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Data Article

Dataset for laboratory treatability experiment with activated carbon and bioamendments to enhance biodegradation of chlorinated ethenes

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ABSTRACT

This dataset describes the outcome of a laboratory trichloroethene (TCE) treatability experiment with liquid activated carbon and bioamendments. The treatability experiment included unamended microcosms, bioamended microcosms with a *Dehalococcoides* containing culture and electron donor, and bioamended microcosms including liquid activated carbon (PlumeStop®). Data were collected frequently over an 85-day experimental period. Data were collected for the following parameters: redox sensitive species, chlorinated ethenes, non-chlorinated end-products, electron donors, compound specific isotopes, specific bacteria and functional genes. The reductive dechlorination of TCE could be described by a carbon isotope enrichment factor (ε_C) of -7.1 ‰. In the amended systems, the degradation rates for the TCE degradation were 0.08–0.13 d^{-1} and 0.05–0.09 d^{-1} determined by concentrations and isotope fractionation, respectively. Dechlorination of cis-DCE was limited. This dataset assisted in identifying the impact of different bioamendments and activated carbon on biodegradation of

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chlorinated ethenes. The dataset is useful in optimising design and setup for future laboratory and field investigations. This study provides novel information on the effect of low dose liquid activated carbon on chlorinated ethenes degradation by applying isotopic and microbial techniques, and by linking the outcome to a field case study. The data presented in this article are related to the research article "Assessment of chlorinated ethenes degradation after field scale injection of activated carbon and bioamendments: Application of isotopic and microbial analyses" (Ottosen et al., 2021).

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Specifications Table

Subject	Environmental Engineering
Specific subject area	Soil and groundwater pollution
Type of data	Tables and figures
How data were acquired	• Gas Chromatography Mass Spectrometry (GC-MS) • Gas Chromatography with Flame Ionization Detector (GC-FID) • Gas chromatography coupled to an isotope ratio mass spectrometer by a combustion interface (GC-C-IRMS) • Ion Chromatography (IC) • Inductively Coupled Plasma with Optical Emission Spectrometry (ICP-OES) • Quantitative Polymerase chain reaction (qPCR)
Data format	Raw and analysed
Parameters for data collection	The laboratory treatability experiment included: • UnAmended microcosms (UA), duplicates • BIOamended microcosms (BIO), duplicates • PlumeStop and BIOamended microcosms (PSBIO), triplicates The seven microcosms were prepared with groundwater and aquifer material, and maintained at groundwater temperature (10°C).
Description of data collection	The microcosms consisted of three compartments: groundwater, gas and sediment. Aqueous and gas samples were analysed frequently. The monitoring procedure was divided into two parts. The first part comprised the first 29 days with frequent sampling, at the end of this part three of the seven microcosms were sacrificed (UA_2, BIO_1, PSBIO_3). Therefore, the second part of the experiment included four microcosms and the sampling frequency was lower. The length of the experiment including both parts was 85 days.
Data source location	Technical University of Denmark, Department of Environmental Engineering, Lyngby, Denmark
Data accessibility	With the article
Related research article	The data article is related to the following research article: Ottosen, C.B., Bjerg, P.L., Hunkeler, D., Zimmermann, J., Tuxen, N., Harrekilde, D., Bennedsen, L., Leonard, G., Brabæk, L., Kristensen, I.L. and Broholm, M.M., 2021. Assessment of chlorinated ethenes degradation after field scale injection of activated carbon and bioamendments: Application of isotopic and microbial analyses. Journal of Contaminant Hydrology, 240, 103794. https://doi.org/10.1016/j.jconhyd.2021.103794.

Value of the Data

- The data provide knowledge on the influence of low concentrations of liquid activated carbon on biodegradation of chlorinated ethenes, which is relevant information in the application of activated carbon as a remedy for groundwater contamination.

