Toxicity-weighted contaminant index for mapping the cumulative release of pollutants to Canadian surface waters using Canada's National Pollutant Release Inventory (NPRI) Database

National Pollutant Release Inventory Academic Challenge

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Abstract

With recent changes to the *Canadian Impact Assessment Act* (2019) there is a reinvigorated push to understand the cumulative effects of industrial activity on the natural world. Using data collected by the National Pollutant Release Inventory (NPRI), a division of Environment and Climate Change Canada for the reporting year of 2019, a substance list of instances of direct effluent release in waterbodies was created. This list of reported substances was then used to create a toxicity-weighted contaminant index allowing substance-to-substance comparison between facilities. This index utilized five well studied variables that best describe a substance's toxicity in relation to aquatic environments and included if the substance recognized as an environmental hazard, a H410 hazard, a H400 hazard, cancer causing, and acute toxicity. The index was then applied to the collected 2019 reported data from the NPRI, to locate areas of concern and highlight waterbodies possibly being stressed by multiple chemical releases. The study identified four major areas of concern, Southern Ontario, Vancouver British Colombia, Calgary and Edmonton, Alberta. A strong trend was observed between large wastewater treatment plants and the above areas of concern. The waterbody experiencing the greatest stress based on our index in 2019 was Lake Ontario located in Southern Ontario.

1. Introduction

With increased industrialization, the management of toxic chemicals and their subsequent environmental release is necessary to mitigate further environmental degradation (UNEP, 2013). Specifically, the environmental effects from cumulative effluent release or spill events is poorly understood and requires greater study (UNEP, 2013). To keep the public informed on local industrial facility emissions, public programs such as Environment and Climate Change Canada’s National Pollutant Release Inventory (NPRI) and the Toxics Release Inventory (TRI) in the United States have been developed to give access to the quantity and types of chemicals being released. The NPRI tracks the release of over 300 substances of concern in Canada, which are required to be reported and tracked under the *Canadian Environmental Protection Act, 1999* (CEPA, 1999). Reported substances include hazardous elements such as heavy metals, polycyclic aromatic hydrocarbons (PAHs), and volatile organic compounds (VOCs). The NPRI does not include every instance of environmental release of a substance of concern in Canada. Only facilities meeting the reporting requirements must submit a NPRI report. The reporting criteria is defined by three major tenets, the activities taking place at the facility, the total number of hours worked by employees, and the substances manufactured, processed, used, and or released (NPRI, 2018). Therefore, any analysis using the database is subject to the reporting limitations and inherent errors in estimation.

Although the NPRI does a good job of making chemical release data available there is a pressing need to turn these data into information about potential environmental impacts, particularly cumulative impacts of release events on waterbodies from multiple facilities. This sentiment is echoed in recent changes in the Canadian Federal mandate and the revitalized *Impact Assessment Act, 2019* where large-scale development projects need to be viewed in their surrounding environmental context. This affords the opportunity to avoid compounding environmental stressors on fixed physical features such as rivers, streams, and lakes (IAA, 2019). Therefore, to aid in this effort, a toxicity weighted contaminant index was created to compare the general toxicity of recorded and tracked chemicals by ECCC's NPRI division. The index scoring system allows for the comparison of the potential environmental impact of various chemicals that may be released in an effort to quantify cumulative impacts on aquatic ecosystems. This is done by factoring in widely studied variables on a per substance basis. These variables included metrics such as LD50 and defined hazard symbols by the National Library of Medicine (NIM) and the Centre for Disease Control (CDC) to allow for substance-to-substance comparisons (PubChem, 2021). This standardization allows for facilities to be viewed in concert regardless of industry or reported released chemicals. This permits the study of the possible cumulative effect of industry on a singular waterbody or feature, which can then be assembled to investigate complete watersheds.

This report specifically investigates substances being released into waterbodies through direct discharge events, either accidental, recurring, or constant. This encompasses a range of reporting sectors and industries in Canada from pulp and paper to wastewater treatment. This highlights the scope of this Canada wide project as well as its possible application in policy making decisions and the project application approval system in Canada. The subsequent rankings of released substances into waterbodies also provides an opportunity for meaningful public engagement. The goal of this index is to simplify complex, multivariate, chemical data, while maintaining accuracy and creating a more digestible value to examine cumulative impacts on aquatic ecosystems.

2. Materials and Methods

2.1 Study Area

The study area includes all of Canada's provinces and territories. The 2019 substance of interest list NPRI reporting year was used for the analysis and the application of the chemical scoring index. This list totaled 84 compounds, which were found to be directly released into Canadian waterbodies.

2.2 Toxicity-Weighted Contaminant Index

The toxicity-weighted contaminant index focused on possible impacts on aquatic life. The index combined the following five variables that were equally weighted in the index score, A) was the substance recognized as an environmental hazard, B) a H410 hazard, C) a H400 hazard, D) cancer causing, and E) acute toxicity. Each variable was then inputted into Formula 1 to create an index score. This score was used for the comparison between substances and facilities regardless of the released substances.

