

# Risk Assessment of Toxic Chemicals in the Environment using Cross-Media Fate Models

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**Abstract** In recent years, the methodologies of risk assessment and risk management regarding toxic chemicals are getting authorized. In the risk assessment process, it is important to know the concentration of each chemical in order to estimate the exposure to human bodies and/or ecosystems. However, measurements with sufficient spatial and temporal coverage are so difficult that model calculations are useful for making up. This paper reports some results of calculations using some numerical models developed by authors. These models are based on the "cross-media approach" including atmosphere, hydrosphere, soil and sediment. Furthermore, the results of some case studies of the risk assessment are shown, in which the importance of the atmospheric process is pointed out. The largest difficulty in such a calculation is the shortage of observation data for validations. In addition, difficulties are also lying in getting emission inventories and in determining the parameters of the intermedia transfer. The perspective of these problems is also discussed.

## 1. INTRODUCTION

It is well known that many kinds of chemical compounds are emitted into the environment by industrial and human activities. Most of them have more or less toxicity. In recent years, the toxicity has been given much attention in association with their effects on human health and ecosystems. The problem of such a chemical risk is one of the most important parts of environmental problems all over the world. From the historical review, one of the typical examples is the death of many seals in North Sea, and another is the appearance of many malformed birds around the Great Lakes in the USA. These are both considered to have originated from polychlorinated biphenyls. These typical examples are lying in the seawater or landwater systems, however, the groundwater contamination and/or atmospheric pollution by these toxic chemicals, especially chlorinated organic compounds, have been getting more serious. Many of them are considered to be carcinogens, however, sufficient countermeasures have not been taken yet.

To plan the effective countermeasures against such problems, some case studies of risk assessments and risk managements have been carried out within these ten or twenty years. The most famous example is the study by US-EPA, in which following points are pointed out:

- 1) The cross-media approach is necessary because these pollutants easily transfer from media to others.
- 2) Model calculations of the concentration of each chemical are useful to know their spatial distribution.

The authors have reported the results of trial calculations of the concentration of some organic chemicals using a three dimensional cross-media model in our previous paper, and the result of a case study for the estimation of human risk by these chemicals was also reported.

In this paper, some recent studies on the risk assessment and risk management in Japan are reviewed. And that is followed by the discussion on the trend of numerical modeling approaches regarding air toxic problems. Finally, some results of modeling studies by authors are shown.

## 2 HISTORY OF RISK ASSESSMENT AND RISK MANAGEMENT IN JAPAN

The concepts of risk assessment and risk management are first proposed in the field of safety engineering, regarding some accidents in the various kind of chemical industries. Such kinds of risk by accidental releases or explosions are much different from the problem discussed here. These activities to prevent accidental risks are of course important, however, the problem described here is also important and more complicated. It usually originates in the regular activities to produce chemicals in the chemical plants and to consume them everywhere including our home. That may be the main reason why such a problem is difficult for governments to act on.

The first example of the integrated risk assessment in Japan using model calculations was appeared in 1989 by Japan Environment Agency. The procedure used in the study was almost same as that in the case study by US-EPA. Some other

studies can be found, however, they can not be called integrated risk assessment because they do not cover all of risk assessment processes.

Furthermore, the risk management process is much more complicated because it relates to many fields such as economics, sociology, jurisprudence, technology etc. Consequently, the methodology on the risk management is not sufficiently studied in Japan. It may take more and more time to establish the method.

Other kinds of studies regarding toxic chemicals are carried out by some Japanese researchers. They are concentrated in the estimation of human risk by the chemicals in the atmosphere on the nationwide basis. In many cases, the risk is represented by cancer risk. Other type of risk can not be quantified because of the lack of the experimental data. Most typical example of such studies is by Nakanishi, showing the life-cycle cancer risk by many chemical species. Table 1 shows a part of her results.

Table 1 Estimated cancer risk throughout life by selected chemical species.(Nakanishi, 1995)

Name of Species	Estimated annual cancer risk (persons/y)	
	United States	Japan
Arsenic	68	14
Chromium(VI)	147ü 255	21
Asbestos	88	--
Benzene	181	133
Chloroform	115	<1
Formaldehyde	124	53
Dioxin	2ü 125	16
1,3-Butadiene	256	--
Gasoline vapor	124	--

### 3. CHEMICAL RISK IN THE ATMOSPHERE

Table 2 Estimated risk for each compound and media, indicated as a probability of getting cancer.

