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Data Article

Dataset describing biodegradation of individual polychlorinated biphenyl congeners (PCBs) by *Paraburkholderia xenovorans* LB400 in presence and absence of sediment slurry

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ABSTRACT

This dataset describes the biodegradation of polychlorinated biphenyl (PCB) congeners by *Paraburkholderia xenovorans* LB400 in absence and presence of PCB-contaminated sediment slurry, over time [1]. In absence of sediment, PCBs were extracted from aqueous bioreactors by liquid-liquid extraction (LLE) with hexane. In presence of sediment, the extraction method used was a modification of U.S. EPA Method 3545 [3]. Sediment slurry samples were extracted from bioreactors using pressurized fluid extraction (Accelerated Solvent Extractor; Dionex ASE-200) with equal parts acetone and hexane. GC–MS/MS triple quadrapole technology in multiple reaction monitoring mode (MRM) was used for identification and quantification of 209 PCBs as 174 chromatographic peaks. Samples were processed in batches of five along with one method blank per batch. All materials used in sample extraction had either been triple rinsed with solvent (methanol, acetone, and hexane) or combusted overnight at 450 °C to prevent background PCB

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contamination. Results from the method blanks were used to determine the limit of quantification (LOQ) as the upper limit of the 95% confidence interval (average mass plus two times the standard deviation). PCB congener masses were corrected for surrogate recoveries less than 100%. The PCB concentration dataset was dichotomized at the threshold of the congener specific LOQ. Concentrations of congeners below the LOQ were treated as zero. During analysis, PCB concentration data was filtered to include only congeners belonging to the commercial PCB mixture, Aroclor 1248. LOQ corrected data can inform future experimental design and be reused by other researchers for further analysis and / or interpretive insights.

Specifications Table

Subject	Environmental Science
Specific subject area	Environmental Engineering - Biodegradation of polychlorinated biphenyls (PCBs) by microorganisms (*Paraburkholderia xenovorans* LB400)
Type of data	Text file and spreadsheets
How data were acquired	Data were acquired using GC–MS/MS Triple Quadrapole Technology following PCB extraction and purification with accelerated solvent extraction (ASE) using a Dionex ASE-200 Instruments: • GC–MS/MS QQQ in multiple reaction monitoring mode (MRM) • Accelerated solvent extractor (ASE-200) Make and model and of the instruments used: • Agilent 7890A GC system, Agilent 7000 Triple Quad, Agilent 7693 autosampler • Dionex ASE-200
Data format	Mixed (raw and preprocessed)
Parameters for data collection	Extraction efficiency, reproducibility, and accuracy was assessed using surrogate standards, replicates of method blanks, development of quality control (QC) acceptance criteria, and analysis of standard reference materials. According to QC criteria, any sample having a recovery less than 50% was excluded from analysis. PCB congener masses were corrected for surrogate recoveries less than 100%.
Description of data collection	Samples were processed in batches of five along with one method blank per batch. Results from the method blanks were used to determine the limit of quantification (LOQ) as the upper limit of the 95% confidence interval (average mass plus two times the standard deviation). Percentage recoveries of surrogate standards were used to correct congener mass as follows: PCB14 recovery was used to correct PCB1 to PCB39, PCB65-d5 was used to correct PCB40 to PCB127 and PCB166 was used to correct PCB128 to PCB209 (sorted by IUPAC number).
Data source location	Institution: University of Iowa City/Town/Region: Iowa City, IA Country: United States of America Latitude and longitude (and GPS coordinates, if possible) for collected samples/data: The sediment used in creating this dataset was taken from a PCB-contaminated emergency overflow lagoon located in Altavista, VA (37°06′52″N, 79°16′21″W).

(*continued on next page*)

Data accessibility	Repository name: Iowa Research Online (IRO) Data identification number: 10.25820/data.006135 Direct URL to data: https://iro.uiowa.edu/discovery/fulldisplay/alma9984002165902771/01IOWA_INST:ResearchRepository The underlying data for this work [3] has been deposited in the Iowa Research Online (IRO) institutional data repository for future reuse under an Open Data Commons Attribution License (ODC-By). There are no registration or fee requirements to download the underlying dataset for this work. Instructions for accessing these data: 1. Visit https://ir.uiowa.edu/ 2. Search the title of the dataset or author names 3. Click on the hyperlink corresponding to the dataset 4. Download associated files
Related research article	Bako, C.M., Mattes, T.E., Marek, R.F., Hornbuckle, K.C., Schnoor, J.L., 2020. Dataset Describing Biodegradation of Individual Polychlorinated Biphenyl Congeners (PCBs) by Paraburkholderia xenovorans LB400 in presence and absence of sediment slurry. Iowa Res. Online V1. https://doi.org/10.25820/data.006135

