

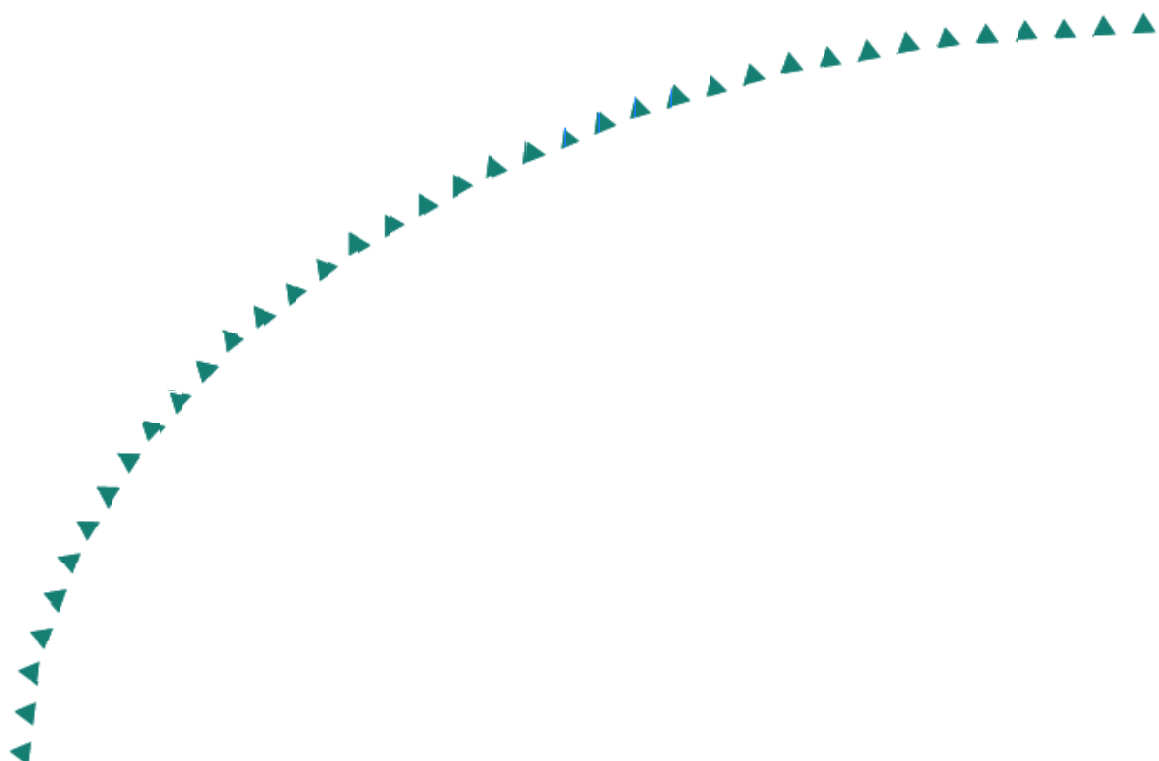
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Final Report

**Environmental Hazard
Assessment for Transportation Related
Chemicals: Development of a
Decision Support Tool**



Research



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16. Abstract (Limit: 200 words) A decision support tool has been developed to estimate the fate and potential risks to ecological receptors posed by chemical contaminants emitted from vehicle emissions. The decision tool has three components derived from the Multimedia Urban Model or MUM and that has been applied to the Minneapolis/St. Paul Twin Cities. The first, MUM-Fate, estimates the long term average concentrations of contaminants in 81 geographic segments and nine media in warm (spring-summer-fall) and cold (winter) scenarios. Secondly, MUM-Exposure estimates the exposure of these contaminants by selected bird and mammal species that are representative of aquatic and terrestrial routes of exposure. Third, MUM-Risk estimates the potential risk posed by the estimated intake of contaminants, as determined by comparison against toxicological benchmarks. The decision tool also estimates the potential risk posed by estimated air, water and sediment concentrations in comparison to media-specific benchmarks. The decision tool is designed to consider volatile and semi-volatile organic compounds that may be persistent or metabolizable, as well as metals. The decision tool is available as a computer program with a user-friendly interface that runs in a Windows™ environment. The decision tool (software program) contains an extensive database of physical-chemical properties, intake rates and diets of species and toxicological benchmarks.			
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ENVIRONMENTAL HAZARD ASSESSMENT FOR TRANSPORTATION RELATED CHEMICALS: DEVELOPMENT OF A DECISION SUPPORT TOOL

Final Report

Miriam L. Diamond
Mehran Monabbati
Josephine A. Archbold

Department of Geography
University of Toronto
Canada

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Executive Summary

With support from the Minnesota Department of Transportation (Mn/DOT), a decision support tool has been developed to assess the fate of and potential risk posed by two classes of chemical contaminants released to the Minneapolis/St. Paul environment from transportation activities. The decision support tool consists of a mathematical model that first estimates the likely fate or distribution of chemicals emitted from vehicles and then, from this distribution, estimates the potential exposure and risk to selected bird and mammal species. The geographic scope of the model is a 45 by 45 km² area within which are the Minneapolis/St. Paul Twin Cities. This area is segmented into 81 geographic segments of 5 by 5 km². Within each segment the model estimates the long-term likely distribution and ecotoxicological effects of semi-volatile organic compounds (e.g., polycyclic aromatic hydrocarbons) and metals (e.g., copper). The model is run on a personal computer platform within a Windows[®] environment.

The decision tool consists of three major modules: environmental fate, exposure pathway analysis, and risk calculation. The fate module is based on the fugacity multimedia fate models developed by Mackay and co-workers (1). Diamond and co-workers adapted this model to consider urban areas by developing the Multimedia Urban Model (MUM) of Diamond (2), (3), hereafter referred to as MUM-Fate. MUM-Fate incorporates characteristics of urban environments, most notably impervious surfaces. The version of MUM-Fate used in the Mn/DOT decision tool has been adapted in several important ways. First, this version of the model considers multiple geographic segments that dissect the entire area considered (Minneapolis/St. Paul is divided into 81 segments or boxes). Second, the movement of chemical via stormwater conduits, which has the potential to transport chemical among segments that are not contiguous, has been added. Third, an air dispersion component has been added to account for lateral dispersion of chemical as well as transport according to advection. Fourth, the model includes two vertical layers of air which improves the estimation of air transport processes. Fifth, the model has been extended to consider metals as well as semi-volatile organic compounds using the “equivalence” formulation of Mackay and Diamond. Sixth, the model has been adapted to provide estimates of contaminant fate in a warm (spring-summer-fall) scenario and a cold (winter) scenario.

MUM-Fate provides estimates of contaminant concentrations in each medium, as well as contaminant mass, and rates of movement among compartments and geographic segments. These estimates are intended to estimate the long term average distribution of semi-volatile organic compounds (SOCs) in a multimedia environment. This is the first generation of multimedia fate models that can accommodate both volatile (SOCs) and involatile (metals) chemicals that experience very different fate processes.

The second module of the decision tool consists of the exposure and risk assessment components. Two levels of risk assessment are offered within the decision tool. In the first, water, sediment and soil concentrations estimated by MUM-Fate are compared with screening level toxicological benchmarks in these media to determine if there are exceedences in any geographic segment. The benchmarks have been taken from first, the Minnesota Pollution Control Agency, and secondly, other regulatory agencies or from the literature. The second and more detailed assessment entails the use of MUM-Exposure to estimate chemical intake by aquatic and terrestrial bird and mammal species (receptors) that represent various trophic levels

and life stages (e.g., adult female and juvenile). The routes of chemical exposure are inhalation and ingestion (drinking and dietary transfer). MUM-Risk compares the estimated exposure or dose with a toxicological reference value (TRV) in order to assess the potential for an adverse health effect. The exposure and risk assessment modules are intended to estimate low level exposures and effects occurring over the life of the receptors. MUM-Exposure and MUM-Risk have been developed for persistent and metabolizable organic contaminants, and metals. To be protective of population-level health effects, the toxicological benchmarks chosen are for growth, development, and reproduction.

The receptors available for the ecological risk assessment are all found within Minneapolis/St.Paul and span a range of exposure routes. MUM-Exposure and MUM-Fate assume that all receptors are resident in each geographic segment.

Overall, the decision tool is intended to identify chemicals emitted by vehicles, which may pose a potential risk to ecological receptors over the long term. MUM-Risk is conservative, designed to conduct screening-level assessments, highlighting areas for further study. The model is not applicable to a site-specific risk or environmental assessment where the aim is to predict the likelihood of an actual effect.

The user-friendly computer model can be run to estimate the fate and potential risk posed by 28 selected volatile and semi-volatile chemicals and 11 metals. The computer program contains a database of physical-chemical properties of all chemicals and temperature corrections for consideration of the warm and cold scenarios. The program also contains databases for intake rates and dietary composition for 15 bird and 9 mammal species. The estimated total daily intake of these receptors can be compared with toxicological benchmarks for all contaminants, where the benchmarks are also compiled in a database in the program.

Chapter 1

Introduction

Human activities release innumerable chemicals into the environment. This is particularly true in urban environments where resource consumption and release of chemicals occur in a relatively restricted geographic area. Over the last decades, increased public pressure has resulted in advancements in our understanding and ability to identify and control point-source emissions of contaminants. This has resulted in an overall reduction in point-source emissions. However, non-point and mobile source emissions remain difficult to characterize, quantify and subsequently control.

In order to develop effective policies for the transportation sector, decision-makers need to know the contaminants emitted from this sector, their sources, fate, and potential current and future impacts. Modeling is a practical method of facilitating decision-making by allowing for the simulation of scenarios, investigating potential impacts of proposed emission scenarios, and rationalizing data collection programs.

The Minnesota Department of Transportation (Mn/DOT) has funded the development of a decision support tool to assess the potential risk posed by chemical contaminants released to the urban environment due to transportation activities. The basis of the decision support tool is a mathematical model that estimates the likely fate or distribution of chemicals emitted from vehicles and from this distribution, the potential health risk posed to non-human species. The model simulates the environment of the Minneapolis/St. Paul Twin City area. This 45 km² area is segmented into 81 boxes of 5 by 5 km². The model estimates the long-term likely distribution and ecotoxicological effects of semi-volatile organic compounds (e.g., polycyclic aromatic hydrocarbons) and metals (e.g., copper) in this area.

This document describes the decision support tool - its basis, assumptions used to construct the model, and data used to apply the model to the Minneapolis/St. Paul area. The model is available from the Minnesota Department of Transportation. The first section of the report provides an overview and description of the decision support tool. Chapter 2 provides details of the fate model and Chapter 3 describes the risk assessment portion of the decision support tool. This report does not focus on results generated by the model. Rather, the intention of the report is to provide background information on the components of the decision support tool.

1.1 Objectives

The goal of this project has been to develop a decision support tool that will assist with assessing the potential risks posed by chemical contaminants released by vehicles. The support tool uses an analysis of ecotoxicological risk to interpret the potential for adverse effects posed by emissions and the distribution of chemical contaminants from vehicles. The decision support tool examines these effects in the Minneapolis/St. Paul area. Specifically, the objectives of this program have been to:

- estimate the concentrations in various media of chemical contaminants emitted by vehicles over the Minneapolis/St. Paul area;
- estimate the potential adverse effects on wildlife exposed to these chemical contaminants; and
- integrate the fate and risk estimation models into a user-friendly computer model that can be used to guide decision-making.

1.2 Model Structure

The model has three major modules: environmental fate (MUM-Fate); exposure pathway (MUM-Exposure); and risk calculation (MUM-Risk). Figure 1.1 indicates the flow of information and the relationship between these modules in the program. MUM-Fate belongs to the family of fugacity-based multimedia fate models developed by Mackay and co-workers (1). Diamond and co-workers adapted this model to consider urban areas by developing the Multimedia Urban Model (MUM) (2), (3). MUM incorporates characteristics of urban environments, notably impervious surfaces, and in this adaptation, the movement of contaminants via stormwater conduits. This version of the model considers the Minneapolis/St. Paul area as comprising 81 geographic segments or “boxes.” The fate model provides estimates of contaminant concentrations in each medium, as well as contaminant mass, and rates of movement among compartments and geographic segments.

MUM-Fate is intended to estimate the long term average distribution of semi-volatile organic compounds (SOCs) in a multimedia environment. In this project, the model was extended to treat metals. This is the first generation of multimedia fate models that can accommodate both volatile (SOCs) and involatile (metals) chemicals, which experience very different fate processes.

The fate model considers contaminants emitted at low concentrations and as such, the model is not capable of estimating the fate of spills. The environment is simulated as well-mixed compartments representing air, water, sediment, soil, terrestrial vegetation, and surface films on impervious surfaces. As such, the model is not intended to estimate phenomena such as plume dispersion or the continuous removal of contaminants emitted from roadways, nor is the model capable of estimating contaminant movement attributable to events such as rain storms.

To treat seasonal changes that alter contaminant fate, MUM-Fate has been developed for a “warm” scenario when trees are in leaf and warm temperatures prevail (i.e., spring, summer and fall). The model also considers winter conditions when the ground is covered in snow and surface waters are frozen over. The model considers contaminant fate under a steady-state condition of constant chemical emissions into a “constant” environment. The model also considers time variant conditions with the simulation moving through seasonally changing environmental conditions.

The other main components of the decision tool are the exposure and risk assessment modules. These two modules have been developed to provide screening-level guidance for the

protection of ecological health. Two levels of risk assessment are available. In the first, water, sediment and soil concentrations estimated by MUM-Fate are compared with benchmark concentrations in these media to determine if there are exceedences in any geographic segment. The benchmark concentrations have been taken from the Minnesota Pollution Control Agency, other regulatory agencies or from the literature. In the second level or lens, MUM-Exposure estimates contaminant intake by individuals of aquatic and terrestrial species (receptors) that are representative of various trophic levels and life stages (e.g., adult female and juvenile). Inhalation and ingestion (drinking and dietary transfer) are the routes of exposure considered. The risk assessment component compares the estimated exposure or dose with a toxicological benchmark in order to assess the potential for an adverse health effect. The exposure and risk assessment modules are designed to estimate low level intakes and effects occurring over the life of the receptors. MUM-Exposure and MUM-Risk have been developed for persistent and metabolizable organic contaminants, and metals. To be protective of population-level health effects, the toxicological benchmarks chosen are for reproduction.

MUM-Exposure and MUM-Fate assume that all receptors are resident in each geographic segment and that exposure occurs during the warm scenario only.

The rationale for providing insight into the long term, average distribution of contaminants and the potential for these concentrations to cause population-level health effects is that this information can be used to guide decisions. The model is not intended to replicate calculations for a site-specific risk or environmental assessment where the aim is to predict the likelihood of an actual effect. Rather, this screening level tool incorporates conservative assumptions that allow consideration of potential adverse effects to a wide range of receptors, caused by a range of contaminants.

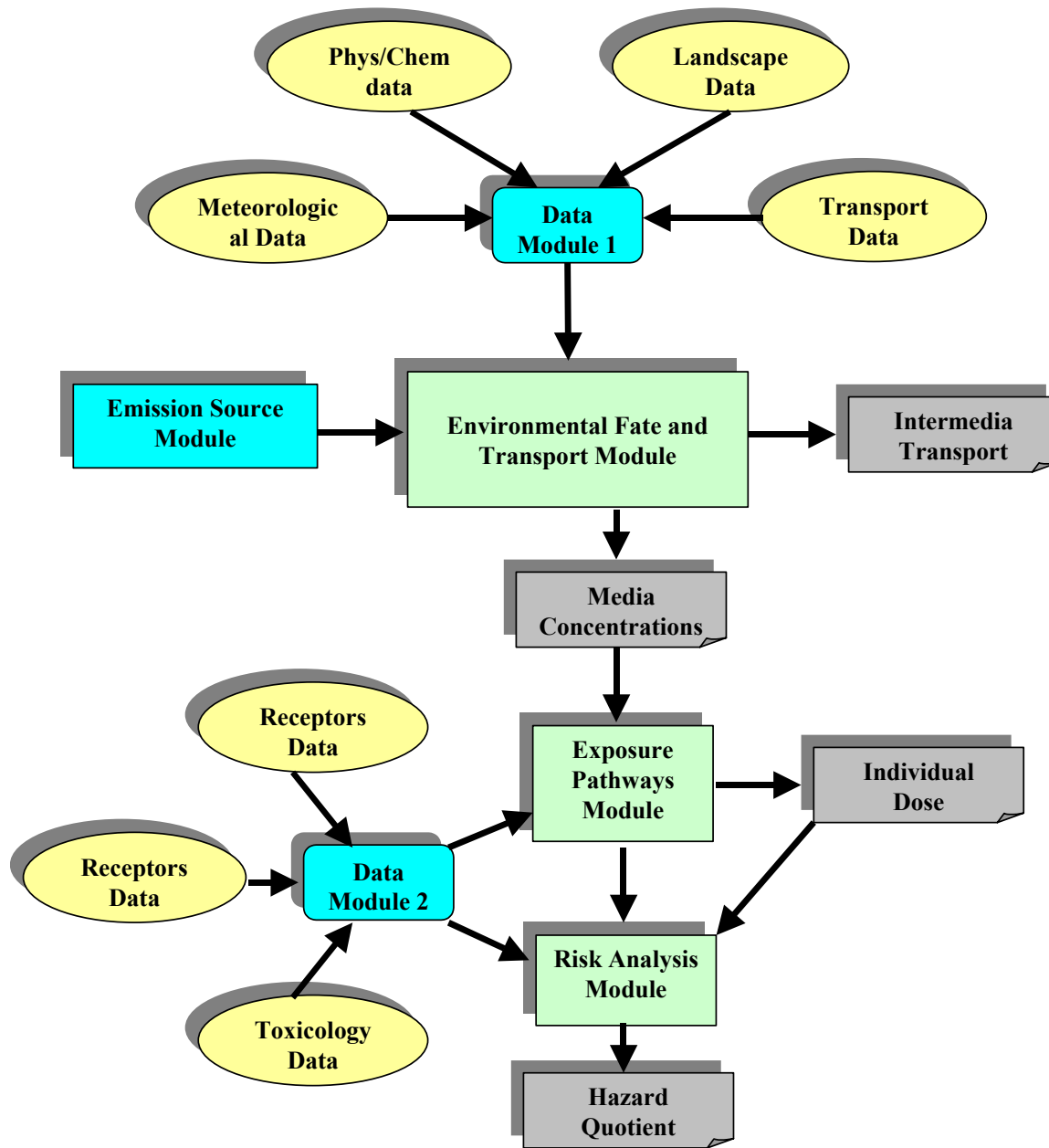


Figure 1.1: Flowchart of integrated fate and risk models.

