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Mechanistic Study on Microbial Degradation and Transformation of Hexachloro-1,3-butadiene under Anoxic Conditions

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ABSTRACT

Hexachlorotrietadiene (HCBD) is a volatile organohalogen commonly found in the environments due to its past applications in products such as transformers, hydraulic oil and heat transfer liquid. Despite regulations prohibiting its intentional production by some countries (e.g., the U.S., Canada, several Europe countries), HCBD continues to be produced and released unintentionally through manufacturing processes of other chlorinated compounds and improper waste disposal. In the year 2015 and 2017, it was listed under Annex A and C of the Stockholm Convention on Persistent Organic Pollutants, respectively. Recently, this pollutant was strictly regulated by the Chinese government in 2023. Studies focusing on the HCBD degradation under oxic conditions or co-metabolic transformation have been reported; nevertheless, research on the environmental fate and transformation of HCBD under the anoxic conditions is still rare. This research project was aimed at improving our understanding of HCBD reductive dechlorination by unraveling the transformation pathway under the anoxic conditions. The main results of this study were as follows: the culture capable of anaerobic transformation of HCBD was enriched, and the anaerobic complete transformation pathway of HCBD was revealed. Microcosms inoculated with Xi river freshwater sediment samples were established with amendments of HCBD as electron acceptor and lactate as carbon source and electron donor. In the microcosms amended with HCBD, 62.5 μmol of HCBD was dechlorinated within 8 months. The daughter products of HCBD reductive dechlorination was identified and monitored by ISQ-LT gas chromatography-mass spectrometry (GC-MS), including (E)-1,1,2,3,4-PCBD (Pentachlorotrietadiene) , (3Z)-1,1,3,4-TeCBD (Techachlorotrietadiene), (E)-1,2,3-TCBD (Trichlorotrietadiene), (E,E)-1,4-DCBD (Dichlorotrietadiene) and 2-CBD (Chlorotrietadiene). In the microcosms amended with HCBD and trichloroethylene (TCE), 62.5 μmol of HCBD and 82 μmol TCE were transformed and dechlorinated also within 8 months; the daughter products of HCBD reductive dechlorination were the same as previously mentioned, and 78.5 μmol ethylene was the end product of TCE reductive dechlorination. Therefore, it is assumed that the pathway for HCBD reductive dechlorination via hydrogenolysis was proposed: HCBD→(E)-1,1,2,3,4-PCBD → (3Z)-1,1,3,4-TeCBD → (E)-1,2,3-TCBD → (E,E)-1,4-DCBD → 2-CBD. To sum up, through monitoring the reductive dechlorination process of hexachloro-1,3-butadiene in this research, the transformation products of the reductive dechlorination of hexachloro-1,3-butadiene were identified, a new anaerobic microbial transformation pathway of hexachloro-1,3-butadiene was analyzed, and our understanding of the reductive dechlorination of hexachloro-1,3-butadiene and its environmental fate was enhanced.

KEYWORDS

Hexachlorotrietadiene; Reductive Dechlorination; Hydrolysis; Anaerobes; Reductive Dehalogenas.

1. BACKGROUND

Hexachloro-1,3-butadiene, as a synthetic organic chloride that does not exist in nature, is a colorless liquid with a similar smell of pine gas(1,2,3,4). It is difficult to dissolve in water at room temperature, and easy to dissolve in organic solvents such as ethanol, diethyl ether and dichloromethane. Persistent organic pollutants (POPs) are difficult to remove in the environment due to their high lipid solubility, obvious bioaccumulative amplification, high toxicity and long-term migration (5). In May 2001, the United Nations Environment Programme hosted the signing of the Stockholm Convention on Persistent Organic Pollutants by more than 100 governments around the world, which entered into force for my country in 2004 (6). Hexachloro-1,3-butadiene, as an emerging POPs, was listed in Annex A (http://chm.pops.int/Countries/StatusofRatifications/Amendmentstoannexes/tabid/3486/Default.aspx) for intentional production control in 2015 and in Annex C (http://chm.pops.int/TheConvention/ConferenceoftheParties/Meetings/COP8/tabid/ 5309/Default.aspx) for unintentional production emissions by the Convention in 2017. In the latest "List of new Pollutants under Key Control" published by the Chinese government in 2023, as a new pollutant, hexachloro-1,3-butadiene has been adopted "Prohibition, Restriction, Discharge Limit" and other four environmental risk control measures (http://www.gov.cn/zhengce/2022-12/30/content_5734728.htm).

As a synthetic halogenated hydrocarbon, hexachloro-1,3-butadiene has been widely used in industrial and agricultural fields in the past, such as as raw materials for the production of aluminum and graphite rods, organic polymer solvents, organic gas cleaning agents, heat conductors, pesticides, herbicides, transformer oil or fumigants in vineyards, etc., becoming a common volatile organic pollutant in groundwater environment(7,8).There are two main sources of hexachloro-1,3-butadiene in the environment: one is as a by-product of chlorinated hydrocarbons (carbon tetrachloride, tetrachloroethylene, trichloroethylene, etc.) manufacturing and electrolytic magnesium processes, and the other is improper discharge during cement manufacturing and waste combustion(9).Data from the United Nations Environment Programme show that from 1975 to 2011, concentrations in the environment in the region of the United Nations Economic Commission(UNECE) for Europe have decreased, with emissions of hexachloro-1,3-butadiene falling from 50,000 kg to 1,064 kg(10). Compared with other countries, hexachlorin-1, 3-butadiene emissions in China have increased, from 60.8 tons in 1992 to 2,871.5 tons in 2016, making China one of the major emitators(1).

Hexachloro-1,3-butadiene, which is normally released into the environment, can enter the body of organisms through ingestion, respiration, and direct skin contact, and can be used as kidney toxins in rodents, aquatic animals, mammals, and other species, causing degradation, necrosis, and regeneration of renal tubular epithelial cells. In addition to nephrotoxicity, hexachloro-1,3-butadiene is mildly hepatotoxic, causing central nervous system lesions, genetic mutations in germ cells, and affecting peripheral lymphocyte function.Based on toxicological studies, the Environmental Protection Agency (USEPA) classifies it as a Class C probable human carcinogen (11).

