Levels and distribution of hexabromocyclododecane (HBCD) in environmental samples near manufacturing facilities in Laizhou Bay area, East China†

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A total of 55 samples including soil, sediment, plants (cypress, reed and seepweed) and aquatic species were collected at locations around hexabromocyclododecane (HBCD) manufacturing facilities in Laizhou Bay area, East China. HBCD was determined at concentrations ranging between 0.88 and 6901 ng g⁻¹ dry weight (dw), 2.93–1029 ng g⁻¹ dw, 8.88–160 241 ng g⁻¹ dw, and 7.09–815 ng g⁻¹ lipid weight (lw), respectively. Significant negative correlations ($r^2 = 0.54$, $p = 0.006$) were observed between HBCD concentrations in soils and the distance from the manufacturing facility, and the concentrations became constant when the distance was >4 km. The calculation results on the bioaccumulation factors (BAFs) suggested that HBCD may be accumulated in plants. Tissue-specific bioaccumulation of HBCD diastereoisomers was found in aquatic species. For example, in crabs the highest concentrations of HBCD (815 ng g⁻¹ lw for female and 446 ng g⁻¹ lw for male) were observed in the gill. Besides the gill, α -HBCD was more preferentially accumulated in the spermary and ovary, while β - and γ -HBCD were more accumulated in the muscle. A similar distribution was also observed in roe and muscle of goby fish.

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† Electronic supplementary information (ESI) available: Sample extraction and cleanup, instrumental analysis, sampling details and concentrations of HBCD isomers (Table S1, S2), BAFs for HBCD in reed, seepweed and cypress species (Table S3), isomer profiles of HBCD in soil, sediment, plants and aquatic species (Fig. S1), principal component analysis of HBCD distribution in soil, sediment, plant samples and aquatic species (Fig. S2). See DOI: 10.1039/c2em30231d

1. Introduction

Hexabromocyclododecane (HBCD) is one of the most widely used brominated flame retardants (BFRs). It is primarily added into expanded and extruded polystyrene (EPS and XPS) which are used in building insulations, and is also employed in back coating of textiles and high impact polystyrene (HIPS). In 2001, the global market demand reached 16 700 tons.¹ As it is mainly used as an additive BFR, HBCD can enter the environment during the production process and upon usage. It was first detected in fish and sediment in 1998,² and has since been detected in various matrices including air, soil, water, sediment, fish, mammals and foodstuffs. Due to its long-range atmospheric transport potential,³ bioaccumulation and biomagnification abilities,^{4,5} neurotoxic effects and endocrine disruptive effects,^{6,7}

Environmental impact

HBCD is a typical brominated flame retardant (BFR) which is widely used in commercial products. To systematically evaluate the impact of manufacturing on the surrounding environment, the levels, distribution and diastereoisomer profiles of HBCD were investigated in various environmental samples near HBCD manufacturing facilities located in Laizhou Bay area, an important HBCD production base in China. The present study provides previously unknown information on HBCD concentrations in environmental matrices near manufacturing sources in China. The high concentrations in the soil and sediment samples reflect the influence from the production activities. Besides, the results revealed that HBCD can be bioaccumulated by plants and aquatic species, therefore increasing the exposure risk of biotic species.

the potential risk of HBCD to the environment has been of increasing concern in recent years. In 2009, HBCD was nominated as a candidate persistent organic pollutant (POP) in the Stockholm Convention.⁸

China is an important producer of HBCD and the production capacity of HBCD reached 7500 tons in 2007.⁹ The emergence of HBCD in the Chinese environment has gradually been studied with respect to the contamination levels and distribution,^{10–12} but studies on HBCD contamination around point sources are still scarce. The Laizhou Bay area is the biggest brominated chemical industry base in China, and many BFR manufacturing facilities are located in the industrial park of Weifang city near Laizhou Bay. This area has a typical temperate monsoon climate. The prevailing wind is from the southeast in summer and autumn, whereas northwesterly winds are more prevalent in winter and spring. In this study, soil, sediment, plant samples and aquatic species were collected around HBCD manufacturing facilities in the Laizhou Bay area, in order to systematically investigate the contamination levels, distribution, and diastereoisomer profiles of HBCD in the environment around manufacturing facilities, and to further evaluate the emission and transport potential of HBCD due to its production. To the best of our knowledge, this is the first study to report on the influence of manufacturing facilities on the HBCD levels in the surrounding environment in China.