Chapter 2

Description of MUM-Fate

2.1 Model Formulation

2.1.1 Introduction

The premise of multimedia models is that a chemical emitted to the environment is distributed among media (e.g., air, water, soil) according to the chemical's physical-chemical properties and the properties of each medium. The distribution of organic contaminants, such as semi-volatile organic compounds or SOCs, is governed by the distribution of organic carbon and lipid, which in turn, is estimated by a series of partition coefficients. The distribution of metals in a multimedia environment is metal-specific where the chemistry of each medium controls speciation and the distribution of metals among media. Mackay (1) provides a complete description of multimedia models for SOCs. Diamond et al. (4) (in press) briefly describes the evolution of these models for metals.

The environmental transport module consists of a set of mass balance equations for each medium and solves them simultaneously to obtain the concentration of the contaminant in each medium, as well as the fluxes of contaminant among media and between adjacent geographic segments. The mass balance equations are based on the balance of inputs and outputs for steady-state conditions, and the balance of inputs, outputs, and accumulation for unsteady-state or transient conditions (Figure 2.1).

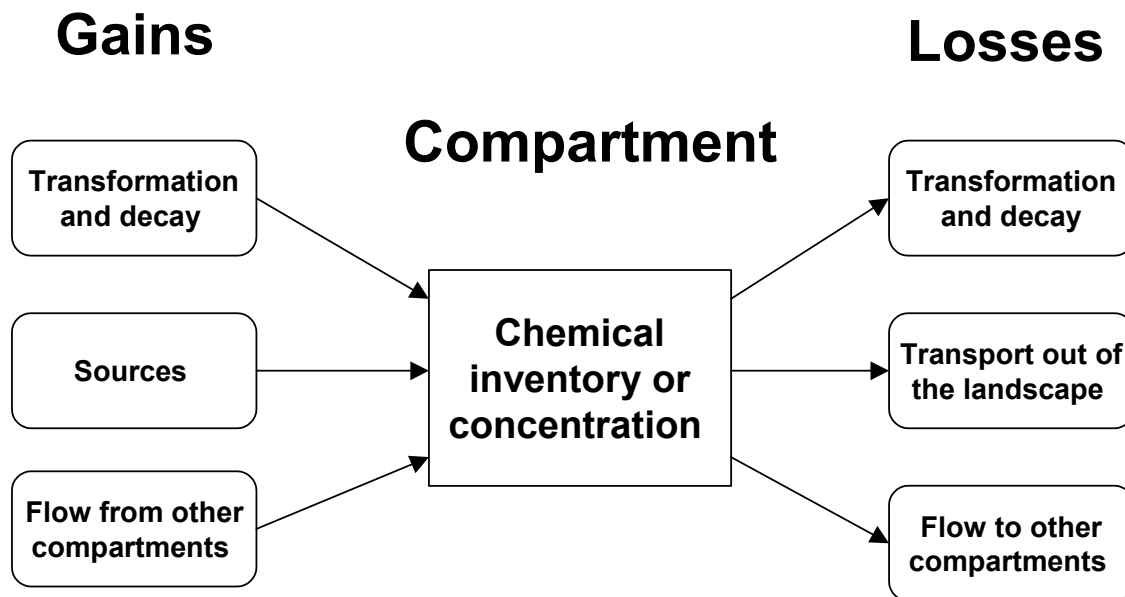


Figure 2.1: Components of general mass balance model.

Generally, n number of equations can be written for n number of media or compartments. These n equations are solved for n number of unknown environmental concentrations. The mathematical formulation for this equation is:

$$V_i \frac{dC_i}{dt} = \sum_{j, j \neq i} G_j C_j + E_i + L_i \quad (2.1)$$

where:

- V_i is compartment i volume (m^3)
- C_i is chemical concentration in compartment i ($mol\ m^{-3}$)
- t is time (h)
- G_j is the bulk flow rate from compartment i to adjacent compartment j ($m^3\ h^{-1}$)
- C_j is the chemical concentration in compartment j ($mol\ m^{-3}$)
- E_i net emission in compartment i ($mol\ h^{-1}$)
- L_i net loss from compartment i ($mol\ h^{-1}$)

Mackay introduced a family of multimedia, mass balance models that use fugacity as an equilibrium criterion (1). Fugacity-based models differ from conventional concentration or mass based models in their mathematical simplicity and elegance. The fugacity approach is suitable for organic compounds with a measurable vapor pressure and that are not highly reactive, such as SOCs. Mackay and Diamond (5) adapted the model to treat involatile chemicals, notably metals, by introducing an analogous equilibrium criterion that is similar to chemical activity, termed “aquivalence.”

The model is based on the Level III (steady state) and Level IV (unsteady state) versions of Mackay’s multimedia model. This model was adapted by Diamond et al. (2) for urban environments and named the Multimedia Urban Model (MUM). MUM-FATE describes the fate of pollutants in an urban environment, stressing the role of vegetation and impervious surfaces.

2.1.2 Fugacity Approach

Fugacity has units of pressure and can be regarded physically as the partial pressure or escaping tendency exerted by a chemical in one physical phase or compartment relative to another (6), (1), (7), (8). When two or more media are in equilibrium the fugacity of a chemical is the same in all media. This characteristic of fugacity-based modeling often simplifies the mathematics involved in calculating partitioning. Fugacity models can also be used to represent a dynamic system in which the fugacities in two adjacent media are changing over time due to an imbalance of gains and losses or to represent a dynamic system that has achieved steady state by balancing gains and losses even though fugacities are not equal.

At low concentrations, like those typical of environmental concentrations C (mol m^{-3}), fugacity, f (Pa), is linearly related to concentration C (mol m^{-3}) through the fugacity capacity, Z ($\text{mol m}^{-3} \text{Pa}^{-1}$), also written as Z in the case of equivalence calculations:

$$C = fZ \quad (2.2)$$

With equivalence, the Z value for water Z_W is defined as 1.00. Subsequent Z values are determined from partition coefficients. The ratio of two Z values in phases 1 and 2 is the dimensionless partition coefficient K_{12} .

All transport and transformation processes are expressed in common mathematical terms as D values ($\text{mol Pa}^{-1} \text{m}^{-3}$). D values are defined as:

$$D = GZ = kVZ = KAZ \quad (2.3)$$

where G (mol h^{-1} or kg h^{-1}) is the flow rate of a medium (e.g., air, water, suspended particles), V (m^3) is volume; k (h^{-1}) is a first order reaction rate constant; K (m h^{-1}) is a mass transfer coefficient; and A (m^2) is the area across which the chemical mass transfer is occurring. The rate of inter-media transport or reaction, (mol h^{-1}) is thus:

$$N = Df = GC \quad (2.4)$$

2.1.3 Equivalence Approach

MUM-Fate is developed to treat both volatile (e.g., semi-volatile organic compounds) and involatile (metals) chemicals. The fugacity approach has been used to describe the multimedia behavior of chemicals with a measurable vapor pressure only, such as most non-polar organic chemicals. For involatile chemicals, such as metals and polymers, an alternative equilibrium criterion is required. Mackay and Diamond (5) introduced “equivalent aqueous concentration” or “equivalence” as an equilibrium criterion suitable for most chemicals. Similarly to fugacity, equivalence, A (mol m^{-3}), is linearly related to concentration

$$C = AZ \quad (2.5)$$

where Z is a dimensionless fugacity capacity.

The equivalence formulation uses D values generated in the same fashion as that for the fugacity formulation; however, the units are $\text{m}^3 \text{h}^{-1}$.

2.1.4 Calculating Z Values

Z values depend on the physical and chemical properties of the chemical and characteristics of the medium such as temperature and density. The fact that fugacities in media are equal at equilibrium allows for the simple determination of Z values from partition coefficients, K_{12} . For example, for two phases in equilibrium (phases 1 and 2):

$$C_1/C_2 = fZ_1/fZ_2 = AZ_1/AZ_2 = Z_1/Z_2 = Z_1/Z_2 = K_{12} \quad (2.6)$$

Z values for the fugacity approach are calculated by first starting with the air compartment, where Z_A is the same as its partial pressure at low chemical concentrations:

$$Z_a = 1/RT \quad (2.7)$$

where R (mol K m⁻³ Pa⁻¹) is the universal gas constant and T (K) is absolute air temperature.

For the equivalence approach, the pure water phase is the starting point for calculating Z values since Z_w is defined as 1. For both approaches, Z values in other phases are calculated as the product of a partition coefficient and the initial Z value. For equivalence, the Z value for the air phase is not calculated as the pure air concentration for metals is zero (with the exception of particular metals such as elemental Hg).

During the last decade researchers have developed relationships that can be used to calculate Z values for other environmental compartments, such as aerosols (9) and vegetation (10). Z values for bulk phases that consist of two or more pure phases are calculated using subcompartmental or pure Z values and volume fractions for each pure phase:

$$Z_{bulk} = \sum Z_i v_i \quad (2.8)$$

where v is the volume fraction of each subcompartment. Examples of bulk phases are: (a) soil that consists of pure phases of soil solids, air and soil pore water, and (b) sediment that consists of sediment solids and pure water. Equation 2.8 is applicable for both fugacity and equivalence formulations.

2.2 Model Structure

2.2.1 Environmental Compartments

The model considers nine bulk compartments: air [A], lake water [L], river water [R], soil [S], sediment underlying the lake water [LS] and river water [RS], vegetation [V], organic film on impervious surfaces [F], and snow pack [SP]. Each bulk medium or phase may consist of sub-phases of specified composition. Chemicals are assumed to be in equilibrium between these sub-phases within each bulk phase (e.g., between gas- and particle-phases within air). Equilibrium is not assumed among compartments.

Briefly, the air compartment consists of gas- and particle-phases of chemical. The compartment consists of two vertical layers where the height of the lower layer fluctuates as a function of the atmospheric mixing height. The mixing height, in turn, depends on meteorological conditions.

The model considers soil as a thin, 5 cm layer from which volatile chemicals can exchange with air and all dissolved chemicals and particulate phases are subject to runoff to

lakes and rivers. Chemicals can ultimately be lost via leaching to groundwater, at which point the chemical is “lost” from the system.

Surface vegetation covers all soil. Vegetation is parameterized to reflect a simple system comprising grass and trees (deciduous and coniferous). This parameterization comes in the value assigned to the leaf area index (LAI) which, in this case, was chosen as 3 (the same value is used for all geographic segments). Volatile chemicals can exchange with leaf surfaces through absorption and volatilization to and from the cuticle and can accumulate on leaves by wet and dry interception. Chemical moves from the leaves to soil through wax erosion, wash-off and leaf fall.

Surface water is conceptualized as lakes and rivers due to the prevalence of small lakes (over 200) in the Twin City area and the location of the Minneapolis/St. Paul area in the path of the Minnesota and Mississippi Rivers. Both river and lake water is underlain by a thin sediment layer of 2 and 5 cm, respectively, from which chemical can re-enter the water or be lost through burial. The difference between lake and river water resides in rates of water and particle (and chemical) transport. For example, the rivers convey water and suspended particles with minimal particle deposition and thus the rivers convey chemical downstream. In contrast, chemical that enters lakes is subject to deposition and net burial, in addition to the potential for downstream movement.

To specifically treat urban areas, the model includes the organic film on impervious surfaces. This is parameterized as a very thin film (e.g., 100 nm) that coats all impervious surfaces. To account for the three dimensional aspect of impervious surfaces (e.g., building walls), we use an Impervious Surface Index (ISI), which is analogous to LAI, of 2 (2). Again, the same value is applied to all geographic segments. Similar to leaves, gas-phase chemical can exchange between the film and air through absorption-volatilization, and particle-phase chemical can accumulate by dry and wet deposition. Chemicals can move from the film to surface waters by wash-off, a process that occurs independently of chemical solubility (11).

The winter scenario includes a snowpack that is a constant 10 cm deep. Since the snowpack is a constant thickness, the rate of snowmelt equals the rate of precipitation of snow. Chemical enters the snowpack through precipitation as well as through absorption-volatilization of gas-phase chemical. With snowmelt the chemical either enters the soil or surface waters.

2.2.2 Model Processes

The model consists of a set of equations that define the Z values, which are the same for all geographic segments (Table 2.1). The set of Z values changes for summer and winter, with the inclusion of Z values for the snowpack and the exclusion of Z values for vegetation in winter. As well, the Z values for the organic chemicals change with each seasonal scenario as the physical-chemical properties from which they are calculated are corrected for temperatures of 20°C and -7°C in summer and winter, respectively. Next, D values are specified. The D values are calculated as products of the Z values and transport/transformation rates. Some of these rates are specific to the particular geographic segment, e.g., advective flow of water, while others are

identical for all segments (e.g., same rates of sediment deposition, resuspension and burial in lakes and soil runoff). Finally, the model consists of a set of mass balance equations that solve for the “equivalence” in each geographic segment, from which segment-specific concentrations, masses, and rates of chemical movement and transformation, are calculated.

Table 2.1: Definitions of Z and Z values for model compartments.

ORGANICS		
Compartment	Phase	Equation
Air	Gas Phase Particulate Bulk	$Z_A = 1/RT$ $Z_Q = 10^{(\log K_{OA} + \log f_{om} - 11.91)} \cdot Z_A \cdot \rho \cdot 10^9$ $Z_{BA} = Z_A + (Z_Q \times v_Q)$
Water	Dissolved Suspended Part. Bulk	$Z_W = 1/H$ $Z_P = Z_W \times \rho \times K_{OC} \times f_{oc}$ $Z_{BW} = Z_W + (Z_P \times v_P)$
Soil	Solids Bulk	$Z_S = Z_W \times \rho \times 0.41K_{OW} \times f_{oc}$ $Z_{BS} = (v_A \times Z_A) + (v_W \times Z_W) + (v_S \times Z_S)$
Sediment	Solids Bulk	$Z_D = Z_W \times \rho \times 0.41K_{OW} \times f_{oc}$ $Z_{BD} = (v_W \times Z_W) + (v_D \times Z_D)$
Vegetation	Leaf Cuticle Bulk	$Z_V = Z_W \times K_{OW} \times f_{oc}$ $Z_{BV} = (v_A \times Z_A) + (v_W \times Z_W) + (v_V \times Z_V)$
Organic film	Dissolved Particulate Bulk	$Z_F = Z_A \times K_{OA} \times f_{oc}$ $Z_Q = 10^{(\log K_{OA} + \log f_{om} - 11.91)} \cdot Z_A \cdot \rho \cdot 10^9$ $Z_{BF} = (Z_F \times \phi_F) + (Z_Q \times \phi_Q)$
Snow	Dissolved Suspended Part. Bulk	$Z_{SN} = 1/H$ $Z_P = Z_W \times \rho \times K_{OC} \times f_{oc}$ $Z_{BW} = (Z_{SN} \times v_{SN}) + (Z_P \times v_P) + (v_A \times Z_A)$

METALS		
Compartment	Phase	Equation
Water	Dissolved	$Z_W = 1$
	Suspended Part.	$Z_P = Z_W \times \rho \times K_{OC} \times f_{oc}$
	Bulk	$Z_{BW} = Z_W + (Z_P \times v_P)$
Soil	Solids	$Z_S = Z_W \times \rho \times 0.41K_{OW} \times f_{oc}$
	Bulk	$Z_{BS} = (v_A \times Z_A) + (v_W \times Z_W) + (v_S \times Z_S)$
Sediment	Solids	$Z_D = Z_W \times \rho \times 0.41K_{OW} \times f_{oc}$
	Bulk	$Z_{BD} = (v_W \times Z_W) + (v_D \times Z_D)$
Vegetation	Leaf Cuticle	$Z_V = Z_W \times K_{OW} \times f_{oc}$
	Bulk	$Z_{BV} = (v_A \times Z_A) + (v_W \times Z_W) + (v_V \times Z_V)$
Snow	Dissolved	$Z_{SN} = 1$
	Suspended Part.	$Z_P = Z_W \times \rho \times K_{OC} \times f_{oc}$
	Bulk	$Z_{BW} = (Z_{SN} \times v_{SN}) + (Z_P \times v_P) + (v_A \times Z_A)$

*Harner and Bidleman (9)

K_{OW} Octanol-water partition coefficient

K_{OC} Organic carbon-water partition coefficient

K_{OA} Octanol-air partition coefficient

f_{om} Organic matter fraction

f_{oc} Organic carbon content

H Henry's law constant

ρ Density of compartment

v volume fraction

ϕ mass fraction

Table 2.2 summarizes the environmental properties used in all geographic segments of the model. Below we describe the model in more detail. Specifically, we describe the model configuration for summer and winter and its application to organic compounds and metals, which are treated differently.

Table 2.2: Parameter values for environmental characteristics.

Parameter	Value	Reference
Leaf Area Index	3	ORNL (12)
Impervious Surface Index	2	Theurer (13)
Number of Growing Days	180	Bennett (14)
Air Density, kg/m ³	1.2	-
Water Density, kg/m ³	1000	-
Sediment Density, kg/m ³	1500	-
Snow Density, kg/m ³	100	assuming 90% porosity
Soil Density, kg/m ³	1500	-
Vegetable Density, kg/m ³	1000	-
Aerosol Density, kg/m ³	1500	Mackay (1)
Sediments Organic Carbon Fraction	0.05	Mackay (1)
Soil Organic Carbon Fraction	0.01	Mackay (1)
Vegetation Organic Carbon Fraction	0.01	Diamond et al. (2)
Suspended Sediment Organic Carbon Fraction	0.08	Mackay (1)
Aerosol Organic Carbon Fraction	0.05	Harner and Bidleman (9)
Suspended Sediment Concentration, mg/m ³	40	MinDNR (15)
Aerosol Concentration, µg/m ³	10	-
Runoff Sediment Concentration, mg/m ³	500	-
Soil Water Volume Fraction	0.2	Mackay (1)
Soil Air Volume Fraction	0.3	Mackay (1)
Sediment Porosity	0.8	Mackay (1)

2.2.2.1 Summer Scenario For Organics

Figure 2.2 illustrates the environmental compartments and transport processes considered in this scenario. Each arrow corresponds to a D value, all of which are listed in Table 2.3. The D values are incorporated into mass balance equations that are solved for steady-state and transient conditions (Table 2.4).

“Warm” or “summer” conditions assume a constant temperature of 20°C. Vegetation and the organic film on impervious surfaces are the key compartments linking air to the other compartments such as soil and water. It is assumed that the canopy drip and wash off from the leaves conveys chemical to the soil, while runoff from impervious surfaces ends up in surface water.

