INTAKE FRACTIONS OF HBCDS

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Introduction

Environmental fate and exposure of hexabromocyclododecanes is important for the characterization of their risks. Arnot et al. [1] 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. In our previous study[2], we assessed the impact of the isomerisation process on the environmental fate model for HBCDs. However, exposure modelling was not included in the study. In this paper, we developed environmental fate and exposure model for HBCDs and calculated the intake fractions (iFs) for these compounds.

Materials and methods

We used a Mackay-type level III multimedia fate model[3] to calculate the steady state concentrations. The model was extended to incorporate the isomerisation process so that isomer specific concentration can be calculated simultaneously. The geographical scale of the model is Japan. Physico-chemical properties of HBCDs was obtained from Arnot et al[1]. The isomer specific degradation rate constants in soil and sediments were obtained from Mitsubishi Chemical Safety Institute[4] and Arnot et al.[1], respectively. Photolytic isomerisation rate constants were calculated based on Harrad et al.[5] To calculate iFs[6] for HBCDs, exposure from inhalation, drinking water, soil ingestion and food were considered. Intake of vegetables, meat and fish were considered.

Results and discussion

Fig. 1 shows the predicted average residence time of HBCDs in each environmental media following emission to air and water. Fig. 2 shows the isomer profile of HBCDs in each media at steady state. For all isomers, the residence time in soil was largest in case of emission to the air and the residence time in sediment was largest in case of emission to water. It seems that these two environmental media has enough long residence time for HBCDs to change to other isomers.

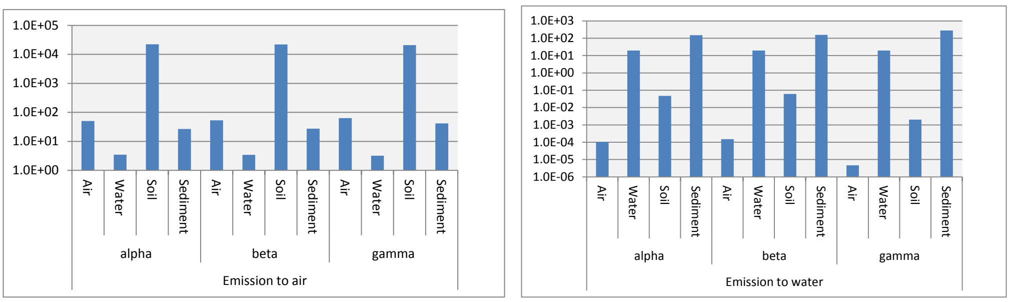

Fig.1 Residence time in each media after emission to air (left) and water (right) (unit: h)

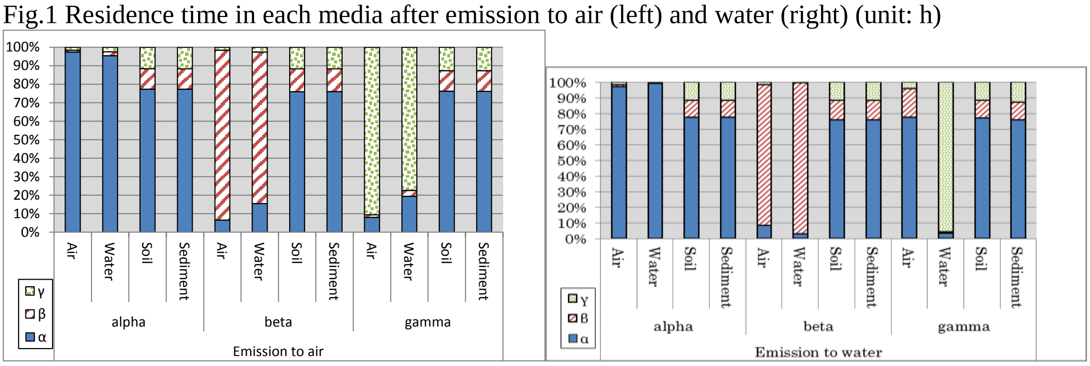

Fig.2 Isomer profile of HBCDs at steady state in each media after emission to air (a) and water (b)

Table 1 shows the intake fractions of HBCDs caused by emission of HBCDs to air and water. The environmental fate model in this paper considers the isomerisation, so not only the original isomer which are released to the environment but also the other isomers are listed in Table 1. Fish was the main exposure route in case of emission to the water, while leafy vegetable was the main expousre route in case of emission to the air.

Table 1 Intake fractions of HBCDs caused by emission to air or water

Exposure route		alpha		beta		gamma	
		Emission to air	Emission to water	Emission to air	Emission to water	Emission to air	Emission to water
alpha	Inhalation	2.48E-06	5.17E-12	2.73E-07	8.92E-13	4.87E-07	1.84E-13
	Drinking water	2.03E-09	1.43E-08	3.93E-10	3.94E-10	5.09E-10	4.92E-10
	Soil ingestion	4.37E-08	9.15E-14	4.12E-08	1.15E-13	3.11E-08	3.89E-15
	Fish	1.28E-05	9.01E-05	2.48E-06	2.49E-06	3.21E-06	3.10E-06
	Leafy vegetable	9.21E-04	1.93E-09	8.23E-04	2.31E-09	6.27E-04	8.11E-11
	Root vegetable	1.75E-04	3.67E-10	1.65E-04	4.63E-10	1.25E-04	1.56E-11
	Meat	1.21E-04	1.04E-09	1.08E-04	3.26E-10	8.26E-05	3.76E-11
	Milk	3.21E-05	2.75E-10	2.87E-05	8.64E-11	2.19E-05	9.97E-12
beta	Inhalation	3.94E-08	1.09E-13	2.43E-06	6.67E-12	8.98E-08	4.40E-14
	Drinking water	5.34E-11	5.53E-11	1.58E-09	1.36E-08	7.97E-11	8.37E-11
	Soil ingestion	6.26E-09	1.31E-14	6.68E-09	1.87E-14	4.54E-09	5.70E-16
	Fish	3.72E-07	3.85E-07	1.10E-05	9.51E-05	5.55E-07	5.83E-07
	Leafy vegetable	1.30E-04	2.73E-10	2.00E-04	5.57E-10	9.59E-05	1.29E-11
	Root vegetable	2.50E-05	5.23E-11	2.66E-05	7.45E-11	1.81E-05	2.27E-12
	Meat	1.88E-05	4.28E-11	2.89E-05	9.01E-10	1.38E-05	6.89E-12
	Milk	4.98E-06	1.13E-11	7.66E-06	2.39E-10	3.67E-06	1.83E-12
gamma	Inhalation	7.55E-08	1.58E-13	8.46E-08	2.37E-13	3.53E-06	1.39E-14
	Drinking water	3.43E-11	5.08E-11	3.53E-11	5.33E-11	6.33E-10	9.28E-09
	Soil ingestion	6.58E-09	1.38E-14	6.30E-09	1.77E-14	5.05E-09	5.87E-16
	Fish	8.16E-07	1.21E-06	8.40E-07	1.27E-06	1.51E-05	2.21E-04
	Leafy vegetable	2.33E-04	4.87E-10	2.23E-04	6.26E-10	1.79E-04	2.08E-11
	Root vegetable	2.49E-05	5.21E-11	2.38E-05	6.68E-11	1.91E-05	2.22E-12
	Meat	9.69E-05	2.12E-10	9.28E-05	2.70E-10	7.46E-05	1.62E-09
	Milk	2.57E-05	5.61E-11	2.46E-05	7.14E-11	1.98E-05	4.29E-10

Acknowledgements
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