2. Materials and methods

2.1. Sampling

Samples from 23 sites around the Laizhou Bay area, East China (Fig. 1) were collected in June 2010 (soil, sediment, plant samples and aquatic species) and January 2011 (aquatic species). S0 and S15 represented two HBCD manufacturing facilities. A control site, S20 (63.8 km from S0), was selected for sediment and plant samples (cypress), S21 (75.7 km from S0) was selected for soil and plant samples (reed), and S22 (Mihe river, one of the drinking water sources of Weifang city) was chosen for aquatic species. S1 to S14 are located at different distances from S0 along a road. Few plant species are able to grow in this area due to the highly saline-alkali soil, and species are limited to a few reeds (*Phragmites*), seepweed (*Suaeda glauca*) and cypress (*Platycladus orientalis*). S16 to S18 are in the centre of the industrial park and S19 (Bailang river) is situated close to the south of the industrial park. Details on the sampling sites and sample information of the soil, sediment, plant samples and aquatic species are provided in Table S1, ESI.†

Undisturbed surface soil (0–20 cm depth) was collected using a clean stainless steel shovel. Surface sediment samples (0–15 cm depth) were collected using a bottom sediment grab sampler (Rickly Hydrological Company, USA). Two to three individual soil or sediment samples collected at one site were combined to form a composite sample. Three to five aboveground tissues of the plants (cypress leaves, reed shoots and seepweed shoots) were combined to form one sample. All the soils were sampled in the same spots as the plants. Crucian carp (*Carassius auratus*), crab (*Eriocheir sinensis*), stone moroko (*Pseudorasbora parva*) and goby (*Acanthogobius hasta*) were collected from S19 in June 2010 by trawling. Freshwater shrimp (*Macrobrachium nipponense*),

goby, loach (*Misgurnus anguillicaudatus*) and silver carp (*Hypophthalmichthys molitrix*) were obtained from S22 in January 2011 with an overnight nylon net.

In total, 57 samples were collected, including commercial HBCD products from the two manufacturing facilities ($n = 2$), soil samples ($n = 15$), sediment samples ($n = 6$), 20 plant samples (5 cypress samples, 11 reed samples and 4 seepweed samples) and 14 aquatic organisms. The aquatic organisms included muscle, gill and ovary/spermary of 28 female crabs and 25 male crabs, muscle and roe of a goby, muscle of 5 crucian carps, muscle of a stone moroko, whole body of gobies ($n > 100$), 25 silver carps, 20 loaches and 12 freshwater shrimps.

All samples were wrapped in aluminum foil, sealed in polyethylene bags, then transported to the laboratory immediately and stored at $-18\text{ }^{\circ}\text{C}$ until pretreatment. Soil and sediment samples were freeze-dried, and both were sieved through a 16-mesh sieve. Cypress, reed and seepweed were washed with high purity water to remove the dust on the surface, then freeze-dried and ground into fine powder using a food blender (HR2870, PHILIPS, Netherlands). All the aquatic species and crab gill were washed with high purity water. Tissues such as muscle, roe, gill, spermary and ovary were separated, then tissue types were pooled and homogenized to form sufficient amounts of each tissue type for analysis. Finally, the samples were freeze-dried and ground into a fine powder.

2.2. Chemicals

Native α -, β -, and γ -HBCD (>98% purity) were purchased from AccuStandard Inc. (New Haven, CT, USA), $^{13}\text{C}_{12}$ - γ -HBCD and d_{18} - γ -HBCD (>98% purity) were from Wellington Laboratories (Guelph, Ontario, Canada). Dichloromethane (DCM) and n -hexane used for extraction and cleanup were pesticide-grade and obtained from Fisher (Fair Lawn, New Jersey, USA), acetonitrile and methanol for HPLC-MS/MS were HPLC-grade and purchased from J.T. Baker (Phillipsburg, NJ, USA). High purity water was produced by Milli-Q system (Millipore, USA). Silica gel was supplied by Merck (Darmstadt, Germany) and was baked at $600\text{ }^{\circ}\text{C}$ for 12 h before use. Anhydrous sodium sulfate (Na_2SO_4) and concentrated sulfuric acid (H_2SO_4) (analytical reagent grade) were obtained from Beijing Chemical Factory (Beijing, China) and the anhydrous Na_2SO_4 was baked at $450\text{ }^{\circ}\text{C}$ for 6 h before use. Acid silica gel was produced from activated silica gel impregnated with 30% (w/w) concentrated H_2SO_4 , basic silica gel was prepared from activated silica gel impregnated with 1.2% (w/w) NaOH (1 mol L^{-1} solution).