Formula 1) $$Index\ Score = \frac{(A+B+C+D+E)}{5}$$

The first variable considered in the calculation was if the chemical being assessed had been designated as an environmental hazard by the Environmental Protection Agency or by the Globally Harmonized System of Classification and Labelling of Chemicals (GHS). This classification acknowledges a chemical or substance unequivocally as an environmental risk either through its innate toxicity, mobility, ability to bioaccumulate, or longevity (UNECE, 2019). An environmental hazard designation refers specifically to possible negative impacts on either aquatic ecosystems or the ozone layer (UNECE, 2019). A substance labelled as an environmental hazard often also pose significant risk to human health with extensive contact and handling (UNECE, 2019). This variable was treated as a binary input in the index calculation, either as a value of 1 for a substance having the designation or a 0 in its absence. An example of a substance with this designation is cadmium. Cadmium has long been identified as an environmental hazard due to its ability to accumulate within the livers and kidneys of mammals and birds (Elinder, 1992, UNECE, 2019). Elevated levels of cadmium in such organs have been linked to chronic interstitial nephritis (Elinder, 1992). This is a form of kidney damage thought to impact survivability at low exposures and higher exposures leading to kidney failure and death (Elinder, 1992). This example demonstrates the significance of a substance receiving this classification in the index score calculation.

The second variable considered was if the substance was designated as an H410 hazard by the GHS classification system. A H410 hazard is given to chemicals which have been assessed through scientific study to be very toxic to aquatic life with long lasting effects (UNECE, 2019). This designation is assigned by the World Health Organization (WHO) and the CDC (UNECE, 2019). This designation is often added to a substance's classification when it exceeds the requirements to be an environmental hazard in these two criteria, toxicity, and longevity. Its inclusion in the calculation allows for a higher degree of accuracy and resolution when comparing substances. This variable was treated as a value between 1 and 0, 1 being a full designation and a 0 stating it does not apply to the substance. In the GHS classification system this variable is assigned along with a level of confidence (UNECE, 2019). This level of confidence was used as the input in the calculation, once again to increase the sensitivity and resolution of the index score. These confidence values may be subject to change as further research is conducted on specific substances, but our index is based on the current understanding of the included chemicals. An example of a substance labelled as a H410 hazard is chrysene also commonly know as creosote. Creosote was used extensively in preserving wooden components such as railway sleepers used to support railroad tracks. Creosote was used because of its ability to penetrate wood grains while being extremely toxic to microbial life and persist in the environment over a rail roads service life (Vilniskis and Vaiskunaite, 2017). These chemical properties work well in preventing rot in the wooden components but poses a real challenge in how to dispose of them in a safe manner after their designed lifetime.

The third variable included in the index calculation was if the individual substance was labelled a H400 hazard, which is a substance designated by the WHO and the GHS classification system to be very toxic to aquatic life (UNECE, 2019). Again, for a substance to receive this designation it must exceed the requirements of the environmental hazard statement in toxicity exclusively related to aquatic species. The H400 hazard is also denoted as a value between 0-1 following its assigned confidence level (UNECE, 2019). An example of a substance with this classification is chlorine, a common chemical used in industrial processes. Chlorine is denoted as both an environmental hazard and a H400 Hazard (NPRI, 2019).

The fourth variable considered was if the observed substance is carcinogenic to aquatic life. This variable was deemed important to consider as carcinogenic growths such as neoplasms can impact fish survivability and successful reproduction (Black and Baumann, 1991; Bunton, 1996). This variable is also a value between 0-1 in the index calculation following the confidence level given to these hazard statements by the NLM, WHO, and GHS classification system (UNECE, 2019). An example of a highly carcinogenic substance monitored by the NPRI is formaldehyde. A once commonly used agent in species sample preservation which has since been linked closely with cancer following prolonged exposures (Blair et al. 1990). The chemical is still used in some industrial production and processes.

The final variable used in the index calculation was acute toxicity. This variable was standardized from the substances known lethal dose (LD50) in ppm by the oral ingestion in either a rat or mouse. The LD50 values of the studied substances were published by the NIM and the CDC and the result of their own rigorous testing process. A LD50 can be described as the amount of substance required to kill 50 percent of a sample often used to quantify common toxicity. The LD50 for rat or mice was used because these data are widely available for a larger suite of chemicals and the LD50 between rats and mice are strongly correlated to LD50 of common aquatic organisms such as *Daphnia Magna* often used in water quality evaluations (Devillers J and Devillers H, 2009; Enslein et al. 1987; Guilhermino et al. 2000). The observed correlation in the three animals' response to large doses of chemicals suggests that LD50 values from rats, mice, and daphnia are related. With that considered, the value was then normalized to a number between 0-1 when compared to the other NPRI tracked substances using Formula 2.