Z values for all organic chemicals are calculated from physical-chemical properties obtained from literature sources. Rates of chemical transformation and degradation in all media are a potentially major source of uncertainty. Appendix A lists the physical-chemical properties of chemicals in the model’s database, as well as rates of transformation and degradation and the sources of these data.

Table 2.3: Inter-compartmental transport processes considered in the summer scenario of the model.

Inter-compartmental transport	Symbol	Individual processes
Air-Vegetation	D ₁₋₅ D ₁₋₅ D ₁₋₅ , D ₅₋₁	Wet deposition Dry deposition Bi-directional diffusion
Air-Film	D ₁₋₆ D ₁₋₆ D ₁₋₆ , D ₆₋₁	Wet deposition Dry deposition Bi-directional diffusion
Air-Soil	D ₁₋₃ D ₁₋₃ D ₁₋₃ , D ₃₋₁ D ₃₋₁	Wet deposition Dry deposition Bi-directional diffusion Soil resuspension
Air-Lake	D ₁₋₂ D ₁₋₂ D ₁₋₂ , D ₂₋₁	Wet deposition Dry deposition Bi-directional diffusion
Air-River	D ₁₋₇ D ₁₋₇ D ₁₋₇ , D ₇₋₁	Wet deposition Dry deposition Bi-directional diffusion
River-Lake	D ₇₋₂	Advection
Vegetation-Lake	D ₅₋₂	Canopy drip/leaf wash off

Inter-compartmental transport	Symbol	Individual processes
Vegetation-Surface soil	D ₅₋₃ D ₅₋₃ D ₅₋₃ D ₃₋₅	Canopy drip/leaf wash off Wax erosion Litter fall Rain splash
Vegetation-River	D ₅₋₇	Canopy drip/leaf wash off
Film-Lake	D ₆₋₂	Film wash off
Film-Surface soil	D ₆₋₃	Film wash off
Film-River	D ₆₋₇	Film wash off
Soil-Air	D ₃₋₁	Bi-directional diffusion
Soil-Lake	D ₃₋₂	Soil run off (dissolved and solid phases)
Soil-River	D ₃₋₇	Soil run off (dissolved and solid phases)
Lake-Sediments	D ₂₋₄ , D ₄₋₂ D ₄₋₂ D ₂₋₄	Bi-directional diffusion Sediment resuspension Sediment deposition
River-Sediments	D ₇₋₈ , D ₈₋₇ D ₈₋₇ D ₇₋₈	Bi-directional diffusion Sediment resuspension Sediment deposition

Table 2.4: Steady- and unsteady-state mass balance equations for environmental compartments in the summer scenario.

No.	Compartment	Mass balance equation
Steady-state mode		
1	Air	$A_1 + E_1 + F_5 \cdot D_{5-1} + F_6 \cdot D_{6-1} + F_3 \cdot D_{3-1} + F_2 \cdot D_{2-1} + F_7 \cdot D_{7-1} = F_1 \cdot (R_1 + S_1 + D_{1-5} + D_{1-6} + D_{1-3} + D_{1-2} + D_{1-7})$
2	Lake water	$E_2 + F_1 \cdot D_{1-2} + F_5 \cdot D_{5-2} + F_3 \cdot D_{3-2} + F_4 \cdot D_{4-2} + F_6 \cdot D_{6-2} + F_7 \cdot D_{7-2} = F_2 \cdot (R_2 + D_{2-1} + D_{2-4})$
3	Soil	$E_3 + F_1 \cdot D_{1-3} + F_6 \cdot D_{6-3} + F_5 \cdot D_{5-3} = F_3 \cdot (R_3 + D_{3-1} + D_{3-2} + D_{3-7} + D_{3-5})$
4	Lake sediments	$F_2 \cdot D_{2-4} = F_4 \cdot (R_4 + B_4 + D_{4-2})$
5	Vegetation	$F_1 \cdot D_{1-5} + F_9 \cdot D_{9-5} + F_3 \cdot D_{3-5} = F_5 \cdot (R_5 + D_{5-1} + D_{5-2} + D_{5-3} + D_{5-7})$
6	Film	$F_1 \cdot D_{1-6} = F_6 \cdot (R_6 + D_{6-1} + D_{6-2} + D_{6-3} + D_{6-7})$
7	River water	$A_7 + E_7 + F_1 \cdot D_{1-7} + F_5 \cdot D_{5-7} + F_3 \cdot D_{3-7} + F_8 \cdot D_{8-7} + F_6 \cdot D_{6-7} = F_7 \cdot (R_7 + D_{7-1} + D_{7-2} + D_{7-8})$
8	River sediments	$F_7 \cdot D_{7-8} = F_8 \cdot (R_8 + B_8 + D_{8-7})$
Unsteady-state mode		
1	Air	$(Z_1/V_1)dF_1/dt = A_1 + E_1 + F_5 \cdot D_{5-1} + F_6 \cdot D_{6-1} + F_3 \cdot D_{3-1} + F_2 \cdot D_{2-1} + F_7 \cdot D_{7-1} - F_1 \cdot (R_1 + S_1 + D_{1-5} + D_{1-6} + D_{1-3} + D_{1-2} + D_{1-7})$
2	Lake water	$(Z_2/V_2)dF_2/dt = E_2 + F_1 \cdot D_{1-2} + F_5 \cdot D_{5-2} + F_3 \cdot D_{3-2} + F_4 \cdot D_{4-2} + F_6 \cdot D_{6-2} + F_7 \cdot D_{7-2} - F_2 \cdot (R_2 + D_{2-1} + D_{2-4})$
3	Soil	$(Z_3/V_3)dF_3/dt = F_1 \cdot D_{1-3} + F_6 \cdot D_{6-3} + F_5 \cdot D_{5-3} - F_3 \cdot (R_3 + D_{3-1} + D_{3-2} + D_{3-7} + D_{3-5})$
4	Lake sediments	$(Z_4/V_4)dF_4/dt = F_2 \cdot D_{2-4} - F_4 \cdot (R_4 + B_4 + D_{4-2})$
5	Vegetation	$(Z_5/V_5)dF_5/dt = F_1 \cdot D_{1-5} + F_9 \cdot D_{9-5} + F_3 \cdot D_{3-5} - F_5 \cdot (R_5 + D_{5-1} + D_{5-2} + D_{5-3} + D_{5-7})$
6	Film	$(Z_6/V_6)dF_6/dt = F_1 \cdot D_{1-6} - F_6 \cdot (R_6 + D_{6-1} + D_{6-2} + D_{6-3} + D_{6-7})$
7	River water	$(Z_7/V_7)dF_7/dt = A_7 + E_7 + F_1 \cdot D_{1-7} + F_5 \cdot D_{5-7} + F_3 \cdot D_{3-7} + F_8 \cdot D_{8-7} + F_6 \cdot D_{6-7} - F_7 \cdot (R_7 + D_{7-1} + D_{7-2} + D_{7-8})$
8	River sediments	$(Z_8/V_8)dF_8/dt = F_7 \cdot D_{7-8} - F_8 \cdot (R_8 + B_8 + D_{8-7})$

A: Advection and inter-compartmental air dispersion term

D: D value

Z: Bulk Z value

V: Volume of the compartment

F: Fugacity

B: Burial

L: Leaching

R: Degradation reactions

S: Vertical Loss

2.2.2.2 Winter Scenario For Organics

Most multimedia models have been developed for summer conditions that do not consider processes that occur during winter, which can be an appreciable portion of the year. Since Minnesota has relatively long, cold winters, it was necessary to include these conditions in the model (Figure 2.3, Tables 2.5 and 2.6). Similar to the summer scenario, the model considers constant “winter” conditions. In this scenario, we assume a constant temperature of -7°C , frozen surface waters, and an absence of leaves on vegetation. Frozen soil is covered by a snow pack and wet deposition is characterized by snowflakes rather than raindrops. The snow pack links air to soil and impervious surfaces. The snowpack is assumed to be of constant depth (10 cm) and inputs of snow to the snowpack are set equal to losses from the snowpack due to melting. Runoff is predominantly in the form of snowmelt from impervious surfaces (e.g. rooves and roadways). Surface waters receive melt water and exchange continues with the sediments.

Z values are calculated from physical-chemical properties as in the summer scenario. Vapor pressures are corrected for the low temperature using the linear relationship between the logarithm of vapor pressure and inverse temperature (Clausius-Clapeyron equation), where heats of vaporization were assumed to be 60 and 30 kJ/mol for PAHs and VOCs respectively. The chemical degradation rates were corrected for winter temperature (-7°C), assuming that the rate decreases by half for every 10°C temperature drop. Although solubility may change with temperature slightly, for this study the solubility is assumed to be independent of temperature.

Table 2.5: Inter-compartmental transport processes considered for organic chemicals in the winter scenario of the model.

Inter-compartmental transport	Symbol	Individual processes
Air-Film	D ₁₋₆ D ₁₋₆ D ₁₋₆ , D ₆₋₁	Wet deposition Dry deposition Bi-directional diffusion
Air-Snow	D ₁₋₉ D ₁₋₉ D ₁₋₉ , D ₉₋₁	Wet deposition Dry deposition Bi-directional diffusion
Air-Vegetation	D ₁₋₅ D ₁₋₅ D ₁₋₅ , D ₅₋₁	Wet deposition Dry deposition Bi-directional diffusion
Snow-Soil	D ₃₋₉ , D ₉₋₃ D ₉₋₃	Bi-directional vapor diffusion Snow melt infiltration
Soil-Lake	D ₃₋₂	Snow melt run off
Soil-River	D ₃₋₇	Snow melt run off
Vegetation-Snow	D ₅₋₉ D ₅₋₉	Wash off Mechanical removal
Film-Lake	D ₆₋₂	Wash off
Lake-Sediments	D ₂₋₄ , D ₄₋₂ D ₄₋₂ D ₂₋₄	Bi-directional diffusion Sediment resuspension Sediment deposition
River-Lake	D ₇₋₂	Advection
River-Sediments	D ₇₋₈ , D ₈₋₇ D ₈₋₇ D ₇₋₈	Bi-directional diffusion Sediment resuspension Sediment deposition

Table 2.6: Steady- and unsteady-state mass balance equations for environmental compartments for organic chemicals in the winter scenario.

No.	Compartment	Mass balance equation
Steady-state mode		
1	Air	$A_1+E_1+F_6 \cdot D_{6-1}+F_9 \cdot D_{9-1}+F_5 \cdot D_{5-1}=F_1 \cdot (R_1+S_1+D_{1-6}+D_{1-9}+D_{1-5})$
2	Lake water	$F_1 \cdot D_{1-2}+F_4 \cdot D_{4-2}+F_7 \cdot D_{7-2}+F_6 \cdot D_{6-2}+F_3 \cdot D_{3-2}=F_2 \cdot (R_2+D_{2-4})$
3	Soil	$E_3+F_9 \cdot D_{9-3}+F_9 \cdot D_{9-3}=F_3 \cdot (R_3+D_{3-7}+D_{3-9}+D_{3-2})$
4	Lake sediments	$F_2 \cdot D_{2-4}=F_4 \cdot (R_4+B_4+D_{4-2})$
5	Vegetation	$F_1 \cdot D_{1-5}=F_5 \cdot (R_5+D_{5-1}+D_{5-9})$
6	Film	$F_1 \cdot D_{1-6}=F_6 \cdot (R_6+D_{6-1}+D_{6-2})$
7	River water	$A_7+F_8 \cdot D_{8-7}=F_7 \cdot (R_7+D_{7-8}+D_{7-2})$
8	River sediments	$F_7 \cdot D_{7-8}=F_8 \cdot (R_8+B_8+D_{8-7})$
9	Snow	$F_1 \cdot D_{1-9}+F_3 \cdot D_{3-9}+F_5 \cdot D_{5-9}=F_9 \cdot (R_9+D_{9-1}+D_{9-3})$
Unsteady-state mode		
1	Air	$(Z_1/V_1)dF_1/dt = A_1+E_1+F_6 \cdot D_{6-1}+F_9 \cdot D_{9-1}+F_5 \cdot D_{5-1} - F_1 \cdot (R_1+S_1+D_{1-6}+D_{1-9}+D_{1-5})$
2	Lake water	$(Z_2/V_2)dF_2/dt = F_1 \cdot D_{1-2}+F_4 \cdot D_{4-2}+F_7 \cdot D_{7-2}+F_6 \cdot D_{6-2}+F_3 \cdot D_{3-2} - F_2 \cdot (R_2+D_{2-4})$
3	Soil	$(Z_3/V_3)dF_3/dt = E_3+F_9 \cdot D_{9-3}+F_9 \cdot D_{9-3} - F_3 \cdot (R_3+D_{3-7}+D_{3-9}+D_{3-2})$
4	Lake sediments	$(Z_4/V_4)dF_4/dt = F_2 \cdot D_{2-4} - F_4 \cdot (R_4+B_4+D_{4-2})$
5	Vegetation	$(Z_5/V_5)dF_5/dt = F_1 \cdot D_{1-5} - F_5 \cdot (R_5+D_{5-1}+D_{5-9})$
6	Film	$(Z_6/V_6)dF_6/dt = F_1 \cdot D_{1-6} - F_6 \cdot (R_6+D_{6-1}+D_{6-2})$
7	River water	$(Z_7/V_7)dF_7/dt = A_7+F_8 \cdot D_{8-7} - F_7 \cdot (R_7+D_{7-8}+D_{7-2})$
8	River sediments	$(Z_8/V_8)dF_8/dt = F_7 \cdot D_{7-8} - F_8 \cdot (R_8+B_8+D_{8-7})$
9	Snow	$(Z_9/V_9)dF_9/dt = F_1 \cdot D_{1-9}+F_3 \cdot D_{3-9}+F_5 \cdot D_{5-9} - F_9 \cdot (R_9+D_{9-1}+D_{9-3})$

A: Advection

D: D value

Z: Bulk Z value

V: Volume of the compartment

F: Fugacity
 B: Burial
 L: Leaching
 R: Degradation reactions
 S: Vertical Loss

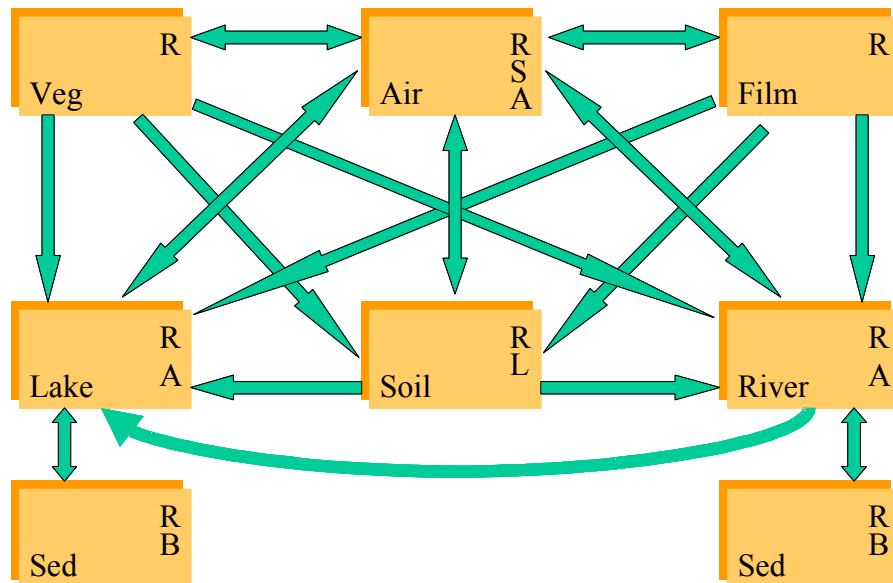


Figure 2.2. Compartments and inter-compartmental transport terms considered for organic chemicals in the summer scenario.

R: Degradation reactions
 B: Sediment burial
 S: Loss to stratosphere
 L: Soil leaching
 A: Advection
 E: Emission

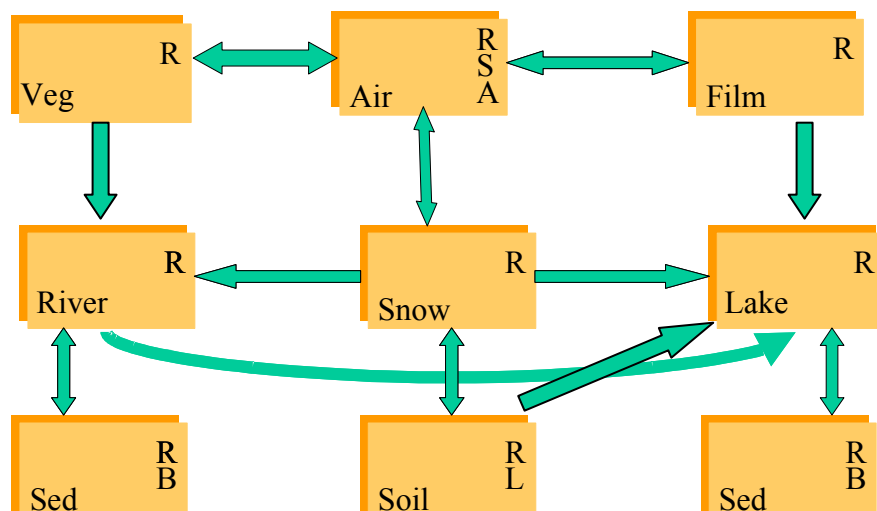


Figure 2.3: Compartments and inter-compartmental transport terms considered for organic chemicals in the winter scenario.

- R: Degradation reactions
- B: Sediment burial
- S: Loss to stratosphere
- L: Soil leaching
- A: Advection
- E: Emission

2.2.2.3 Summer Scenario For Metals

As mentioned above (Section 2.1.3), the equivalence formalism was used to develop the mass balance equations for all compartments except air. Since metals do not have vapor pressures (i.e., are not volatile, except for Hg), an equivalence value cannot be defined for air, however, metals exist in particulate form. To account for this behavior in air, we considered the atmospheric compartment in terms of particulate matter only, i.e., the metal is emitted from a vehicular source as a fine particle that is then subject to air advection and dispersion, as well as depositional processes. The other difference in the metal formulation is the exclusion of bi-directional diffusive processes between air and other compartments (e.g., eliminate air-vegetation, air-film, and air-water diffusive exchange). Tables 2.7 and 2.8 list the D values and mass balance equations used to model metal fate under summer conditions.