Value of the Data

- These data represent the most detailed dataset, to date, of individual congener biodegradation by the well characterized PCB-degrading microorganism, *Paraburkholderia xenovorans* LB400.
- The data describe the biodegradation process by which LB400 preferentially biodegrades low molecular weight (LMW) congeners, over time, in presence and absence of PCB-contaminated sediment slurry.
- Researchers and practicing engineers will benefit from these data when making risk-based decisions regarding in situ remediation options as alternatives to traditional treatment technologies (such as environmental dredging) which are widely regarded as ecologically invasive and costly.
- This dataset may be used/reused to gain further insights and/or develop of PCB biodegradation experiments using microorganisms with or without LB400-type congener specificity.
- Data described in this article may better inform bioremediation/augmentation/stimulation strategies to decrease human exposure to PCBs.

1. Data Description

This dataset describes results from two experiments designed to assess the biodegradation of polychlorinated biphenyl (PCB) congeners by *Paraburkholderia xenovorans* LB400 in absence and presence of PCB-contaminated sediment slurry, over time [2]. The first lab-scale bioreactor experiment was conducted in absence of sediment. The bioreactors in the first experiment contained a mixture of analytical standards (AccuStandard Inc; New Haven CT) representing commercial PCB mixture Aroclor 1248. The raw data from the first experiment can be found in the spreadsheet file titled “LB400_Biodegradation_NoSed_2020–11–17.xlsx”.

The second lab-scale bioreactor experiment was conducted in presence of sediment. The bioreactors in the second experiment contained PCB-contaminated sediment gathered from a field site. No additional PCB congeners were added to the bioreactors in the second experiment. The raw data from the first experiment can be found in the spreadsheet file titled “LB400_Biodegradation_WithSed_2020–11–17.xlsx”. A list and description of the ‘sheets’ contained in both spreadsheet files can be found in the ‘ReadMe’ text file titled “LB400_Biodegradation_ReadMe_2020–12–03.txt”.

The dataset has been deposited in the Iowa Research Online (IRO) institutional data repository [1]. The dataset contains results of both lab-scale bioreactor experiments so that the data can be reused, and further interpretive insights can be made by other researchers. The 'ReadMe' text file describes the contents of each sheet in the data spreadsheets. The sheets labelled "Data Dictionary" in each data spreadsheet define all column headings, abbreviations, and variables used.

Measurements of PCB congeners were made using an Agilent GC–MS/MS Triple Quad ran in multiple reaction monitoring mode (MRM). PCB mass values (nanograms; ng) were calculated for all 209 congeners from 174 chromatograph peaks using the internal standard method.

2. Experimental Design, Materials and Methods

2.1. Bacterial strain and growth conditions

Paraburkholderia xenovorans LB400 was grown aerobically at 30 °C on a platform shaker in a 500 mL Erlenmeyer flask containing 250 mL of K1 medium and solid biphenyl crystal (5 mM; 0.19 g; Acros Organics) as a sole carbon and energy source until mid-exponential phase ($OD_{600} = 0.8$). Cells were harvested by centrifugation (5000 × g, 15 min), washed twice with sterile K1 medium, resuspended in K1 medium, and inoculated into bioreactors using a 1 mL pipette. The recipe for K1 medium can be found in the supplemental information.

2.2. Experimental design of PCB biodegradation assay without sediment

Bioreactors were 9 mL Pyrex® test tube with PTFE-lined screw caps [2]. Live-cell treatments and dead-cell controls were added to the bioreactors. First, 1 mL of K1 bacterial medium was transferred to the bioreactor and spiked with Aroclor 1248 in acetone (3 µL; 25 ng/mL final concentration). The Aroclor 1248 stock solution was created with analytical standard obtained from AccuStandard, Inc. (New Haven, CT) suspended in acetone (pesticide grade; Fisher Scientific). Aroclor 1248 stock solution (3 µL) was added to 1 mL K1 medium already inside the bioreactors using a 10 µL syringe for a final concentration of 25 ng/mL as Aroclor 1248. PCBs equilibrated with the aqueous phase by shaking on a platform shaker table at 150 rpm for 48 h prior to the addition of LB400 cells. The biodegradation reaction was started by adding 2 mL of live LB400 cells ($OD_{600} = 0.8$) suspended in K1 medium to the bioreactor. Dead-cell controls were inactivated by adding 60% perchloric acid (20 µL; final concentration 0.7%; Fisher Scientific). Time-zero samples were prepared to equal volume but did not contain LB400 cells. Bioreactors were incubated at room temperature (~25 °C) for one week on a platform shaker table at 150 rpm. All treatments were prepared in quintuplet ($n = 5$) but two samples were lost at $T = 48$ h due to a faulty equipment sensor which led to the complete evaporation of one sample each in the live and dead-cell treatments resulting in $n = 4$ at the 48 h time point.