Formula 2) $$Normalized\ Toxicity\ Value = \frac{a-Max}{Max-Min}$$

The variable a in the equation represents the known LD50 of the substance under investigation. This value was then compared to the largest LD50 of the NPRI's 84 reported substances released directly into waterbodies, denoted by the variable Max. The variable Min in the equation represents the lowest or most toxic substance's ppm value to achieve LD50. This formatting allows the five variables to be compared in equation 1 as the variables are all equally weighted by a value between 0-1. Of the index's 84 included substances monitored by the NPRI and released into the Canadian environment in the reporting year of 2019, antimony had the lowest LD50 value of 0.43 ppm to kill a rat (NIM). Although having the highest general toxicity, as reported by the LD50 of all the substances, antimony ranked 24th on our toxicity-weighted contaminant index list due to the fine resolution which can be achieved using the five variables to rank the substances. As antimony, while extremely toxic, had a medium to low confidence of being assigned as a H410 and H400 hazard designation. This indicates that it may not be as hazardous in an aquatic environment than other recorded substances.

The five outlined variables were chosen to be included in the index score as they maximize the number of substances that can be compared and included in the index based on available data and the current toxicological understanding. Utilizing the selected variables 76 of the 84 (~90%) recorded chemicals released directly into waterbodies in 2019 were accounted for in the index and scoring list (Table 1). The use of five variables allows for a finer level of detail when comparing substances, as each variable adds additional information. This is necessary as substances such as Chlorine can be classified as an environmental hazard and a H400 Hazard but not a H410 hazard.

Application of the Scoring Index in a Canadian Context

The resulting index score (between 0 and 1) for each NPRI listed chemical was then multiplied by the quantity of the chemical released at each listed location, creating an adjusted quantity of release for each reported chemical. These adjusted quantity values for each chemical released were then able to be totaled for a specific facility, assigning a single value based on its possible impact to aquatic ecosystems. These facilities were then plotted in ArcMap's 10.7.1 using associated coordinates and superimposed on Canada's waterbodies shapefile from Natural Resource Canada (NRCAN, 2019). Adjusted facility chemical releases were then able to be totaled for specific waterbodies based on the reported 2019 data. The waterbodies were then sorted by total adjusted environmental release resulting in a list of the top 20 most impacted Canadian waterbodies (Table 2). The adjusted quantity of direct water release per facility was also mapped for all of Canada (Figure 1).

A point value density analysis was also conducted in ArcMap's, limiting noise, and showing broad areas of concern (Figure 2). This analysis calculates the magnitude of supplied datapoints per unit area, highlighting areas where environmental release occurred at the greatest rate in 2019 (Esri, 2021). Specific areas of interest were then selected based on the results of the point value density analysis. The first area being facilities which released substances directly into Lake Ontario, Ontario (Figure 3). The second area of interest being the Fraser River in British Columbia (Figure 4).

3. Results and Discussion

The result of the toxicity-weighted contaminant index for reported substances directly released into Canadian waterbodies in the reporting year of 2019, is that 76 of the reported 84 chemicals had sufficient information to be included in the analysis. The top five substances on the toxicity index, Benzo[k]fluoranthene, Benzo[e]pyrene, Dibenz[a,h]anthracene, Benzo[a]pyrene, and Hydrazine (and its salts), were all within 0.00001 units of each other in their index score (Table 1). The lowest ranking reported substance was methanol with an index value of 0.15520 (Table 1). Other notable substances were ranked with lower-level scores such as lead with a value of 0.39200 (Table 1).

The top grouping of the first five substances were indicative of the nature of the index scoring system. As the top 5 substances ranked near or at the highest possible value of 1, in all five considered variables. It is also notable that four of these first five substances were classified as PAHs apart from hydrazine. PAHs are often associated with the creation and combustion of fossil fuels (Pickering, 1999). Secondary oxygenated products of PAHs, or oxy-PAHs are recognized as an associated environmental contaminant to PAHs (Lundstedt et al. 2007). It has been argued that this secondary product of PAHs is both more mobile and stable in surface waterbodies than PAHs (Lundstedt et al. 2007). This possesses a significant environmental risk as it then becomes more likely for the contaminated site to have a greater spatial influence (Lundstedt et al. 2007). This increases the subsequent risk of compounding environmental stressors as the result of the cumulative effects of pollutants being released from multiple reporting facilities.

From the 2019 NPRI reporting data the substance recorded with the greatest adjusted quantity considering its index score was the nitrate ion in solution at a pH >= 6.0. It was noted that this substance also had the greatest release quantity with an approximate 80000 tons released across Canada. Therefore, it is not unexpected that even with a lower index score the sheer quantity of the released substance surpasses the other substances in potential impact.

The results of this analysis display a dark picture of Southern Ontario as it indicated the top 20 waterbodies in Canada experienced the highest inflow of adjusted effluent for the 2019 reporting year. Seven of the top ten impacted waterbodies in the list are located in in Southern Ontario. The waterbody experiencing the greatest adjusted chemical release being Lake Ontario with 7924.78 units (Table 2), which was then followed by the Humber River with 1201.06 units (Table 2), which eventually flows into Lake Ontario. This also clearly displays a large disparity between the two waterbodies experiencing the largest quantity of adjusted release in both the quantity and the types of substances being released.