Unlike the fugacity formulation for organic chemicals with a measurable vapor pressure, i.e., where Z values are calculated from physical-chemical properties, the formulation for metals relies on empirically derived partition coefficients, e.g., the distribution of metals between

sediment and dissolved phases in water, K_d . The partition coefficients depend upon the ambient chemistry in the system in which they were measured: methods are not yet available to reliably predict partition coefficients based on fundamental properties of each metal. As a result, the use of literature-derived partition coefficients is another source of uncertainty in the model.

Table 2.7: Inter-compartmental transport processes considered for metals in the summer scenario.

Inter-compartmental transport	Symbol	Individual processes
Aerosol-Vegetation	G_{1-5} G_{1-5}	Wet deposition Dry deposition
Aerosol-Film	G_{1-6} G_{1-6}	Wet deposition Dry deposition
Aerosol-Soil	G_{1-3} G_{1-3} D_{3-1}	Wet deposition Dry deposition Soil resuspension
Aerosol-Lake	G_{1-2} G_{1-2}	Wet deposition Dry deposition
Aerosol-River	G_{1-7} G_{1-7}	Wet deposition Dry deposition
River-Lake	D_{7-2}	Advection
Vegetation-Soil	G_{5-3} G_{5-3} G_{5-3}	Canopy drip/leaf wash off Wax erosion Litter fall
Film-Lake	G_{6-2}	Film wash off
Film-River	G_{6-7}	Film wash off
Soil-Lake	D_{3-2}	Soil run off (dissolved and solid phases)
Soil-River	D_{3-7}	Soil run off (dissolved and solid phases)
Lake-Sediments	D_{2-4} , D_{4-2} D_{4-2} D_{2-4}	Bi-directional diffusion Sediment resuspension Sediment deposition
River-Sediments	D_{7-8} , D_{8-7} D_{8-7} D_{7-8}	Bi-directional diffusion Sediment resuspension Sediment deposition

Table 2.8: Steady- and unsteady-state mass balance equations for environmental compartments for metals in the summer scenario.

No.	Compartment	Mass balance equation
Steady-state mode		
1	Aerosol	$E_1 + A_3 \cdot D_{3-1} = C_1 \cdot (G_{1-5} + G_{1-6} + G_{1-3} + G_{1-2} + G_{1-7})$
2	Lake water	$E_2 + C_1 \cdot G_{1-2} + A_3 \cdot D_{3-2} + A_4 \cdot D_{4-2} + C_1 \cdot G_{6-2} + A_7 \cdot D_{7-2} = A_2 \cdot D_{2-4}$
3	Soil	$C_1 \cdot G_{1-3} + C_1 \cdot X \cdot G_{5-3} = A_3 \cdot (D_{3-1} + D_{3-2} + D_{3-7} + L_3)$
4	Lake sediments	$A_2 \cdot D_{2-4} = A_4 \cdot (B_4 + D_{4-2})$
7	River water	$E_7 + C_1 \cdot G_{1-7} + A_3 \cdot D_{3-7} + C_1 \cdot G_{6-7} + A_8 \cdot D_{8-7} = A_7 \cdot (D_{7-2} + D_{7-8})$
8	River sediments	$A_7 \cdot D_{7-8} = A_8 \cdot (B_8 + D_{8-7})$
Unsteady-state mode		
1	Air	$(1/V_1)dC_1/dt = E_1 + A_3 \cdot D_{3-1} - C_1 \cdot (G_{1-5} + G_{1-6} + G_{1-3} + G_{1-2} + G_{1-7})$
2	Lake water	$(Z_2/V_2)dA_2/dt = E_2 + C_1 \cdot G_{1-2} + A_3 \cdot D_{3-2} + A_4 \cdot D_{4-2} + C_1 \cdot G_{6-2} + A_7 \cdot D_{7-2} - A_2 \cdot D_{2-4}$
3	Soil	$(Z_3/V_3)dA_3/dt = C_1 \cdot G_{1-3} + C_1 \cdot X \cdot D_{5-3} - A_3 \cdot (D_{3-1} + D_{3-2} + D_{3-7} + L_3)$
4	Lake sediments	$(Z_4/V_4)dA_4/dt = A_2 \cdot D_{2-4} - A_4 \cdot (B_4 + D_{4-2})$
7	River water	$(Z_7/V_7)dA_7/dt = E_7 + C_1 \cdot G_{1-7} + A_3 \cdot D_{3-7} + A_8 \cdot D_{8-7} - A_7 \cdot (D_{7-2} + D_{7-8})$
8	River sediments	$(Z_8/V_8)dA_8/dt = A_7 \cdot D_{7-8} - A_8 \cdot (B_8 + D_{8-7})$

A: Aquivalence

D: D value

Z: Bulk Z value

V: Volume of the compartment

B: Burial

L: Leaching

E: Combined advection and emission terms

C: Concentrations

G: Total molar flux

2.2.2.4 Winter Scenario For Metals

The same assumptions that were made in developing the winter scenario for organic contaminants were used to develop the winter scenario mass balance equations for metals, e.g., the inclusion of the snowpack and the frozen state of surface waters. Tables 2.9 and 2.10 list the inter-compartmental transport processes and the steady- and unsteady-state mass balance equations for metals in the winter scenario.

Table 2.9: Inter-compartmental transport processes considered for metals in the winter scenario.

Inter-compartmental transport	Symbol	Individual processes
Aerosol-Vegetation	G_{1-5} G_{1-5}	Wet deposition Dry deposition
Aerosol-Film	G_{1-6} G_{1-6}	Wet deposition Dry deposition
Aerosol-Soil	G_{1-3} G_{1-3} D_{3-1}	Wet deposition Dry deposition Soil resuspension
Aerosol-Lake	G_{1-2} G_{1-2}	Wet deposition Dry deposition
Aerosol-River	G_{1-7} G_{1-7}	Wet deposition Dry deposition
Aerosol-Snow	G_{1-9} G_{1-9}	Wet deposition Dry deposition
River-Lake	D_{7-2}	Advection
Vegetation-Surface soil	G_{5-3} G_{5-3} G_{5-3}	Canopy drip/leaf wash off Wax erosion Litter fall
Film-Lake	G_{6-2}	Film wash off
Soil-Lake	D_{3-2}	Soil run off (dissolved and solid phases)
Soil-River	D_{3-7}	Soil run off (dissolved and solid phases)
Lake-Sediments	D_{2-4} , D_{4-2} D_{4-2} D_{2-4}	Bi-directional diffusion Sediment resuspension Sediment deposition
River-Sediments	D_{7-8} , D_{8-7} D_{8-7} D_{7-8}	Bi-directional diffusion Sediment resuspension Sediment deposition
Snow-Soil	D_{3-9} , D_{9-3} D_{9-3}	Bi-directional vapor diffusion Snow melt infiltration
Snow-Lake	D_{9-2}	Snow melt run off

Table 2.10: Steady- and unsteady-state mass balance equations for environmental compartments for metals in the winter scenario.

No.	Compartment	Mass balance equation
Steady-state mode		
1	Aerosol	$E_1 + A_3 \cdot D_{3-1} = C_1 \cdot (G_{1-9} + G_{1-5} + G_{1-6} + G_{1-3} + G_{1-2} + G_{1-7})$
2	Lake water	$E_2 + C_1 \cdot G_{1-2} + A_3 \cdot D_{3-2} + A_4 \cdot D_{4-2} + C_1 \cdot G_{6-2} + A_7 \cdot D_{7-2} + A_9 \cdot D_{9-2} = A_2 \cdot D_{2-4}$
3	Soil	$C_1 \cdot G_{1-3} + C_1 \cdot X \cdot G_{5-3} + A_9 \cdot D_{9-3} = A_3 \cdot (D_{3-1} + D_{3-2} + D_{3-7} + L_3)$
4	Lake sediments	$A_2 \cdot D_{2-4} = A_4 \cdot (B_4 + D_{4-2})$
7	River water	$E_7 + C_1 \cdot G_{1-7} + A_3 \cdot D_{3-7} + A_8 \cdot D_{8-7} = A_7 \cdot (D_{7-2} + D_{7-8})$
8	River sediments	$A_7 \cdot D_{7-8} = A_8 \cdot (B_8 + D_{8-7})$
9	Film	$C_1 \cdot G_{1-9} = A_9 \cdot (D_{9-3} + D_{9-2})$
Unsteady-state mode		
1	Air	$(1/V_1)dC_1/dt = E_1 + A_3 \cdot D_{3-1} - C_1 \cdot (G_{1-5} + G_{1-6} + G_{1-3} + G_{1-2} + G_{1-7})$
2	Lake water	$(Z_2/V_2)dA_2/dt = E_2 + C_1 \cdot G_{1-2} + A_3 \cdot D_{3-2} + A_4 \cdot D_{4-2} + C_1 \cdot G_{6-2} + A_7 \cdot D_{7-2} + A_9 \cdot D_{9-2} - A_2 \cdot D_{2-4}$
3	Soil	$(Z_3/V_3)dA_3/dt = C_1 \cdot G_{1-3} + C_1 \cdot X \cdot G_{5-3} + A_9 \cdot D_{9-3} - A_3 \cdot (D_{3-1} + D_{3-2} + D_{3-7} + L_3)$
4	Lake sediments	$(Z_4/V_4)dA_4/dt = A_2 \cdot D_{2-4} - A_4 \cdot (B_4 + D_{4-2})$
7	River water	$(Z_7/V_7)dA_7/dt = E_7 + C_1 \cdot G_{1-7} + A_3 \cdot D_{3-7} + A_8 \cdot D_{8-7} - A_7 \cdot (D_{7-2} + D_{7-8})$
8	River sediments	$(Z_8/V_8)dA_8/dt = A_7 \cdot D_{7-8} - A_8 \cdot (B_8 + D_{8-7})$
9	Snow	$(Z_9/V_9)dA_9/dt = C_1 \cdot G_{1-9} - A_9 \cdot (D_{9-3} + D_{9-2})$

A: Aquivalence

D: D value

Z: Bulk Z value

V: Volume of the compartment

B: Burial

L: Leaching

E: Combined advection and emission terms

C: Concentrations

G: Total molar flux

2.2.3 Spatial Resolution / Scale

The results of environmental fate models are sensitive to the total size and spatial resolution of the area considered. In this application, the decision tool considers the metropolitan Minneapolis/St. Paul region, a 45 x 45 km² area. This area includes the three rings of urban and suburban development in the Twin Cities.

To account for spatial differences, this area is divided into 81 geographic segments or “boxes” of 5 x 5 km². The model uses landscape data specific to each segment, e.g., area of impervious surface and lake and river water volumes. The multi-segment approach requires employing a simple air dispersion model to predict the flux of chemicals across the boundaries of each segment (Section 2.5.1). Stormwater also conveys contaminants across segment boundaries (Section 2.5.2). Appendix B lists the segment-specific data used in the model.

2.2.4 Temporal Resolution / Scale

The model is capable of carrying out both steady-state and unsteady-state or transient calculations. Whereas steady-state calculations deal with snapshots in time during which conditions are constant (not to be confused with equilibrium conditions that are not assumed to prevail), the transient calculations accommodate monthly and seasonal changes in environmental conditions, e.g., values of temperature, precipitation, wind speed and direction, and river discharge volume are varied in the model. Since the environmental behavior of contaminants in cold climates differs between summer and winter, the model has two independent routines for summer and winter calculations (as described above). The minimum time scale over which environmental parameter values are changed is bi-weekly.

The steady-state formulation is suitable in circumstances where model parameters are relatively constant and where detailed temporal information are lacking. However, as Mackay (1) argues, steady-state models provide most of the information needed, including estimates of the response time of the system. Mathematically, the assumption of steady-state conditions is reasonable for soil and sediment, which respond slowly to changes such as variations in loadings. In contrast, air, water, vegetation and organic film compartments respond quickly to environmental changes and may not achieve steady state. The steady-state version of the model assumes pseudo-steady-state conditions over a short time in order to overcome the difficulties arising from the large differences in time constants among the compartments that respond “slowly” and “quickly.” Figure 2.4 depicts a simplified flow chart for the steady-state calculations.

The transient model accounts for temporal changes in temperature, precipitation, wind speed and direction, and river discharge volume. The entire time domain for the transient model is broken into two-week periods. For each two-week period, the parameters are assigned values representative of constant, seasonal conditions. After this two-week period the values are updated. The model uses the previous and new sets of data in the discretized transient mass balance equations for the new period to solve the equations. This iterative procedure continues to the end of the model run. Thus, the model is intended to simulate shifts in average conditions;

the model does not track events such as storms. The results from the steady-state calculations are used to initialize the unsteady-state version (Figure 2.5).

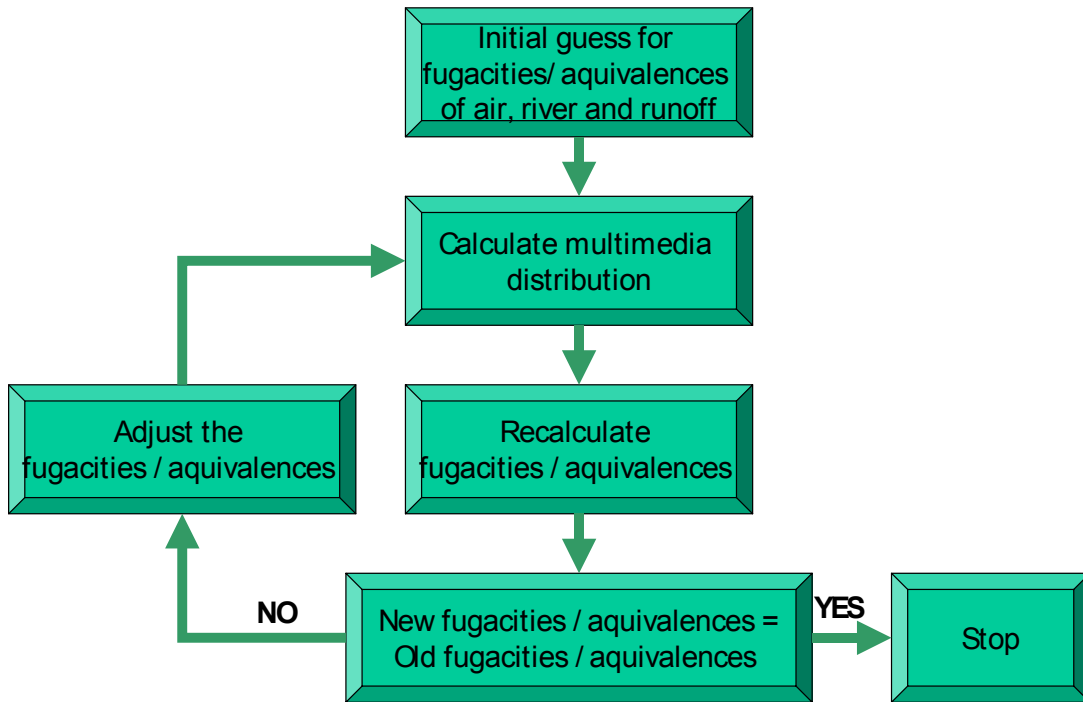


Figure 2.4: The simplified flow chart for steady-state calculations.

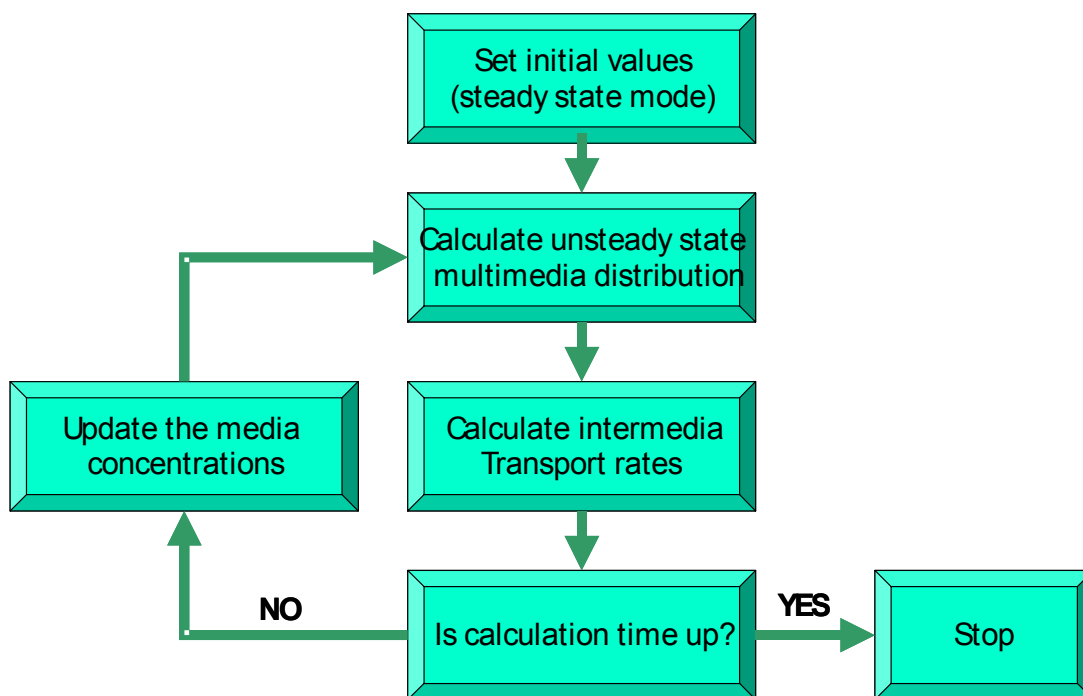


Figure 2.5: The simplified flow chart for unsteady-state or transient calculations.

Simultaneously solving the steady-state and transient mass balance equations for all boxes requires numerical methods. The method of successive iteration was used to obtain the simultaneous solution of the steady-state mass balance equations. The model is first initialized with chemical concentrations in air, river water, and runoff in all boxes. These three media control inter-box transport of chemicals. Using these initial values allows the model to solve the equations for each segment independently. For computational purposes, a relaxation parameter is used to slow down the convergence and to avoid divergence.

For the unsteady-state version, the set of differential equations are solved on a time-step basis using an explicit finite difference method. The time steps for the calculations are in the order of 5-20 seconds to ensure the stability of the solution. The steady-state results are used as the initial values for the unsteady-state calculations.

2.3 Multimedia Transport Processes

2.3.1 Air

Air is the medium into which all chemicals are emitted. Organic chemicals, e.g., formaldehyde, can be emitted in the gas-phase. Organic chemicals and metals can be emitted as fine particulate matter. Chemicals, or any particular chemical, are assumed to be emitted into the air of a particular box and instantaneously achieve a constant concentration in that box and, for volatile chemicals, an instantaneous equilibration between gas- and particle-phases. From that

geographic segment, chemical can move within air among segments or to other media (e.g., vegetation, water) within the box.

