Study of Indicator Isomer in Dioxin Analysis

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Introduction

Analytical results of polychlorinated dibenzo-*p*-dioxins and polychlorinated dibenzofurans (PCDDs/PCDFs) are reported by the summation of toxic equivalents, expressed as 2,3,7,8-TeCDD (TEQ), of 2,3,7,8-PCDDs/PCDFs. These TEQ values are obtained through the complicated pretreatment and analysis procedures, which require the high-cost chemicals and equipment such as labeled isotopes and high resolution gas chromatograph/high resolution mass spectrometer (HRGC-MS). Due to these reasons, simple analytical or substituting methods, which are quicker than conventional methods, have been proposed in order to save the analytical time and cost.
Authors reviewed the past several years' data of PCDDs/PCDFs from a variety of environmental media such as flue gases and ambient air, so that we could find that an established distribution profiles existed among 17 kinds of 2,3,7,8-congener by environmental media. Thus, in this study, we would suggest any possibility to find the representative indicating congener, which is available for simply estimating TEQ or total concentrations of PCDDs/PCDFs and developing the fate model for PCDDs/PCDFs in environment. In addition, conversion coefficient of I-TEQ value into WHO-TEQ also reviewed through the correlation analysis for the comparison of TEQ data, because many countries use WHO-TEQ value as PCDDs/PCDFs concentrtion, including co-planar PCB's WHO-TEQ as well. [1)]

Material and Methods

PCDDs/PCDFs concentrations of incinerators, either controlled or uncontrolled, and ambient airs, listed in this paper, were the results analyzed by Korean Standard Testing Method for Dioxins and Furans.[2)] PCDDs/PCDFs were analyzed by HRGC/HRMS (Micromass Co., Autospec Ultima) above 10,000 resolution with an SP-2331 column of 60m × 0.32mm ID × 0.25um for PCDDs/PCDFs. Toxic equivalents, expressed as 2,3,7,8-TeCDD (TEQ), were calculated by using the international toxicity equivalency factor (I-TEF).[3)]

Table 1. PCDDs/PCDFs data, used in this study

	Period	Number of data	Unit
Incinerator	1997 ~ 2002	Emission Gases: 587 Uncontrolled Gases: 94	ng I-TEQ/Nm^3 [O_2 = 12%]
Ambient air	1999 ~ 2002	219	pg I-TEQ/Nm^3

And, all PCDDs/PCDFs TEQ values of incinerators were to be converted into the normal state of 0°C and 1 atm, and corrected by 12 % of O_2. Types and numbers of data, used in this study, were listed in Table 1.

Results and Discussion

A. Distributing pattern of congeners

Distributing pattern of 2,3,7,8-PCDDs/OCDFs as I-TEQ values from incinerators was a similar to that in ambient air, as shown in Figure 1. Major contributing congeners were 2,3,4,7,8-PeCDF and 2,3,4,6,7,8-HxCDF, which were 35 ~ 39% and 11 ~ 13% of total TEQ values, respectively. In case of total concentration, a slightly different distributing pattern of congener from TEQ case was found in that major contributing congener were in order of OCDF, 1,2,3,4,6,7,8-HpCDF and OCDD in ambient air, and OCDD, OCDF and 1,2,3,4,6,7,8-HpCDF. Theses three dominant congeners averaged 64% to 68% of total 2,3,7,8- PCDDs/PCDFs concentrations, as shown in Figure 2.

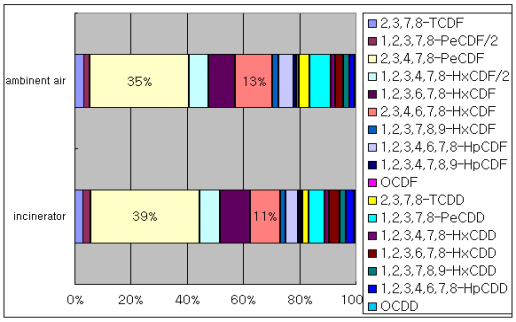

Figure 1. Distribution of 2,3,7,8-PCDDs/PCDFs as a TEQ concentration.

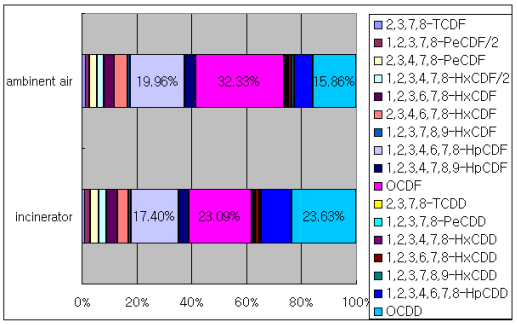

Figure 2. Distribution of 2,3,7,8-PCDDs/PCDFs as a total concentration.