The waterbodies which experienced the greatest amount of adjusted chemical release at large resided in Southern Ontario near Lake Ontario. This may be due to both the industrial activity occurring in the region as well as the large populations from major Canadian cities such as Toronto and Hamilton. The resulting data also suggests that wastewater treatment plants are a major source of these reported pollutants. This may be due to multiple factors such as the ability for these facilities to closely follow the outlined protocol from the NPRI in reporting pollutants in comparison to a commercial business. It also may be related to the volume of the waste being processed on a constant basis. Built in bias in the treatment process may also lead to the differential treatment of contaminants. As the focus of wastewater treatment plants is to break down and sterilize potentially harmful organic material and settle suspended sediments and not remove VOCs (Zhou et al. 2019). Therefore, substances which can stay in solution would be released along with the treated wastewater. This possess environmental concern in two main aspects, one being the current failure to capture these contaminants from a centralized point source. The second area of concern being the possible impact of emerging environmental pollutants such as pharmaceutical drugs and their release from urban wastewater treatment plants (Sayadi et al., 2010, Wennmalm and Gunnarsson, 2005). This pattern of wastewater treatment plants being a major source for released substances is consistent across the NPRI Canadian dataset for 2019. This raises concern over the current limited success of implementing wastewater treatment plants that are able isolate and remove these pollutants.

The mapping products highlight four major areas of concern in Canada (Figures 1 and 2). The first area located in Southern Ontario around the cities of Toronto and Hamilton with the highest levels of adjusted environmental release occurring in all of Canada (Figure 2, Figure 3). This is followed by Calgary and Edmonton, both areas displaying a high density of release in both the number of facilities reporting as well as their associated magnitude (Figure 2). The final area of concern is Vancouver, British Columbia. This area is of particular concern due to the number of facilities releasing effluent into the Fraser River, BC (Figure 4).

The four areas of concern all coincide with Canada's largest urban centres, with the exception of Montreal. This pattern is not unexpected as these areas house most of Canada's manufacturing facilities as well as large wastewater treatment plants. Lake Ontario is of particular concern as the reporting data from the NPRI only provides half of the picture regarding released substances of concern. This is due to the fact that Lake Ontario is an international boarder between Canada and the United States of America and the NPRI only describes Canadian based facilities. Therefore, to get a better understanding of the released pollutants in Lake Ontario data from the EPA must be considered.

The Fraser River highlights a waterbody where multiple facilities have been recorded releasing substantial amounts of adjusted pollutants from a range of facilities (Figure 4). This as an example provides a use case for the developed scoring index and its application in transforming and standardizing NPRI data. The adjusted scores allow for a better understanding of the possible impacts direct water release has on aquatic environments and species. The facilities releasing pollutants into the Fraser River can be viewed individually or as a collective unit of stressors on the waterbody (Figure 4). This could not be done without the use of the index system as chemicals could only be accurately compared to like chemicals. The standardization of the index permits such a wide view and scope of analysis.

3.1 Limitations and uncertainty analysis

Utilizing such a broad system to standardization data does come with its limitations and assumptions, as when data are simplified information is often lost. As through the selection of the five variables in the index score calculation information used must be limited. The selection of the variables was also limited by the known and foundational ecotoxic studies of the substances of concern. If information was missing or incomplete from the used sources such as NLM, CDC, WHO, or GHS hazard statements they could not be included as variable in the index scoring calculation. Therefore, a balance had to be achieved between including known information and excluding partial or missing information. As a result, ~90% of the substances recorded to be directly released to waterbodies were included in the final analysis.

Another limitation of the current study is the lack of consideration of chemical fate. To simplify the study quantity of reported substances was only recorded as it left the point source. This creates some unknowns when investigating the possible cumulative effect of multiple facilities on a single waterbody. As the current study does not account for alterations that may occur in solution such as photochemical decomposition or the creation secondary biproducts. The exclusion of chemical fate in the study also leaves the area of effect unknown. With the area of effect from the point source of pollution unknown it can only be assumed that the impact of multiple facilities is cumulative on a single waterbody. While this may not be the case, as given the appropriate spacing between facilities, chemical stressors may degrade or fall out of solution limiting their associated negative environmental impacts. This issue could be addressed through ground truthing studies, sampling for the recorded substances and establishing areas of effect. The final limitation of the study is not factoring in the residence time of the substances or the volume of the waterbodies. This was not included in the analysis as this information is not widely available for all the NPRI tracked substances. If the information does become widely available, it would be an excellent additional variable to the index score calculation. A similar issue arises for the volume of waterbodies, as this information is not available for all waterbodies investigated. The current study provides areas of interest which would greatly benefit from further study where and when this information is available.

