Assessment of environmental behavior of PCDD/F using mathematical models

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Abstract

We applied the ISCLT3 model and the PRZM2 model to estimate the behavior of PCDD/F in air and the soil around a municipal solid waste incinerator without an electrostatic precipitator or a multicyclone in a rural area. By comparing calculated and monitored data, the transport process is confirmed as the dominant fate process in air. Although some uncertainty still remains, transformation and volatilization are the dominant fate processes in the soil. Based on the calculated soil accumulation factors, it is suggested that fly ash with aerodynamic diameters of 5～7 μm are emitted from the simulated incinerator. Generally, particles with aerodynamic diameters less than 10 μm can contribute to human exposure via inhalation.

1. INTRODUCTION

Because of their high toxicity, the assessment of the human health risk of polychlorinated dibenzo-*p*-dioxins (PCDDs) and dibenzofurans (PCDFs) released from municipal solid waste (MSW) incinerators has become an urgent issue for scientists and environmental regulators. Although some monitoring data on PCDD/F around MSW incinerators have been reported, it may be important not only to track their environmental behavior but also to assess risk of human exposed to them.

In this study, we apply computer simulation models to estimate the environmental behavior of PCDD/F around a MSW incinerator without an electrostatic precipitator or a multicyclone in a rural area (disposable capacity: 60 ton/day).

2. MODEL SIMULATION

The Industrial Source Complex Long Term model, version 3 (ISCLT3)[1] was used to simulate the annually averaged atmospheric behavior of PCDD/F around a MSW incinerator. These chemicals have been detected in the fly ash and flue gases of actual MSW incinerators, and the source profiles are characterized by an almost uniform profile of PCDD/F[2,3]. Therefore, we simulated atmospheric concentrations of PCDD/F in both gas and particle phases under the conditions listed in Table 1. The meteorological data file for the ISCLT3 model was prepared from data measured by the Tokyo District Meteorological Observatory from 1991 to 1996. The atmospheric transformation process was not considered in the model calculation.

Table 1 Input parameters for ISCLT3 model simulation

Parameter	Value
Release rate, μg(PCDD/F)/s	25
Stack height, m	55
Inner stack top diameter, m	4.0
Stack gas temperature, K	593
Stack gas exit velocity, m/s	0.4
Particulate diameter, μm	0(gas), 1～20
Particulate density, g/cm^3	1.5

Table 2 Soil parameters for PRZM2 model simulation

Parameter	Value
Pan factor	0.72
Minimum depth for evaporation, cm	15.0
Monthly daylight hour, hr	5.64 5.36 5.32 5.37 5.87 4.10 4.42 5.71 3.67 4.16 4.57 5.35
Soil erodibilty for USLE	0.30
Topographic factor for USLE	0.14
Practice factor for USLE	1.00
Average duration of rainfall, hr	4.00
Runoff curve number	64
Cover management factor for USLE	0.1
Total depth of soil core, cm	20.0
Diffusion constant, m^2/day	4.3×10^3
Enthalpy of vaporization, kcal/mole	20
Bulk density, g/cm^3	1.35
Initial soil water content, cm^3/cm^3	0.257
Field capacity, cm^3/cm^3	0.257
Wilting point, cm^3/cm^3	0.148
Organic carbon, %	4.5

The Pesticide Root Zone Model, version 2 (PRZM2)[4] was applied to estimate the behavior of PCDD/F in the soil. The values of input parameters for the soil are listed in Table 2.

The meteorological data file for the PRZM2 model was also prepared using data measured by the Tokyo District Meteorological Observatory. Chemical parameters for PCDD/F are listed in Table 3.

Table 3 Chemical parameters for PRZM2 model simulation[5]

Chemical	Henry's constant*	Koc, l/kg	DT50, days
2,8-DCDD	8.7×10^{-4}	1.6×10^{5}	230
2,3,7,8-TCDD	4.1×10^{-4}	1.2×10^{6}	710
1,2,3,4,7,8-HxCDD	1.9×10^{-4}	1.7×10^{6}	2290
OCDD	2.8×10^{-4}	1.2×10^{7}	2290
2,8-DCDF	2.6×10^{-3}	1.1×10^{5}	230
2,3,7,8-TCDF	6.0×10^{-4}	5.0×10^{5}	710
1,2,3,6,7,8-HxCDF	3.0×10^{-4}	4.0×10^{6}	2290
OCDF	7.9×10^{-5}	5.2×10^{6}	2290

*:Henry's law constant was calculated from water solubility and vapor pressure.

