SIMULATION OF MULTI-MEDIA TRANSFER AND FATE OF PCDD/Fs IN CHINA

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Abstract

The environmental behaviors of PCDD/Fs in China are simulated by level Ⅲ fugacity model. The considered compounds are 2,3,7,8-TCDD and OCDD, they are chosen among all 17 toxic PCDD/Fs for great physiochemical properties discrepancy. All simulated results are consistent with the measured ones. It shows that advection inflow of PCDD/Fs from atmosphere is main source. Our result also suggests that soil is the main sink of PCDD/Fs, and transportation from air to soil is dominating process. PCDD/ Fs concentrations in environmental media are sensitive to the temperature and precipitation through analyzing the sensitivity of all inputs. It can be predicted the variation of concentration and transport, by simulating the change of temperature and precipitation according the climate of China.

Introduction

With the performance of Implementation Plan for the Stockholm Convention on Persistent Organic Pollutants, the routine monitor of PCDD/Fs gradually plays an important role. While it is lack of enough data of PCDD/Fs in China at present, model becomes a fast and effective method. So far, it has developed a number of model approaches that broadly fall into two categories, box and chemistry transport models. An example of the former class is fugacity model. The models have been widely used. Such as, it is applied to simulate the concentrations in various bulk media with seasonal variation or emission rate in different regions (Chang et al., 2007) and other aspects (Mackay et al. 2000; MacLeod et al., 2001). The study mainly shows the work of using the level Ⅲ fugacity model to simulate the fate of PCDD/Fs in China and analyzes the influence of advection inflow and the process of transport.

Materials and Methods

Level Ⅲ fugacity model considers the whole region as a system, dividing it into four compartments (air, water, soil and sediment). The assumption that all environmental compartments are at thermodynamic equilibrium with respect to the chemical is now removed, but the system is still assumed to be at steady-state. The fugacity of each compartment isn't equal (Mackay et al., 2002; Yuan et al., 2002).

In this research, China is considered as investigated area. In the whole country, the environment reaches an approximate steady-state and non-equilibrium state on the condition of long-term stability of emissions. The data of emission is obtained from the PCDD/Fs inventory of The People's Republic of China National Implementation Plan for the Stockholm Convention on Persistent Organic Pollutants. The advection inflow parameter is set to 50fg I-TEQ/m^3 according to the minimum value of the ambient in Asia, which published in the First Regional Monitoring Report Asia-Pacific Region of Global Monitoring Plan for Persistent Organic Pollutants.

For the great discrepancy environmental fates between .2, 3, 7, 8-TCDD and OCDD, both of them are selected to stand for the whole instance of the environmental fate of PCDD/Fs in China.

The input parameters are list in Table1.

Regional parameter

	Area($10^{12}m^2$)	Depth(m)
Air	960	1500
Soil	942.53	0.22
Water	17.47	15.44
sediment	17.47	0.13

Emission (g TEQ/a)

Release	Total (g TEQ/a)	Rate (g TEQ/h)
Air	5042.4	0.5756
Water	41.2	0.0047
Soil	993	0.1134
Total	6076.6	0.6937

Advection inflow=50 fg I-TEQ/m3

Volume fractions (%)

Air	aerosol	5E-11
Water	Suspend particles	5E-06*
	fish	1E-06*
Soil	vapor	0.2*
	water	0.3*
	solid	0.5*
sediment	water	0.8*
	solid	0.2*

* is default value

Transport velocity（m/h）

Air side air-water MTC	2.25	Rain rate	6.28E-05
Water side air-water MTC	0.018	Aerosol dry deposition	10.8
Soil-air boundary layer MTC	5	Sediment deposition rate	0.0000005
Sediment-water diffusion MTC	0.0001	Sediment resuspension	0.0000002
Soil-air diffusion MTC	0.02	Soil-water runoff rate	0.00005
Soil-water diffusion MTC	0.00001	Soil-solids runoff rate	1E-08

The influential parameters of the model are identified by sensitivity analysis. The sensitivity coefficient is defined as

$$S = \frac{|Y_{1.01} - Y_{1.00}|/Y_{1.00}}{X_{1.01} - X_{1.00}/X_{1.00}}$$

$X_{1.00}$ and $Y_{1.00}$: values of input and output, $|Y_{1.01} - Y_{1.00}|$: variation of output when input vary 1%.

The results simulated by model，which depend on the input environmental parameters of the investigated area, could show the influence of the advection inflow and the main process of transport and the fate of PCDD/Fs. Through the sensitivity analysis, the sensitive parameters are temperature and precipitation; when they changed with the climate of China, the trends of concentration in air and amount of residue are predicted.