4. Conclusion

Though the creation and adaptation of the chemical scoring index based on the 2019 reported substance list, there is now a robust way to compare substance to substance release to aquatic ecosystems. The scoring system was applied to 2019 reporting data from the NPRI to highlight areas of concern across Canada. As a result of the analysis, it was determined that wastewater treatment plants constitute a large proportion of the adjusted quantity of substances released into surface waterbodies. Wastewater treatment plants, manufacturing facilities and a dense population lead to 7 of the top 10 waterbodies experiencing the greatest amount of adjusted effluent in Southern Ontario. This substance-to-substance comparison allows a direct linkage between multiple reporting facilities on the same waterbody.

Table 1. Toxicity weighted contaminant index for reported chemicals found in direct water release

Chemical Name	Index Score
Benzo[k]fluoranthene	0.99994
Benzo[e]pyrene	0.99993
Dibenz[a,h]anthracene	0.99992
Benzo[a]pyrene	0.99960
Hydrazine (and its salts)	0.99953
Hexavalent chromium (and its compounds)	0.99880
Benz[a]anthracene	0.99840
Chrysene	0.99744
Naphthalene	0.99536
Cadmium (and its compounds)	0.99288
Hexachlorobenzene	0.96800
5-Methylchrysene	0.85440
Dioxins and furans - total	0.80000
Benzo[b]fluoranthene	0.79994
Arsenic (and its compounds)	0.79990
Mercury (and its compounds)	0.79976
Quinoline	0.79736
Biphenyl	0.78480
Pyrene	0.76578
Acenaphthene	0.76188
Cyclohexane	0.76000
Zinc (and its compounds)	0.76000
Silver (and its compounds)	0.74754
Antimony (and its compounds)	0.72678
Nonylphenol and its ethoxylates	0.70282
Anthracene	0.69414
Benzo[ghi]perylene	0.69414
Fluoranthene	0.67556
Fluorene	0.67288
Copper (and its compounds)	0.62540
Phosphorus (total)	0.59996
Thallium (and its compounds)	0.59995
Sodium nitrite	0.59860
Chlorine	0.59766
Hydrogen sulphide	0.58672
Cobalt (and its compounds)	0.55063
Dibutyl phthalate	0.54001
Chromium (and its compounds)	0.46462
Phenanthrene	0.45602
1,2,4-Trimethylbenzene	0.45600
n-Hexane	0.40000

Aluminum (fume or dust only)	0.39989
Molybdenum trioxide	0.39925
Formaldehyde	0.39920
Acetaldehyde	0.39864
Catechol	0.39803
Nickel (and its compounds)	0.39800
Indeno[1,2,3-cd]pyrene	0.39720
Vinyl chloride	0.39600
Chloroform	0.39437
Lead (and its compounds)	0.39200
Chloromethane	0.38102
Manganese (and its compounds)	0.37354
1,4-Dioxane	0.35864
Selenium (and its compounds)	0.34640
Benzene	0.32016
Diethanolamine (and its salts)	0.20000
Cyanides (ionic)	0.19998
Nitric acid	0.19947
Nitrate ion in solution at pH >= 6.0	0.19932
Fluorine	0.19852
Phenol (and its salts)	0.19784
Toluene	0.19492
Bisphenol A	0.19328
Hydrochloric acid	0.19280
Xylene (all isomers)	0.19106
Cresol (all isomers, and their salts)	0.18848
Acenaphthylene	0.18592
Methyl isobutyl ketone	0.18480
Sulphuric acid	0.18288
Calcium fluoride	0.17890
Ethylbenzene	0.17200
Isopropyl alcohol	0.17120
Methyl ethyl ketone	0.16760
Ethylene glycol	0.15600
Methanol	0.15520

Table 2. Top 20 waterbodies experiencing the largest amount of adjusted direct water release in Canada using multipliers from the toxicity weighted contaminant index for 2019 reported data

Name of Waterbody	**Total Adjusted Chemical Release**
Lake Ontario, ON	7924.78
Humber River, ON	1201.06
Speed River, ON	872.64
Highland Creek, ON	863.04
Fraser Rive, BC	608.68
Etobicoke Creek, ON	554.46
Annacis Channel, BC	405.49
Redhill Creek, ON	399.84
Thames River, ON	369.81
Wabush Lake, NL	333.74
Grand River, ON	301.70
South Saskatchewan River, AB, SK	256.73
St. Lawrence River, ON, QC	239.90
Lake St. Francis, ON, QC	203.02
Ottawa River, ON, QC	195.13
Hillsborough River, PE	189.60
Welland Canal, ON	186.42
Lac Dollard-des-Ormeaux, QC	177.37
The Cove, ON	155.21
St. Marys River, ON	148.44

