COMPARISON OF OBSERVED AND ESTIMATED CONCENTRATIONS OF PERFLUOROOCTANE SULFONATE (PFOS) USING A FATE MODEL IN TOKYO BAY OF JAPAN

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Introduction

Perfluorinated compounds (PFCs) such as perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA) have received worldwide attention because of their environmental persistence and widespread distribution. Fire-fighting foam formulations, including aqueous film forming foams (AFFFs) containing perfluoro-alkanesulfonate salts and perfluorocarboxylates are well-known as an potential source of PFCs[1]. Due to fire accidents where large amounts of AFFFs were used, PFCs have been accidentally released to soil and water matrices, particularly to the bays and oceans[1-3]. In that case, it required monitoring surveys of PFCs for long periods of time to assess the water contamination by the accidentally release of PFCs. Thus, there is a need to estimate the concentrations of PFCs continuously after the accidents. One possibility for the effective estimation of concentrations is the use of a simulation model combined with information on the amount of emission or usage. Although a fate model, which is capable of estimating the concentrations of tributyltin[4,5], copper pyrithione[6], and polychlorinated dioxins[7] in Tokyo Bay, Ise Bay, and Seto Inland Sea, have been developed at the National Institute of Advanced Industrial Science and Technology, Japan (AIST), the estimation accuracy of surfactants such as PFOS still remains unclear.

In this study, the fate model (National Institute of Advanced Industrial Science and Technology - The Risk Assessment Model: AIST-RAM) and PFOS fluxes from certain river to Tokyo Bay were used for the estimation of PFOS concentrations in water and sediment of Tokyo Bay. The observed concentrations of PFOS were compared with the estimated concentrations from the AIST-RAM for Tokyo Bay combined with the PFOS flux data. The accuracy of estimation by the AIST-RAM was determined.

Materials and Methods

Sampling and calculating point. Tokyo Bay was selected as calculation area for estimating PFOS concentration in water and sediment, due to the wealth of information on PFOS fluxes from major rivers, such as Edo River, Naka River, Ara River, Sumida River, Tama River, and Tsurumi River, to Tokyo Bay. Samples of water and sediment in Tokyo Bay were collected by Odaka and Masunaga[8], and the sampling and calculating points are shown in Figure 1.

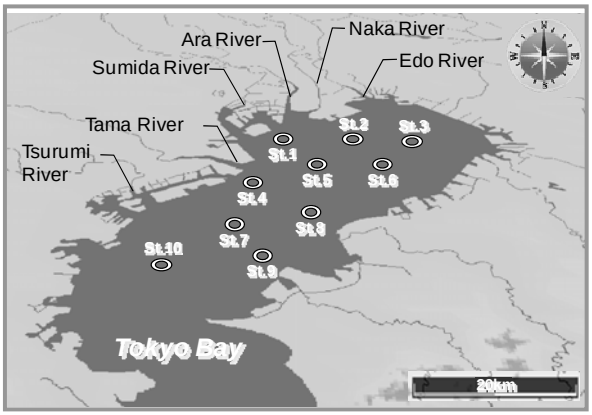

Figure 1 Sampling and calculating points

Estimation model of PFOS concentration. The AIST-RAM (National Institute of Advanced Industrial Science and Technology - The Risk Assessment Model) for Tokyo Bay (Ver. 1.3) was one of the 3-D chemical fate prediction model, by incorporating the chemical fate model, the databases of seasonal flow fields, and distributions of organic substances (phytoplankton and detritus) in Tokyo Bay. The AIST-RAM was used for calculating the concentrations of PFOS in the water and sediment of Tokyo Bay. For the calculation, the AIST-RAM required parameters such as PFOS flux, biodegradation rate, decomposition rate in sediment, sinking rate of phytoplankton, detritus, and inorganic suspended substances, logarithmic partition coefficient normalized to organic carbon content (log Koc), and adsorption rate of phytoplankton, detritus, and inorganic suspended substances.

Results and Discussion

Input parameters for calculating concentrations using the AIST-RAM. The PFOS fluxes calculated from the values described in the literature[8] were used. The biodegradation rate and decomposition rate in sediment used in this study were 0 s^{-1}, because it has not shown any degradation for PFOS in tests of hydrolysis, photolysis or biodegradation in any environmental condition tested[9,10]. The default values in the AIST-RAM were selected for the sinking rate of phytoplankton, detritus, and inorganic suspended substances, due to no effect of physicochemical properties of chemicals to these values. The log Koc for PFOS was reported to be 2.57–3.1[11] and 2.98–3.49[12]. A value of 3 within the range of reported values was selected. The adsorption rate for PFOS has been previously unreported. In the case where the value varied from 2×10^{-7} to 2×10^{-1} s^{-1}, the estimated concentrations of PFOS in seawater varied only slightly within approximately 8%. Therefore, the value of 2×10^{-5} s^{-1} was used as the default value for tributyltin (log Koc = 5)[5] was selected for the adsorption rate of PFOS. However, the values for the adsorption of PFOS on inorganic suspended substances were set to be 0 because the adsorption on inorganic suspended substances was negligible compared with those on phytoplankton or detritus. The input parameters for the calculations by the AIST-RAM are given in Table 1.

Table 1 Input parameters for calculating concentrations using the AIST-RAM.