In recent years, the research on hexachloro-1,3-butadiene at home and abroad mainly focuses on the source, distribution, toxicity and detection methods, but there are few reports on the degradation and transformation of hexachloro-1,3-butadiene. The research of degradation and transformation in environment mainly focuses on biodegradation, photodegradation and other physicochemical degradation. This study focused on the microbial degradation and transformation pathway and mechanism of hexachloro-1,3-butadiene. By using the sediment of Xi River in Shenyang as the inoculation source, the microspace culture system for anaerobic conversion of hexachloro-1,3-butadiene was established, the intermediate metabolites of hexachloro-1,3-butadiene were identified, and the anaerobic conversion pathway of hexachloro-1,3-butadiene was elucidated. This study improves the understanding of the pathways and mechanisms of dechlorination in the anaerobic reduction of hexachloro-1,3-butadiene, and enriches the microbial resources for the anaerobic transformation of hexachloro-1,3-butadiene.

2. MATERIALS AND METHODS

The environmental samples used in this experiment are sediments from Xi River (N 41°37 '4 ", E 123°3' 13 ") in Shenyang, Liaoning Province (Figure 1). In the Xi River area, 22.18 km of water was severely black and smelly. The water quality monitoring results showed that the chemical oxygen demand (COD), biochemical oxygen demand (BOD), ammonia nitrogen and total phosphorus (TP) indexes of the fine river were lower than the standard value of Class V water quality, which was severely polluted (12,13).Before sampling, the shovel was sterilized with alcohol, the bottom mud was excavated with the shovel, the bottom mud was quickly loaded into the No. 12 ziploc bag, and the ziploc bag was squeezed to discharge the air in the bag, and then it was sealed to maintain an anaerobic environment. The ziplock bag marked with longitude and latitude coordinate information was stored in an ice box and stored in the refrigerator at 4 ℃ after being transported back to the laboratory.

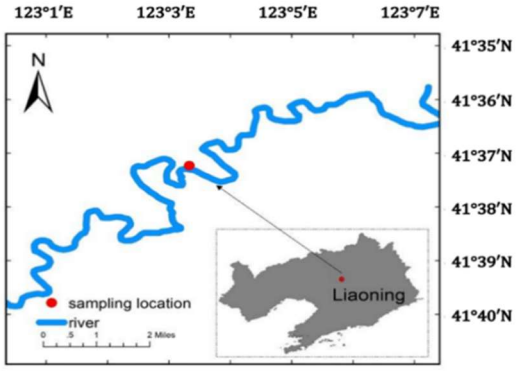


Figure 1. Sampling location of Xi River sediment

The basic inorganic salt (DCB-1) anaerobic culture medium (14) was prepared according to the method of Löffler et al., and ultra-pure water and basic mother liquor were added to the three-neck round-bottom flask according to the actual required dosage. A 5 L three-neck round-bottom flask was used and 2 L DCB-1 anaerobic culture base was configured. The aluminum cover of the anaerobic medium was opened on a super-clean work table, and then placed in an anaerobic glove box overnight with a sample of Xi River sediment preserved at 4 ℃, a sampling spoon and a balance cleaned by ultrasound, to remove oxygen. 5 g Xi River sediment samples (fresh weight) were taken in the anaerobic glove box for inoculation, and then removed from the anaerobic glove box. Carbon source, electron donor, electron acceptor and nutrients were added to the medium.

In this study, the experimental group and the control group were set up (negative control). The experimental group were treated with (1) 5 mM lactic acid as electron donor and carbon source, 10 μL hexachloro-1,3-butadiene as electron acceptor, and 0.1 mL Wolin complex vitamin as nutrient; (2) 5 mM lactic acid as electron donor and carbon source, 10 μL hexachloro-1,3-butadiene and 8 μL trichloroethylene as electron acceptor, 0.1 mL Wolin complex vitamin as nutrient. In the negative control group, the medium added with mud was autoclaved under the same sterilization conditions as the inorganic salt medium, and other components of the same concentration were added after sterilization and cooling. The above experimental groups were treated with four parallel sets respectively, and the information was marked and put into a constant temperature incubator at 30 ℃.

The degradation and transformation of hexachloro-1,3-butadiene and trichloroethylene were monitored regularly. When the substrate electron acceptor was depleted and the product did not change significantly, the microcosm culture system was transferred to the anaerobic medium DCB-1 with the same composition by 5 % (V/V) volume transfer, and the culture conditions were unchanged.

All bacteria-free syringes involved in the operation must be washed with nitrogen first to prevent oxygen from entering and maintain the anaerobic nature of the medium to the greatest extent.

The detection of substances involved in this study mainly included hexachloro-1,3-butadiene, trichloroethylene and their dechlorination products. Qualitative measurements of hexachloro-1,3-butadiene and their daughter products were performed using ISQ-LT purse-catch-Gas chromatography-mass spectrometry (GC-MS) using TRACE 1300 series gas chromatography systems. The volatile sample (10 μL) was injected at a separation ratio of 1:30. Trichloroethylene and its degradation and conversion products, cis-dichloroethylene, monovinyl chloride and ethylene, were qualitatively and quantitatively determined using a gas chromatograph (Agilent 7890B) equipped with a serial flame ionization detector (FID) and a DB-624 capillary column. The injection port temperature was maintained at 200 ℃ and the detector temperature was 300 ℃ with high-purity helium as the carrier gas.

