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Fate Prediction Model of Organic Chemicals in Coastal Bay Estuaries

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Abstract—A fate and exposure of industrial organic chemicals has been developed for Japan and its coastal sea. Chemicals flowing into the water should be considered to be in the process of adsorption to suspended solids and sedimentation. These chemical processes are incorporated into the model. The field data slightly exceed the simulated concentrations for the Tama River estuary, but otherwise results fall between the maximum and minimum concentrations. In addition, the field concentration of TBT in Yokohama Port was over 30 ng/L, which was reproduced by the model.

The loading fluxes of dioxins were high during summer and consequently the amount of particulate-phase dioxins was large during that period. However, the amount of dissolved-phase dioxin was also high during winter.

Keywords: organic chemicals, TBT, dioxins, prediction model, Tokyo Bay

INTRODUCTION

A fate and exposure of industrial organic chemicals has been developed for Japan and its coastal sea (Horiguchi *et al*., 2001, 2006; Yamamoto *et al*., 2009). First, the model was focused on the fate of Tributyltin (TBT), which has been used as antifouling paint on vessel hulls and fishing nets, and can be particularly hazardous to humans and the surrounding environment.

MODEL

The concept for predicting the fate of a chemical contaminant such as TBT is shown in Fig. 1.

Chemicals flowing into the water should be considered to be in the process of adsorption to suspended solids and sedimentation. These chemical processes are incorporated into the model as follows:

1) Inflow load

   Chemicals flow into the sea system in a dissolved state. The source of TBT inflow to Tokyo Bay was assumed to consist solely of direct leaching from antifouling paints. In the case of Dioxin, sources are from

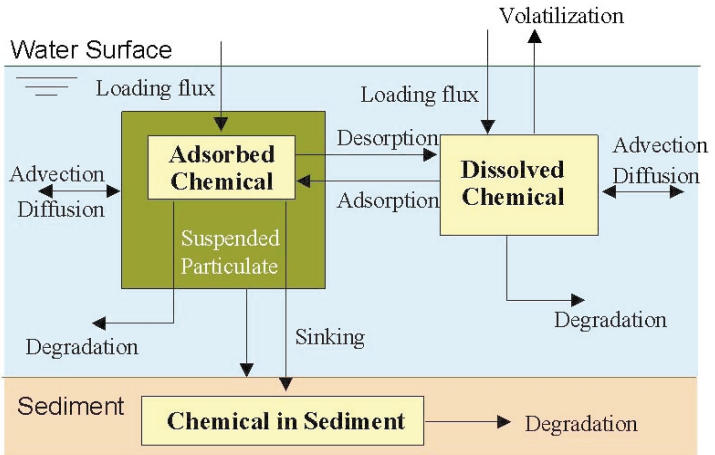

Fig. 1. Model concept for predicting the fate of a chemical contaminant.

rivers and the atmosphere.

2) Equilibrium between forms (adsorption and desorption)
   The processes of adsorption and desorption of dissolved chemicals and those adsorbed to organic particle are specified by the partition coefficient of these two forms and by the rate of adsorption.
3) Horizontal and vertical transfer of chemicals
   Chemicals adsorbed to suspended solids, and dissolved chemicals, are transported by advection and diffusion in Tokyo Bay.

The model system consists of a hydrodynamic model, ecosystem model (Taguchi and Nakata, 1998) and chemical fate model. The model was applied to TBT and Dioxin in Tokyo Bay. Simulation of the model was performed over 1 year using a fine mesh system.

For TBT, loading distribution along the navigation route and in port areas are shown in Fig. 2 based on shipping census data (The Japan Port and Harbour Association, 1990).