2.3. Sample extraction and cleanup

Approximately 1 g of a homogenized sample was mixed with 10 g of anhydrous Na_2SO_4 and spiked with 10 ng $^{13}\text{C}_{12}$ - γ -HBCD as internal standard, then extracted with n -hexane : DCM (1 : 1, v/v) using an accelerated solvent extractor (ASE 300, Dionex, USA). The detailed extraction and cleanup processes are given in the ESI.†

2.4. Instrumental analysis

Samples were analyzed using a Micromass Quattro Premier XE triple quadrupole MS spectrometer (Micromass, Manchester,

Fig. 1 Map of the sampling sites around the Laizhou Bay area in East China. The map on the bottom-left details the sampling locations near the HBCD manufacturing facility (S0) and along a road. The green crosses depict manufacturing facilities at the locations S0 and S15.

UK) equipped with an Alliance 2695 LC system (Waters, Milford, MA.). Analysis of three HBCD diastereoisomers was performed following a method reported elsewhere,¹³ with some modifications to the gradient program of HPLC and source parameters of MS. Details of the instrumental analysis are provided in the ESI.†

2.5. Quality control

One procedural blank (anhydrous Na_2SO_4) was included in each batch of 6–10 samples. HBCD in all blank samples was below the limit of detection (LOD). Methanol was injected before the sample analysis to ensure no contamination during the instrumental analysis. A duplicate HBCD standard mixture (10 ng g^{-1} α -, β -, and γ -HBCD) was analyzed for each ten samples to check the stability of the instrument and repeatability of the analytical method. The internal standard $^{13}\text{C}_{12}$ - γ -HBCD was used to quantify the concentrations of α -, β -, and γ -HBCD, and the injection standard d_{18} - γ -HBCD was used to calculate the recovery of $^{13}\text{C}_{12}$ - γ -HBCD. Native α -, β -, and γ -HBCD standard mixtures at eight concentration levels (2.5, 5, 10, 25, 50, 75, 100, 200 ng mL^{-1}) were used to obtain the calibration curve. The RSD of the relative response factors (RRFs) were $<25\%$ for α -, β -, and γ -HBCD. Recoveries of $^{13}\text{C}_{12}$ - γ -HBCD were $83.5 \pm 12.2\%$ (mean $\pm$ SD, $n = 55$). Method detection limits (MDLs) were defined as signal to noise (S/N) = 3/1 in procedural blanks, and the MDLs for α -, β -, and γ -HBCD were 0.2 ng g^{-1} ,

0.1 ng g^{-1} , and 0.1 ng g^{-1} , respectively. Limits of quantification (LOQ) were set as eight times S/N in the samples.

3. Results and discussion

3.1. Levels and spatial distribution of HBCD in soil and sediment

The total HBCD (sum of α -, β -, and γ -HBCD) concentrations in the soils are summarized in Table S1.† HBCD was detected in all the samples, and the levels ranged from 0.88 to $6901 \text{ ng g}^{-1} \text{ dw}$. The concentration in the soil near the manufacturing facility (S15) showed the highest level ($6901 \text{ ng g}^{-1} \text{ dw}$), which was the same order of magnitude as that at the other manufacturing facility S0 ($2295 \text{ ng g}^{-1} \text{ dw}$). However, both of these soil samples were lower than the reported highest value ($23200 \mu\text{g kg}^{-1} \text{ dw}$) from HBCD-processing plants in European countries.¹⁴ The ΣHBCD concentration ($0.88 \text{ ng g}^{-1} \text{ dw}$) in the soil from the control site (S21) was much lower than those from other sites. This concentration was at the same level as those from urban areas in South China (1.7 – $5.6 \text{ ng g}^{-1} \text{ dw}$)¹⁵ and other countries, such as Belgium (from below LOD to $6.6 \text{ ng g}^{-1} \text{ dw}$),¹⁶ India, Vietnam, Malaysia, Indonesia and Cambodia (from below LOD to $2.5 \text{ ng g}^{-1} \text{ dw}$),¹⁷ but higher than those from Chongming Island in East China (from below LOD to $93.8 \text{ pg g}^{-1} \text{ dw}$).¹²