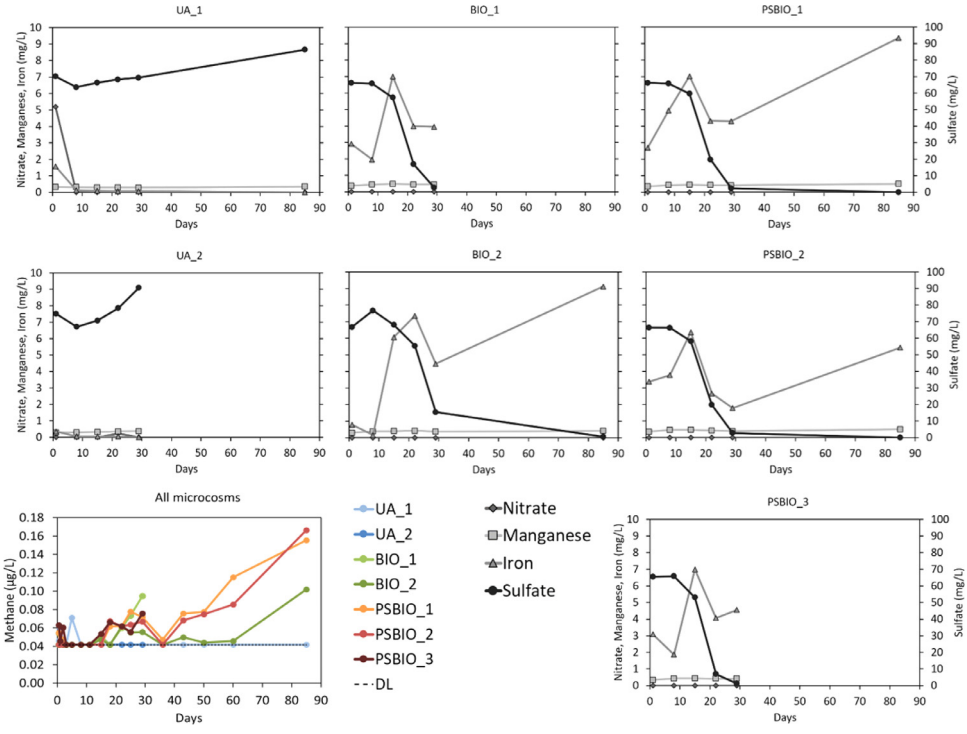

Fig. 1. Development in redox sensitive parameters in the different microcosms. Methane was measured in the headspace and converted to aqueous concentrations. The raw data are provided in Tables S1, S2.

- The data are helpful for professionals in order to comprehend and monitor processes at field scale remediation.
- The data provide insights on how the design and experimental setup can be optimised in future laboratory and field projects.

1. Data Description

In this article a collection of experimental results are provided for the three different types of microcosms. Information on the experimental design is provided subsequent to the results. The development in redox sensitive parameters (nitrate, manganese, dissolved iron, sulfate and methane) are provided in Fig. 1 (raw data in Tables S1,S2). The concentrations of volatile fatty acids, measured by the end of the experiment at day 85, are presented in Table 1. The

Table 1
Concentration (mg/L) of volatile fatty acids in the microcosms by the last sampling round at 85 days. The method quantification limits were 17 mg/L for acetic acid, 8.9 mg/L for propionic acid, 5.0 mg/L for iso-butyric acid, 4.7 mg/L for butyric acid and valeric acid, and 4.5 mg/L for iso-valeric acid.

	Acetic acid	Propionic acid	Iso-butyric acid	Butyric acid	iso-valerid acid	Valeric acid
UA_1	196	16.1	<QL	<QL	<QL	<QL
BIO_2	350	254	<QL	<QL	<QL	<QL
PSBIO_1	614	577	<QL	<QL	<QL	<QL
PSBIO_2	241	217	<QL	<QL	<QL	<QL

Table 2
Abundance (cells/mL) of specific bacteria and functional genes in microcosms selected for analysis and the culture. For *Dehalococcoides* (DHC) and the related functional genes *tceA, bvcA* and *vcrA* the detection limits were in the range of 7.0E + 00 to 8.3E + 01 cells/mL. For *Dehalogenimonas* (DHG) and the related functional gene *cerA* the detection limits were in the range of 7.0E + 01 to 8.3E + 02 cells/mL. The abundances of these biomarkers were below the detection limits in the well, where the groundwater for the microcosms was collected.