3. RESULTS

Figures 1 and 2 show annually averaged distribution of atmospheric concentrations of PCDD/F in gas and particle phases (diameter: 10 μm). As shown in the two figures, a high-concentration area appeared within 2km from the source. Furthermore, the annual concentration-distribution pattern for all years are very similar. The highest concentration of PCDD/F is about 12 pg/m^3 for gas and particle ($\leqq$ 10 μm) phases, which is in agreement with the concentrations measured around the simulated MSW incinerator (25 and 29 pg/m^3).

The PRZM2 calculations suggest that concentrations of less-chlorinated PCDD/F in the surface soil reach a steady state within 5 years; conversely, more than 10 years are required for HxCDD/F and OCDD/F. The dominant fate processes of PCDD/F in the soil are volatilization and transformation. Other processes such as leaching, surface runoff, and erosion do not contribute to its fate in the soil. Less-chlorinated PCDD/F tends to be more volatile and more degradable than more-chlorinated PCDD/F. Therefore, more-chlorinated PCDD/F tends to be more accumulative in the surface soil (Figure 3).

Although most of the TCDD/F, HxCDD/F and OCDD/F were suggested to be distributed in the surface soil layer (0～2 cm) in our simulation, Brzuzy and Hites reported that greater than 80% of the total PCDD/F was found in the upper 15 cm of soils collected from two geographical regions[6]. This discrepancy implies contributions of the macropore water flow and biological turbulence to the vertical transport of PCDD/F in the actual soil.

As described above, a precipitator such as EP or MC is not included the simulated MSW incinerator. Therefore, fly ash with large diameter is probably emitted. As shown in Figure 4, we relate soil accumulation factors to aerodynamic diameters of fly ash, based on the calculated concentrations of particle-phase PCDD/F in air and the soil. The soil accumulation factors measured around the simulated MSW incinerator are 1.0×10^7 and 1.7×10^7, which correspond to aerodynamic diameters of 5.3 and 7.0 μm , respectively. Generally, particles with aerodynamic diameters less than 10 μm can contribute to human exposure via inhalation.

4. CONCLUSIONS

By comparison of our calculation results and the monitoring data, it is confirmed that the transport process is the dominant fate process of PCDD/F around MSW incinerators. The transformation processes such as OH radical oxidation and direct photolysis might be significant during atmospheric transport of PCDD/F over long distances.

The rates of atmospheric deposition of PCDD in gas and particle phases are the key factors in determining the concentration of PCDD in the soil.

Although transformation and volatilization may be the dominant fate processes in the soil, some uncertainty still remains. Further studies are needed to obtain reliable values of some physicochemical properties and rate constants of transformation for typical homologues of PCDD/F.

5. REFERENCES

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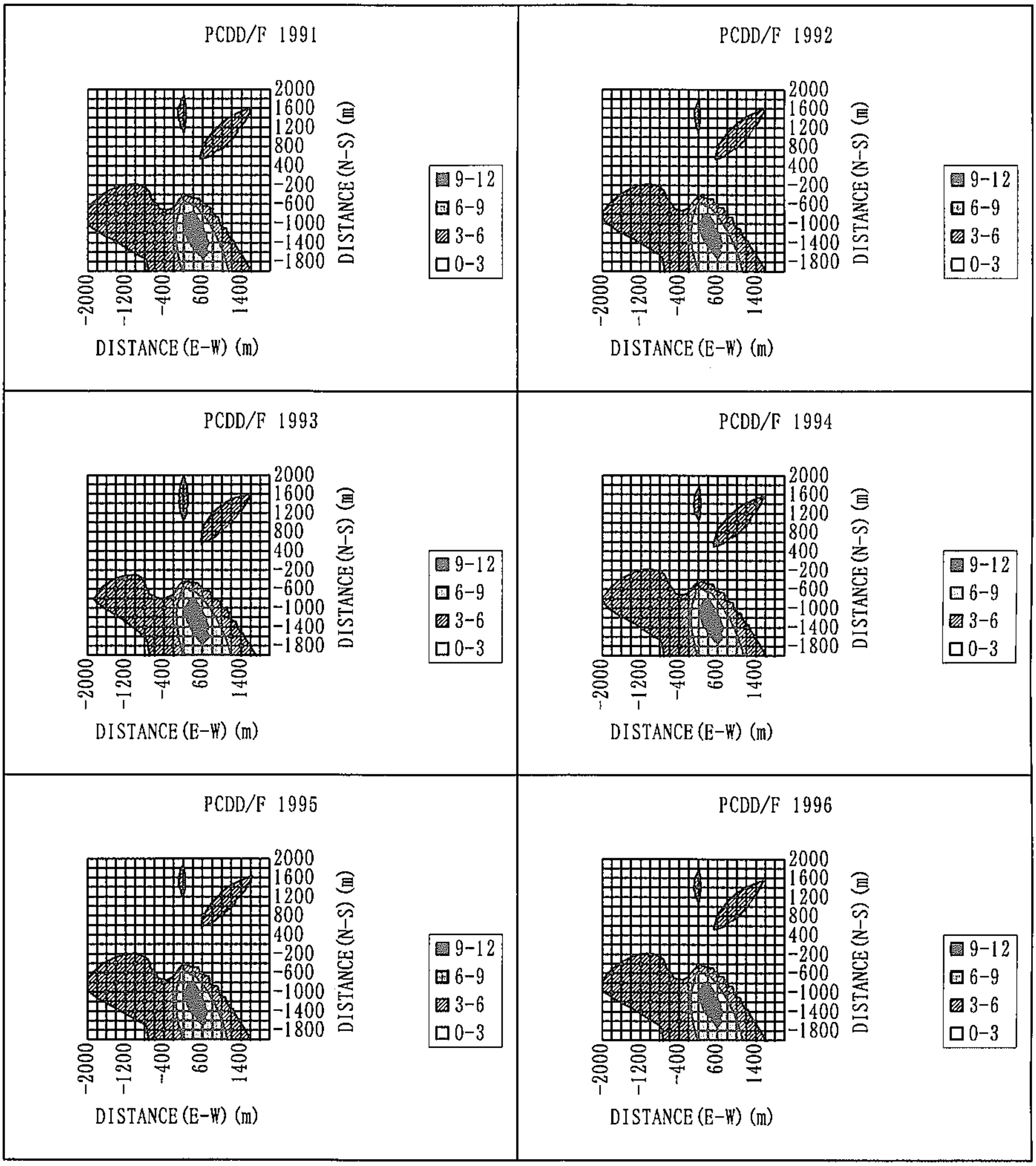