The spatial distribution of HBCD in the soil samples around the manufacturing facility S0 is given in Fig. 2. Sampling sites at distances $>4 \text{ km}$ from S0 showed concentrations decreasing to

Fig. 2 Spatial distribution of HBCD in the soil samples around the manufacturing facility (S0).

the same level as that at S16 (13 ng g⁻¹ dw). A significant negative correlation ($r^2 = 0.54$, $p = 0.006$) was found between the HBCD concentrations and the distance from the point source (S0), as shown in Fig. 3. Similar spatial distribution of HBCD around potential point sources was also observed in soil samples collected near an XPS-producing facility in Sweden¹⁸ and HBCD processing plants in European countries.¹⁴ Gao *et al.*¹⁹ investigated the HBCD concentrations in soils from e-waste recycling areas in South China and reported that the concentrations decreased dramatically with increasing distance from the recycling site, which is also considered as a typical point source of HBCD entry into the environment.

For sediment samples, HBCD concentration at site S9 (1029 ng g⁻¹ dw) was significantly higher than those at the other sites (2.93–64.2 ng g⁻¹ dw). As shown in Fig. 1, S9 was very close to the manufacturing facility and the water body can be easily affected by the emission source. The sample from a drainage river (S17) also showed a relatively higher level (64.2 ng g⁻¹ dw), whereas the

Fig. 3 The correlation between the distance from the point source (S0) and HBCD concentration in the soil samples.

samples from other locations (S14, S18 and S19) were at the same level as the control site S20 (8.69 ng g⁻¹ dw). Compared to other studies around the world, the levels (except for S9) were comparable with those from coastal waters in Korea (0.39–59 ng g⁻¹ dw)²⁰ and downstream from the textile industry in Sweden (1–25 µg kg⁻¹ dw),¹⁸ but higher than those from the Detroit River (ranged from <0.075 to 3.7 ng g⁻¹ dw),²¹ Swiss lakes (2.5 ng g⁻¹ dw in 2001)²² and English lakes (0.88–4.8 ng g⁻¹ dw).²³

3.2. Diastereoisomer profiles of HBCD in soil and sediment

Typically, commercial HBCD mixtures mainly consist of three diastereoisomers, α -HBCD (10–13%), β -HBCD (1–12%), and γ -HBCD (75–89%).¹ The distribution and environmental fate of these isomers in various environmental matrices can be quite different. γ -HBCD is the major diastereoisomer in abiotic environmental samples, such as soil, sediment, air and water, whereas α -HBCD is the predominant diastereoisomer in aquatic organisms, birds and mammals.¹ In the present study, γ -HBCD was the most abundant isomer in all soil samples (Fig. S1, ESI†), followed by α -HBCD and β -HBCD, with mean contributions of 67.3%, 20.4%, 12.3%, respectively. Similar diastereoisomer profiles were also observed in the sediment samples, all of which were comparable to those in the two commercial HBCD products (Table S2, ESI†) from HBCD manufacturing facilities S0 (70% γ -HBCD) and S15 (60% γ -HBCD).

HBCD profiles in the soil samples were somewhat different among the sampling sites. The highest γ -HBCD contribution reached 87% at sampling site S4, whereas at sampling sites S7, S11 and S13, γ -HBCD ratios were below 50%. This extent in variation has also been found in soils from other studies. γ -HBCD contribution ranged from 33.3% to 90.8% in soils from e-waste recycling areas and industrial areas in South China.¹⁹ In soils from Asian developing countries,¹⁷ the average contribution of γ -HBCD was only 52%, which was much lower than that in the commercial mixtures. The variations were generally considered to be the results of thermal isomerization during the processing of final products and isomer-specific processes in environmental media. Rearrangement of HBCD isomers takes place at temperatures above 160 °C, and decomposition occurs above 240 °C.²⁴ The different physicochemical properties of the three isomers (e.g. thermal stabilities and photodegradation characteristics) can give rise to isomer-specific transport, partitioning, degradation and metabolism of HBCD in environmental media. Zhao *et al.*²⁵ investigated the thermodynamics and photochemical properties of α -, β - and γ -HBCD and found that α -HBCD was the most stable isomer. Harrad *et al.*²⁶ determined HBCD diastereoisomers in indoor dust and found that there was a rapid photolytically mediated shift from γ -HBCD to α -HBCD after one week of exposure to light, whereas no significant change was found in the control samples.