In order to maintain the reliability of the experimental results, the standard curves of trichloroethylene and its degradation and transformation products cis-dichloroethylene, monovinyl chloride and ethylene were drawn. The specific operation was as follows: ultra-pure water (80 mL) with the same volume as the medium was added into the 120 mL clean serum vial, and the standard substance was added with a microinjection needle at a certain concentration gradient (2 μL,4 μL, 6 μL,8 μL,10 μL or 0.5 mL,1.0 mL,1.5 mL,2.0 mL,2.5 mL）.After the standard substance was dissolved with an ultrasonic cleaner, it was placed in a 30 ℃ constant temperature incubator overnight. Three parallels were set for each gradient, and a standard curve was drawn as shown in Figure 2.

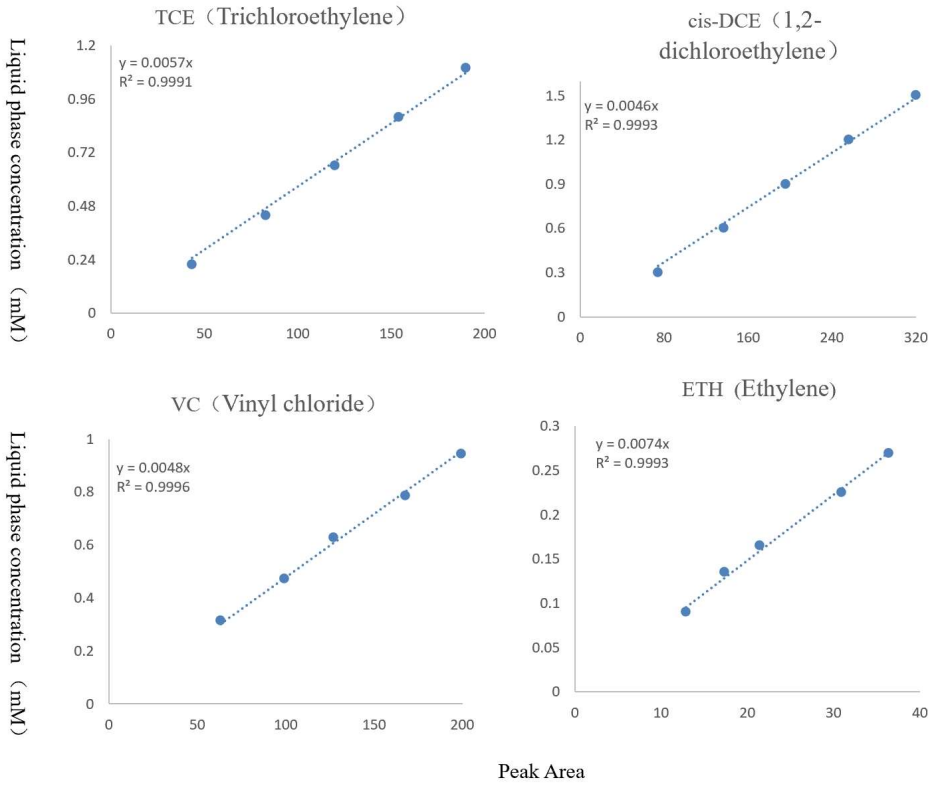


Figure 2. Standard curves of Trichloroethylene(TCE), cis-Dichloroethylene(cis-DCE), Vinyl chloride(VC) and Ethylene(ETH)

3. RESULTS AND DISCUSSION

Two different culture conditions were set up in this experiment, respectively: (1) hexachloro-1,3-butadiene as electron donor, lactic acid as carbon source and electron donor; (2) hexachloro-1,3-butadiene and trichloroethylene as electron donor, lactic acid as carbon source and electron donor treatment group. Due to the unknown degradation products and the lack of standard products, in order to identify the anaerobic conversion products of hexachloro-1,3-butadiene, ISQ-LT purse-catch-gas chromatography-mass spectrometry (GC-MS) was used to identify the conversion products in the culture system. In the microcosmic culture system with hexachloro-1,3-butadiene as electron donor, 62.5 μmol of hexachloro-1,3-butadiene could be completely converted within eight months. In addition to hexachloro-1,3-butadiene with chromatographic retention time of 21.50 min, two substances with chromatographic retention time of 20.86 min and 20.14 min were also observed at 30 days of culture. After 30 days of continuous culture, three substances with retention time of 21.50 min, 20.86 min and 20.14 min were still observed in the system, and two new substances with retention time of 20.03 min and 17.19 min were also observed. After the monitoring every 30 days, the above five substances could still be observed in the microuniverse culture system with hexachloro-1,3-butadiene as electron donors at 90-210 days, and the composition of the substances did not change, and no new substances were produced. At 210 days, the chromatographic retention time of 5.64 min was detected. At 240 days of culture, substances with chromatographic retention time of 20.86 min and 21.50 min were not observed, and the other 4 substances could be observed. After that, they were observed every 30 days, the composition remained stable, no new substances with peak emergence time were observed, and no substances with chromatographic retention time of 5.64 min, 17.19 min, 20.03 min and 20.14 min were found to disappear.

The culture medium inoculated with sediment was sterilized and the same components as the microspace culture system in which hexachloro-1,3-butadiene was used as the electron donor were added as the negative control. The total ion flow chromatogram extracted by GC-MS was shown in Figure 3. Only hexachloro-1,3-butadiene with chromatographic retention time of 21.50 min was detected. The total ion flow chromatogram of hexachloro-1,3-butadiene anaerobic conversion system extracted by GC-MS at the culture stage was shown in Figure 4. The gas chromatogram (A), mass spectrometry (B) and structural formula of the ion flow captured and extracted from substances 1 to 6 by GC-MS were shown in Figure 5-10. The specific analysis results of each substance are as follows:

The chromatographic retention time of substance 1 was 5.64 min, the m/z value of parent ion was 88, and the m/z values of characteristic fragment ions were 53 and 88, respectively. By comparing with the proton database, substance 1 was determined to be monochlorobutadiene (2-CBD), the end product of dechlorination by anoxylative reduction of hexachloro-1,3-butadiene. The retention time of substance 2 was 17.19 min, the m/z value of parent ion was 122, and the m/z values of characteristic fragment ions were 51, 87 and 122, respectively. Substance 2 was confirmed to be dichlorobutadiene ((1E,3E)-1,4-DCBD), an intermediate product of anaerobic conversion of hexachloro-1,3-butadiene by comparing with proton database. The chromatographic retention time of substance 3 was 20.03 min, the parent ion m/z value was 156, and the characteristic fragment ions m/z values were 50, 85 and 121, respectively. Substance 3 was identified as the intermediate trichlorobutadiene ((E)-1,2, 4-tcBD) by comparison with the proton database. The chromatographic retention time of substance 4 was 20.14 min, the m/z value of parent ion was 190, and the m/z values of characteristic fragment ions were 50, 119 and 155, respectively. Substance 4 was determined to be the intermediate product tetrachlorobutadiene ((3Z)-1,1,3, 4-TECBD) by comparing with the proton database.The chromatographic retention time of substance 5 was 20.86 min, the m/z value of parent ion was 224, and the m/z values of characteristic fragment ions were 84, 191 and 226, respectively. By comparing with the proton database, substance 5 was determined to be the intermediate product pentachlobutadiene (1,1,2,4,4-PCBD).The chromatographic retention time of substance 6 was 21.50 min, the m/z value of parent ion was 258, and the m/z values of characteristic fragment ions were

118, 190 and 225, respectively. Substance 6 was confirmed to be the substrate hexachloro-1,3-butadiene by comparing with the proton database.

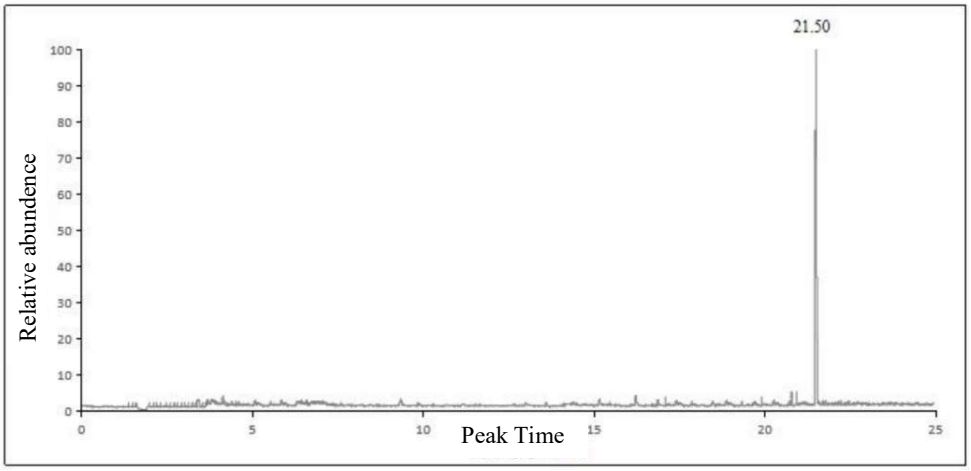


Figure 3. Extracted total ion chromatogram of the chemicals from sterilized medium amended with hexachlorobutad

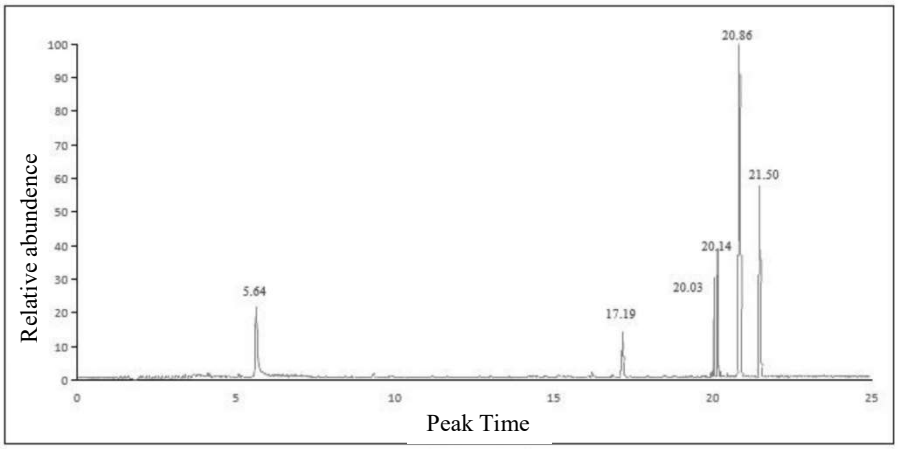


Figure 4. Extracted total ion chromatogram of the chemicals from hexachloro-1,3-butadiene anaerobic transformation system

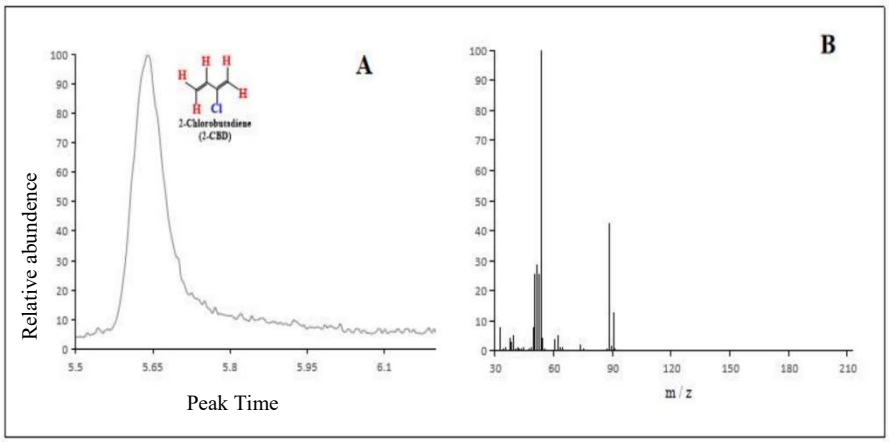


Figure 5. The extracted ion current chromatogram (A) and mass spectrum (B) of substance 1