Input	Contents		Unit
PFOS flux	**Edo River**	0.026	kg/day
	Naka River	0.026	kg/day
	Ara River	0.093	kg/day
	Sumida River	0.073	kg/day
	Tama River	0.287	kg/day
	Tsurumi River	0.093	kg/day
Biodegradation rate		0	1/s
Decomposition rate in sediment		0	1/s
Sinking rate	**Phytoplankton**	0.000200	cm/s
	Detritus	0.000579	cm/s
	Inorganic suspended substances	0.000579	cm/s
Logarithmic partition coefficient normalized to organic carbon content [Log Koc]*	**Phytoplankton**	3	-
	Detritus	3	-
	Inorganic suspended substances	0	-
Adsorption rate**	**Phytoplankton**	0.00002	1/s
	Detritus	0.00002	1/s
	Inorganic suspended substances	0	1/s

***** : This value was described in 3M (2000) and Yu et al. (2009)

****** : The default value in the AIST-RAM model was used.

Comparison of observed concentration with estimated concentration.

The observed and estimated concentrations of PFOS in the surface, intermediate, and bottom seawaters and sediment in Tokyo Bay are summarized in Table 2. The distributions of PFOS concentrations in the surface seawater estimated by the AIST-RAM is shown in Figure 2 as an example.

The observed concentrations of PFOS ranged from 2.0 to 7.3 ng/L for surface seawater, 2.2 to 5.7 ng/L for intermediate seawater, 1.5 to 5.7 ng/L for bottom seawater, and 0.3 to 0.9 ng/g for sediment. Location St.1, was close to the estuary of Ara River, Sumida River, and Tama River which are main emission source of PFOS, was shown to be the most contaminated area. The concentrations of PFOS at Location St.7, St.9, and St.10 were relatively lower in seawater and sediment from other locations, due to the connection with the Pacific Ocean.

The ratios of the calculated concentrations to the observed concentrations ranged from 0.79 to 1.8 for surface seawater, 0.73 to 1.4 for intermediate seawater, and 0.59 to 1.3 for bottom seawater. The margins of error were relatively unaffected by a change in layers of seawater. Results indicated that the AIST-RAM involved a high degree of accuracy for estimating the concentrations of PFOS in seawater. In the case of sediment, the ratios of the calculated concentrations to the observed concentrations ranged from 0.88 to 2.8, the estimations of PFOS concentrations in sediment by the AIST-RAM had a relatively larger margin of error than those in seawater. However, our results indicated that the AIST-RAM allowed the estimations of PFOS concentrations in seawater and sediment in Tokyo Bay with satisfactory accuracy.

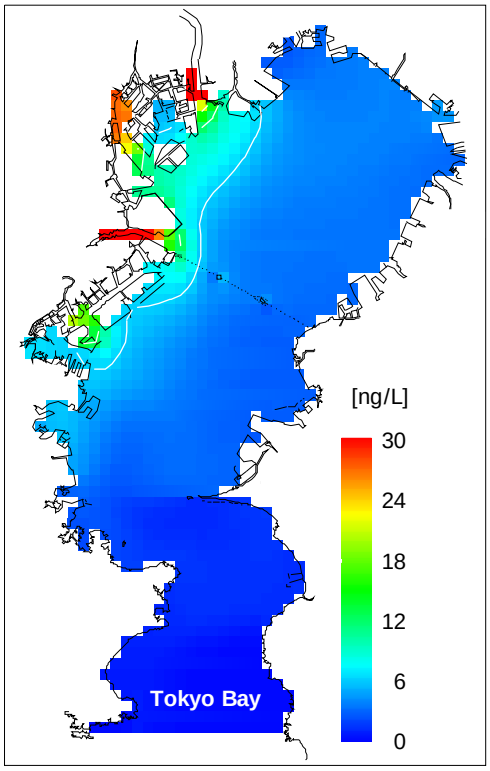

Figure 2 The distributions of PFOS concentrations in the surface seawater estimated by the AIST-RAM

Table 2 Observed and calculated concentrations of PFOS in water and sediment of Tokyo Bay

	Observed concentration				Estimated concentration			
	Surface [ng/L]	Middle [ng/L]	Bottom [ng/L]	Sediment [ng/g]	Surface [ng/L]	Middle [ng/L]	Bottom [ng/L]	Sediment [ng/g]
St.1	7.3	5.7	5.7	0.4	8.1	6.3	3.3	1.03
St.2	-	-	-	0.9	-	-	-	0.79
St.3	3.0	4.8	3.4	0.7	3.7	3.5	2.6	0.70
St.4	3.4	3.6	2.0	0.4	4.9	4.6	2.1	0.64
St.5	3.8	3.4	2.9	0.6	4.1	4.2	2.2	0.62
St.6	-	-	-	0.6	-	-	-	0.53
St.7	2.0	2.6	1.5	0.4	3.7	3.5	2.1	0.66
St.8	5.0	3.3	2.8	0.4	3.9	3.1	2.0	0.57
St.9	3.4	3.5	1.8	0.5	3.3	3.2	2.1	0.64
St.10	2.6	2.2	1.8	0.3	2.9	2.8	2.4	0.85

Furthermore, because the observed concentrations of PFOS in Tokyo Bay were comparable to the concentrations estimated from the PFOS fluxes of 6 major rivers such as Tama River and Tsurumi River, other emission sources of PFOS such as rain directly falling in Tokyo Bay could be negligible compared with the PFOS fluxes from the major rivers to Tokyo Bay.

Acknowledgement

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