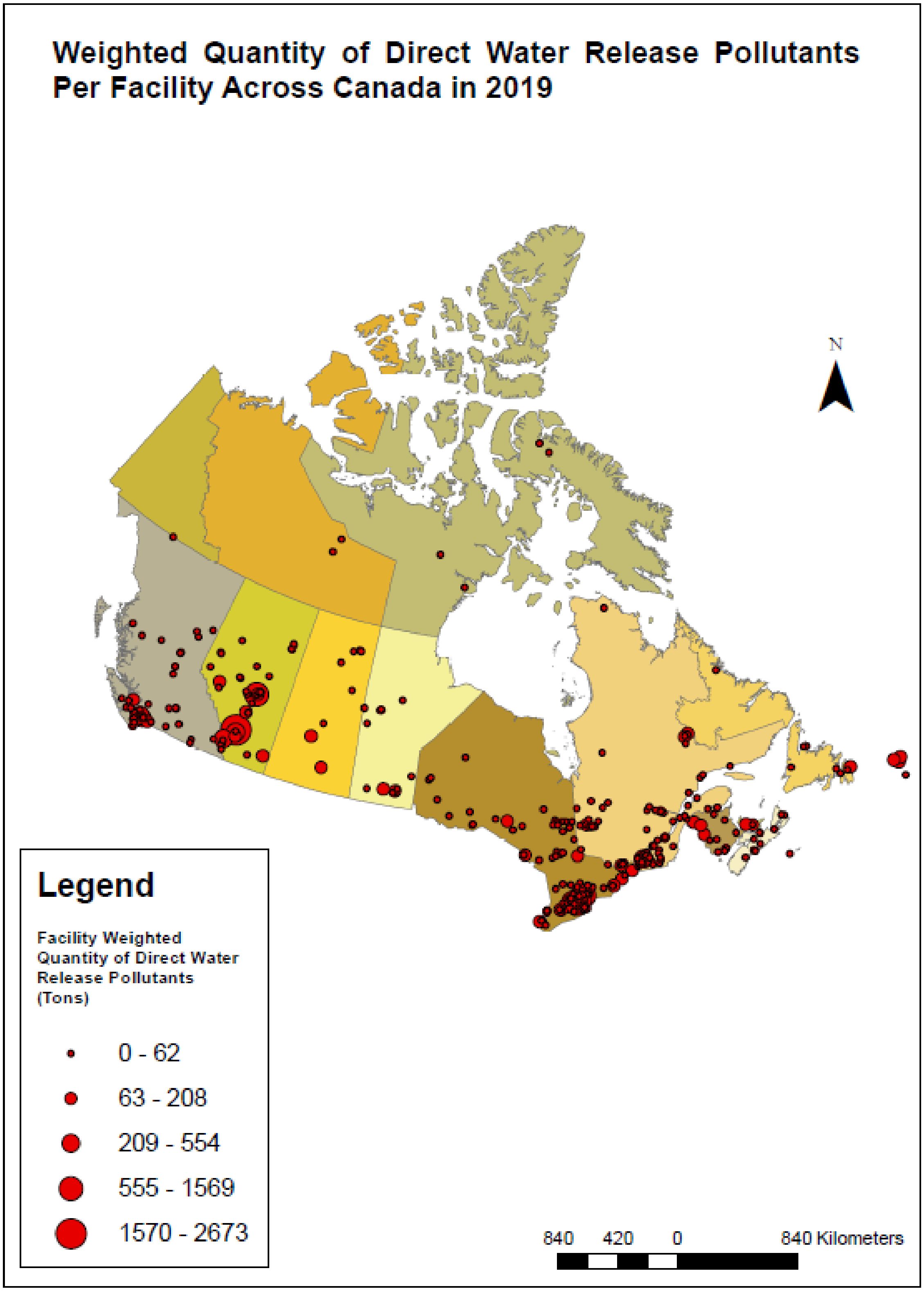

Figure 1. Weighted quantity of direct water release pollutants per facility using 2019 reporting data from the NPRI