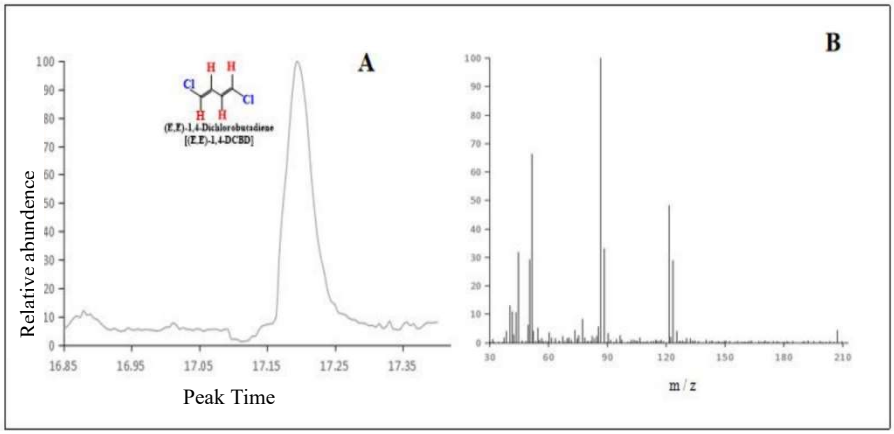


Figure 6. The extracted ion current chromatogram (A) and mass spectrum (B) of substance 2

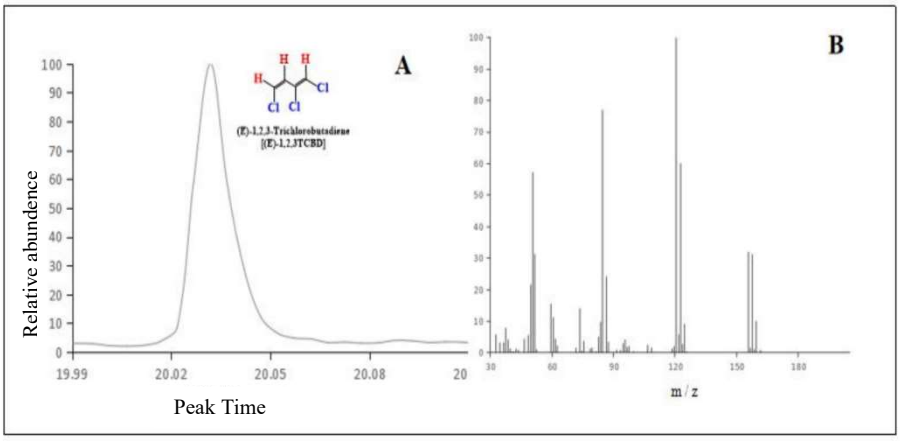


Figure 7. The extracted ion current chromatogram (A) and mass spectrum (B) of substance 3

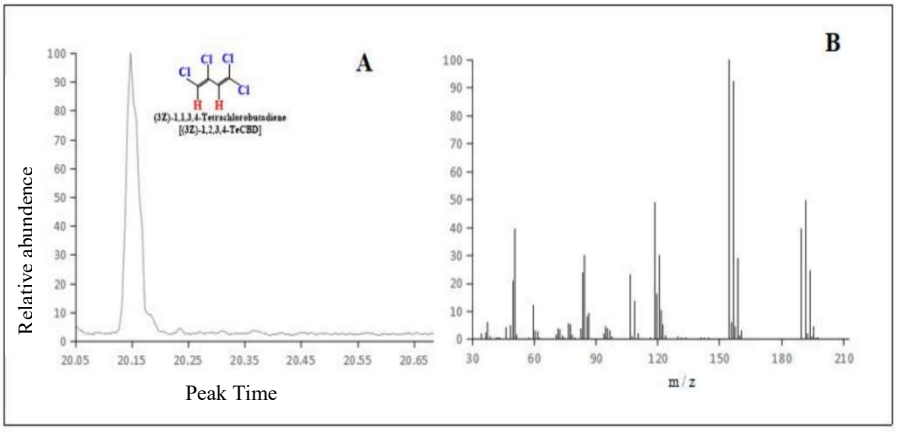


Figure 8. The extracted ion current chromatogram (A) and mass spectrum (B) of substance 4

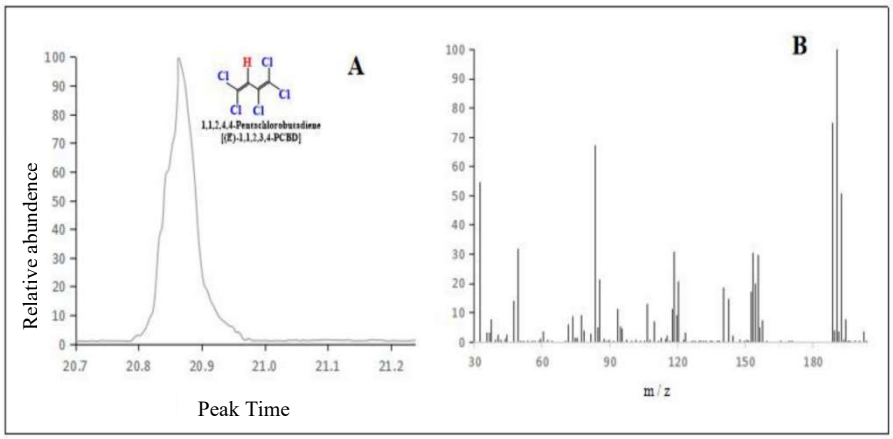


Figure 9. The extracted ion current chromatogram (A) and mass spectrum (B) of substance 5

