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ARTICLE INFORMATION

Article title

"Zooplankton community composition data after chronic exposure to benzalkonium chloride"

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Keywords

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Abstract

Benzalkonium chloride (BAC) is a potent antimicrobial currently listed as the number one active ingredient in disinfectants approved by the Government of Canada for use against the COVID-19 virus. Consequently, BAC use has increased in industrial, clinical, and household settings since the onset of the pandemic. Such ubiquitous usage has led to the continuous discharge of these compounds into surface waters primarily via wastewater treatment plant effluent. The perpetual input of BACs into freshwater systems creates pseudo-persistence, potentially exposing downstream aquatic biota. In June of 2023, a mesocosm experiment was conducted at the International Institute for Sustainable Development – Experimental Lakes Area to determine the ecosystem level effects of five nominal concentrations of BAC. Eight 2 m diameter, 1.75 m deep circular enclosures were deployed approximately 3 m apart on a sandy flat bar in the north basin of Lake 375. BAC treatments were assigned randomly to the enclosures and followed a regression design with target concentrations of 20 ng/L, 112 ng/L, 632 ng/L, 3,556 ng/L, and 20,000 ng/L, plus three control enclosures (0 ng/L). A technical mixture of BAC homologs with varying alkyl chain lengths (C10 to C18) was used to spike the enclosures for 16 weeks to simulate pseudo-persistence and maintain target concentrations. Actual BAC concentration, dissipation rate (half-life), and composition of BAC homologs in the enclosures were determined by taking grab samples of water at 6 time points over the duration of the experiment. A YSI water quality meter was used to measure chlorophyll a, DO, pH, and specific conductance weekly throughout the experiment. Zooplankton samples were collected from each of the eight enclosures one day prior to the first BAC addition (day 0), then every two to three weeks after using a 15 L

Schindler-Patalas plankton trap. Samples were filtered through 53 µm mesh and preserved in 5% sugar-formalin solution after narcotization in methanol in the field. Zooplankton were identified to species and life stage using light microscopy and subsequently counted. Eggs were counted to determine reproductive rates of abundant zooplankton taxa. Thus, the dataset contains the site metadata, treatment enclosure key, and raw zooplankton community composition counts, including eggs. This data set may be used for comparisons between mesocosm studies or to determine appropriate target concentrations for future in-situ experiments on the effects of chronic BAC exposure.

SPECIFICATIONS TABLE

Subject	*Ecology*
Specific subject area	*Chronic toxicity of the disinfectant benzalkonium chloride on crustaceous zooplankton communities in a mesocosm experiment*
Type of data	*Table (.csv format)* *Raw*
Data collection	*Data were collected by using light microscopy to count and identify crustaceous zooplankton community samples taken from eight mesocosm enclosures dosed with benzalkonium chloride to achieve five nominal target concentrations, plus three controls. Water quality data was collected weekly using a YSI water quality meter.*
Data source location	*International Institute for Sustainable Development – Experimental Lakes Area (Northern Ontario, Canada; 93°30'–94°00'W, 49°30'–49°45'N)*
Data accessibility	Repository name: my-GEOG717-repository Direct URL to data: https://github.com/claireestey/my-GEO712-repository Instructions for accessing these data: Raw data are located under the 'data_raw' folder. Details on the dataset are located under "Data Description" below.
Related research article	*none*

VALUE OF THE DATA

- This dataset is valuable as a need has been identified for increased study on the effects of benzalkonium chloride on aquatic biota since the onset of COVID-19.

- The majority of research on BACs are acute lab exposure studies, which lack the ability to capture environmental variability and complex ecological interactions that only an *in-situ* study can achieve.
- This dataset can be reused by other researchers to:
    - Perform an entire food web analysis (including biofilm, algae, benthic invertebrates, etc.)
    - Compare results of other experiments using a mesocosm design
    - Develop additional experiments that build on in-situ chronic BAC exposure, such as a whole lake addition experiment.