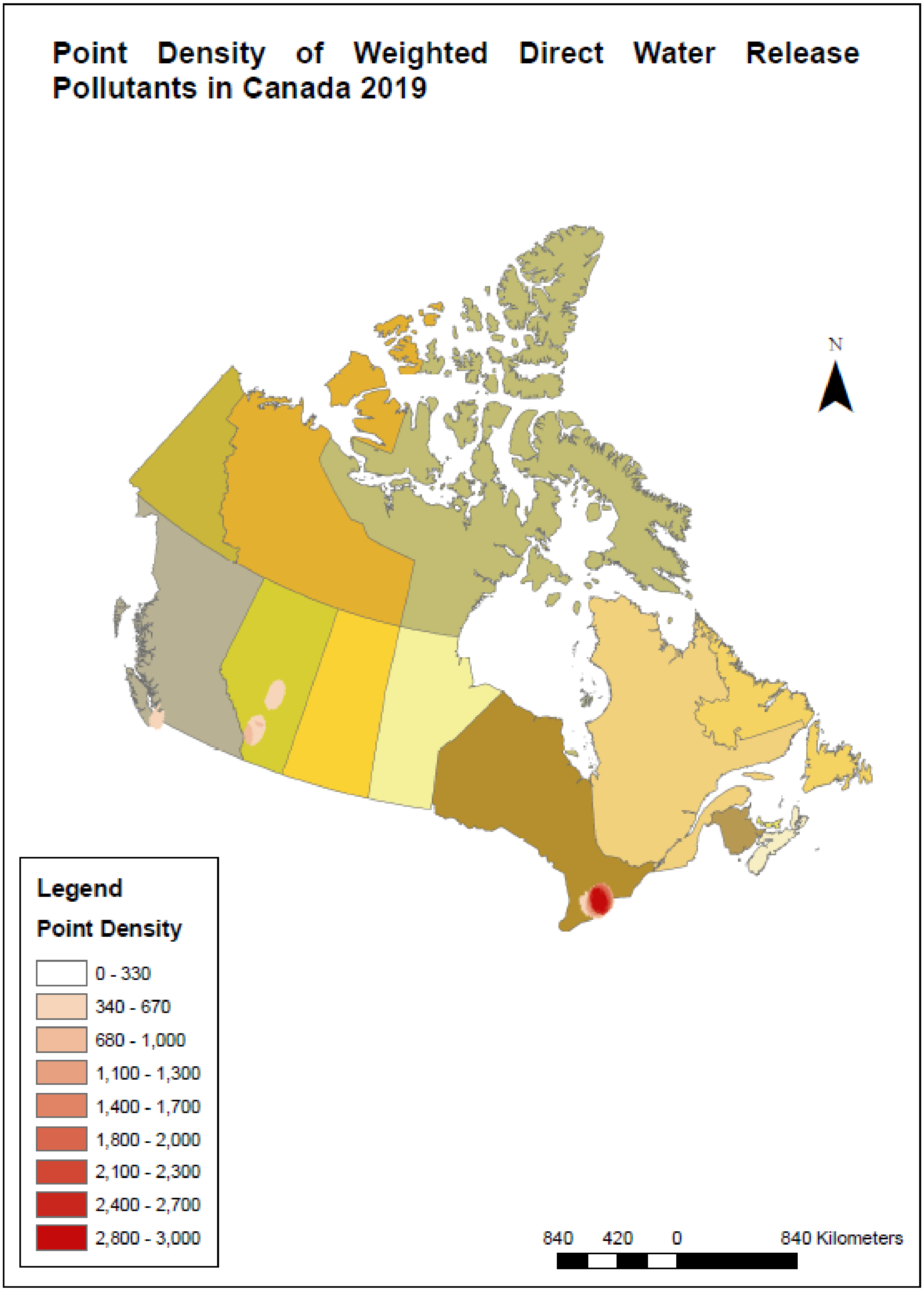

Figure 2. Point density analysis of facilities weighted contaminant release using 2019 reporting data from the NPRI