Figure 1 Concentration-distribution profiles of gaseous PCDD/F around the MSW incinerator

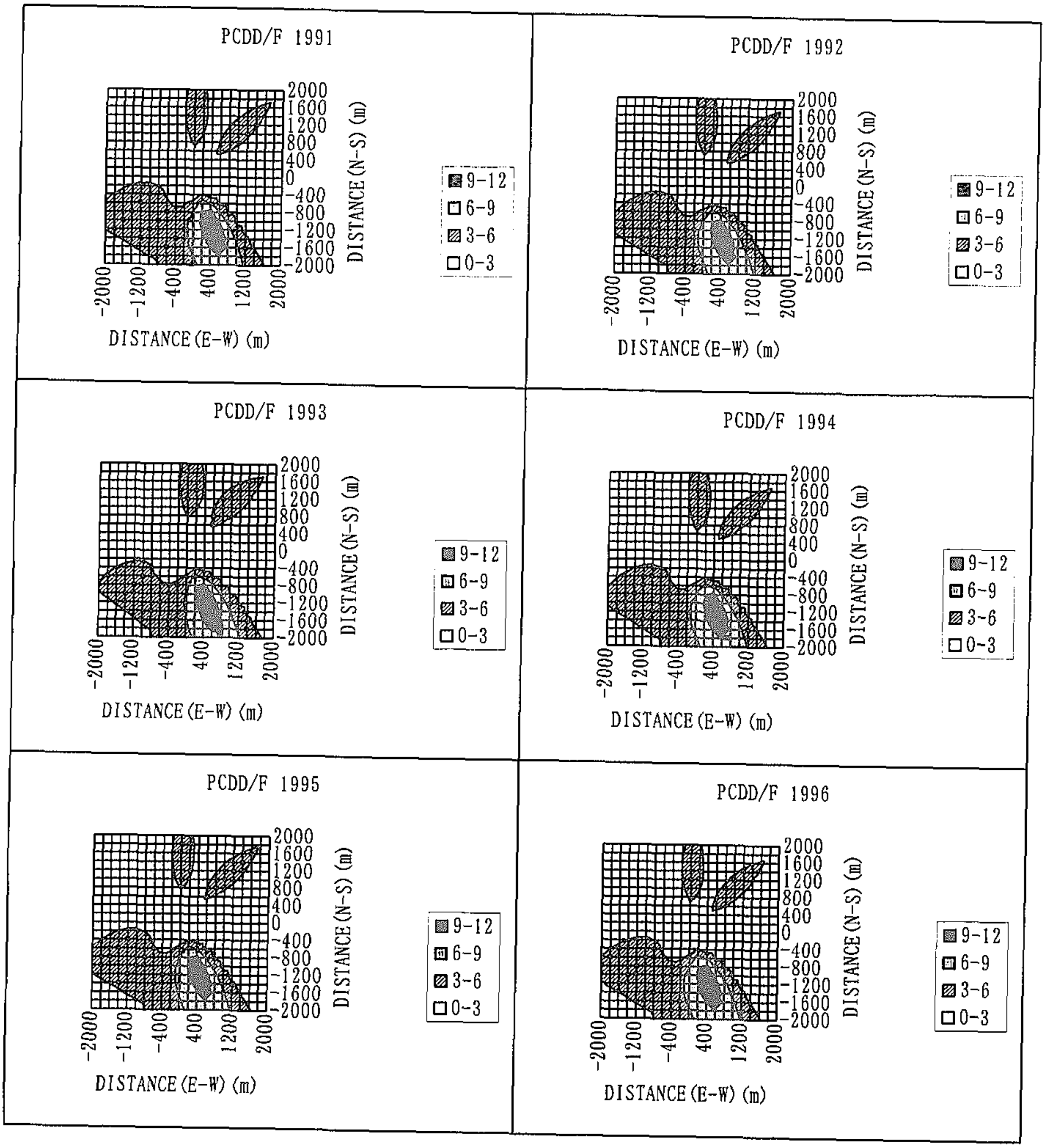

Figure 2 Concentration-distribution profiles of PCDD/F adsorbed onto 10 μm-diameter particles around the MSW incinerator

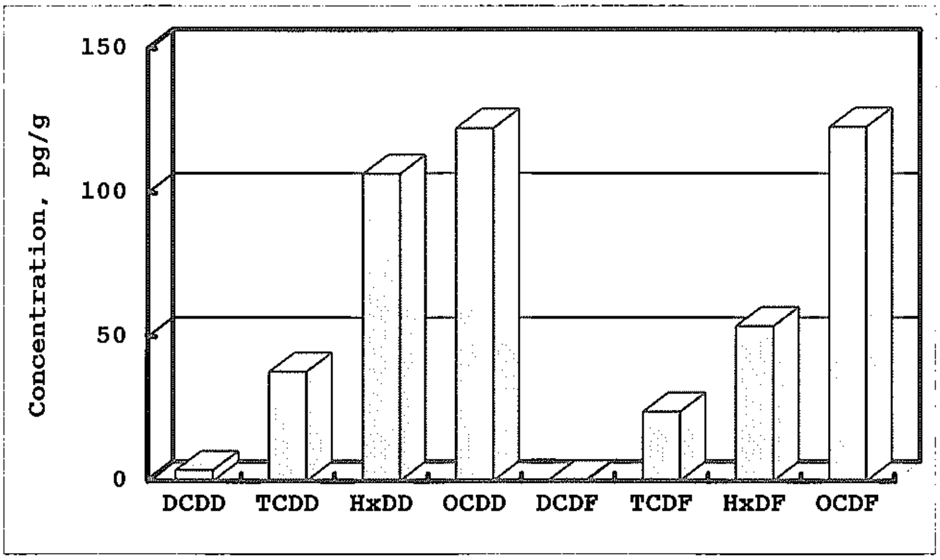