As discussed in Section 2.2.1, air is divided into two vertical layers among the 81 geographic segments. Intra-segment movement of chemical between the two vertical layers and movement between adjacent segments is discussed below. In addition to these processes, chemical can exchange between the atmosphere and the other compartments through depositional and diffusive processes.

Bi-directional diffusive transfer is modeled using the conventional two-film theory. When two compartments, such as surface water and air, are in contact, the mass transfer from air to water (or from water to air) depends on mass transfer through both the air-side and water-side boundary layers. The overall resistance to mass transfer through the two boundary layers is the sum of the two resistances through the air and water boundary layers. The mass-transfer resistance is proportional to the inverse of the mass transfer coefficient:

$$U = [1/(U_a) + 1/(U_w)]^{-1} \quad (2.9)$$

The mass transfer coefficient at each side can be written as a function of the effective diffusion coefficient and boundary layer thickness of each side:

$$U_a = D_a / \delta_a \quad (2.10)$$

$$U_w = D_w / \delta_w \quad (2.11)$$

where D_a is the diffusivity in the air compartment, m^2/d ; δ_a is the boundary-layer thickness in the air above water, m; D_w is the effective diffusivity in the water compartment, m^2/d ; and δ_w is the boundary-layer thickness in the water below the air, m. The relationships derived in this section for mass transfer at the air-water interface can be generalized to mass transfer at air-soil, soil-soil, and water-sediment interfaces.

There is a discontinuity in concentration at this boundary because the concentration at the interface reflects the equilibrium partitioning of contaminant concentrations in the different phases. In contrast, the fugacity is continuous across this interface. Thus, the above equations can be modified for use in the fugacity approach:

$$U_z = [1/(Z_a U_a) + 1/(Z_w U_w)]^{-1} \quad (2.12)$$

Dry deposition of particulates from air is calculated using a dry deposition velocity and the following equation:

$$\text{Dry deposition} = V_d \times A \times v_p \times C_p \quad (2.13)$$

where :

V_d is dry deposition velocity, m/h

A is the deposition area, m²

v_p is particulate volume fraction in air

C_p is concentration of chemical in particulate phase.

Wet deposition comprises two processes of rain dissolution and wet particulate scavenging. Rain dissolution removes the chemicals from air by dissolving the gaseous chemicals in raindrops. In the winter scenario, this term is assumed to be zero, because of the limited ability of snow flakes to dissolve chemical. The following equation is used to calculate rain dissolution:

$$\text{Rain dissolution} = P \times C_r \times A \quad (2.14)$$

where P is the precipitation rate (m/h), C_r is the equilibrium concentration of chemical in raindrops (mole/m³), and A is the deposition area.

Wet particulate scavenging is calculated using scavenging factors of 200,000 (1) for raindrops in summer and 1,000,000 (16) for snowflakes in winter. The equation that is used is:

$$\text{wet scavenging} = P \times v_p \times C_p \times R \times A \quad (2.15)$$

where R is the scavenging ratio.

2.3.2 Water

Surface water occurs as lakes and rivers and the dimensions of each are defined by site-specific data retrieved from the Lakefinder database of the Minnesota Department of Natural Resources (15). Concentrations of suspended particles are constant across all lakes at 40 mg/L and across all river compartments at 60 mg/L. All particles have a defined fraction of organic carbon that controls the partitioning of organic chemicals. Chemical enters lake and river water from the air through adsorption and wash-out of gas-phase chemical and wet and dry deposition of chemical in the particle phase. Chemical (dissolved and particle-phase) can enter the river water through advective flow from other geographic segments. Lakes can receive chemical inputs from the wash-off of the organic film on impervious surfaces via stormwater outfalls.

The diffusive exchange of volatile and semi-volatile organic chemicals between air and surface water depends on both the physicochemical properties of the contaminant and the physical properties of the air and water compartments. Important physicochemical properties include solubility, molecular weight, vapor pressure, and diffusion coefficients in air and water. The important landscape properties include temperatures of air and water, wind speed, water-flow velocity, water depth, and water turbulence.

Lyman et al. (17) have reviewed several methods for estimating water-side and gas-side mass transfer coefficients for atmosphere-surface water exchange of organic chemicals. The

estimation of the air-side and water-side boundary mass-transfer coefficient, D_w/δ_w , can be based on methods developed by Southworth (18) from laboratory data. In this method the mass transfer coefficient is a function of current and wind velocity as well as chemical molecular weight.

Chemical can be lost from surface waters by water-air diffusive exchange (as mentioned above), sediment-water diffusive exchange (below), advective loss to downstream segments (the latter applies to dissolved and particle-phase chemicals in river water), and sediment deposition of particle-phase chemicals. Loss via sediment deposition is parameterized according to a bulk rate of sediment loss taken from values typical for lakes and rivers in the area. Rates of net deposition are minimal for the river, i.e., deposition is balanced by resuspension. Lakes do have net deposition of material, with deposition exceeding resuspension.

2.3.3 Sediment

Sediment is parameterized as a 5 cm layer of solids and pore water within which chemical is assumed to exchange with the overlying water. Beneath this layer are buried sediments that are a sink or ultimate loss for chemicals (Section 2.4.3). Partitioning between sediment solids and pore water is defined by K_{OW} and K_d for organics and metals, respectively.

Chemical exchanges between sediment and the overlying water through deposition and resuspension. Dissolved chemicals exchange through bi-directional diffusion. Formica et al. (19) have described a method for calculating the effective diffusivity of the sediment layer based on corrections for the solids content of sediment. This approach is similar to that used by Jury et al. (20) for soil with the volume fraction of the gas phase set to zero. Boundary layer thickness can be calculated using the method of Jury et al. (20).

2.3.4 Soil

The model considers the top 5 cm of soil. Chemical enters soil from air and vegetation, and is lost from soil via volatilization, via run-off of dissolved and particle-sorbed chemical and via leaching to deeper soils. Since the layer is less than 5 cm deep, it is considered to lie above the water table and thus to be fully aerated. Soil is the most complex of compartments since it is composed of water, air, and soil solids, with the latter having a defined organic carbon fraction.

The diffusive flux between air and soil is in part controlled by the boundary layer thickness that, for well mixed compartments, is on the order of centimeters. Cohen et al. (21) have noted that the soil compartment in a multimedia model should use a spatial diffusion model. Jury et al. (22) have shown that the limiting soil depth varies from 0.001 m (for chrysene) to 160 m (for dichlorodifluoromethane) in sandy soil and from <0.001 to 61 m for the same compounds in clay soil. The limiting soil depth is defined as the thickness of soil that is required to limit volatilization loss over an infinite time to less than 1% of the initial concentration. This is the depth at which volatilization at the surface has essentially no impact on concentration.

There have been several approaches to the problem of devising a simple but accurate model of diffusive exchange between air and soil. In one of the more simple approaches, Mackay (1) uses a diffusion-path length that is half the depth of the soil compartment, which in their case was 0.1 m, and in this model is assumed to be 2.5 cm, as the boundary-layer thickness in their regional fugacity model. The diffusion coefficient is independent of which chemical is modeled. Mackay (1) notes that using a single soil layer and a half-depth boundary layer can significantly underestimate volatilization at the soil surface. He suggests two potential remedies for this situation: (1) use more than one soil-layer compartment in the multimedia model, and (2) use the geometric-mean value of the soil-layer depth as an approximation for boundary layer.

Jury et al. (20) have developed a comprehensive analytical expression for estimating the flux and concentration of a contaminant at any point at or above the initial depth of contaminant incorporation. Jury et al. (22) have also developed a version of this model that can be applied to contaminants buried at some depth below the surface. These models have the advantage of being analytical solutions and of having been evaluated against field experiments with pesticides. In this model the method developed by Jury et al. (20) is used to calculate the mass transfer coefficient in soil and consequently the leaching rate.

Diffusive mass transfer at the soil-air interface accounts for both net volatilization of contaminants from soil and deposition of gas-phase contaminants to the ground-surface-soil layer. Once again, net mass transfer depends on mass transfer through both the air-side and soil-side boundary layers. The mass transfer coefficient in the soil side is calculated using the effective diffusion coefficient, which in turn is calculated using the diffusion coefficient through pore water and air in the soil as described in Section 2.3.1. The mass transfer coefficient in the air side is assumed to be constant and equal to 3 m/h.

The transport of chemical from soil to surface water occurs through the runoff process. While some of the rainfall infiltrates the soil and subsequently leaches chemicals from soil to groundwater, some runs over the soil as runoff and carries chemicals to surface water. For this study it was assumed that 50% of rain infiltrates soil while only 10% of the rain to impervious surfaces infiltrates.

2.3.5 Film

It is assumed that impervious surfaces are covered by an organic coating derived from both natural and anthropogenic sources (2), (23). The organic film accumulates chemicals beyond that of clean surfaces due to its “sticky” nature (24). The total area of impervious surfaces is calculated similarly to that of leaf area by using aerial estimates of impervious surface area and an impervious surface index (ISI) developed for typical building arrangements and dimensions by Theurer (13) and adapted by Diamond et al. (2). The total interfacial area of impervious surfaces was assumed to be 50% two-dimensional surfaces (e.g., roadways and sidewalks) and 50% three-dimensional structures.

Chemicals accumulate in the film through wet and dry deposition of particle-sorbed phases and absorption of gas-phase constituents, processes described by Priemer and Diamond

(3). Chemical loss is through wash-off and volatilization (Figure 2.6). Bi-directional gas-phase transfer is modeled using the conventional two-film theory. The air-side mass transfer coefficient, k_A (m/h), is calculated as the ratio of the mean diffusivity of the contaminant in air to the boundary layer thickness, δ_a (mm), adjacent to the film surface as outlined in Nobel (25):

$$\delta_{bl} = \beta \times \sqrt{\frac{l}{v}} \quad (2.16)$$

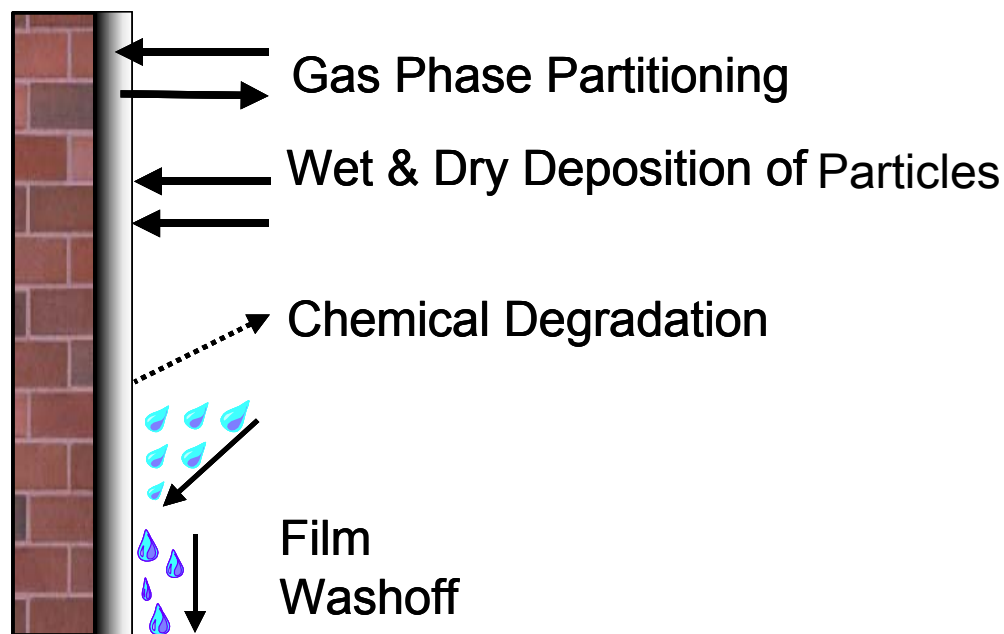


Figure 2.6: Transport processes for the organic film on impervious surfaces.

where l (m) is the mean length of the surface in the direction of the wind, v (m/s) is the wind speed, and β ($\text{mm}\cdot\text{s}^{-1/2}$) is assigned a value of 6 (in accordance with hydrodynamic theory for an air current adjacent to a flat plate). The film-side mass transfer coefficient, k_F (m/h), is calculated according to Trapp (26):

$$\text{Log}[U_F] = (0.704 \text{ Log } K_{OW} - 11.2) / K_{AW} \quad (2.17)$$

where K_{AW} is the air-water partition coefficient.

The film facilitates the transfer of chemicals accumulated from the atmosphere to surface waters through film wash-off. The wash-off process occurs independently of chemical solubility (11), a feature presumably attributable to the high concentration of polar compounds in the film (27). Precipitation conveys film constituents to surface waters. It is assumed that the extent of

wash-off is related to the intensity of the precipitation up to a maximum rate of removal and results in a portion of the film remaining. Consequently, film-water transfer is estimated as a bulk removal process of a fraction of the film, independent of the physical-chemical properties of chemicals. The process is controlled by a mass transfer coefficient, U_{FW} (m/h):

$$U_{FW} = T_F \times W \quad (2.18)$$

where T_F is the film thickness (m), and W is the wash-off rate constant (h^{-1}). Currently it is believed that the value of W reaches an asymptote but the exact nature of the relationship between wash-off and precipitation rate is now being investigated (Labencki, unpubl. data). To estimate a reasonable value applicable to steady-state rather than event-specific conditions, W can be determined empirically by comparing measured contaminant loadings from sewer outfalls in Toronto (28) with measured chemical concentrations in the organic film (23), hydrological data, and impervious surface coverage (11).

On a steady-state basis, the yearly average film thickness and volume are assigned a constant value. For metals, since they do not degrade and do not undergo diffusive exchange with gas-phase chemical, chemical accumulation is equal to the removal of particles from the film. Thus, an overall mass balance for particles in the film can be written as follows:

$$G_i = G_o \quad (2.19)$$

where G_i is the total particulate matter input and G_o is total solids output from the film.

The mass balance for the metal can be written as follows:

$$C_p G_i = C_{film} G_o \quad (2.20)$$

where C_p and C_{film} are metal concentrations in atmospheric particulate matter and film, respectively. Comparing Equations 2.19 and 2.20 result in the following:

$$C_p = C_{film} \quad (2.21)$$

which means that the concentration of the metal in the film is the same as the concentration of the metal in the atmospheric particulate matter.

2.3.6 Vegetation

Diamond et al. (2) summarize the treatment of air-vegetation-soil transfer that incorporates vegetative canopy interception (29), (30), (31) and contaminant partitioning between air and leaves and air and soil (32), (33). These processes are illustrated in Figure 2.7.

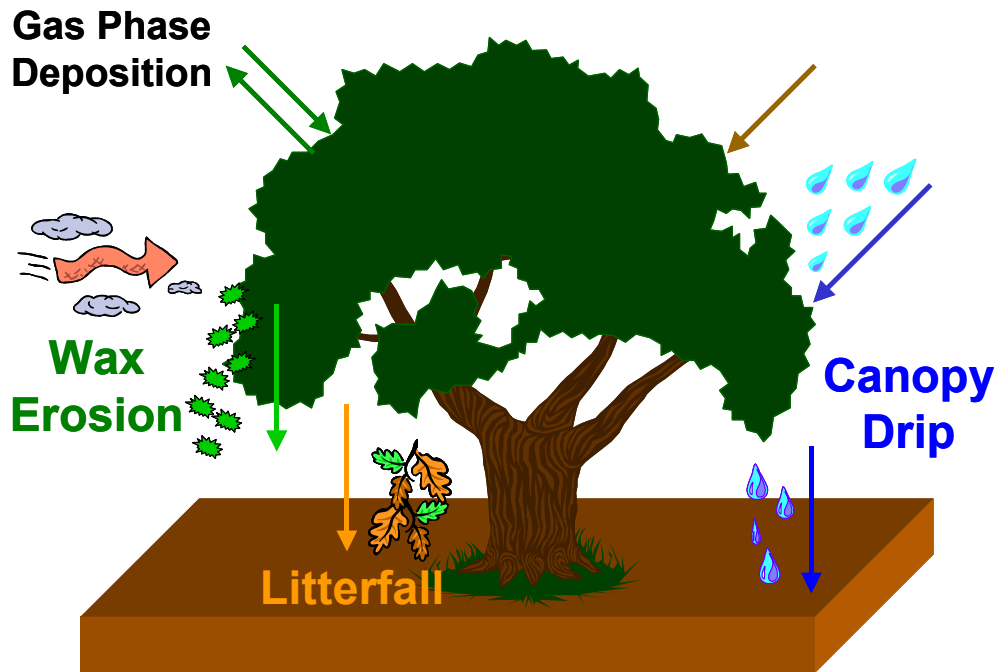


Figure 2.7: Transport processes for vegetation.

Similar to the film, the cuticle of leaves mediate air-leaf exchange of gas-phase chemical. This bi-directional diffusion is described using the Whitman two-film theory. The air-side mass transfer coefficient for vegetation is calculated similarly to that for the film, substituting a value of 4 for β for vegetative surfaces (25).

Canopy interception of atmospherically deposited chemical under wet and dry conditions is described as the fraction of chemical, on an aerial basis, that is deposited on leaves. The dry deposition interception fraction, I_{fD} , is from Whicker and Kirchner (34):

$$I_{fD} = 1 - \exp(-2.8 \cdot B) \quad (2.22)$$

where B is the above ground biomass of vegetation (kg dry mass/m^2). The wet deposition interception fraction, I_{fW} , is a function of leaf area index (LAI), and the interception coefficient, α . I_{fW} can vary considerably with meteorological conditions and canopy density (35):

$$I_{fW} = LAI \times \alpha \times (1 - \exp(-\ln 2/3 \cdot 1/\alpha)) \quad (2.23)$$

I_{fD} and I_{fW} are then multiplied by terms for dry and wet particle deposition to a surface, respectively. The wet deposition interception loss fraction, I_{lW} , is defined as the fraction of total incident precipitation that evaporates off the leaf surface and as such does not enter the soil below. Throughfall is the fraction of contaminants not intercepted by the vegetative canopy, but rather are transported directly from the air to soil (29).

