Development of Environmental Fate Model for Hexabromocyclododecanes(HBCDs) with Isomerisation Process

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Introduction

Environmental fate of hexabromocyclododecanes is important for the characterization of their risks. Arnot et al. 2009 presented a comprehensive collection and critical review of available physical-chemical property and transformation data for technical-HBCD, α-HBCD, β-HBCD and γ-HBCD. However, due to the limited availability of data, isomerisation process was not included in the model calculation. The purpose of this study is to assess the impact of the isomerisation process on the environmental fate model for HBCDs.

Materials and Methods

We used a Mackay-type level III multimedia fate model (Mackay et al. 1996) to calculate the steady state concentrations. The model was extended to incorporate the isomerisation process so that isomer specific concentration can be calculated simultaneously.

Table 1 shows the partitioning coefficients and half lives for HBCDs. The degradation rate constant in air for technical HBCD was obtained from Arnot et al. 2009. No distinction among the isomers was made for the degradation rate constant in air. Degradation rate constant in water for technical HBCD (Arnot et al. 2009) was adjusted to obtain the isomer specific degradation rate constants by assuming that the isomer specific degradation rates in water were proportional to those in methanol and that half life of technical HBCD calculated by the isomer specific degradation rates in water equals the half life observed in water. The isomer specific degradation rate constants in soil and sediments were obtained from Mitsubishi Chemical Safety Institute 2009 and Arnot et al. 2009, respectively.

Photolytic isomerisation rate constants were calculated based on Harrad et al. 2009 (Table 2). Harrad et al. reported the changes of diastereomer specific HBCD concentrations in Methanol over 7 days. We assumed 5 cases for the isomerisation processes in the environment. In case 1 and 2, isomerisations occur in all media. In case 3 and 4, isomerisations occur only in air and water. In case 5, isomerisations are not considered. In case 1 and 3, the isomerisation rate constants are the same as those in methanol. In case 2 and 4, the rate constants are one-tenth of those in methanol.

Table 1: Partitioning coefficients and half lives for HBCDs

Diastereomer	Log Kow	Log Kaw	Log Koa	Half lives [days]			
				air	water	soil	sediment
α-HBCD	5.75	-6.34	12.09	1.34	98.8	113	128
β-HBCD	5.79	-6.20	11.99	1.34	91.9	68	72
γ-HBCD	6.25	-9.17	15.42	1.34	68.3	104	92

Table 2: Isomerisation rate constants for HBCDs in methanol [h^{-1}]

From α to β	From α to γ	From β to α	From β to γ	From γ to α	From γ to β
2.03×10^{-4}	2.77×10^{-4}	1.42×10^{-3}	2.91×10^{-4}	1.78×10^{-3}	3.13×10^{-4}

Results and Discussion

Figure 1 shows the predicted steady-state amount of HBCDs in air and soil after continuous emission of each HBCD isomers to air. The predicted steady state concentration in air was not affected by the isomerisation process (Figure 1 left). On the other hand, the predicted steady state concentration in soil was affected if we assume that isomerisation process occurs in all media (case 1 and 2). In case 3 and 4, where we assumed that isomerisation process occurs only in air and water, the results for soil concentrations were virtually the same for case 5, where we assumed no isomerisation. Similar results were observed in water and sediment concentrations after continuous emission to water.

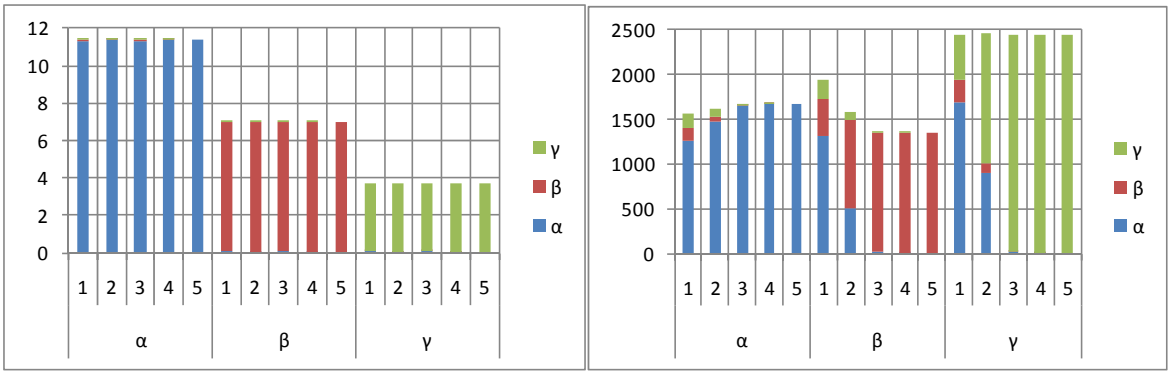

Figure 1: Predicted steady-state amount [mol] of HBCDs in air (left) and soil (right) after continuous emission [1mol/h] of each HBCD isomers to air. The values can be interpreted as the average residence time in air and soil. The bottom labels indicate the assumption on isomerisation process (case 1-5) and source isomers (α, β, γ). See text for the explanation of case 1-5.

Acknowledgement

This research was funded by Japan Ministry of Environment, Waste Management Research Grant (K2121).

References

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