BACKGROUND

Quaternary ammonium compounds (QACs) are a group of high production volume chemicals known for their efficacy as antimicrobials, antistatic and softening agents, and emulsifiers[1]. Among QACs, benzalkonium chloride (BAC) is a potent antimicrobial currently listed as the number one active ingredient in disinfectants approved by the Government of Canada for use against the COVID-19 virus[2]. Consequently, BAC use has increased in industrial, clinical, and household settings since the onset of the pandemic[3]. Such ubiquitous usage has led to the continuous discharge of these compounds into surface waters primarily via wastewater treatment plant effluent, with surface water QAC concentrations being found to range from < 1 µg/L to ~100 µg/L globally[3]. Though the half-life of BAC in aqueous form is estimated to be around 5 to 7 days, it's perpetual input into freshwater systems creates pseudo-persistence, potentially exposing downstream aquatic biota[4]. A regression design was used to determine the target concentrations of BAC (20 ng/L, 112 ng/L, 632 ng/L, 3,556 ng/L, and 20,000 ng/L, plus three controls). These values cover both the range of concentrations that have been found in surface waters globally, as well as those that have been shown to have chronic effects on test organisms in laboratory studies.

DATA DESCRIPTION

Within the repository, the *data_raw* folder contains the five .csv files that make up this dataset. 240816_qac_main_logbook.csv is the master list of all samples that were taken as part of this project as well as the sample metadata (including sample type, sample ID, collection method, location, coordinates, date collected, and date entered). R_formatted_raw_counts.csv is the raw zooplankton community composition data as zooplankton per L. Within this file, the study day, day of year, sample code, and zooplankton group are recorded followed by the raw counts of zooplankton in each category. Treatments.csv is the key used to link which 'location' in the master list corresponds to which concentration of BAC, and therefore which sample came from which mesocosm enclosure. Similarly, taxon_codes.csv is the key to interpreting the short-formed zooplankton group used in the r_formatted_raw_counts.csv. Finally, ysi.csv contains the study day, treatment enclosure, and corresponding dissolved oxygen, pH, and chlorophyll concentration.

EXPERIMENTAL DESIGN, MATERIALS AND METHODS

Sample Collection

In June 2023, eight 2 m diameter, 1.75 m deep circular enclosures (Curry Industries) were deployed approximately 3 m apart on a sandy flat bar in the north basin of Lake 375 (Figure 1). Treatments were assigned randomly to the enclosures and followed a regression design with target concentrations of 20 ng/L, 112 ng/L, 632 ng/L, 3,556 ng/L, and 20,000 ng/L, plus three control enclosures (0 ng/L).

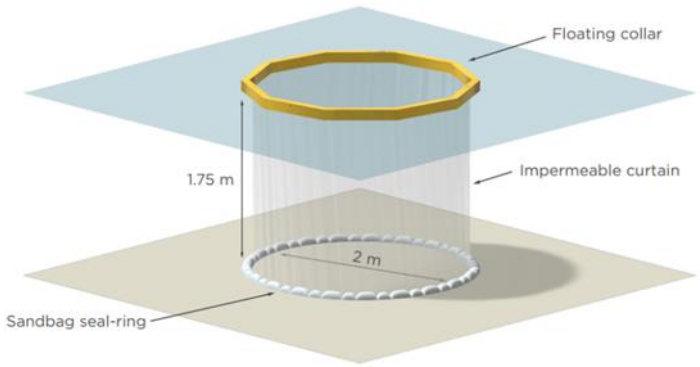

Figure 1. Schematic of mesocosm enclosure design (Curry Industries)

A technical mixture of BAC homologs with varying alkyl chain lengths (C10 to C18) was used to spike the enclosures, with BAC C12 and C14 making up most of the mixture (Toronto Research Chemicals). This mixture was dissolved and homogenized in methanol before being added to ensure proper dissolution in the water column. The enclosures were first dosed on June 22nd, 2023, and were spiked weekly for 16 weeks (except for September 28th). An additional 2 m diameter, 1 m deep, closed-bottom enclosure was deployed with tritium isotope (H_3) to determine the evaporative water loss occurring within the enclosures.