RESULTS AND DISCUSSION

In order to quantitatively examine the reproducibility of TBT concentrations in Tokyo Bay, the field data in rivers (estuaries) and ports in Tokyo Bay compiled by the Ministry of the Environment were compared with the model results (Fig. 3). The field data were obtained in 1990, before TBT regulation. The maximum and minimum levels of TBT in Tokyo Bay for each year, as predicted by the model, are shown with the corresponding data in this figure. The field data slightly exceed the simulated concentrations for the Tama River estuary, but otherwise results fall between the maximum and minimum concentrations. In addition, the field concentration of TBT in Yokohama Port was over 30 ng/L,

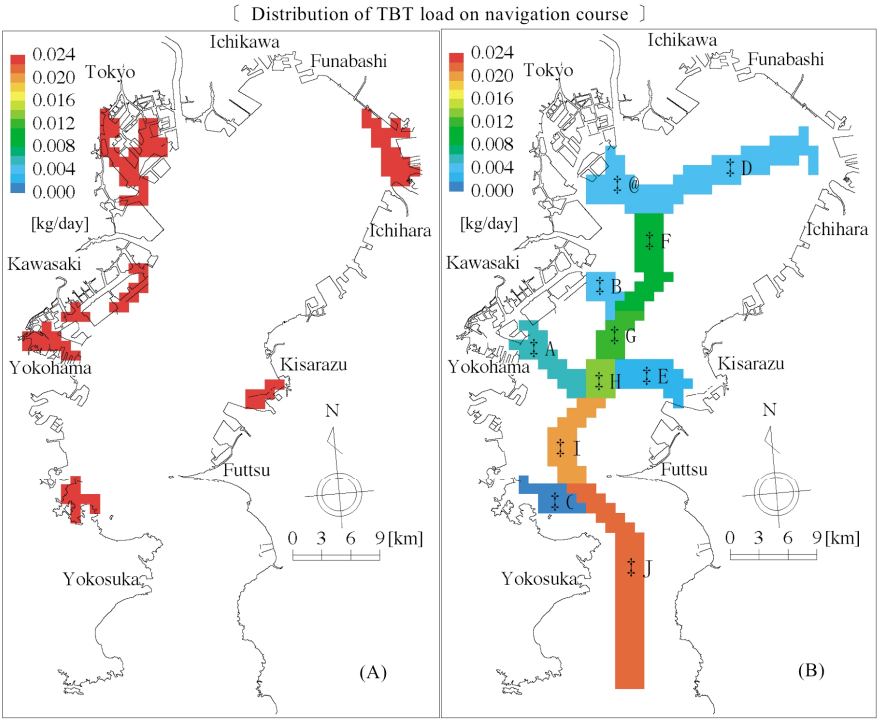

Fig. 2. Estimate of the distribution of TBT load along navigation routes and in ports of Tokyo Bay. (A): Distribution within each port, and (B): distribution along shipping navigation course.

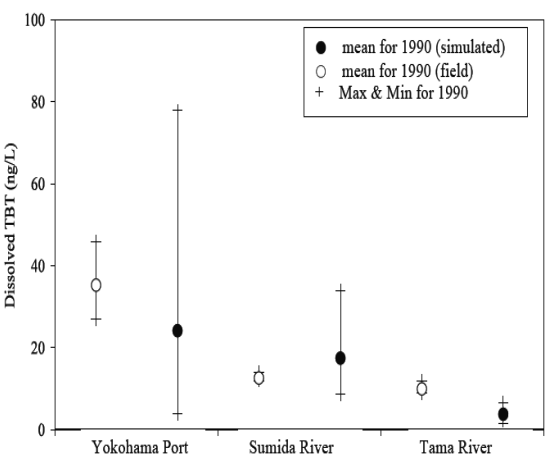

Fig. 3. Comparison of dissolved TBT concentrations between field data collected from rivers (estuaries) and ports (Ministry of the Environment, 1999) and model results.