Under wet conditions contaminant transport between vegetation and soil occurs via canopy drip, the removal of particulates from vegetation by rainfall. The mass transfer coefficient for this process, U_{CD} (m/h), is defined as:

$$U_{CD} = R_R \cdot (I_{fW} - I_{lW}) \cdot \lambda \quad (2.24)$$

where R_R is the rain rate (m/h) and λ is the canopy drip parameter, which is related to the efficiency of the removal of particulates from the leaf surface. It is assumed that a fraction of the leaf surface is covered by particles of which only a small fraction are removed in any given rain event.

Litterfall and wax erosion convey chemicals from vegetation to soil under dry conditions. Litterfall occurs when dead or decaying leaf matter falls from trees to the ground. Litterfall is estimated using a first order rate constant, (R_{LF}) which is parameterized as $1/L_G$ where L_G is the length of the growing season (14). In urban centers litterfall is typically collected and disposed of outside city boundaries, making it a permanent removal process for chemicals in the system. Wax erosion transports contaminants from vegetation to soil when portions of the waxy cuticle, which contains chemical, are physically removed.

Particle-sorbed chemical can move from soil to vegetation through rainsplash (34). This process is estimated as the product of the bulk Z value for soil, the soil volume (v_s), and a first order rate constant, R_S (h^{-1}).

Metals are treated similarly to organic compounds with the exception of diffusive processes. Similar to the formulation for metals in the organic film, a simple mass balance equates metals in vegetation (or on leaves to be precise) and the concentration of metal in atmospheric particulate matter. Because of the removal of litter fall from cities, the total input and total output do not balance on a yearly basis. The mass balance equation for metals can be written as follows:

$$C_p G_i = C_{veg} G_o \quad (2.25)$$

where C_{veg} is metal concentration in vegetation, G_i is the atmospheric particulate matter input attributable to wet and dry deposition, and G_o is the output of particulate matter through wash-off and litter fall from the vegetation compartment.

Rearranging equation 2.25 provides:

$$C_{veg} = (G_i/G_o) C_p = X C_{SS} \quad (2.26)$$

where X is defined as:

G_i = wet and dry deposition

G_o = wash off and litterfall

2.3.7 Snow

Snow and the snow pack that accumulates in winter significantly affect chemical fate through wet deposition and air-surface exchange (36), (16). In winter, wet deposition occurs as snowflakes, which scavenge the gas- and particle-phases of chemicals. Franz and Eisenreich (16) found that the scavenging rates for snowflakes can be 10 times greater than those for raindrops, a phenomenon which they attributed to the large surface area of snowflakes, which are coated with a thin film of liquid water. This film is capable of dissolving vapor phase contaminants as well as capturing particle-borne contaminants. Similar to the summer scenario, wet deposition in the winter scenario is calculated using the precipitation rate and a snow scavenging factor (16).

After deposition, the snowflakes in the snow pack age and undergo compaction due to the weight of the snow pack. Snow pack aging and compaction reduce the capacity of the snow to hold chemical (36). This phenomenon results in a “pseudo-volatilization” process that adds to snow-to-air diffusion. The rate of volatilization N_{v-s} (mole/h) is calculated using the difference in the surface sorption capacity of the fresh and aged snow (36):

$$N_{v-s} = D_v f_s = PSA(C_{sf} - C_{sa}) \quad (2.27)$$

where D_v is the transport parameter for volatilization ($\text{mole m}^{-3} \text{ Pa}^{-1}$), f_s is the fugacity of snow (Pa), P is the precipitation rate (m/h), S is the specific surface area of fresh snow (m^2/m^3), A is the landscape area (m^2), and C_{sf} and C_{sa} are the sorption capacities of fresh and aged snow, respectively (mol/m^2).

The snow pack is defined by a specified and constant thickness for both steady-state and transient calculations. This necessitates that the rate of snowmelt equals the precipitation rate of snow. The rate of snowmelt infiltration to soil is approximately 70% while the remaining 30% runs off to surface water (37). It was further assumed that 90% of the snowmelt from impervious surfaces (e.g. roofs and roads) runs off to surface waters and rivers and 10% infiltrates the soil under impervious surfaces through cracks.

The bidirectional diffusion process between soil and snowpack is treated by the method described in Section 2.3.1 for air-soil exchange, with the exception that the snow side mass transfer coefficient is calculated using an effective diffusion coefficient, which in turn is calculated using the diffusion coefficient through pore water and air in the snowpack.

2.4 Loss Mechanisms

2.4.1 Chemical Transformation

Organic chemicals undergo transformation through various reaction mechanisms such as photolysis, oxidation and biodegradation. Organic chemical transformation is assumed to occur only in the dissolved or gas-phase, but not when organic chemicals are sorbed to particles. Transformation processes can occur in all compartments, including snow. Organic chemical

transformations in each environmental compartment are estimated using a first-order degradation rate. The rate constant is calculated using the available half-life time for each organic chemical:

$$k_R = 0.693/t_{1/2} \quad (2.28)$$

This rate constant, k_R (h^{-1}) is used to calculate the mass of organic chemical that is transformed:

$$\text{rate of decomposition} = k_R \times V_c \times C \quad (2.29)$$

The rates of decomposition in winter were corrected for the winter scenario as described in Section 2.2.2.2. Snow is assumed to be 30°C colder than surface water in summer. The rate of degradation in snow is assumed to be 1/8th of that in water.

2.4.2 Soil Leaching

Precipitation to the soil is divided into two portions. The first portion runs off the surface and enters surface waters, carrying with it particle-sorbed chemical. The second portion infiltrates the soil and transfers a fraction of chemical in the aqueous phase from the soil layer to the ground water. It was assumed that 50% of the precipitation infiltrates the soil. The following equation is used to calculate the rate of soil leaching:

$$\text{soil leaching} = 0.1 \times P \times A \times C_1 \quad (30)$$

where C_1 is the equilibrium concentration of chemical in the aqueous phase of infiltrating water.

2.4.3 Sediment Burial

Suspended sediments in surface water settle to the bottom while some of the bottom sediments are resuspended to the water column. The net deposition rate is the difference between the deposition and resuspension rates between the water column and the bottom sediments. Sediment mineralization and decomposition are not considered. The newly deposited layer pushes part of the sediment layer below the active depth of the sediment compartment. This part of the sediment and its associated chemical content is assumed to be buried and is not capable of exchanging the chemicals with the surface water.

2.4.4 Loss To Stratosphere

The air compartment is divided into two vertical layers in each geographic segment. The heights of these two layers are fixed in the steady-state version and vary in the transient version. The height of each layer is determined as follows. The minimum and maximum mixing height in the morning and afternoon were obtained from meteorological data (38). The height of the lower layer equals the minimum mixing height and the upper layer height equals the difference between the maximum and minimum mixing height minus the height of the lower layer. In the afternoon, the mixing height increases resulting from the thermal expansion of the atmosphere. Overnight, the mixing height decreases, resulting in the loss of some of the chemicals. This cyclic “ventilation” mechanism results in net loss of chemical from the air compartment to the

stratosphere. This diurnal loss of chemicals was selected as the steady-state rate of loss to the stratosphere. In the model the cyclic ventilation process is modeled as an average loss mechanism whereby chemicals in the gas- and particle-phases are lost to the air above the two air layers considered.

2.5 Intersegment Transport

2.5.1 Air Dispersion

Since the model considers multiple geographic segments, a simple air dispersion module is needed to estimate chemical transport across segment boundaries and chemical loss to the stratosphere (Section 2.4.4). The Minneapolis/St. Paul area is divided into 81 geographic segments of equal horizontal and vertical dimension. The concentration within each segment is assumed to be uniform and is a function of the segment volume, as well as the rates of chemical emission, import via air advection, and export via air advection.

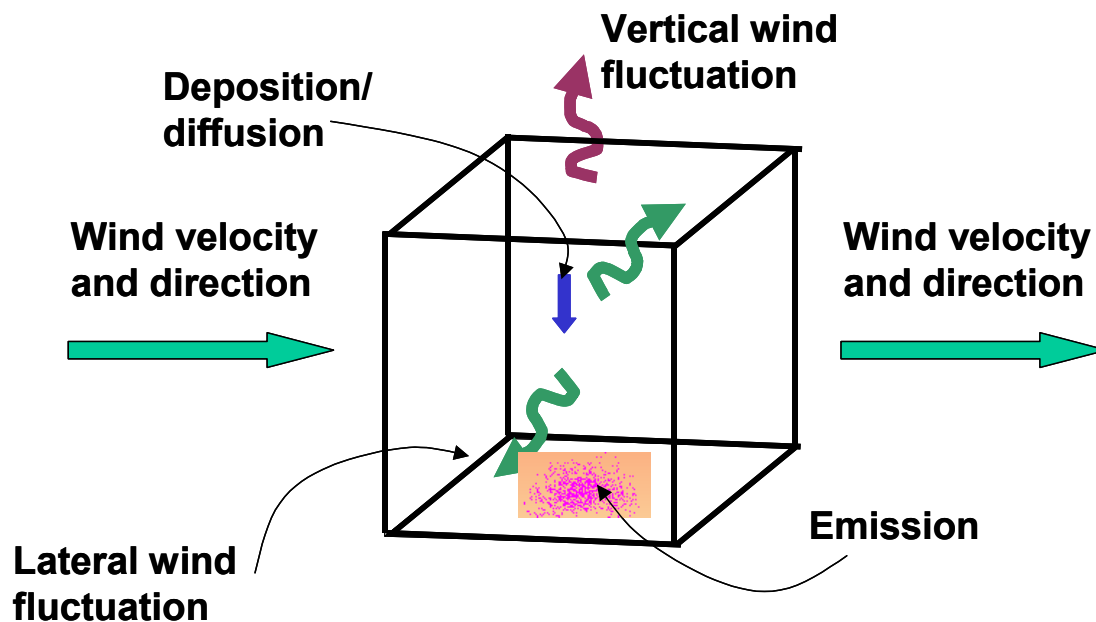


Figure 2.8: Transport processes involving the air compartment.

The atmospheric advection for each segment has two components, one parallel to the wind direction and the other a cross-wind direction which is perpendicular to the wind direction. The average, predominant wind direction is used to calculate dispersion along with the wind direction. The cross-wind dispersion is calculated using the K method (39). Figure 2.8 illustrates these processes.

In this model, turbulent fluxes of chemical C are assumed to be proportional to the mean gradient of C for both gas- and particle-phases. The continuity equation for two-dimensional

(the vertical direction is assumed to be well-mixed), time-independent, and continuous ground-level sources can be written as follows:

$$u \frac{\partial C}{\partial X} = K_Y \frac{\partial^2 C}{\partial Y^2} \quad (2.31)$$

For a simple case of constant u and K_Y , the solution for this equation follows a Gaussian distribution:

$$C = \frac{Q}{1.23u} \left(\frac{u}{4K_Y X} \right)^{1/2} \exp\left(-\frac{uY^2}{4K_Y X} \right) \quad (2.32)$$

The standard deviation of the Gaussian distribution (σ_Y) is given by:

$$\sigma_Y = \left(\frac{2K_Y X}{u} \right)^{1/2} \quad \text{or} \quad K_Y = \frac{u\sigma_Y^2}{2X} \quad (2.33)$$

The following empirical formula was used to calculate σ_Y in urban conditions:

$$\sigma_Y = mX(1 + 0.0004X)^{-1/2} \quad (2.34)$$

For distances greater than 5 km (the size of the segments in the study), the addition of 1 can be neglected and Equation 2.31 reduces to:

$$\sigma_Y = 50mX^{1/2} \quad (2.35)$$

Substituting Equation 2.32 into Equation 2.30 yields:

$$K_Y = 1250m^2u \quad (2.36)$$

Thus the crosswind dispersion term can be formulated as:

$$\text{Crosswind dispersion} = K_Y A \frac{C_1 - C_2}{\Delta X} \quad (2.37)$$

2.5.2 Interbox Transport

Although mass balance equations are written for each segment, they are not independent as they include inter-segment transport processes in the form of air and water advection. Each segment receives chemicals from some of the adjacent geographic segments through air

advection, surface water advection, and runoff, and chemicals exit each segment by means of the same processes to adjacent segments.

Interbox air transport is calculated using the simplified air dispersion scheme described in Section 2.5.1. Surface water transport from each segment to another occurs predominantly by river water flow. Average water flow rates of rivers within the domain were used to calculate the quantity of dissolved and particle-sorbed chemicals moving from segment-to-segment. Finally, information on storm water management was used to model the movement of film wash-off from segment-to-segment.

2.6 Emissions

The major purpose of the model is to estimate the fate of chemicals associated with transportation emissions. As such, it was necessary to estimate “line” emissions for each segment. Specifically, emissions were assumed to enter the lower atmospheric layer of each geographic segment.

Emission rates were estimated using GIS information on road density (road number and length), average daily traffic (ADT) counts, and emission factors for total and individual PAH (US EPA 2000) for light and heavy duty vehicles and for VOCs and metals (Great Lakes Emission Inventory).

Based on this information, the emissions E ($\text{mg}\cdot\text{km}^{-1}$) to air from vehicles in each segment are calculated as:

$$E = \sum L \times ADT_{LDV} \times EF_{LDV} + \sum L \times ADT_{HDV} \times EF_{HDV} \quad (38)$$

where E (mg/d) is the emission rate for each segment, L (km) is road length, ADT_{LDV} is the average daily traffic count for light duty vehicles, ADT_{HDV} is average daily traffic count for heavy duty vehicles, EF_{LDV} ($\text{mg d}^{-1} \text{km}^{-1}$) is the emission factor for light duty vehicles, and EF_{HDV} ($\text{mg d}^{-1} \text{km}^{-1}$) is the emission factor for heavy duty vehicles.

2.7 Spatial Data and Link to GIS

2.7.1 Link to GIS

For this model, the use of multiple geographic segments demands a large amount of spatial data in order to calculate the interfacial surface areas, compartmental volumes, and emissions. For example, each segment requires the area of impervious surface, water and vegetation coverage. In addition, an estimate of leaf area index is needed to calculate the air-vegetation interfacial area. Estimating chemical emissions also requires spatial data on road densities.

In order to efficiently obtain this spatial information and to facilitate the display of model results, the fate model is loosely coupled to the GIS ArcView (Version 3.1). Intermediate data files are used to transfer spatial data between the model and GIS.

Collected spatial data (described in Section 2.7.2) are used to define areal proportions of land cover, which were used to estimate, for each segment, surface coverage of soil, impervious surfaces and lake and river water. The area of impervious surface for each segment was estimated using proportional estimates of impervious surface per land use developed by the US Soil Conservation Service (1986). For each land use, we computed the area of impervious surface as the product of the proportional estimate of impervious surface and the total area of a land use in a box. The area of the water is explicit in the dataset and used directly to calculate the water surface area in each segment. The area of soil per segment land use was computed by taking the difference of the total area of land use and impervious surface. The estimated land cover is used as input data to be considered in the model. Appendix B summarizes the land use coverage of each segment.

2.7.2 Spatial Datasets

The following data sets were used to complete the spatial analysis necessary for parameterizing the model for Minneapolis/St. Paul:

- 1997 generalized land use data for the Twin Cities Metropolitan Area (Metropolitan Council),
- 1996 city streets for Minnesota municipalities (Mn/DOT). City streets only include Municipal State-Aid Streets (MSAS).

After obtaining the land use dataset in vector format, an 81 km² grid was established for the study area. The grid could be no larger than the spatial extent of the land use coverage and needed to encompass all of the sampling sites.

When the grid was established, both the land use, roads, and grid datasets were converted to a raster format so that the area of each land use and the length of all roads within each of the 81 boxes could be calculated. These values were exported into a table with each record of the table representing a segment in the grid. The land cover for each segment was estimated based on the types and areal extent of land use occurring in each box as discussed above. Road density for each segment was estimated based on the area of the segment and the length of roads. The table for land use measurements and land cover estimates for each of the 81 segments is in Appendix B.

2.8 Input Data

While most of the data required to run the program is provided by the data base as default values, the user has a chance to modify or change the data based on specific needs. The input data are classified into five groups:

- Landscape data (user input or data base or GIS)

- Meteorological data (user input or data base)
- Receptor data (user input)
- Physical/chemical data (data base)
- Toxicological and regulatory data (data base)
- Transport and transformation parameters (data base)
- Exposure data (data base)
- Average Daily Traffic data (ADT) (user input or GIS)

In terms of the landscape data, depth profiles for the lakes were obtained from the information for more than 250 lakes provided by Minnesota Department of Natural Resources (15). The stage and flow rates for the rivers were obtained from a real-time database maintained by USGS. Meteorological data were downloaded from the NOAA web site for three local weather stations.

The database contains physical/chemical data for the chemicals considered, landscape information for selected sites, and meteorological data for selected regions. A complete list of the database files and the structure of the data are provided in the Appendices A to C.

Chapter 3

MUM-Exposure and MUM-Risk

3.1 Introduction

In contrast to substantial improvements in the control of point source emissions to the environment over recent decades (40, 41), emissions from mobile and other non-point sources remain challenging to characterize, monitor and control. Modelling the potential toxicological impacts of contaminant releases can facilitate developing rational and effective policies to respond to the challenge posed by non-point source emissions.

The purpose of this chapter is to present an environmental risk assessment (ERA) decision-support tool that facilitates the assessment of toxicological impacts on biota from chemicals originating from the transportation sector. We introduce a generic screening-level, semi-empirical ERA model applicable to multi-media, multi-receptor assessments for non-point source emissions. The model can address metal and organic contaminants, integrate terrestrial and aquatic environments, incorporate wildlife juvenile life stages, examine winter and summer scenarios, spatially resolve the landscape, consider urban characteristics, investigate multiple contaminants, and integrate contaminant fate and transport, exposure and risk modeling into one decision-support tool. The model is deterministic, tracks parent contaminant but not transformation products, and is applicable to chemical stressors only.

This chapter describes the risk assessment component of the Multimedia Urban Model or MUM. MUM-Exposure and MUM-Risk estimate the potential risk to ecological receptors arising from contaminant concentrations estimated by MUM-Fate, a Level III fugacity and equivalence model developed for urban/suburban environments (2). Figure 3.1 illustrates the MUM modeling components, their inter-relationships, and the necessary input and output parameters.

3.2 Background

ERA is a process that evaluates the potential adverse effects that human activities have on our ecosystems (42). It is a tool that systematically gathers the available information on exposure and toxicity potential while explicitly identifying data gaps and the limitations in the current scientific knowledge (43). By using conservative assumptions, screening-level ERAs are typically used to identify or “screen” contaminants or highlight areas that are potentially at risk using information that is readily available in the literature. The goal of the MUM-series is to screen a large number of contaminants for their potential environmental impacts and to identify Contaminants of Potential Ecological Concern (COPECs). Contaminants which are classified as COPECs are recommended as candidates for additional research, for more detailed ERAs, or for environmental monitoring.