Component	Media			
	Atmosphere	Surface Water	Ground Water	Sea Water
Trichloroethene	2.1×10(-7)	2.6×10(-10)	3.8×10(-9)	4.8×10(-9)
Tetrachloroethene	3.1×10(-7)	1.2×10(-9)	5.9×10(-9)	1.2×10(-7)
Benzene	7.2×10(-5)	6.6×10(-10)	9.8×10(-10)	1.1×10(-9)
Carbontetrachloride	4.3×10(-5)	--	--	--
1,2-dichloroethane	5.6×10(-5)	--	--	--
Chloroform	3.1×10(-5)	1.4×10(-8)	2.3×10(-7)	2.1×10(-8)
Benzo(a)pyrene	8.2×10(-6)	--	--	--
Total	2.1×10(-4)	1.6×10(-8)	2.4×10(-7)	1.5×10(-7)

### 4. STATUS OF MODELING STUDIES ON AIR TOXICS IN JAPAN

Risk assessment should be ideally based on the measurement of each toxic chemical in the actual environment, however, it is very difficult to satisfy the temporal and spatial coverage only by the measurements. Computer calculations using numerical models are suitable, at least partly, for fulfilling the shortage of measurements.

As previously described, risk by toxic chemicals was first noticed as a problem in the hydrosphere. Before 1980s, at least in Japan, most events of contamination or pollution by toxic chemicals reported by mass-media are dominated by hydrosphere problems. However, some results of the case studies indicate that such a risk is dominated by atmospheric processes rather than hydrospheric or other processes. In recent years, the chemical risk is getting popular and it is considered as an "atmospheric problem". A case study was carried out by authors. Table 2 shows the typical result of our study. This result is calculated using some measurement data and some estimated value by model calculations. The detail of our model calculation is described in our previous paper and briefly explained in the following section.

From these results, the priority of the risk can be assessed as follows:

1) Compounds:

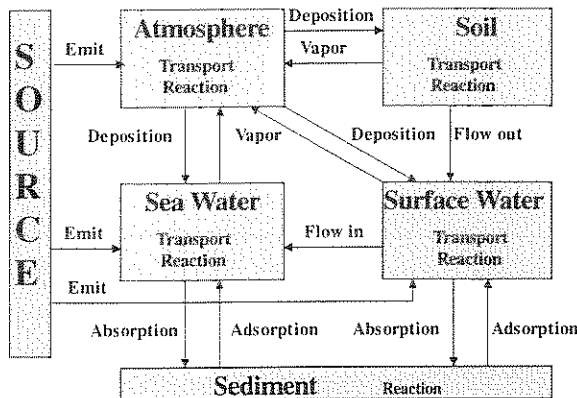
Benzene ≅ 1,2-Dichloroethane >> Chloroform  
 ≅ Carbontetrachloride > Benzo(a)pyrene  
 > Trichloroethene ≅ Tetrachloroethene

2) Media:

Atmosphere >> Groundwater ≅ Seawater  
 > Surfacewater > Marine products

As well known, the atmospheric pollution problems are mainly dominated by automobile exhausts, which include remarkable concentration of benzene. This fact strongly supports the hypothesis that the atmospheric process is dominant among many media regarding toxic chemicals' problem.

Modeling studies are widely used in atmospheric sciences in Japan. However, very few studies can be found regarding the modeling on the behavior of air toxics. In this section, a history of such a modeling study is firstly described, and a recent model by authors is shown as an example.



#### 4.1 History of the Modeling Studies on Air Toxics in Japan

As previously described, numerical models on the behavior of toxic chemicals are necessary to include cross-media approach. Such a model is called "fate model". The first example of the fate model in Japan is developed by Environment Agency of Japan. This model includes six media such as atmosphere, surface water, groundwater, seawater, soil and sediment. Case studies were carried out in the spatial scale of 100km×100km with the grid size of 5km×5km. Relatively large numbers of studies have been reported regarding the transfer of chemicals through the boundary of two media such as water surface.

The second model was developed by authors. The outline of the model is described in Figure 1.

