Comparison of Various Approaches to Simulate Dioxins/Furans Environmental Fate and Transport

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Introduction

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Polychlorinated dibenzodioxin and dibenzofuran compounds (hereafter referred to as dioxins and furans) are released into the environment from a variety of sources and, because of their propensity to bioaccumulate, may expose individuals to doses of concern. Consequently, it is necessary to assess the human health risks that may be associated with human exposure to dioxins/furans. Several health risk assessment models have been developed that simulate the fate and transport of these compounds in the multimedia environment. Those models differ widely in their approach to the physical transport, chemical transformations, and bioaccumulation of dioxins/furans.

We present here a comparison of two different modeling approaches. First, we describe the formulations of the two modeling approaches. Next, we provide values for the various environmental fate and transport parameters needed to apply the model. Finally, the two modeling approaches are applied to simulate the potential impacts of a coal-fired power plant and the results are discussed in terms of the relative advantages and disadvantages of the two approaches (e.g., accuracy versus computational requirements).

Formulation of the Modeling Approaches

The two approaches considered here are referred to as screening and refined. They can be summarized as follows.

<u>Screening Approach</u>: In the screening approach, the emissions of dioxins/furans are converted to an emission of 2,3,7,8-TCDD equivalent by means of toxicity equivalent quotients (TEQ). Then, the environmental fate and transport calculations are conducted for 2,3,7,8-TCDD and the potential health risks are calculated for this 2,3,7,8-TCDD equivalent. Therefore, it is assumed that all dioxins/furans behave in the environment in the same manner as 2,3,7,8-tetrachlorodibenzodioxin (2,3,7,8-TCDD).

<u>Refined Approach</u>: In the refined approach, the individual dioxin and furan congeners are treated separately throughout the environmental fate and transport calculations. The

ORGANOHALOGEN COMPOUNDS Vol. 36 (1998) TEQs are used only when calculating the toxicity of the congeners, i.e., at the point of human exposure.

<u>Environmental Fate and Transport Model</u>: The general model formulation is based on that of the Total Risk of Utility Emissions (TRUE) model, a multimedia health risk assessment model. The processes modeled include the following:

- Atmospheric transport and dispersion.
- Dry and wet atmospheric deposition to the earth's surface.
- Surface water runoff to water bodies.
- Transport, dispersion and first-order decay in rivers.
- Dilution, sedimentation and first-order decay in lakes.
- Infiltration, percolation, retardation processes and first-order decay in soils.
- Transport, dispersion and first-order decay in groundwater.
- Bioaccumulation in fish.
- Bioconcentration in cattle, dairy cows, vegetation, and mother's milk.
- Human exposure through inhalation, ingestion, and dermal absorption.
- Carcinogenic and chronic non-carcinogenic health effects.

A detailed description of the model formulation is presented by Constantinou and Seigneur¹.

Environmental Fate and Transport Parameters

The environmental parameters that are required as inputs to the fate and transport model are presented in Table 1. The values of these parameters for 2,3,7,8-TCDD are also listed in that table. Other dioxin and furan congeners typically have parameter values that differ from those of 2,3,7,8-TCDD. Concentrations of dioxins/furans in mother's milk are treated with a mass balance model rather than a bioconcentration factor.

Parameter	Value for 2,3,7,8-TCDD
Solubility ²	1.93 x 10 ⁻⁵ μg/ml
Henry's Law Constant 3	1.60 x 10 ⁻⁵ m ³ -atm/mol
Organic Carbon Adsorption Coefficient ²	4.57 x 10°
Molecular Diffusion Coefficient in Air ²	0.047 cm ² /s
Surface Soil Decay Rate ²	3.5 x 10 ⁻³ day ⁻¹
Surface Water Decay Rate ²	$1.2 \ge 10^{-3} \text{ day}^{-1}$
Groundwater Decay Rate ²	3.5 x 10 ⁻⁶ day ⁻¹
Soil-to-Grass Bioconcentration Factor ³	5.6 x 10 ⁻³
Soil-to-Root Vegetable Bioconcentration Factor ³	3.92 x 10 ³
Biotransfer Factor for Beef Cattle ³	0.57 day/kg
Biotransfer Factor for Dairy Milk 3	0.52 day/kg
Biota Sediment Accumulation Factor ⁴	0.06

Table 1. Environmental fate and transport parameters for 2,3,7,8-TCDD

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Application to a Power Plant Case Study

The two model formulations (i.e., screening and refined) are applied to the simulation of the potential public health impacts of dioxin/furan emissions from a coal-fired power plant. The results are compared in terms of the calculated health risks and the computational requirements. The relative difference in health risks between the two approaches depends on the initial composition of the dioxin/furan emissions. If the dioxin/furan speciation of the emissions is available, we recommend that the refined approach be used. Clearly, if only a TEQ emission value is available (e.g., no sampling data are available and an emission factor was used to obtain the emissions), then the screening method must be used. However, if the screening calculations suggest that there may be some potential health risk calculated in the local region, then, a stack emission sampling program should be conducted using best available methods and a refined health risk assessment should be conducted using the stack-specific sampling data. The screening risk assessment should be used to determine the detection limits needed to ensure an accurate risk assessment⁵.

Acknowledgements

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References

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