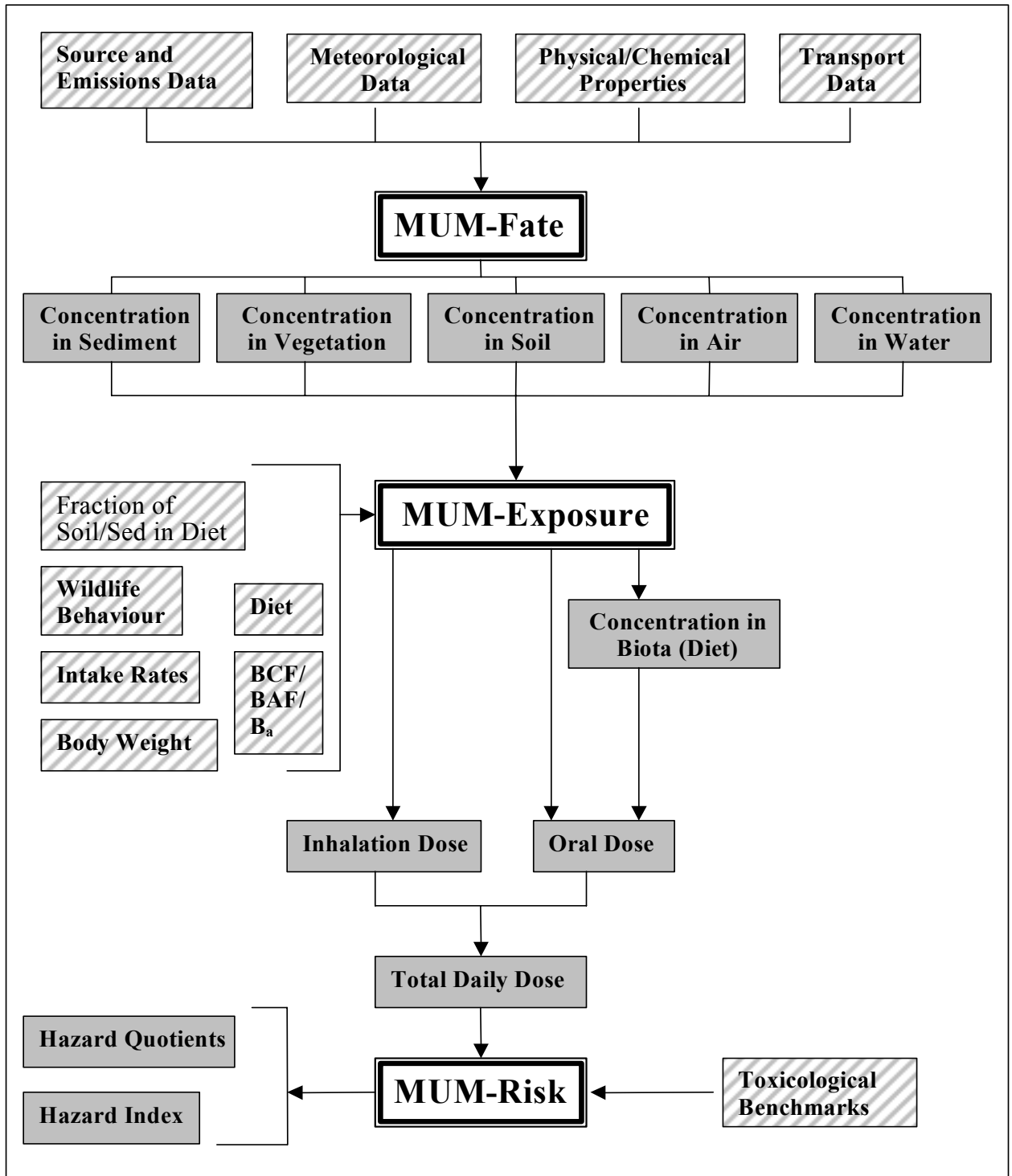


Figure 3.1: Multi-media Urban Model (MUM) – structure and input and output parameters.

3.3 Development of MUM-Exposure

MUM-Exposure describes the course a contaminant takes from the abiotic environment to wildlife (i.e., the exposure pathway), and describes the spatial intensity of co-occurrence or contact. The utility of MUM-Exposure is that it calculates potential contaminant doses to wildlife and it elucidates the relative importance of different exposure pathways.

3.3.1 Wildlife Receptors

Total daily dose (TDD) (oral and inhalation, addressed separately) is calculated from wildlife's exposure to contaminants in a multi-media environment. MUM-Exposure consists of species-specific and generic exposure models for mammals (rodents, herbivores, and non-herbivores) and birds (passerine and non-passerine). These generalized exposure models can be applied to most wildlife species by inputting species-specific parameters, such as body weight, behaviour and diet. For each receptor, the exposure is calculated for an adult (female) and a juvenile. Species-specific exposure models were developed for (Appendix D):

- Great Blue Heron, (*Ardea herodias*)
- American Robin (*Turdus migratorius*)
- Canada Goose (*Branta canadensis*)
- Bald Eagle (*Haliaeetus leucocephalus*)
- Mallard Duck (*Anas platyrhynchos*)
- Lesser Scaup (*Aythya affinis*)
- Osprey (*Pandion haliaetus*)
- Red-tailed Hawk (*Buteo jamaicensis*)
- American Kestrel (*Falco sparverius*)
- American Woodcock (*Scolopax minor*)
- Spotted Sandpiper (*Actitis macularia*)
- Herring Gull (*Larus argentatus*)
- Belted Kingfisher (*Ceryle alcyon*)
- March Wren (*Cistothorus palustris*)
- Northern Bobwhite (*Colinus virginianus*)
- Red Fox (*Vulpes vulpes*)
- River Otter (*Lutra canadensis*)
- Muskrat (*Ondatra zibethicus*)

- Short-Tailed Shrew (*Blarina brevicauda*)
- Meadow Vole (*Microtus pennsylvanicus*)
- Raccoon (*Procyon lotor*)
- Mink (*Mustela vison*)
- Eastern Cottontail (*Syvilagus floridanus*)
- Deer Mouse (*Peromyscus maniculatus*)

3.3.2 Routes of Exposure

The exposure media considered are soil, sediment, water, air, and biota (diet). Routes of exposure considered are ingestion and inhalation. Typically in ERAs, the oral route of exposure is considered dominant and all other routes are considered to be negligible (44), (45). This assumption simplifies the exposure calculations and allows for the comparison of total dose to toxicity tests that are based on oral exposure only (8). This assumption may not be appropriate for emissions from the transportation sector, where air emissions are the dominant route of entry into the environment, and continual emittance may result in air concentrations that could be an important source of potential risk for urban wildlife. Therefore, we retain both routes of exposure and calculate an estimated total daily dose (TDD_{oral}) (g-contaminant/g-body weight wet weight/day) and $TDD_{inhalation}$ (g-contaminant/day).

Dermal exposure is not considered because there are inadequate data available to model this route (45), (47). In addition, there is a general lack of understanding of the ecological relevance and mechanisms of wildlife dermal exposure. We justify its exclusion from this screening-level analysis because it is generally not considered a significant route of exposure for wildlife (45), (48), and it would dramatically increase the level of uncertainty in our results. However, studies have shown that the potential importance of the dermal exposure pathway (49), particularly for amphibians (50), may be significant. This is a critical data gap and should be a priority for research.

3.3.3 Contaminant Concentration and Dose

MUM-Exposure was developed by using allometric equations that relate body weight to intake rates for oral ingestion and inhalation (47). Allometric equations are built on the relationship (51):

$$a = b \cdot BW^{1-c} \quad (3.1)$$

where a is a biological variable, b is a constant characteristic of wildlife, BW is body weight, and c is a scaling factor.

Body weight or size has been shown to be related to many biological processes by a quarter power of body mass (51), based on the assumption that all organisms maximize their

energy dispersal mechanisms and this system of dispersal is constrained by the same physical and geometric parameters across all biological systems (51). While the use of these allometric equations, in place of species-specific intake rates, introduces uncertainty, this uncertainty is assumed to be no greater than the natural variability within species (52).

3.3.4 Bioavailability

For metals, it is often assumed that the dissolved free metal ion is available to move across biological membranes and is thus, bioavailable (53). For organics, it is the truly dissolved phase in aquatic systems that is generally considered bioavailable (54). In the aquatic environment, MUM assumes that fraction of organic contaminant in water that is dissolved is bioavailable. For metals, it is the total dissolved metal concentration that we consider bioavailable. When calculating the wildlife exposure dose, we assume that the contaminant's bioavailability is the same as the bioavailability of the chemical used in the toxicity test from which the toxicological benchmark is derived. Because toxicity tests typically use highly bioavailable forms of chemicals, this is a conservative assumption. Our method does not use any modifying factors (e.g. metabolism, assimilation, absorption) to account for the bioavailability of the contaminant. This is a conservative assumption typical for a screening-level ERA (48), (55).

3.3.5 Input: Abiotic and Biotic Contaminant Concentrations

The input parameters required for MUM-Exposure are contaminant concentrations in air (bulk, particle and gas phases), surface water (lake and river water in dissolved and particulate forms), lake and river sediment (dissolved and particulate forms), soil (soil water dissolved solids, and gas-phase), and terrestrial vegetation (bulk). Using these values, empirically and semi-empirically derived biotransfer factors (B_a), bioconcentration factors (BCF), and bioaccumulation factors (BAF) are used to calculate average dietary contaminant concentrations in fish (forage fish and piscivorous fish), aquatic invertebrates, small birds, small mammals, terrestrial invertebrates, earthworms, and aquatic vegetation. BCF describes an organism's uptake of a contaminant from its surrounding media (water, soil or sediment) and is defined as the ratio of the contaminant concentration in an organism (C_{organism}) to the contaminant concentration in the medium (e.g. C_{water}).

$$C_{\text{fish}} = C_{\text{water}} \cdot BCF \quad (3.2)$$

where C_{fish} is g-contaminant/g-fish, C_{water} is g-contaminant (dissolved)/L, and BCF is L/g fish.

BAF and B_a describe the uptake of contaminants from all routes of exposure for aquatic and terrestrial environments, respectively, and are defined as the ratio of the contaminant concentration in the organism to the particular medium contaminant concentration measured for the study (e.g. water, soil, or diet). For example,

$$C_{\text{fish}} = C_{\text{water}} \cdot BAF \quad (3.3)$$

$$C_{bird/mammal} = TDD_{oral} \cdot BW \cdot Ba \quad (3.4)$$

where BAF is L/g-fish, B_a is day/g-tissue, $C_{bird/mammal}$ is g-contaminant/g-bird/mammal, TDD_{oral} is total daily oral dose, g-contaminant/g-bird/mammal/day, and BW is body weight, g.

3.3.6 Exposure Duration (ED)

In the urban environment, transportation-related contaminants are emitted continuously, therefore, we assume that exposure duration is for the life span of the wildlife. Daily consumption of chronically contaminated food, water, soil/sediment, and air can be compared to repeatedly administered single doses in chronic toxicity studies (44).

The exposure duration is critical to characterizing the nature and magnitude of risk (44). Temporal dynamics impacting risk include the reproductive cycle of the receptor, seasonal changes in behaviour and physiology (migration/hibernation), development and maturation, and changes in the external environment of the receptor (e.g. drought conditions, floods, unusually long winter, etc.). Seasonal allometric equations have not been developed for intake and metabolic rates (52). In order to address seasonal changes in contaminant concentrations, MUM-Fate is run for a spring/summer/fall scenario and a winter scenario (leafless deciduous trees, presence of snow and frozen surface water).

The exposure duration term (ED) is used to incorporate migration or hibernation into the exposure calculation (Equation 3.5). For example, a bird migrating from the area for 6 out of 12 months per year, would have an ED of 0.5 as a fraction of 1. The assumption is that the receptor is not exposed to the contaminant for the remainder of the year. This assumption is appropriate for a source-specific ERA because migration removes the receptor from the system of study. The model is either run for a summer or winter scenario, therefore, the model's results are interpreted as representing either an average summer scenario or an average winter scenario.

$$TDD = TDI \cdot ED \quad (3.5)$$

where TDD is total daily dose (g-contaminant/g-body wt-day), TDI is total daily intake (g-contaminant/g-body wt-day), and ED is exposure duration (dimensionless).

3.3.6.1 Foraging Range

Many ERA methods developed for contaminated waste sites apply an exposure factor to address the spatial aspects of exposure (i.e. the proportion of time that the wildlife spends foraging in the contaminated area) (43), (56). This is appropriate for an assessment of a contaminated site where there may be high concentrations of a contaminant in a portion of the wildlife's foraging area. However, this approach is not appropriate for an urban environment where contaminants are ubiquitously distributed over a large spatial scale. In order to characterize the geographic variation in exposure in an urban environment, we have spatially resolved the urban/suburban environment into boxes. Contaminant concentrations within each compartment within each segment are considered to be homogenous. Since the receptors are

assumed to forage and live within each box, the model calculates an exposure scenario specific to the box.

3.4 Dose Calculations: the Building of MUM-Exposure

Wildlife contaminant doses are calculated as a wet weight intake normalized by wet body weight of receptor (g-contaminant/g-body wet weight-day). Dry weight data and factors are converted to their wet weight equivalents using the percentage water content for the given medium or biota (Appendix E lists water contents and Appendix F lists conversion equations).

3.4.1 Total Daily Dose (g/g-day)

The use of a TDD calculation for oral and inhalation (Equations 3.6 and 3.7) assumes that absorption efficiencies are equal for media with equivalent routes of exposure. It is also assumed that these efficiencies are equivalent to the absorption efficiency of the test species and exposure route that was used to derive the toxicological benchmark against which it will be compared (48), (55), (57). For example, the same amount of chemical will reach the target site if ingested through water or food. This assumption introduces uncertainty into the model's estimates.

$$TDD_{oral} = (TDI_{water} + TDI_{food} + TDI_{soil} + TDI_{sed}) \cdot ED \quad (3.6)$$

$$TDD_{inhalation} = (TDI_{gas} + TDI_{particulate}) \cdot ED \quad (3.7)$$

3.4.2 Routes of Exposure

3.4.2.1 Inhalation Exposure

For many ERAs, inhalation of contaminants is assumed to be negligible for birds and mammals (45). This assumption is based on contaminated waste sites where it is appropriate to assume that wildlife exposure to de-gassing contaminated soil and water is negligible compared to wildlife consumption of contaminated soil, sediment, water and diet. However, many contaminants are emitted directly to air from transportation activities and hence, this assumption may not hold for the urban environment. A limitation to assessing risk due to inhalation is a lack of avian data, although data are available for mammalian test species.

TDI for inhalation of contaminant gas- and particle-phases is calculated by (58).

$$TDI_{air} = (IR_{air} \cdot C_{gas}) + (IR_{air} \cdot C_{particulate}) \quad (3.8)$$

Where IR_{air} = intake rate (m^3/day), C_{gas} and $C_{particulate}$ = concentration of contaminant in gas and particle phases, (g/m^3).

Lasiewski and Calder (59) developed an allometric equation for the inhalation rate of non-passerine bird species (Appendix G), which we applied to all birds (47). A factor of 3 was

used to translate this laboratory-derived inhalation rate to a field inhalation rate (47). Stahl (60) developed allometric equations for mammals (Appendix G). This equation was also corrected for free-living metabolic rate by using a factor of 3 (47).

3.4.2.2 Oral Routes of Exposure

3.4.2.2.1 Water Ingestion

An organism's daily water requirements are met by the receptor's intake of drinking water, water contained in food sources, and water produced by metabolism. The physiology of the organism and external circumstances, including temperature, level of stress, and time of year, determine these requirements. Calder and Braun (61) developed an allometric equation for drinking water intake of birds and mammals (Appendix G).

TDI for water ingestion is calculated as:

$$TDI_{water} = NIR_{water} \cdot C_{water} \cdot FR \quad (3.9)$$

where NIR_{water} is body weight normalized water intake rate (g-water/g-body weight-day), C_{water} is water contaminant concentration (g-contaminant/g-water), and FR is fraction of total water ingestion.

It is assumed that each wildlife receptor will receive half of its water intake from lake water and half from river water (FR= 0.5). This assumption can be examined in further assessments on a species and site-specific basis.

3.4.2.2.2 Soil and Sediment Ingestion

Soil and sediment ingestion can occur accidentally or intentionally and can be a critical route of exposure. This is particularly relevant for animals that inadvertently or purposely consume soil or sediment as part of the dietary intake or to aid in digestion (47). For example, wildlife can have high soil/sediment ingestion rates if they primarily eat earthworms due to the high soil content in the gut of the worms (62), (63) or if they hunt by probing or pecking in the sediment to find their prey (47).

Experimentally derived soil or sediment ingestion rates have been determined for few species (47). To generalize to all species we assume that soil/sediment ingestion is a fraction of wildlife's food intake (47). (56). Fractions of soil and sediment in species' total diet have been estimated using wildlife scat analysis (63)-(65) (Appendix H). Where the soil/sediment fractions were unavailable, related wildlife data were used. Literature-derived values were rounded to the nearest whole percentage.

Nagy (52) calculated steady-state food ingestion rates (dry matter per day) on an allometric basis (Appendix G) for broad classes of wildlife based on calculated, free-living metabolic rates and average dietary values (metabolizable energy).

Wildlife ingestion of soil and sediment is calculated as:

$$TDI_{soil/sed} = NIR_{food} \cdot CF \cdot C_{soil/sed} \cdot FR_{soil/sed} \quad (3.10)$$

where NIR_{food} is body weight normalized food (soil/sediment) intake rate (g-soil dw/g-body weight ww-day), CF is a conversion factor for intake rate dry weight to wet weight (95% water content for lake sediment and 80% for river sediment; 30% for soil), $C_{soil/sed}$ is contaminant concentration in bulk soil/sediment (g-contaminant/g-soil/sediment ww), and FR is the fraction of sediment or soil in total dry matter diet of receptor (dimensionless).

Uncertainties arise from the use of highly generalized food intake rates and the assumption of homogenous concentrations of soil and sediment within each geographic box, when in reality these concentrations are highly heterogeneous. Nagy (52) developed the food intake allometric equations for large classes of wildlife (e.g. rodents, herbivores, all mammals). He estimated that variations between species and within the species would result in an under- and over-prediction of -63% to +169% for all mammals, -64% to +176% for rodents, -62% to +161% for herbivores, -55% to +135% for all birds, and -31% to +45% for passerine birds. These confidence ranges also reflect natural variations in age, season, habitat, microclimate, and behaviour (52).