Results and Discussion

Table 2 two scenarios are compared.

	air(fg/ m^3)	soil(pg/g)	sediment(pg/g)
Prediction values(advection inflow=0)	1.23-7.75	0.00199-0.0199	0.00202-0.00794

Prediction values(advection inflow=50fg)	3.76-23.6	0.00375-0.0532	0.0562-0.194
Measured values	18-3030	0.017-7.307	1.91-3289600

From the table one can find the concentrations of PCDD/Fs considered advection inflow are about three times than the value of not considered advection inflow. It is obvious that the results of considered advection inflow are close to the minimum measured values. Advection inflow from other regions is a main source. It is coincide with Ruth's study. In the further study, more data should be collected about advection inflow to enhance the accuracy of the input, especially for the study in large scale and low inter-emission.

The inter-media transportation from air to soil is up to 93.1-94.5%, while the total transport rate is 1.492-1.15 E-03Kg/h, so the transportation from air to soil is the main process. It is because that, PCDD/Fs in air are mainly exist in aerosol particle (Li Y. M. 2008), it is easy to fall down by wet and dry deposition, and the soil area accounted for 98.18% of China land. So the PCDD/Fs are deposited from air and then mainly fall on the soil. At the same time, PCDD/Fs in soil have relatively low reaction and transport rate, so soil becomes the central reservoir of PCDD/Fs in China. It can be proved by the result of the model, 96.0%--98.3% of the residual PCDD/Fs are in the soil, while the others bulk only account for 1.7%-4%. So monitoring the concentration of PCDD/Fs in soil can reflect the pollution of the whole region.

The sensitivity analysis (Fig.1) shows that the sensitivity coefficients are temperature, precipitation, scavenging ratio and advection inflow concentrations. Temperature and precipitation are the most sensitivity parameters of meteorology (Fig.2). Obviously, the precipitation determines the wet deposition process.

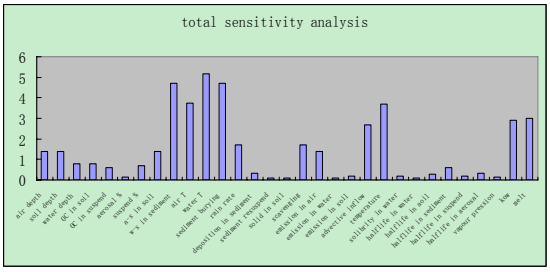


Fig.1

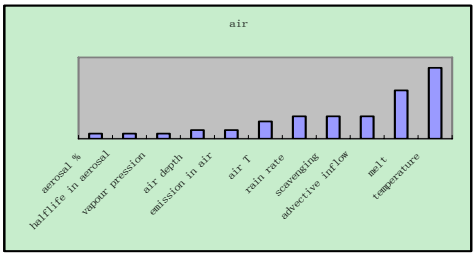
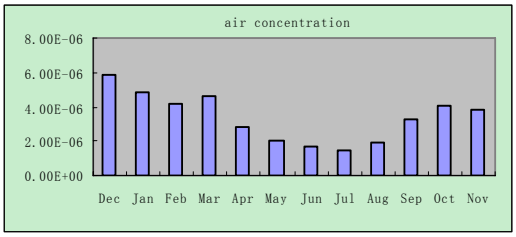
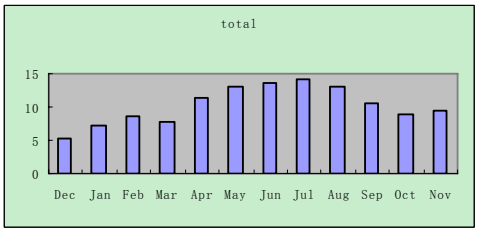


Fig.2

Considered the influence to the concentration of air from precipitation, the under graph shows that the concentration of the air goes down with the increase of the precipitation. As the wet deposition velocity of air goes up with the increased of the precipitation, the transportation of PCDD/Fs from air to soil is improved. As a result, the PCDD/Fs concentrations rose in the soil, water and sediment. At the other hand, the total burden of the environment in investigated area is increased, because the mobility of the other bulk was weaker than air. The follow plots illustrate that the concentration of PCDD/Fs in the water, soil and sediment, increase with the precipitation, but it shows inverse trend in the air.

The mean of monthly temperature and precipitation in china, is used to simulate the variation of concentration and transport along with the change of temperature and precipitation in China. It was found that under the climate condition of July, the PCDD/Fs concentration in air reaches minimum, and the amount of residue reaches maximum, and in the condition of Dec, the results are on the contrary. The PCDD/Fs concentration in air is law in the weather of higher temperature and more precipitation.





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