3.3. HBCD in plants

The levels of Σ HBCD in the 18 plant samples from 17 sampling sites (S0–S8, S10–S16, S18) ranged from 110 to 160 241 ng g⁻¹ dw (Table S1, ESI†), which were much higher than those at control site S21 (reed sample, 8.88 ng g⁻¹ dw) and S20 (cypress sample, 84.2 ng g⁻¹ dw). Because of the limited number of

sampling sites for cypress and seepweed samples, reed was used to investigate the spatial distribution of Σ HBCD in plants around the manufacturing facility S0. Similar to the soils, the highest concentration was also found at S0 (84227 ng g⁻¹ dw), after which the levels decreased with increasing distance from S0, although no significant relationship was found ($p > 0.1$).

The relationship between HBCD concentrations (log-transformed) in the soil and reed samples from the same sampling site was also investigated (Fig. 4). HBCD concentrations in the reed showed a significant positive correlation with those in the soil ($r^2 = 0.86$, $p < 0.01$). Unlike seepweed and cypress, reed is a perennial herb having hair roots mainly distributed in the upper soil.²⁷ On the other hand, the positive correlation also implied that reed might be exposed to a similar extent to soil at different locations.

Bioaccumulation factors (BAFs) are usually used to reveal bioaccumulation abilities by biota, which could be defined as $[\Sigma\text{HBCD}]_{\text{plant}}/[\Sigma\text{HBCD}]_{\text{soil}}$ in this study. As shown in Table S3, ESI,† except for sampling site S10, all the BAF values exceeded 1.0 with the highest value at 1047 in the cypress sample from S5. Even at the control site S21, the value was greater than 10. A recent study²⁸ reported the uptake of HBCD from experimental soil by cabbage and radish, the results showed that both plant species could uptake HBCD, and cabbage showed greater accumulation ability. In the present study, the high BAF values implied that HBCD might be accumulated in plants in the field environment. On the other hand, for plants, deposition or adsorption on the leaf surface and absorption from air could also be important pathways to result in the exposure to persistent semi-volatile organic contaminations. Further studies on HBCD concentrations in the atmosphere are needed to investigate the effect of atmospheric deposition on HBCD levels in plants.

Very similar isomer profiles of HBCD were found in the plant samples in spite of the different species studied (Fig. S1, ESI†). γ -HBCD accounted for 77.0% of Σ HBCD in all samples, followed by α -HBCD and β -HBCD with average ratios of 12.2% and 10.8%, respectively. The isomer profiles were also similar to the two commercial HBCD products (Table S2, ESI†). A limited number of studies on the isomer profiles of HBCD in plant species indicated that the contribution of γ -HBCD in grains and plant leaves were 38% and 53%, respectively.²⁹ Li *et al.*²⁸

investigated the distribution of the three HBCD isomers in cabbage and radish plants, and found the predominance of α -HBCD in shoot tissues and γ -HBCD in root tissues.

3.4. HBCD in aquatic species

HBCD concentrations and individual diastereoisomer patterns in aquatic species are summarized in Table S1, ESI.† The concentrations ranged between 7.09–128 and 72.8–815 ng g⁻¹ lw in the samples from S22 (four aquatic species) and S19 (ten tissues of four aquatic species), respectively. The levels in the aquatic species were slightly lower than those in the marine species near known point sources in the Netherlands (9–1110 ng g⁻¹ lw)³⁰ and the freshwater species near the textile industry in Sweden (downstream industrial effluents 970–1800 ng g⁻¹ dw).¹⁸ However, they were at the same level as in other freshwater fish, *e.g.*, in crucian carp in South China (21–378 ng g⁻¹ lw)²⁹ and in fish from English lakes (14–290 ng g⁻¹ lw).²³

Σ HBCD concentrations varied significantly in the different aquatic species and tissues. Among the four species at the sampling site S19, loach exhibited the highest concentration of HBCD (128 ng g⁻¹ lw), which was 18 times higher than that in silver carp (7.09 ng g⁻¹ lw). Furthermore, the highest value was found in the gills (815 ng g⁻¹ lw for female crab and 446 ng g⁻¹ lw for male crab) followed by muscle, spermary and ovary in the crab tissues, without any obvious difference in between the sexes. Crabs are benthic animals and usually burrow in sediment. As the organ of respiration, the gill is easily exposed to contaminants in sediment and water, which may explain the high concentrations in this organ.