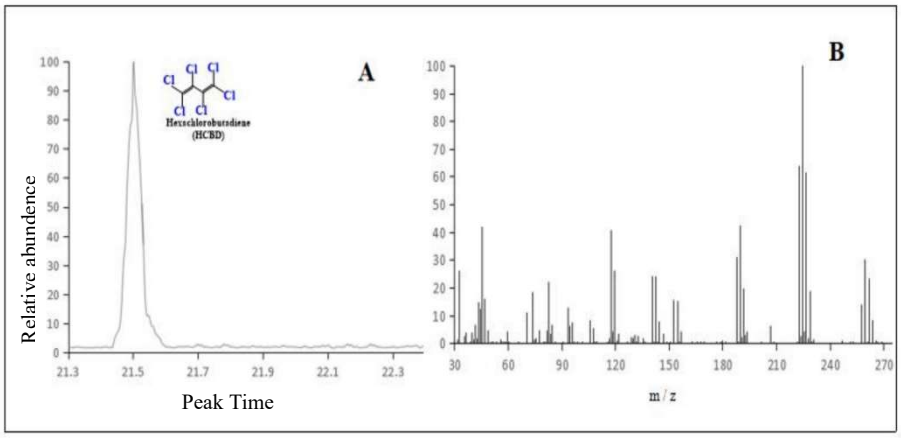
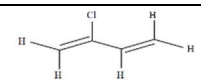
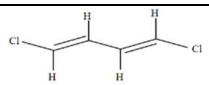
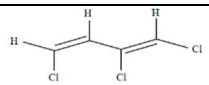
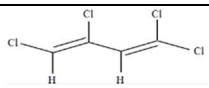
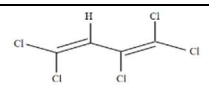
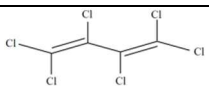


Figure 10. The extracted ion current chromatogram (A) and mass spectrum (B) of substance 6

Table 1. Composition of hexachloro-1,3-butadiene anaerobic transformation system

Compound	Peak time	Molecular mass	Molecular formula	Characteristic ion fragment	Molecular structure
2-CBD	5.64	88	C_4H_5Cl	53,88	
(1E,3E)-1,4-DCBD)	17.19	122	$C_4H_4Cl_2$	51,87,122	
(E)-1,2,4-TCBD)	20.03	156	$C_4H_3Cl_3$	50,85,121	
(3Z)-1,1,3,4-TeCBD)	20.14	190	$C_4H_2Cl_4$	50,119,155	
(1,1,2,4,4-PCBD)	20.86	224	C_4HCl_5	84,191,226	
Hexachloro-1,3-butadienee	21.50	258	C_4Cl_6	118,190,225	

When the SI (Standard Index) and RSI (Reverse standard index) values of GC-MS identified substances were both greater than 700, the structure of the substances can be determined (15,16). Table 1. listed the basic information such as SI and RSI values of hexachloro-1,3-butadiene reduction dechlorination products captured by ion flow chromatography after proton library comparison. According to the results obtained from the analysis, the components of each organic chlorine compound in the anaerobic conversion system of hexachloro-1,3-butadiene coulde be obtained as shown in Table 1. The anaerobic conversion system of hexachloro-1,3-butadiene contains its step-by-step dechlorination products: Pentachlorobutadiene (1,1,2,4,4-PCBD), tetrachlorobutadiene ((3Z)-1,1,3, 4-TECBD), trichlorobutadiene ((E)-1,2,4-TCBD), dichlorobutadiene ((1E,3E)-1, 4-dCBD), and monochlorobutadiene (2-CBD).

Based on 16S rRNA gene high-throughput sequencing analysis of the microbial community structure in the hexachloro-1,3-butadiene anaerobic microuniverse, combined with real-time quantitative PCR (qPCR) analysis, it was inferred that the microorganisms responsible for the reduction and dechlorination of hexachloro-1,3-butadiene were Dehalococcoides. Therefore, three treatment groups with hexachloro-1,3-butadiene as electron acceptor, hexachloro-1,3-butadiene and trichloroethylene as electron acceptor and trichloroethylene as electron acceptor were set respectively during the third conversion of the culture system with hexachloro-1 and 3-butadiene as electron donor, and the other conditions were the same as the first and second conversion.

The conversion products of trichloroethylene were detected by gas chromatography, and the peak times of methane, trichloroethylene and their degradation and conversion products cis-dichloroethylene were determined by standard samples, which were 2.792 min, 6.275 min, 5.384 min, 3.354 min and 2.836 min, respectively. The anaerobic degradation of trichloroethylene by the third transition using trichloroethylene as electron acceptor was shown in Figure 11. In this culture system, 81 μmol trichloroethylene was completely degraded within 80 days, and three substances were detected in the culture system. The retention times of gas chromatography were 2.792 min, 5.384 min and 6.275 min, corresponding to the retention time of methane, cis-dichloroethylene and trichloroethylene standard samples, respectively. Monitoring results showed that cis-dichloroethylene production began at day 31, and 5 μmol of methane was detected at day 46, 46 μmol of dichloroethylene and 15 μmol of methane were detected in the culture system when the trichloroethylene was exhausted after further culture.

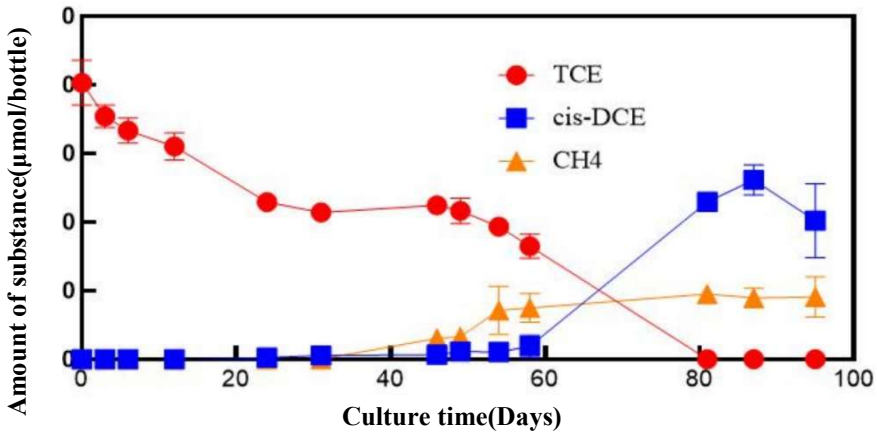


Figure 11. Trichloroethylene biodegradation in the third transferred enrichment cultures