	BIO_1 (day 29)	BIO_2 (day 85)	PSBIO_3 (day 29)	PSBIO_1 (day 85)	Culture (day 29)
DHC	7.6E+02	<DL	9.1E+02	3.1E+03	1.8E+08
tceA	1.1E+03	<DL	5.4E+02	1.7E+03	6.4E+07
bvcA	<DL	<DL	<DL	1.1E+02	<DL
vcrA	3.1E+02	<DL	2.1E+02	7.3E+02	2.7E+07
DHG	<DL	<DL	<DL	<DL	<DL
cerA	<DL	<DL	<DL	<DL	<DL

Table 3
$\delta^{13}C$ values (‰) for TCE and cis-DCE in the aqueous phase for all microcosms. The standard deviation for the analysis was 0.2 ‰.

	UA_1	UA_2	BIO_1		BIO_2		PSBIO_1		PSBIO_2		PSBIO_3	
Day	TCE	TCE	TCE	cis-DCE	TCE	cis-DCE	TCE	cis-DCE	TCE	cis-DCE	TCE	cis-DCE
0.5	-27.9	-27.8	-27.7		-27.9		-27.0		-26.9		-26.3	
1	-27.5	-27.5	-27.6		-27.3		-26.8		-26.6		-26.4	
4	-27.3	-26.9	-27.2		-27.1		-26.3		-25.9		-25.9	
8	-27.2	-26.5	-26.8		-26.7		-26.7		-25.9		-25.7	
15	-26.7	-26.2	-26.4		-26.3		-26.2		-26.3		-25.7	-37.3
22	-26.7	-25.8	-23.5	-35.8	-26.3		-23.9	-36.1	-21.3	-37.0	-22.4	-34.7
29	-26.2	-26.0		-29.3	-25.4	-37.6		-29.0	-18.0	-31.9		-27.9
60	-26.3					-27.2		-27.0		-27.5		
85	-26.4					-26.8		-26.7		-27.1		

Table 4
Degradation rates and corresponding half-lives, $T_{½}$, for the reductive dechlorination of TCE determined by isotope fractionation (*I*) (Eq. (1)) and concentrations (*C*) (Fig. S2).

	BIO_1		PSBIO_1		PSBIO_2		PSBIO_3	
Method	I	C	I	C	I	C	I	C
Period (d)	15-22	18-25	15-22	18-25	15-29	18-29	15-22	18-25
Rate (d^{-1})	0.06	0.09	0.05	0.09	0.09	0.08	0.07	0.13
$T_{½}$ (d)	12	8	15	8	8	9	10	5

microbial abundances, measured by the end of the two experimental parts, at day 29 and 85, are presented in Table 2. The development in TCE, cis-1,2-dichloroethene (cis-DCE) and vinyl chloride (VC) aqueous concentrations are presented in Fig. 2 (raw data in Tables S3–S5). The non-chlorinated end-products ethene, ethane and acetylene were not detected. Further, a mass balance for TCE in the unamended microcosms, where sampling was the only mass removal process, is presented in Fig. 3. In the mass balance figure, estimated concentrations are plotted against the actual measured concentrations, where the first assumes immediate equilibrium. The mass balance estimated a TCE aqueous concentrations decrease of around 12% in the unamended microcosms by the end of the experiment (85 days). The aqueous carbon isotope values for TCE and cis-DCE for all microcosms are presented in Table 3. Finally, degradation rates and the corresponding half-lives, estimated from isotope and concentration results, are presented in Table 4.