Regarding the isomer profile, significant species-specific and tissue-specific accumulations of the three diastereoisomers were also observed in the samples. α -HBCD dominated in all the fish samples, of which the ratios were in the range of 47.8–92.2%, followed by 6.44–43.3% and 2.72–12.4% for γ - and β -HBCD, respectively (Fig. S1, ESI†). However, at sampling site S22, a lower contribution of α -HBCD was found in the freshwater shrimp (29.6%), which was consistent with the results in an early study.³⁰ Species-specific accumulations of the three isomers have previously been reported in aquatic food webs.^{4,31} Tissue accumulation ratios³⁰ of the three HBCD diastereoisomers in crabs and goby are given in Fig. 5. All three isomers were easily accumulated in gill tissue in both male and female crabs. Besides the gill, α -HBCD was more preferentially accumulated in the spermary and ovary, while β - and γ -HBCD were accumulated more in the muscle. This distribution was also observed in the roe and muscle of the goby (Fig. 5). Tissue-specific accumulation of α - and γ -HBCD was also reported in the study of bib and whiting³⁰ and juvenile rainbow trout,³² in which a preferential accumulation of α -HBCD was found in the liver. In addition, the apparent concentrations in these tissues could also be affected by biotransformation, metabolism, biodegradation and more, which were previously discussed in the studies on cytochrome P450 mediated biotransformation in marine mammals,³³ metabolites and biodegradation of HBCD in rats^{34,35} and bioisomerization of HBCD isomers in fish.³⁶

Compared with the distribution in other environmental matrices, the elevated ratio of α -HBCD in the aquatic species could probably be affected by factors such as physical–chemical

Fig. 4 Correlations of HBCD concentrations (log-transformed) in the soil and reed samples from the same sampling site.

Fig. 5 Tissue accumulation ratios of the three HBCD diastereoisomers in female crab (A), male crab (B) and goby (C).

properties (aqueous solubility and half life in the environment) of the three isomers and isomer-specific bioavailability in the organisms. The higher aqueous solubility of the α isomer ($48.8 \mu\text{g L}^{-1}$) versus the β ($14.7 \mu\text{g L}^{-1}$) and γ ($2.08 \mu\text{g L}^{-1}$) isomers³⁷ can facilitate the bioaccumulation of α -HBCD in aquatic species. Biotransformation from β -HBCD and γ -HBCD to α -HBCD^{36,38} and isomer-specific metabolism (β and γ isomers are more easily metabolized than the α isomer)³⁸ could further confirm the predominance of the α isomer in aquatic species.

3.5. Multivariate statistical analysis for HBCD diastereoisomers in environmental samples

Principal component analysis (PCA) was also employed to further study the different accumulation of HBCD diastereoisomers in the abiotic matrices and biotic species. As shown in Fig. S2, ESI,† two distinctive clusters were classified for α -HBCD and γ -HBCD. PC1 was positively correlated to γ -HBCD contribution and explained 83.3% of the variance, and PC2 was positively correlated to α -HBCD contribution and explained 16.7% of the variance. Commercial HBCD products, soil, sediment and plant samples showed significant predominance of γ -HBCD, whereas α -HBCD predominated in the aquatic species, which was in agreement with many other studies.^{11,23,39}

Overall, the same distribution pattern of HBCD isomers in the commercial products and abiotic matrices indicated a significant effect of the emission source on the surrounding areas, even though it may also be affected by individual differences, species differences and transformation process differences of HBCD isomers in the environment.

4. Conclusions

This study investigated the levels and distribution of HBCD in the soil, sediment and biotic samples around HBCD manufacturing facilities. The high concentrations in the soil and sediment samples reflected the influence from the production activities. Besides, higher HBCD levels in the three plant species compared to those in the surrounding soils implied that HBCD might be accumulated in the plant. Species-specific and tissue-specific accumulations of HBCD isomers were evidently observed in the aquatic species. Diastereoisomer profiles of HBCD reflected that γ -HBCD was the major diastereoisomer in the abiotic samples and plants, which was similar to the two commercial HBCD products, whereas α -HBCD predominated in the aquatic species. These results further confirm the transport potential of HBCD from production facilities to the surrounding environment, as well as the changes in HBCD diastereoisomer profiles during transport and bioaccumulation in aquatic species.

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