Figure 1 Outline of the non-equilibrium model

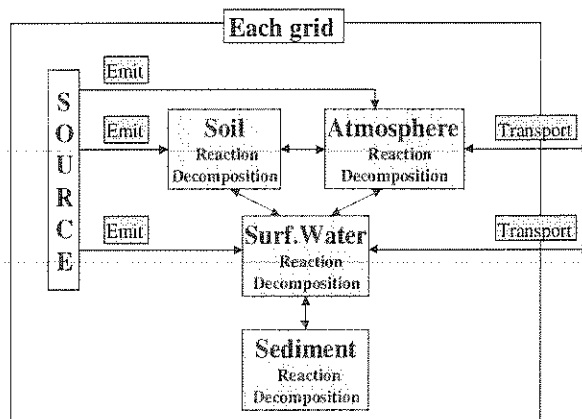
A case study was carried out using the model in the scale of 12km×12km with the grid size of 1km×1km. The result is summarized in Table 2. This model is based on the atmospheric transport model with high spatial resolution. These two models can give a temporal variation of the concentrations of chemicals, however, such a variation is not very important when the long term risks such as carcinogenicity are discussed. In addition, the characteristic of these models is the necessity of a large volume of calculation and computation time. From these viewpoints, the authors started to develop another type model that aims to calculate the long term average concentrations of chemicals based on the assumption of the equilibrium between media. Such a trial was formerly carried out by some researchers in Japan, however, most of them are aimed at spatially averaged concentrations, and are not suitable for the assessment of spatial distribution of the risk. In general, the concentration of air toxic has steep spatial variation. That is why the spatial resolution is necessary for model calculations. The example by

the authors has a feature that the spatial distribution is considered in the equilibrium model.

#### 4.2 Semi-Equilibrium Model with Spatial Resolution

In general, the equilibrium type model has an assumption that the concentrations of the species are spatially uniform. The authors tried to develop another type model. In this model, the objective area is divided by the grids and the assumption of equilibrium holds good in each grid. Such a subgrid equilibrium is disturbed by the transportation between a pair of grids and emission from the sources, then the equilibrium is calculated again. The basic concept of this "semi-equilibrium model is shown in Figure 2. Four media, atmosphere, surface water, soil and sediment were considered. Of course, groundwater is also an important environmental medium. However, it was neglected because the model development is still on the preliminary stage.

The compartment of atmosphere was assumed vertical uniformity. The size of the whole area of trial calculation is approximately 12km×12km and the size of each grid is approximately 1km×1km. The atmospheric transport was calculated using the meteorological data obtained from three stations in the objective area, and the surface water transport was calculated using water flow data of each river.



The typical results of the trial calculations are shown in Figure 3(a) and 3(b). From these figures, following points can be said.

1) Calculation is generally under-estimating. The underestimation seems to be mainly related to following items:

- # Missing data in the emission inventory
- # Background concentration that is originated in the sources in other areas.

2) Calculated spatial variation is fairly consistent with observations. That means the propriety of the transport calculation in the model.

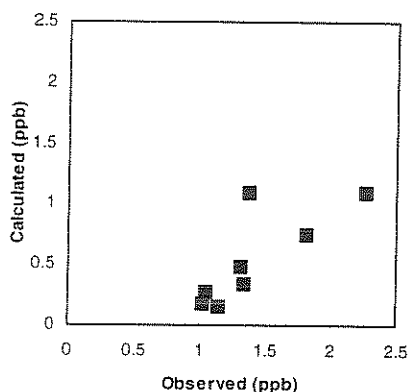


Figure 3(a). Comparison of observation and calculation (Benzene)

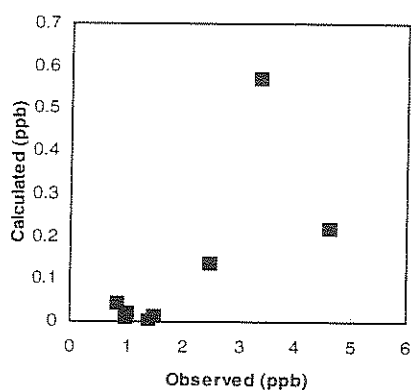


Figure 3(b). Comparison of observation and calculation (1,1,1-Trichloroethane)

#### 4.3 Remaining Problems

The largest difficulty in developing a model is the shortage of observational data for the model validation. They are ideal when sufficient coverage and resolution both spatially and temporally is available. Recently, some high performance analyzers such as GC/MS have been generally used. However, it is not easy to satisfy the above-mentioned necessities because it takes much labor and much cost. Developments in the analytical techniques are highly desired.

Second problem related to data availability is the shortage of emission inventories. However, since the PRTR (Pollutant Release and Transfer Register) system was implemented in Japan in 1999, it is expected that the availability is highly improved.

To increase the reliability of the model, it is necessary to quantify the inter-media transfer with high accuracy. At present, very few experimental data are available for the model calculations as the parameters expressing the transfer of species. Not only the experimental approaches but some estimation methods are important to fill the necessity.

## 5 CONCLUSION

The current status of the risk assessment and risk management in Japan was summarized and the modeling studies regarding air toxics were briefly reviewed. The methodologies of risk assessment and risk management are not sufficiently established and further studies are necessary. Modeling studies regarding toxic chemicals are not enough at present, especially focusing the validations of existing models using observation data. The largest problem is that there are very few scientists who are involved in such a modeling study.

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