In the third generation transfer culture system with hexachloro-1,3-butadiene and trichloroethylene as electron acceptor, 78 μmol of trichloroethylene was completely degraded within 95 days, and a total of four substances were detected in the culture system. The retention time was 2.836 min, 3.354

min, 5.384 min and 6.275 min respectively, corresponding to the retention time of ethylene, monovinyl chloride, cis-dichloroethylene and trichloroethylene standard samples. Monitoring results showed that after a stagnation period of 58 days, 2.4 μmol cis-dichloroethylene was observed by gas chromatography at 58 days, and 2 μmol monovinyl chloride and 20 μmol ethylene were detected at 81 days of culture. After further culture monitoring, trichloroethylene was consumed at 95 days of culture. In the culture system, 48 μmol ethylene was detected, no methane was observed, and only trace amounts of cis-dichloroethylene and monovinyl chloride were observed during the whole degradation process, as shown in Figure 12.

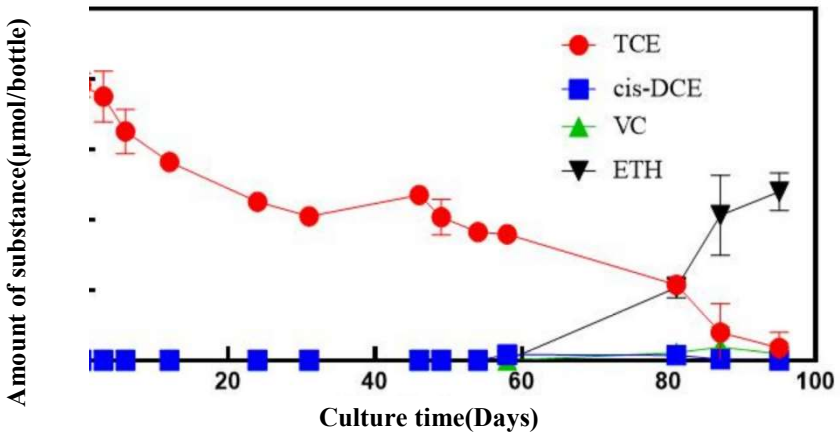


Figure 12. Trichloroethylene biodegradation in the third transferred enrichment cultures supplemented with hexachloro-1,3-butadiene and trichloroethylene as electron acceptor

In the group treated with both hexachloro-1,3-butadiene and trichloroethylene as electron donors and lactic acid as carbon source and electron donor, no hexachloro-1,3-butadiene was detected after 8 months, and its step-by-step dechlorination products were detected: tetrachlorobutadiene ((3Z)-1,1,3, 4-TECBD), trichlorobutadiene ((E)-1,2,4-TCBD), dichlorobutadiene ((1E,3E)-1, 4-dCBD) and monochlorobutadiene (2-CBD). At the same time, trichloroethylene can be completely transformed into ethylene by anaerobic degradation after a stagnation period of 24 days. After all the organic chlorine compounds were degraded and transformed, 3 % conversion was carried out under the same conditions, and the anaerobic degradation and transformation of trichloroethylene was regularly monitored by gas chromatography, as shown in Figure 13. In the first generation of anaerobic culture system with hexachloro-1,3-butadiene and trichloroethylene, it was observed that cis-dichloroethylene began to be produced at 24 days of culture, and trace amounts of monovinyl chloride (2 μmol) and ethylene (1.3 μmol) were observed at 46 days of culture. At 58 days of culture, the accumulation of cis-dichloroethylene reached a peak of about 25 μmol, and then began to gradually decrease, and at 81 days of culture, all trichloroethylene was degraded, at which time 80.5 μmol ethylene, 10.5 μmol monovinyl chloride and 9 μmol dichloroethylene were observed in the system. In the subsequent observation, the amount of dichloroethylene, monovinyl chloride and ethylene of trichloroethylene degradation and conversion products remained basically unchanged, and the product and the amount of trichloroethylene added in the initial culture basically maintained the material balance.

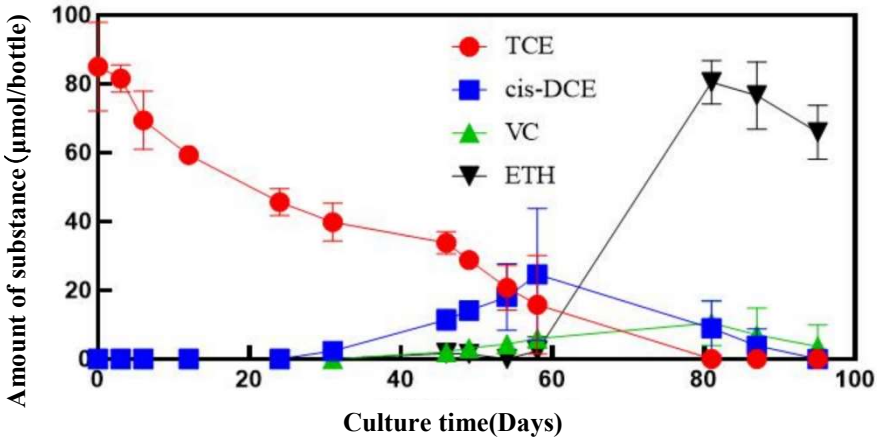


Figure 13. Trichloroethylene biodegradation in the first transferred enrichment cultures supplemented with hexachloro-1,3-butadiene and trichloroethylene as electron acceptor

Hexachloro-1,3-butadiene is chemically stable and has a long half-life. At present, only Serratia marcescens HL1 and Agrobacterium sp. BJ-04 strains of aerobic bacteria that degrade hexachloro-1,3-butadiene have been isolated. No organic halogen breathing bacteria have been identified that can anaerobically degrade and convert hexachloro-1,3-butadiene and obtain energy for growth (17,18). As for the anaerobic degradation and conversion of hexachloro-1,3-butadiene, Bosma and Shen Rui et al. proposed that the anaerobic conversion mechanism of hexachloro-1,3-butadiene is step-by-step dechlorination based on the experimental observation and theoretical study (19, 2). In this experiment, according to the comparison of ion fragments captured by GC-MS and the proton database results combined with the existing research results, we proposed a new anaerobic conversion pathway, as shown in Figure 14: Hexachloro-1,3-butadiene can be progressively dechlorinated to monochlorobutadiene (2-CBD) by replacing the chlorine atom on the carbon skeleton with a hydrogen atom through hydrogenolysis.