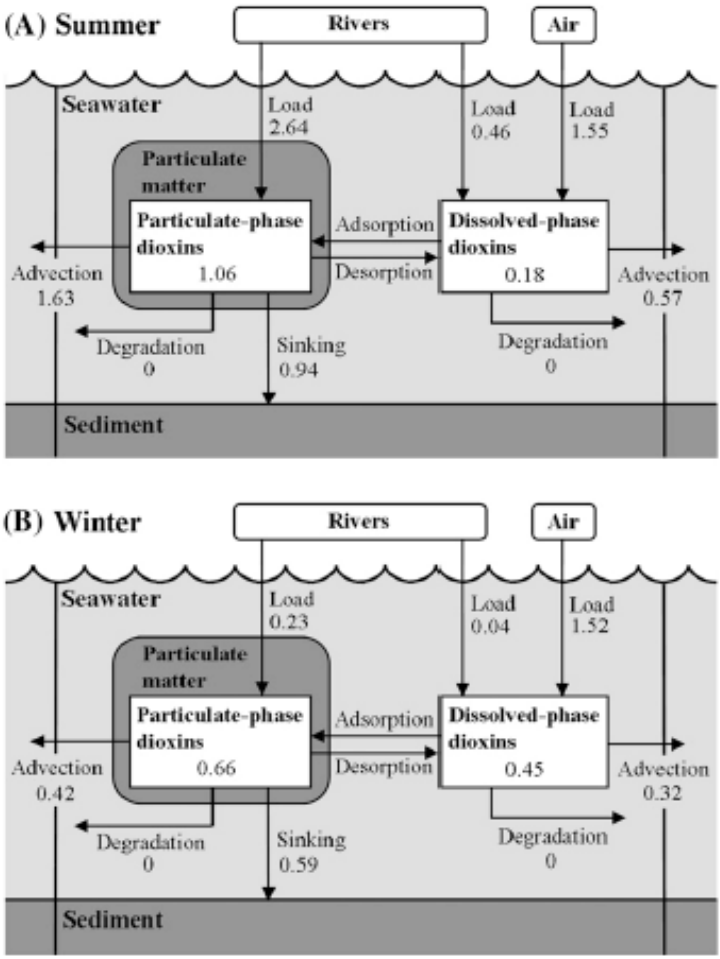

Fig. 4. Budget of the dioxins in the Tokyo Bay during summer and winter from the model simulation results (expressed in g-TEQ).

which was reproduced by the model. The model is also applied for Dioxin distribution in Tokyo Bay (Kobayashi *et al*., 2006).

In Fig. 4, the budget of dioxins in seawater of Tokyo Bay is shown during summer and winter, as analyzed from the simulation results. The loading fluxes of dioxins were high during summer and consequently the amount of particulate-phase dioxins was large during that period. However, the amount of dissolved-phase dioxin was also high during winter. The model results suggested that the loading flux of dioxins from rivers was the most important factor affecting the particulate-phase dioxin concentrations and that the seasonal cycle of the concentrations of organic particulate matter, which is related to primary production

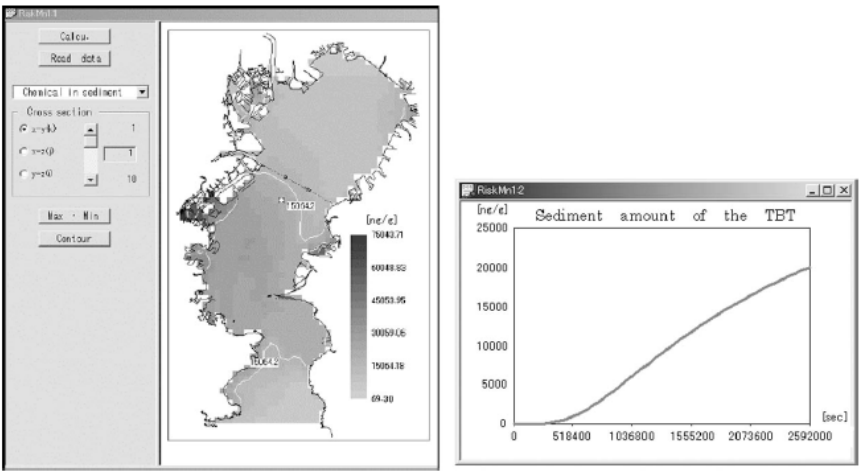

Fig. 5. Example of predicted TBT concentrations in Tokyo Bay in Windows version.

in the water column, was the most important factor affecting dissolved-phase dioxin concentrations in the bay.

Next we developed a simplified version of the fate prediction model of the chemicals in a coastal bay system. The hydrodynamic and ecosystem model results for each season were stored in a database, and then combined with the chemical fate prediction model for a specified coastal bay system. This model can be adapted for operation in a Windows system so that such an analysis is more accessible to other operators. Using a simple input of parameters, this prototype modeling system enabled detailed prediction of environmental concentrations and ecosystem exposure in a coastal area (in Fig. 5).

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