Figure 3 Relative concentrations of some PCDD/F compounds under the steady state

assumed deposition rate: 8.8 $\mu g/m^2$/year for each PCDD/F

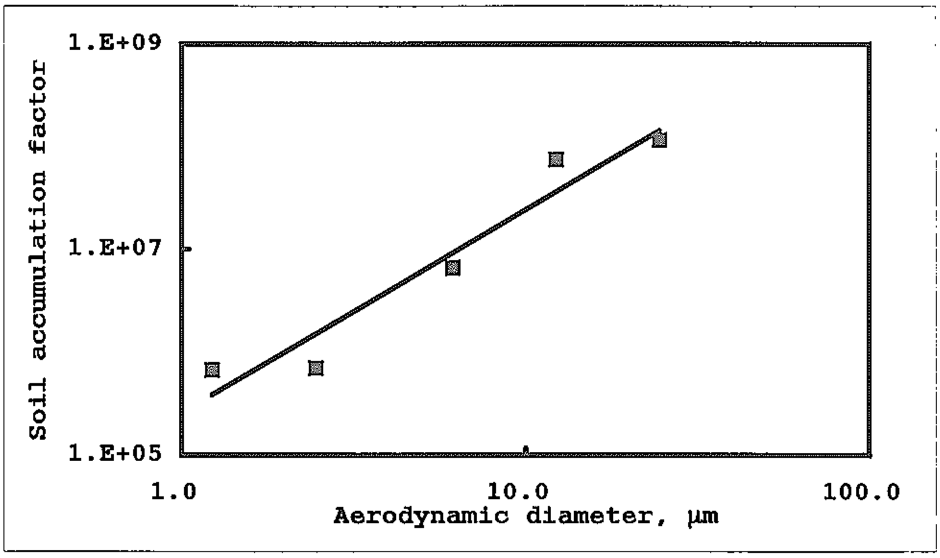

Figure 4 Relationship of soil accumulation factor to aerodynamic diameter of fly ash