2.3. Sediment homogenization and characterization

Sediment gathered from the field site was transferred to a 20gal drum and thoroughly homogenized for approximately 15 min using a mud mixer attached to a power drill before use in experiments.

2.4. PCB quantification

GC–MS/MS (Agilent 7890A GC system, Agilent 7000 Triple Quad, Agilent 7693 autosampler) in multiple reaction monitoring mode (MRM) was used for identification and

quantification of 209 PCBs as 174 chromatographic peaks. The GC was equipped with a Supelco SPB-Octyl capillary column (50% n-octyl, 50% methyl siloxane, 30 m × 0.25 mm ID, 0.25 µm film thicknesses) with helium as the carrier gas flowing at 0.75 mL/min and nitrogen/ argon as the collision gas. The GC operated in solvent vent injection mode at the following injection conditions: initial temperature 45 °C, initial time 0.06 min, ramp 600 °C/min to inlet temperature 325 °C at 4.4 psi. The GC oven temperature program was 45 °C for 2 min, 45 to 75 °C at 100 °C/min and hold for 5 min, 75 to 150 °C at 15 °C/min and hold for 1 min, 150 to 280 at 2.5 °C/min and final hold 5 min (total run time 70.86 min). The triple quadrupole MS electron ionization source was set to 260 °C. PCB mass values (nanograms; ng) were calculated for all 209 congeners from 174 chromatograph peaks using the internal standard method.

2.5. Quality assurance & quality control (QA/QC)

Extraction efficiency, reproducibility, and accuracy was assessed using surrogate standards, replicates of method blanks, development of QC acceptance criteria, and analysis of standard reference materials. Standard reference material purchased from the National Institute of Standards and Technology (NIST SRM 1944, New York, New Jersey Waterway sediment; Gaithersburg, MD, USA) was analyzed in quintuple. The mean percent difference between the measured and certified values (27 congeners) was 13% ± 14%. Mean and standard deviation percentage recoveries of PCB14, PCB65-d5 and PCB166 were 97 ± 1%, 94 ± 4% and 114 ± 4%, respectively. According to QC criteria, any sample having a recovery less than 50% was excluded from analysis. Percentage recoveries of surrogate standards were used to correct congener mass as follows: PCB14 recovery was used to correct PCB1 to PCB39, PCB65-d5 was used to correct PCB40 to PCB127 and PCB166 was used to correct PCB128 to PCB209 (sorted by IUPAC number). PCB congener masses were corrected for surrogate recoveries less than 100%. Samples were processed in batches of five along with one method blank per batch. All materials used in sample extraction had either been triple rinsed with solvent (methanol [optima grade, Fisher scientific], acetone [pesticide grade, Fisher Scientific], and hexane [pesticide grade, Fisher Scientific]) or combusted overnight at 450 °C to prevent background PCB contamination. Results from the method blanks were used to determine the limit of quantification (LOQ) as the upper limit of the 95% confidence interval (average mass plus two times the standard deviation).

2.6. Description of PCB extraction method in experiment without sediment

PCBs were extracted from the aqueous bioreactor using a liquid-liquid extraction (LLE) with an equal volume of hexane (3 mL; pesticide grade, Fisher Scientific) added to each bioreactor. Prior to extraction, the bioreactor was spiked with surrogate standards PCB 14 (50.81 ng; 3,5-dichlorobiphenyl), deuterated PCB 65-d5 (52.5 ng; 2,3,5,6-tetrachlorobiphenyl-d5, deuterated) and PCB166 (52.56 ng; 2,3,4,4′,5,6-hexachlorobiphenyl; Cambridge Isotope Laboratories, Inc.). The bioreactor was vortexed and centrifuged. The hexane layer containing the sample extract was transferred to a TurboVap (Biotage, Uppsala, Sweden) tube. The LLE process was repeated three times. The resulting volume of solvent containing the sample extract was concentrated to approximately 1 mL using a TurboVap II Concentration Workstation (Caliper Life Sciences).