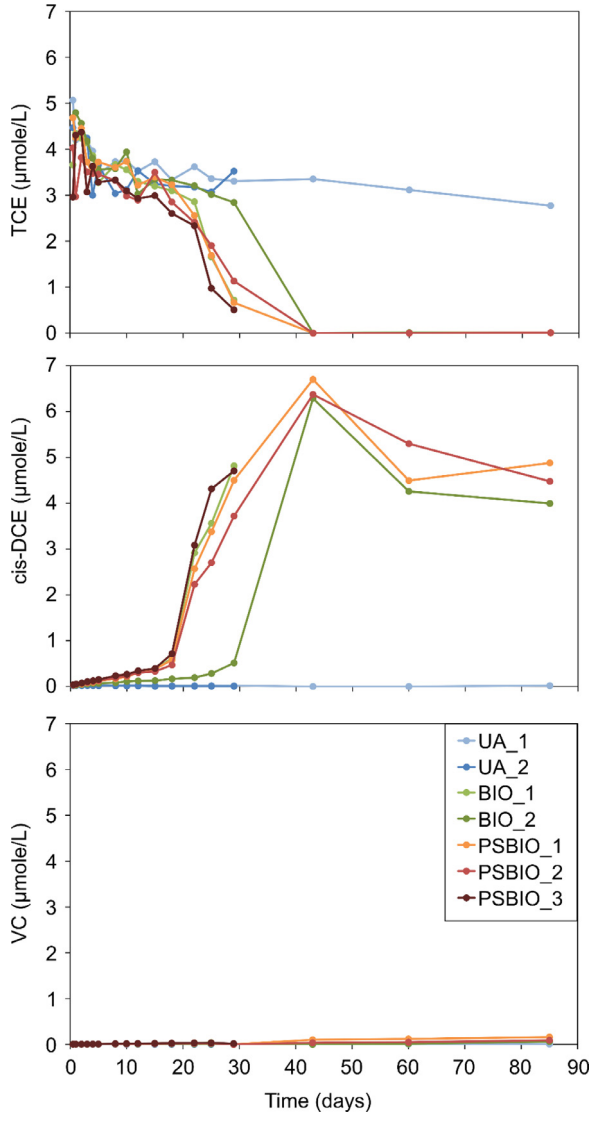

Fig. 2. Development in aqueous concentrations of TCE, cis-DCE (measurements at day 43 are analytical outliers) and VC. The raw data are provided in Tables S3–S5.

2. Experimental Design, Materials, and Methods

2.1. Collection of materials

Groundwater and aquifer material were collected at the field site, in an industrial area (Vassingerød, Denmark) described in [1], to represent realistic conditions. Prior to groundwater sampling, the groundwater well was purged until the field parameters (electrical conductivity (EC), pH, oxygen concentration (O_2) and temperature (T)) were stable. The groundwater was collected in 1.1 L autoclaved glass flasks. During sampling the flasks were flushed with nitrogen

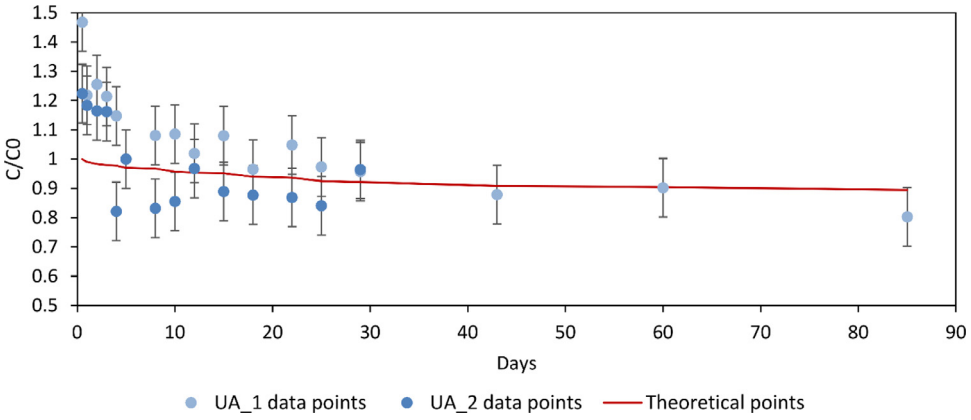

Fig. 3. Measured water concentrations for TCE in the unamended microcosms against the estimated water concentrations (see Eqs. (3)–(5)) based on mass balance calculations (normalized with the assumed equilibrium concentration from day 5).