To determine the actual BAC concentration, dissipation rate (half-life), and composition of BAC homologs in the enclosures, grab samples of water were taken at 6 time points over the duration of the study; five times during the first week of additions (study days 0, 1, 2, 4, and 7), and once near the conclusion of the study (day 75). Water quality data, including total dissolved nitrogen and phosphorus (TDN and TDP), dissolved organic and inorganic carbon (DOC and DIC), and chlorophyll a were measured two days prior to the first addition, as well as on study days 12, 33, and 54 (integrated sampling of epi- and hypolimnion). Dissolved oxygen (DO) was monitored continuously in each enclosure throughout the study using a HOBO dissolved oxygen data logger. A YSI water quality meter was used to measure chlorophyll a, DO, pH, phycocyanin, and specific conductance weekly throughout the study.

Zooplankton samples were collected from each of the eight enclosures one day prior to the first BAC addition (June 21st; day 0), two weeks after the first addition, then every three weeks for the remainder of the study (study days 14, 35, 56, and 77). A 15 L Schindler-Patalas plankton trap lowered

to 0.5 m was used for all collections. Samples were filtered through 53 µm mesh and preserved in 5% sugar-formalin solution[5] after narcotization in methanol in the field for later laboratory analysis[6].

Laboratory and Statistical Analysis

Preserved zooplankton samples were prepared for analysis by rinsing though a 53 µm sieve using deionized (DI) water, then washed into a graduated vial and made up to a known volume. This volume depended on the visual density of the sample and was recorded. 1 mL subsamples were drawn up using a wide mouth pipette, deposited into a Bogorov counting chamber, and suspended in DI water for identification and counting.

Zooplankton were identified to species using light microscopy with the help of several keys [7, 8] (with the exceptions of *Bosmina sp.* and *Chydorus sp*., which were identified to genus). Stage CI to CIII copepodids were identified to order (Calanoida or Cyclopoida), but copepod nauplii were not. Adult copepods (CVI) were identified as male or female. The target number of adult and CIV to CV individuals was 300, though the entire sample was scanned for rare species even after this target was met. Abundance was calculated from raw counts as zooplankton per L using the following equation, where n is the raw count, K is the fraction of subsample counted, and V is the volume of water filtered through the trap:

$$zooplankton\ L^{-1} = nK^{-1}V^{-1}$$

Eggs were counted to determine reproductive rates of abundant zooplankton taxa and will be used to calculate the ratio of eggs per female[9], with loose eggs being distributed proportionally between abundant copepod taxa. Community diversity will be calculated using the Inverse Simpson Index (^2D), where S is the species richness, n_i is the number of individuals of species i, N is the total number of individuals of all species, and therefore $n_i/N = p_i$, the proportion of individuals of species i:

$$^2D = \frac{1}{\sum_{i=1}^{S}\left(\frac{n_i}{N}\right)^2}$$

LIMITATIONS

A limitation associated with this dataset is the variable density of individuals in zooplankton samples, with some samples containing thousands of individuals per litre, and others containing less than 10. Additionally, all zooplankton samples were collected during the day, contrary to the standard practice of sampling zooplankton at night due to their diel migration. Because of this, larger, predatory zooplankton such as *Mysis sp.* were not found in the samples though they are known to be present in the lake.

ETHICS STATEMENT

The authors have read and followed the ethical requirements for publication in *Data in Brief* and confirm that this work does not involve human subjects, animal experiments, or any data collection from social media platforms.

CRediT AUTHOR STATEMENT

Jose Luis Rodriguez: Conceptualization, methodology, validation, investigation, data curation.

Karen A. Kidd: Conceptualization, methodology, supervision.

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DECLARATION OF COMPETING INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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