The final hexane extract was passed through a Pasteur pipette filled with 0.1 g of combusted silica gel (70–230 Mesh, Fisher Scientific) and 1 g of acidified silica gel (2:1 silica gel:sulfuric acid by weight) and eluted with approximately 10 mL of hexane. Samples were concentrated to approximately 1 mL and transferred to a gas chromatography vial. The final sample was spiked with internal standards deuterated PCB 30-d5 (19.6 ng; 2,4,6- trichlorobiphenyl-2′,3′,4′,5′,6′-d5, deuterated) and PCB 204 (19.6 ng; 2,2′,3,4,4′,5,6,6′-octachlorobiphenyl; Cambridge Isotope Laboratories, Inc.).

2.7. Description of PCB extraction method in experiment with sediment

The sediment was not spiked with any additional PCB congeners. The biodegradation reaction was started by adding 2 mL of live LB400 cells ($OD_{600} = 0.8$) in K1 medium to the incubation vessel containing Aroclor 1248-contaminated sediment slurry (1 mL K1 medium with 0.3 g PCB-contaminated sediment). Dead-cell controls were inactivated by adding perchloric acid (20 µL; final concentration 0.7%). Cells were incubated at room temperature (~25 °C) for one month ($T = 28$ days) on a platform shaker table at 150 rpm. All treatments were performed in quintuplet ($n = 5$).

The analytical method employed for sample extraction is a modification of U.S. EPA Method 3545 [3]. Sediment slurry samples were extracted using pressurized fluid extraction (Accelerated Solvent Extractor; Dionex ASE-200) with equal parts acetone and hexane. At the time of sampling, contents of the bioreactor were poured into a mortar and pestle containing approximately 7 g combusted diatomaceous earth (ASE® Prep DE, Thermo Scientific/Dionex). The mass of sediment remaining in the bioreactor after pouring was determined gravimetrically. The diatomaceous earth containing the sample was ground to a fine powder and transferred to a 33 mL ASE-200 cell containing approximately 3 g silica gel sorbent. The sample was spiked with surrogate standards PCB 14 (50.81 ng; 3,5-dichlorobiphenyl), deuterated PCB 65-d5 (52.5 ng; 2,3,5,6-tetrachlorobiphenyl-d5, deuterated) and PCB166 (52.56 ng; 2,3,4,4′,5,6-hexachlorobiphenyl; Cambridge Isotope Laboratories, Inc.). The sample extract resulting from pressurized fluid extraction was concentrated within the collection vial to approximately 1 mL and transferred to a 15 mL Pyrex® test tube with PTFE-lined screw cap.

Polar interferences and other compounds were removed by extraction with 2 mL sulfuric acid (99% purity, certified ACS plus, Fisher Scientific). The final hexane extract was passed through a Pasteur pipette filled with 0.1 g of combusted silica gel and 1 g of acidified silica gel (2:1 silica gel:sulfuric acid by weight) and eluted with approximately 10 mL of hexane. Samples were concentrated to approximately 1 mL and transferred to a gas chromatography vial. The final sample was spiked with internal standards deuterated PCB 30-d5 (19.6 ng; 2,4,6- trichlorobiphenyl-2′,3′,4′,5′,6′-d5, deuterated) and PCB 204 (19.6 ng; 2,2′,3,4,4′,5,6,6′-octachlorobiphenyl; Cambridge Isotope Laboratories, Inc.).

All treatments were prepared in quintuplet ($n = 5$) but, due to surrogate recoveries below established QA/QC criteria in the time-zero measurement, two samples were excluded from the analysis, resulting in $n = 3$ at the time-zero time point. Additionally, one sample from the live cell treatment at the 1-month timepoint was excluded from analysis because it had low surrogate recoveries due to an instrumentation error during PCB extraction resulting in $n = 4$ at the one-month time point, for the live cell treatment.

CRediT Author Statement

Christian M. Bako: Conceptualization, data curation, formal analysis, investigation, methodology, validation, visualization, writing (original draft, reviewing, and editing); **Timothy E. Mattes:** Conceptualization, funding acquisition, methodology, project administration, resources, supervision, writing (reviewing and editing); **Rachel F. Marek:** Funding acquisition, methodology, project administration, resources, software, writing (review and editing); **Keri C. Hornbuckle:** Funding acquisition, project administration, resources, writing (review and editing); **Jerald L. Schnoor:** Conceptualization, funding acquisition, methodology, project administration, resources, supervision, writing (review and editing).

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have or could be perceived to have influenced the work reported in this article.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2021.106821.

References

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