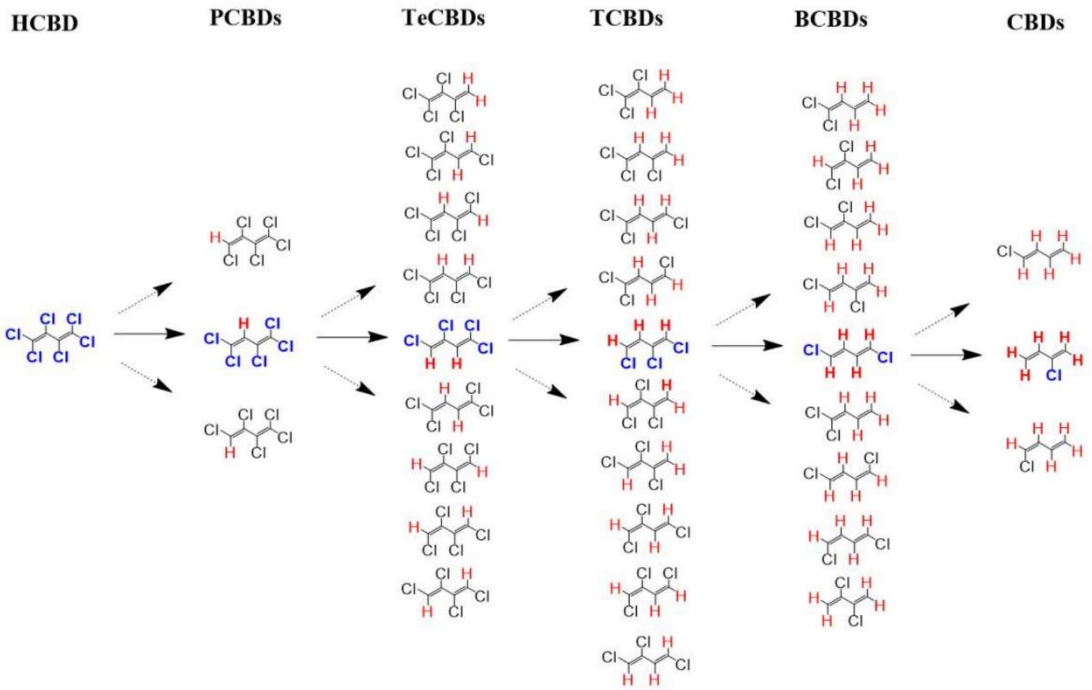


Figure 14. Anaerobic transformation pathways of hexachloro-1,3-butadiene

4. DISCUSSION

In this study, a new mechanism of microbial reduction and dechlorination of hexachloro-1,3-butadiene under anaerobic conditions was explored. Firstly, the enrichment culture of hexachloro-1,3-butadiene was established from the sediment of Xi River as the source. The reduction dechlorination products were identified by monitoring the anaerobic conversion process of hexachloro-1,3-butadiene and using ISQ-LT purge and capture gas chromatography mass spectrometry, and the anaerobic conversion mechanism of hexachloro-1,3-butadiene was analyzed.

Using Xi River sediment as inoculation source, lactic acid as electron donor and carbon source, the anaerobic enrichment culture system for conversion of hachloro-1, 3-butanedium was successfully established. Due to the lack of standards, the intermediates could not be quantitatively analyzed and only qualitative tests could be performed. The results showed that 62.5 μmol of hexachloro-1,3-butadiene could be completely dechlorinated by this system within 8 months, and the microbial anaerobic conversion pathway was as follows: consumed two electrons by hydrogenolysis to form one molecule of hydrogen chloride to successively reductive dechlorination to pentachlorobutadiene (1,1,2,4,4-PCBD), tetrachlorobutadiene ((3Z)-1,1,3, 4-TECBD), trichlorobutadiene ((E)-1,2,4-TCBD), dichlorobutadiene ((1E,3 E)-1, 4-dCBD) eventually produces monochloroprene (2-CBD). The conversion pathway of hexachloro-1,3-butadiene under anaerobic conditions was revealed, which improved our understanding of hexachloro-1,3-butadiene reducing dechlorination and its environmental trend.

However, due to the limited research time, there are still some problems that need to be further explored in the future. In the process of anaerobic conversion of hexachloro-1,3-butadiene, because of the lack of standards, only ISQ-LT purge and trap gas chromatography-mass spectrometry can be used to qualitatively measure the reduction and dechlorination products, and there is a lack of research on the material balance of the whole reduction and dechlorination process. Therefore, future studies can be conducted by synthetic synthesis of pentachlorobutadiene (1,1,2,4,4-PCBD), tetrachlorobutadiene ((3Z)-1,1,3, 4-TECBD), trichlorobutadiene ((E)-1,2,4-TCBD), dichlorobutadiene ((1E,3E)-1,4-DCB, and monochlorobutadiene (2-CBD),which are the conversion product of hexachloro1, 3-butadiene, using these products as standards, and combining with isotope labeling methods to establish the material and electron balance in the anaerobic conversion process of hexachloro-1,3-butadiene.

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