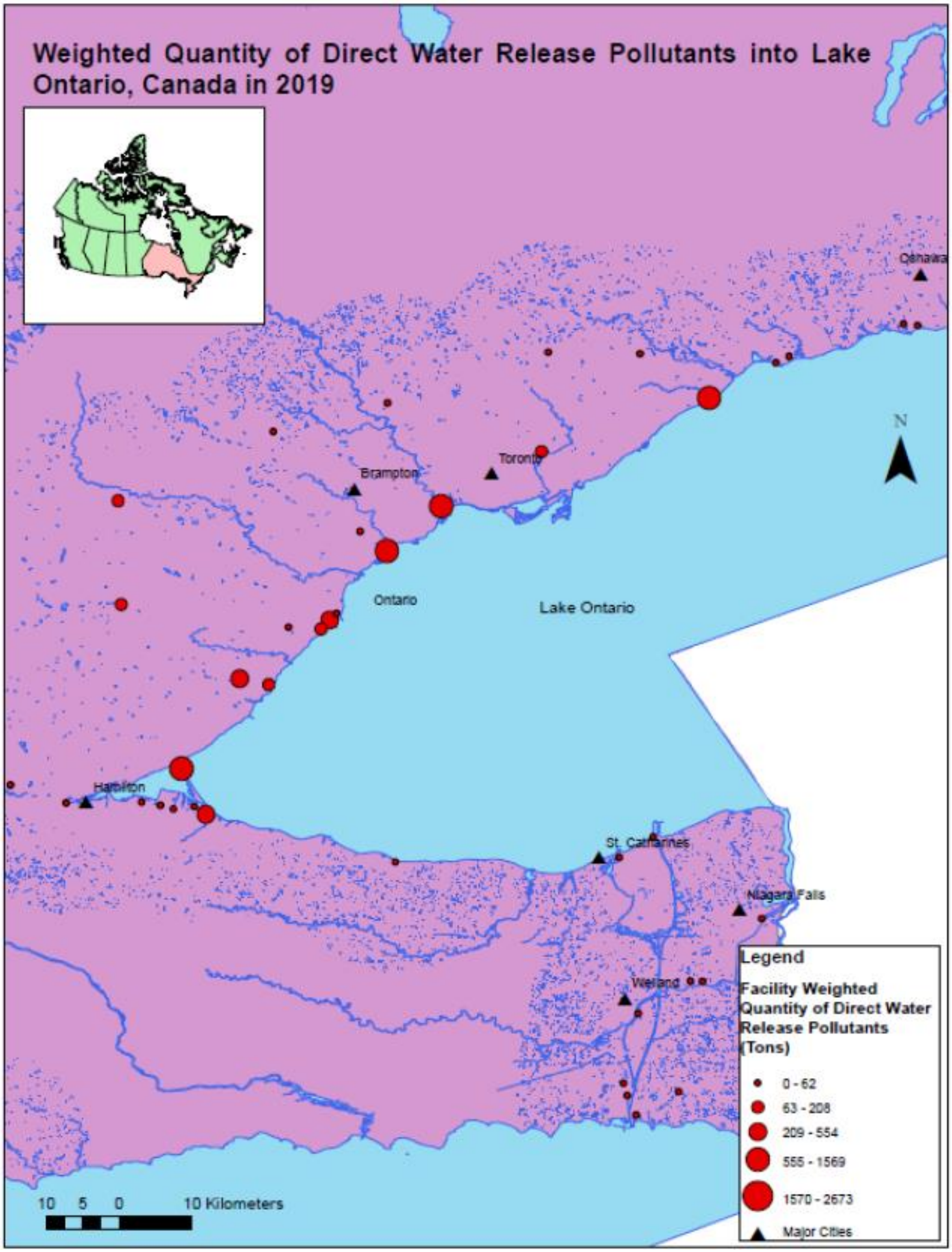

Figure 3. Facility weighted contaminant release in Lake Ontario, ON in 2019

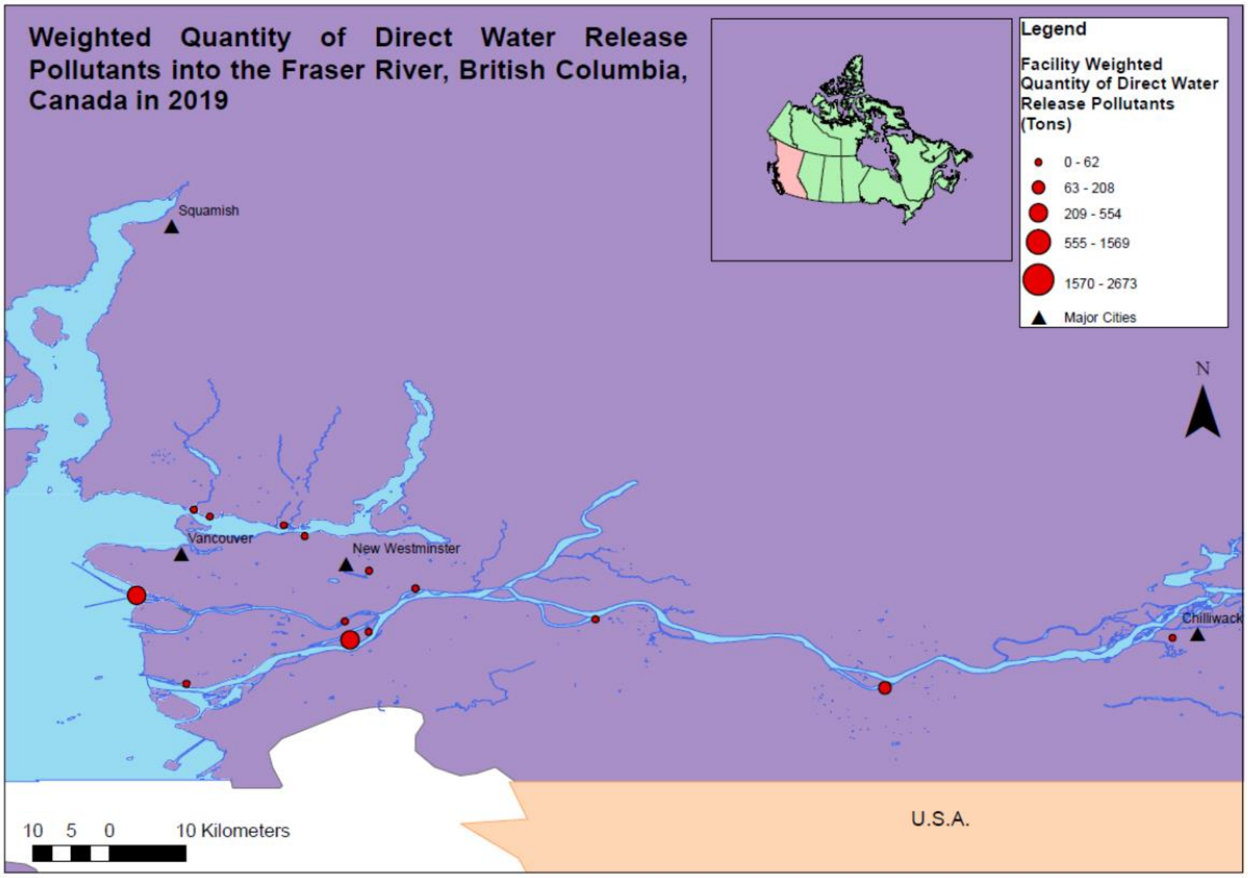

Figure 4. Facility weighted contaminant release in the Fraser River, BC in 2019

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