B. Correlation of measured concentration with TEQ concentration

Good correlations with 0.92 ~0.94 of R^2 were observed between total and TEQ concentrations of PCDDs/PCDFs in both cases, as shown in Table 2.

Table 2. Correlations between total and TEQ concentration

	a	b	R^2
Incinerator	24.54	11.08	0.9474
Ambient air	25.16	-1.01	0.9216

$Y = ax + b$
y = Total concentration of 2,3,7,8-PCDDs/PCDFs (ng or pg/Nm^3)
x = TEQ concentration of 2,3,7,8-TCDDs/PCDFs (ng or pg I-TEQ/Nm^3)

C. Correlation of TEQ concentration of each isomer with total TEQ concentration

As shown in Table 3, correlations between each congener's TEQ value and total TEQ value were as good as more or less than 0.9 of R^2 in most congeners of both cases, except for OCDF in incinerator case and some congeners with about 0.75 of R^2 in ambient air case. The most correlating congener to total TEQ value, which had a highest R^2 value, was 1,2,3,6,7,8-HxCDF in

incinerator case and 2,3,4,7,8-PeCDF in ambient air case. In addition, correlation equation was expressed as y = ax + b, where x means TEQ value (ng or pg I-TEQ/Nm^3) of each congener, and y means total TEQ concentration.

Table 3. Correlations between each congener TEQ value and total TEQ value

	Incinerator			Ambient air		
	a	b	R^2	a	b	R^2
2,3,7,8-TCDF	39.50	-0.48	0.9857	33.33	-0.02	0.8945
1,2,3,7,8-PeCDF	31.54	0.59	0.9875	39.77	0.03	0.9773
2,3,4,7,8-PeCDF	2.53	0.12	0.9973	3.23	-0.05	0.9835
1,2,3,4,7,8-HxCDF	11.64	0.88	0.9935	10.28	0.10	0.9295
1,2,3,6,7,8-HxCDF	9.08	0.22	0.9981	10.86	-0.01	0.9667
2,3,4,6,7,8-HxCDF	10.57	-0.77	0.9760	6.77	0.03	0.9480
1,2,3,7,8,9-HxCDF	47.37	0.60	0.9924	19.01	0.21	0.7686
1,2,3,4,6,7,8-HpCDF	21.98	-0.03	0.9730	16.74	0.03	0.9173
1,2,3,4,7,8,9-HpCDF	95.55	0.39	0.9792	75.09	0.09	0.9343
OCDF	104.31	2.36	0.3257	76.56	0.13	0.8054
2,3,7,8-TCDD	59.08	-1.89	0.8927	20.56	0.08	0.7565
1,2,3,7,8-PeCDD	19.64	-0.80	0.9808	11.51	0.04	0.8757
1,2,3,4,7,8-HxCDD	70.99	0.06	0.9936	60.29	0.05	0.8522
1,2,3,6,7,8-HxCDD	21.85	0.78	0.9782	32.99	0.02	0.9501
1,2,3,7,8,9-HxCDD	50.42	-0.21	0.9828	32.89	0.09	0.9109
1,2,3,4,6,7,8-HpCDD	29.20	1.02	0.9687	51.02	0.02	0.9473
OCDD	137.29	0.96	0.9616	181.24	0.07	0.7601
PCDFs	1.22	0.05	0.9995	1.25	0.00	0.9944
PCDDs	5.39	-0.12	0.9897	4.48	0.03	0.9233

D. Correlations between I-TEQ and WHO-TEQ values

Conversion factors, expressed as y = ax + b, were obtained for purpose of converting a I-TEQ into a WHO-TEQ, and its values were 1.04 in incinerator case and 1.06 in ambient case with R^2 of 0.999.

Table 4. Correlations between I-TEQ and WHO-TEQ values

	a	b	R^2
Incinerator	1.04	0.03	0.9999
Ambient air	1.06	0.00	0.9991
WHO-TEQs = a × (I –TEQs) + b			

Reference

1. About Indicator of Dioxin Analysis, Japan Society for Environmental Chemistry, 2000, pp170-171
2. Ministry of Environment, Republic of Korea, 1996. The Korean standard testing method for dioxins and furans.

3. U.S. EPA Method 1613 Revision B, (1996) Tetra-Through Octa-Chlorinated Dioxins and Furans by Isotope Dioxins and Furans by Isotope Dilution HRGC/HRMS.