till there was no headspace. The groundwater was collected shortly before the start of the laboratory experiment. The aquifer material was collected at a similar depth as the groundwater, with a Geoprobe® rig applying a sediment core sampler system. The cores were capped immediately after sampling and placed in aluminium bags flushed with nitrogen. The materials were stored cold until use.

2.2. Setup of laboratory microcosms

An overview of the setup for the different microcosms (UnAmended (UA), BIOamended (BIO), and PlumeStop and BIOamended (PSBIO)) is provided in Table 5. The microcosms were prepared in infusion glass flasks (1100 mL) with thick rubber stoppers. The sediment was homogenised and added to the infusion flasks inside an anaerobic glove box. The groundwater was added to the infusion flasks with a dispenser on a sterile bench. While adding the groundwater, the flasks were continuously flushed with a N_2/CO_2 mixture (80:20) to remove H_2 from in the anaerobic box atmosphere.

At the start of the experiment, 10 days after addition of the field materials, the remaining materials were added through the rubber stopper. A stock solution with an initial concentration of ~3.5 mg/L TCE was prepared, and added to all microcosms, resulting in an expected initial aqueous concentration of ~580 µg/L for TCE. Subsequently, sodium lactate was added to the amended microcosms. Sodium lactate was used as a donor, as it is an immediately available donor, which was ideal for the length of the experiment. To avoid donor depletion, sodium lactate was added in excess by three to four times the required level for reduction of

Table 5
Overview of the setup for the three different types of microcosms.

	Replicates	Sediment	Groundwater	TCE stock	Donor	Culture	Liquid activated carbon
UnAmended (UA)	2	300 g	500 mL	100 mL	-	-	-
BIOamended (BIO)	2	300 g	500 mL	100 mL	0.75 mL	65 µL	-
PlumeStop and BIOamended (PSBIO)	3	300 g	500 mL	100 mL	0.75 mL	65 µL	5 mL (0.04% AC solution)

Table 6
Sampling scheme for the experiment. *X*: all microcosms sampled and Y: selected microcosms sampled at that particular time. Please note that due to the sacrifice of three microcosms during the experiment, the two parts have a different number of microcosms monitored, and the notation relates to the individual parts.

	Day	CE *water*	Redox *water*	MEAE *gas*	Isotopes *water*	Microbial *water*	VFA *water*
First part (7 microcosms:	½	X	X	X	X		
UA_1, UA_2, BIO_1,	1	X		X	X		
BIO_2, PSBIO_1, PSBIO_2	2	X		X			
and PSBIO_3)	3	X		X			
	4	X			X		
	5	X		X			
	8	X	X	X	X		
	10	X					
	11			X			
	12	X					
	15	X	X	X	X		
	18	X		X			
	22	X	X	X	X		
	25	X		X			
	29	X	X	X	X	Y: UA_2, BIO_1, PSBIO_3	
Second part (4 microcosms:	36			X			
UA_1, BIO_2, PSBIO_1	43	X		X			
and PSBIO_2)	50			X			
	60	X		X	X		
	85	X	X	X	X	X	X

CE = chlorinated ethenes. MEAE = methane, ethene, acetylene and ethane. VFA = volatile fatty acids.

the redox species and for complete reductive dechlorination. A *Dehalococcoides* containing culture (Bio-Dechlor Inoculum® plus, BDI+) with a cell count of 10^8 cells/mL, was added to the amended microcosms, resulting in an expected initial count of 10^4 cells/mL. Liquid activated carbon (PlumeStop®, 4% AC content) was diluted with anaerobic groundwater (1:100) and 5 mL (~2 mg) colloidal activated carbon was added to selected microcosms. The culture and the liquid activated carbon were supplied by Regenesis, USA. No other nutrients or bio-stimulants were added to the microcosms.

