chemicals industry; seventy-seven percent is emitted from point sources, i.e., stacks. Carbon tetrachloride is used as cleaning and degreasing solvents; extraction, paint, and coating solvents; and as a feedstock to produce other chemicals [29]. Carbon tetrachloride can cause liver cancer and is classified as a probable human carcinogen [30,31].

Chromium, which is a significant contributor to cancer potential for air, especially in Pennsylvania, is emitted primarily by the industry sectors of primary metals (37%), transportation manufacturing (20%), fabricated metals (19%), and machinery (14%). More chromium emissions come from fugitive sources than from point sources, indicating the need to tightly regulate both. Chromium can cause respiratory diseases such as asthma [32].

Formaldehyde is a significant contributor to the eco-toxicity potential for water, especially in Alabama, Louisiana, New York, and North Carolina. The formaldehyde is emitted primarily by the paper (81%) and chemical (16%) industry sectors. Formaldehyde hydrates, polymerizes, and forms a variety of compounds, which have the potential to impact aquatic species [33].

Hexachlorobenzene, which is emitted primarily by the chemical (62%) and petroleum (38%) industry sectors, is a significant contributor to cancer potential in water, especially in Illinois. According to the results of animal experiments, hexachlorobenzene can cause liver, thyroid, and kidney cancers [30].

Mercury is a significant contributor to non-cancer potential for both air and water, as well as to ecotoxicity for air; ecotoxicity potential for water is not significant because of a low emission to water and a low characterization factor compared to those for air. The states of West Virginia, Louisiana and Ohio are most affected. As an air pollutant, mercury is emitted primarily by the electric utility (28%), chemical (25%), cement (17%), and primary metals (13%) industry sectors. Mercury is emitted primarily from point sources related to coal combustion in power plants [34]. As a water pollutant, mercury is emitted primarily by the chemical (56%), primary metals (21%), and petroleum (18%) industry sectors. Mercury can be converted to a potent neurotoxin impairing the lipid-rich neurons of the central nervous system and the immune response in humans [35]. Mercury can also affect ecosystems through transformation, transport, bioaccumulation, and fate [36,37].

Lead is a significant contributor to non-cancer potential for both air and water, especially in Illinois and Ohio, respectively. As an air pollutant, lead is emitted primarily by the primary metals (62%) industry sector; 81% of the lead is emitted from point sources. As a water pollutant, lead is emitted primarily by the primary metals (32%), chemical (29%), and paper (12%) industry sectors. Lead affects the nervous, cardiovascular, immune, and hematological systems [38,39].

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	3% ≤ Share < 10%				10% ≤ Share	< 30%	Share ≥ 30%				
	Q	uantity-base	ed			Toxicit	y-based				
Chemical	Total Releases and Disposals	Air Emission	Water Emission	Cancer Potential for Air	Cancer Potential for Water	Non-cancer Potential for Air	Non-cancer Potential for Water	Ecotoxicity Potential for Air	Ecotoxicity Potential for Water		
Aluminum											
Ammonia											
Arsenic											
Barium Compounds*											
Benzo(g,h,i)Perylene											
Carbon Tetrachloride											
Chromium											
Copper											
Copper Compounds*											
Ethylene Oxide											
Formaldehyde											
Hexachlorobenzene											
Hydrochloric Acid											
Hydrogen Cyanide											
Hydrogen Fluoride*											
Lead											
Lead Compounds*											
Manganese Compounds*											
Mercury											
Methanol											
Naphthalene											
Nitrate Compounds*											
Sulfuric Acid*											
Toluene											
Vanadium											
Zinc Compounds*											

Fig. 5. Chemical-level analysis comparing quantity-based results with toxicity-based results.

Vanadium, which is emitted primarily by the primary metals (74%) and chemical (18%) industry sectors, is a significant contributor to ecotoxicity for water, especially in Texas. The aquatic toxicity of vanadium is a risk to fish in watersheds [40], and vanadium transforms and accumulates in biological systems [41].

Clearly, these chemicals, which are emitted in small quantities (each less than 3% of the TRI releases to either air or water), present ecological and human health concerns that should not be overlooked by focusing on quantity-based evaluation methods. Furthermore, the states in which these chemicals are emitted also represent different states than those identified by quantity-based evaluation, although the aggregation does lead to more overlap of priorities. Interestingly, with further aggregation to the industry sector level, the sectors of priority are identified more consistently, regardless of whether quantity-based or toxicity-based evaluation methods are used.

For the toxicity potential evaluation, besides TRACI, two other environmental impact assessment tools were considered for this study: USETox and RSEI. USETox is a recently developed toxicity model created by UNEP-SETAC (United Nations Environmental Program-Society for Environmental Toxicology and Chemistry) that provides characterization factors for both human toxicity and freshwater ecotoxicity derived from scientific consensus among international toxicity experts [42]. It was not employed for the current study, however, because characterization factors for metals and metal compounds are not yet available. The U.S. EPA Risk-Screening Environmental Indicators (RSEI) [43] method uses a risk assessment approach to complement the TRI by taking into account the human health risk from chemicals based on site-specific air and water modeling, and affected population. The primary reason why RSEI was not used in the current study is because it does not account for ecotoxicity. In addition, the RSEI does not differentiate metals and metal compounds [43].

## 7. Conclusions

The results of this study can contribute to enhanced environmental management for individual facilities and environmental policy for local, state, and federal governments. Individual facilities can strive to reduce the releases of the priority chemicals; to effectively mitigate toxicity potentials on neighboring communities, occupational workers, and ecosystems; and to enhance corporate sustainability. Government can be proactive in targeting priority chemicals, industries, and states when establishing environmental policy and regulations. Government can also financially assist in the development of cleaner technology and safer products to minimize emissions of priority chemicals, and to improve the overall environmental performance within the United States.

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## Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jhazmat.2010.01.041.

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