2.3. Monitoring and sampling procedure

The microcosms were stored upside down at 10 °C, and were shaken by hand before and after sampling. The sampling scheme for the experiment is presented in Table 6. After each sampling, the microcosms were compensated for the extracted volume with nitrogen gas. The chlorinated ethenes were analyzed by GC–MS headspace analysis. The cations were analysed by ICP-OES and the anions by IC. Methane, ethene, acetylene and ethane (MEAE) were analyzed by GC-FID. The carbon isotopes were analyzed by GC-C-IRMS and the biomarkers by qPCR as described in [1]. The different samples were stored and conserved in different ways to preserve the individual parameters optimally (Table S6).

2.4. Data treatment

The isotope values were used to quantify the degradation by Eq. (1) [2].

$$k = \frac{-\left(\frac{1000}{\varepsilon}\right) \cdot \ln\left(\frac{\delta^{13}C/1000+1}{\delta^{13}C_0/1000+1}\right)}{t} \quad (1)$$

Where k is the degradation rate and t is the time between the isotope sampling events. The enrichment factor, ε, was determined following the Rayleigh equation [3], see Eq. (2).

$$\left(\ln\left(\delta^{13}C_t + 1000\right) - \ln\left(\delta^{13}C_0 + 1000\right)\right) \cdot 1000 = \varepsilon \cdot \ln(f) \tag{2}$$

Where $\delta^{13}C_t$ and $\delta^{13}C_0$ are the carbon isotope ratios in ‰ and f is the fraction of substrate (C_t/C_o) remaining after time t. A double logarithmic plot (Fig. S1) was used to find the enrichment factor of -7.1 ‰.

A mass balance was set up for the unamended microcosms, Eq. (3). The known input mass, M_T, was converted to a concentration in water, C_W, Eq. (4). For each sampling step, where mass was removed, a new M_T applies, Eq. (5), which was converted to a new water concentration. This way a stepwise curve could be made over the expected concentration trend for TCE (Fig. 3).

$$\begin{aligned} M_T &= C_W * V_W + C_S * M_S + C_A * V_A \\ M_T &= C_W * V_W + K_D * C_W * M_S + K_H * C_W * V_A \\ M_T &= C_W * (V_W + K_D * M_S + K_H * V_A) \end{aligned} \tag{3}$$

$$C_W = M_T / \left(V_W + K_D * M_S + K_H * V_A\right) \tag{4}$$

$$M_{T,NEW} = M_{T,BEFORE} - \left(C_W * V_{W,out}\right) - \left(C_W * K_H * V_{A,OUT}\right) \tag{5}$$

Where V_W is the water volume in the system, C_S is the sediment concentration, M_S is the sediment mass in the system, C_A is the air concentration, V_A is the volume of headspace in the system, K_D is the distribution coefficient between sediment and water and K_H is the Henry's law constant.

CRediT Author Statement

Cecilie B. Ottosen: Conceptualization, Methodology, Investigation, Writing - Original Draft, Visualization, Writing - Review & Editing; **Melissa Skou:** Conceptualization, Methodology, Investigation, Visualization, Writing - Review & Editing; **Emilie Sammali:** Methodology, Investigation, Visualization, Writing - Review & Editing; **Jeremy Zimmermann:** Investigation, Writing - Review & Editing; **Daniel Hunkeler:** Supervision, Writing - Review & Editing; **Poul L. Bjerg:** Supervision, Writing - Review & Editing; **Mette M. Broholm:** Conceptualization, Methodology, Supervision, Writing - Review & 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.2021.107291.

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