3.4.2.2.3 Diet

The diet is considered the dominant route of exposure for most organic contaminants and has been suggested as a potentially important route of exposure for metals (53). The approach we use to calculate dietary contaminant exposure uses species-specific dietary composition and food intake rates that are calculated using the metabolizable energy (ME) of the dietary item. This method is less uncertain than the allometric equations for food ingestion rates that are used in the soil/sediment ingestion calculations (47) (52).

We calculate the ME using the gross energy (GE) of the dietary item and the assimilative efficiency (AE) for the wildlife species (Equation 3.11):

$$ME = AE \cdot GE \quad (3.11)$$

where ME is metabolizable energy (kcal/g), AE is assimilative efficiency (dimensionless), and GE is gross energy (kcal/g).

GE is the total energy content of a food item and AE is the fraction of GE that the animal is able to absorb for use for respiration, growth and reproduction. AE is governed by the physiology of the consumer and the characteristics of the prey species. Thus, ME is the energy remaining after losses to feces and urine and is the energy available to fulfill metabolic needs, most of which escapes as heat (otherwise known as respired energy) (66). ME and the field free-living metabolic rate (FMR) govern the rate of consumption of the individual food item.

Therefore, the dietary route of exposure is calculated as (47):

$$TDI_{diet} = NFMR \cdot \sum_{i=n}^n \left(\frac{C_i \cdot FR_i}{ME_i} \right) \quad (3.12)$$

where NFMR is body weight normalized free-living metabolic rate of consumer (kcal/g-body weight-day), n is number of dietary items, i is dietary item (e.g. small mammal, earthworms, terrestrial vegetation), C_i is concentration in food item (determined from BAF, BCF, or B_a) (g-contaminant/g-organism ww) and FR is the fraction of each prey item in the total diet (%).

Appendix I and J list generalized AE and GE values across broad consumer/prey relationships (e.g., bird eating terrestrial invertebrates) calculated as the geometric mean of literature-derived AE and GE values (47). Applying generalized AE values to calculate ME is a reasonable approach because it has been shown that AE values are relatively constant among groups of similar avian and mammalian functional feeding groups (i.e. carnivore, herbivore, omnivore, insectivore) (52), (67), (68).

If a particular prey dominates a receptor's dietary composition (criteria: >50 %), then the prey-specific values of GE and AE are used for that food item category rather than the geometric mean for the category. The prey species are assumed to be homogeneous (45), (55), (56).

3.4.2.2.3.1 Normalized Free-living Metabolic Rate (FMR)

Nagy developed allometric equations based on the FMR of 23 species of placental mammals, 13 species of marsupials, and 25 species of birds (Appendix G). The FMR rate is a more accurate metabolic rate to describe wildlife behaviour compared to laboratory-derived rates because FMR incorporates the metabolic cost of basal metabolism, thermoregulation, locomotion, feeding, predator avoidance, alertness, posture, digestion and food detoxification, reproduction, and growth (52). Allometric equations for the FMR do not include representative large, non-passerine, terrestrial birds (>500 g), very small mammals or large ruminants (52). Nagy estimated the 95% confidence intervals of the predicted FMR for mammals (non-marsupials) and birds to be approximately 50% to 60%, 45% to 55%, respectively.

3.4.2.2.3.2 Juvenile Receptors

Juvenile life stages have unique exposure and toxicological profiles, often making them more vulnerable than their parents. It has been shown in human (Mes et al 1984 *in*(69)), rodent (Gallenberb and Vodcink 1989 *in* (69)), dolphin (Cockcroft et al. 1989 *in* (69)), grey seal (Addison and Stobo 1993 *in* (69)), and fur seals (69) that offspring received the bulk of their contaminant burden in the first few months of nursing. By body weight, juvenile fat contaminant concentrations can exceed their mother's after a few months of nursing (69). This potential of receiving high doses of contaminant at a sensitive developmental stage makes this an important route and life stage to consider. Unfortunately, there are limited data with which to assess potential risk to the juvenile life stage.

The exposure and toxicological profiles for juvenile birds and mammals are allometrically scaled using the body weight of juvenile receptors and the same methods as

outlined for the adult females. The important difference in the treatment of juveniles is the introduction of contaminant intake through milk ingestion for mammalian receptors. Many of the toxicity benchmarks are based on studies that incorporated multi-generational studies. Thus, the sensitivity specific to the juvenile is incorporated into the risk characterization. The juvenile bird species' dietary exposure route is modeled using parental dietary composition (i.e. regurgitated food) with juvenile-specific, food intake rates. The juvenile wildlife's source of dietary contaminants is through regurgitated food or milk ingestion, calculated as:

$$TDI_{food/milk} = NIR_{food} \cdot C_{food} \cdot CF \quad (3.13)$$

where NIR_{food} is food intake rate normalized to body weight, (g-food dw/g-body weight ww day), C_{food} or C_{milk} is food or milk contaminant concentration (g-contaminant/g-food or milk ww), and CF is a conversion factor that converts intake rate from dry weight to wet weight (70).

We use Nagy's (52) food ingestion rates in place of the FMR/ME method described above because of the absence of AE or GE values for juvenile wildlife. We assume that the water content of wildlife's milk is the same as cow's milk. We do not model the transfer of contaminants to avian egg yolk, which can be a significant route of exposure for some contaminants (e.g. selenium).

Uncertainties are introduced by the use of Nagy's (52) food intake allometric equations which represent the feeding rates required to achieve energetic steady-state, and do not characterize the increased metabolic cost of growth. However, the food intake equations were developed using the FMR of many wildlife species that were growing (juveniles) and reproducing, therefore, the extra metabolic costs of growth and reproduction are implicitly addressed (52). Juvenile, species-specific food ingestion rates are a critical data gap for ERA.

3.4.2.2.3.3 Milk

B_a for milk from dairy cows are developed for organic contaminants using Equation 3.14 that estimates the biotransfer of contaminants from the cow's feed and water to the milk of the cow (71). This relationship was developed using 28 contaminants that range in metabolic half-lives. We use Equation 3.14 because it is the only method that is available to predict milk-contaminant concentrations, because there is a lack of empirical data, and because of the precedence of its use in human health risk assessments (72).

$$\log Ba_{milk} = -8.1 + \log K_{ow} \quad (3.14)$$

Wildlife milk contaminant concentrations are calculated by applying B_a to the adult female total oral dose (TDD) (Equation 3.15).

$$C_{milk} = TDD_{oral} \cdot BW \cdot Ba \cdot CF \quad (3.15)$$

where C_{milk} is milk concentration (g-contaminant/g-milk ww), TDD is total daily intake (g-contaminant ww/g-body weight adult female wildlife ww-day), BW is body weight of the adult female (g), $B_{\text{a-milk}}$ (day/kg), and CF is a conversion factor (1kg/1000g).

To estimate milk ingestion by juveniles, the milk concentration calculated by Equation 3.15 is applied to the food intake allometric equation used for wildlife, adjusted to a juvenile life stage by using the juvenile's body weight (Appendix G). This is a source of uncertainty because the food intake rate may be much greater for nursing juveniles, but is used in the absence of direct estimates of juvenile intake rates. The juvenile IR_{food} must be converted from dry weight to wet weight using a milk moisture content of 87% (Appendix F).

3.4.2.2.3.4 Metals

Values of $B_{\text{a-milk}}$ for metals are taken from an extensive review of the literature by Baes *et al.* (73).

3.5 Calculating Contaminant Concentration in Wildlife Foods: Tissue Uptake Factors

Tissue concentrations are calculated by MUM-Exposure as follows: the wildlife foods are classified and generalized into aquatic invertebrates, forage and piscivorous fish, small birds, small mammals, terrestrial invertebrates, earthworms, and aquatic vegetation. The contaminant concentrations in terrestrial vegetation are estimated by MUM-Fate. We use three methods to characterize uptake by biota of: 1) non-metabolizable organics, 2) metabolizable organics, and 3) metals (Figure 3.2).

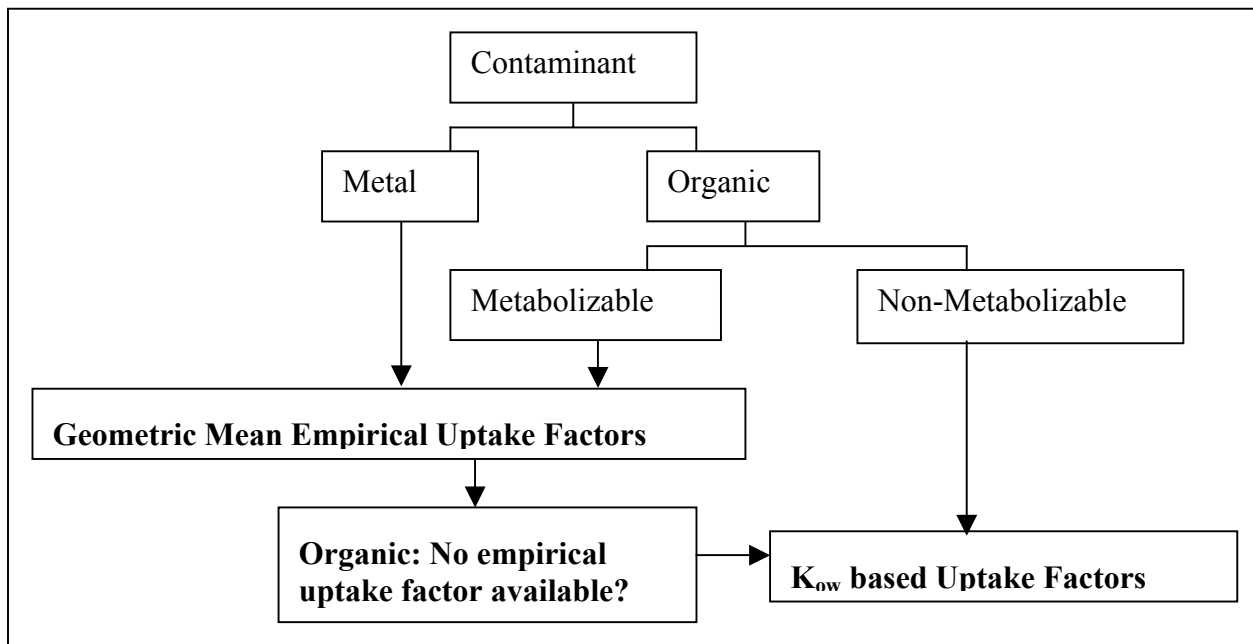


Figure 3.2: Uptake Factor Decision Tree.

Many methods exist for estimating the movement of contaminants from the abiotic environment into biota. For metals and metabolizable organics we use experimentally determined B_a , BCFs and BAFs. For non-metabolizable organic contaminants, we use semi-empirical uptake models based on the octanol-water partition coefficient ($K_{ow} = (g\text{-contaminant}/L\text{-octanol})/(g\text{-contaminant}/L\text{-water})$).

e.g. $BCF = L \cdot K_{ow}$ (74) (3.16)

* recommended for substances with a $\log K_{ow} > 1$. $BCF = 1 + (L \cdot K_{ow})$ recommended for contaminants with $\log K_{ow} < 1$ (75).

where L is lipid content of fish and aquatic invertebrates. We assume that the lipid content of fish and aquatic invertebrates is 5% (54).

Organics whose vertebrate biota (bird, fish or mammal) half-life is less than 100 hours are defined as metabolizable. Vertebrates possess a mixed function oxidase (MFO) system to metabolize organics (e.g. PAHs), whereas invertebrates have a less well developed system resulting in contaminant bioaccumulation (76). Metabolizable organics should be modeled using empirically-derived uptake factors for both invertebrate and vertebrate biota. If biota half-lives are unavailable, then the vertebrate biota half life may be inferred by the abiotic half-life of the contaminant. Under Canada's Persistence and Bioaccumulation Regulations a substance is considered persistent when it has a half-life greater or equal to 2 days in air, greater or equal to 182 days in water or soil, and greater or equal to 365 days in sediments. Therefore, if a contaminant is considered persistent in the abiotic environment, then it may be considered non-metabolizable in the MUM method.

The advantage of using K_{ow} -based models is that they have a mechanistic basis, their use avoids uncertainty and inaccuracy associated with extrapolating laboratory and field studies conducted under specified conditions, and the approach avoids the problem that test organisms may not reach equilibrium concentrations due to kinetic limitations and growth dilution (77). However, the K_{ow} approach is only applicable to non-ionizing organic contaminants that do not appreciably metabolize (78). For metabolizable organics (e.g. benzo(a)pyrene, B[a]P), a K_{ow} -based model overestimates body burden when compared to non-metabolizable organic pollutants (e.g. PCB congeners) (Table 3.1).

Table 3.1: Model-derived BCFs using Equation 3.15 (74) compared to Empirically-derived BCFs.

Contaminant	Log K_{ow}	Organism	Ratio of Model-derived to Empirically-derived BCF
B[a]P	6.04	Fish	35 X larger ^a
PCB congener 47	6	Fish	2.4 X larger ^b
PCB congener 52	6.1	Fish	2.3 X smaller ^b

^a Experimentally-derived BCFs from (79)

^b Experimentally-derived BCFs from (80)

A more accurate means of estimating body burden is using a mechanistic model (e.g. Mackay, Gobas)(77). However, these models require species-specific physiological rates (e.g. uptake, depuration) that are available for only a few species and contaminants (45). While the mechanistic approach is most rigorous, it is not practical for a screening-level risk assessment (45). Until such time that the uptake and depuration kinetics are calculated for a wide range of contaminants, we propose the use of empirical and semi-empirical models that are appropriate for use in a broadly applicable, screening-level tool.

Because the K_{ow} -based approach overestimates body burdens for metabolizable organics, we use empirically-determined BCFs and B_a . For metals, we use empirically-derived values of BCF, B_a and BAF. This approach does not account for the biological complexities associated with metal accumulation, which include biologically-regulated uptake (both active transport and exclusion) and reduced uptake due to toxicity (81). The exception to this is the methods available for metal uptake by earthworms presented by Oak Ridge National Laboratory (81).

3.5.1 Fish

3.5.1.1 Non-metabolizable Organics

Many models have been developed to calculate fish tissue uptake using the contaminant's K_{ow} (74),(17), 82), (83), (84) (85). Gobas (77) extensively reviewed aquatic bioaccumulation models and reported that for non-metabolizable organic pollutants, K_{ow} -based models can underestimate BCFs and BAFs by factors up to 400 times (77). Gobas found that Equation 3.16 only underestimated field values by 8 to 12 times. Equation 3.16 is considered appropriate for screening-level assessments (86) Therefore, we use Equation 3.16 to assess the uptake of non-metabolizable organic contaminants by fish and aquatic invertebrates.

In order to account for dietary transfer of non-metabolizable organic contaminants we use a food chain multiplier (FCM) to calculate a BAF for non-metabolizable organics (72).

$$BAF = FCM \cdot BCF \quad (3.17)$$

Where FCM = food chain multiplier (dimensionless) (Appendix K).

The common guidance is to assume that tissue concentrations are derived as the product of the BCF and the dissolved water concentration of the contaminant when $\log K_{ow}$ is < 4 , and BAF and the dissolved water concentration for contaminants with $\log K_{ow} > 4$ (70), (55). This assumes that the uptake of contaminants with $\log K_{ow} < 4$ is primarily through the respiratory surface and skin, and that uptake of contaminants with $\log K_{ow} > 4$ is through the respiratory surface, skin and diet (72). This approach cannot be used for organics where appreciable metabolism is known to occur.

FCMs were taken from those published in the EPA Great Lakes Water Quality Initiative (87), which were developed using the Gobas model (54). FCMs were developed for forage and piscivorous fish. The FCMs assume no metabolism of the contaminant.

3.5.1.2 Metabolizable Organics and Metals

For metabolizable organics and metals, we use geometric means of empirically derived BCFs.

3.5.2 Aquatic Invertebrates

3.5.2.1 Non-metabolizable Organics

Contaminant concentrations in pelagic aquatic invertebrates are estimated as (54):

$$BCF = L_a \cdot K_{ow} \quad (3.18)$$

where L_a is the lipid content of aquatic invertebrates.

We assume that the lipid content of aquatic invertebrates is 5% (54). The BCF value is applied to dissolved water contaminant concentrations. Sediment is a significant sink for many hydrophobic contaminants, and consequently we calculate benthic aquatic invertebrate concentrations using an approach that uses sediment contaminant concentrations and assumes equilibrium partitioning between the sediment and benthos (Equation 3.19) (54).

$$C_{invertebrates\ benthic} = \frac{L_B}{f_{OC}} \cdot C_{sed} \quad (3.19)$$

Where $C_{invertebrates\ benthic}$ = g-contaminant/g-benthos wet weight, L_B = lipid fraction of benthos (g-lipid/g-benthos ww), f_{OC} = organic carbon fraction of sediment (g-organic carbon/g-sediment dw), and C_{sed} = sediment contaminant concentration (g-contaminant/g-sediment dw).

We assume that the lipid fraction of wet benthos is 6% (54) and the fraction of organic carbon in the dry sediment is 2% (54).

3.5.2.2 Metabolizable Organics and Metals

For metabolizable organics and metals we use geometric means of empirically derived BCFs.

3.5.3 Terrestrial Invertebrates and Earthworms

The terrestrial invertebrates are divided into two groups, earthworms and other terrestrial invertebrates. Earthworms are considered separately because of their critical importance as a dietary route of exposure (88) and because their uptake differs from that of other terrestrial invertebrates.

3.5.3.1 Non-metabolizable Organics

We use the model recommended by EPA (1999) (55) to determine the BCF for non-earthworm, terrestrial invertebrates:

$$\log BCF = 0.819 \cdot \log K_{ow} - 1.146 \quad (89) \quad (3.20)$$

The earthworm BCF is determined by (90):

$$BCF = \frac{K_{worm-water}}{\rho_{worm}} \quad (3.21)$$

where BCF is L-water/g-worm wet weight, $K_{worm-water}$ is a partition coefficient (g-contaminant/L-worm/g-contaminant/L-water), and ρ_{worm} is the bulk density of the worm (g-worm wet weight/L-worm).

We assume that the bulk density of the worm (g-worm wet weight/L-worm) is 1 (90).

$K_{\text{worm-water}}$ is determined by (90):

$$K_{\text{worm-water}} = F_{\text{water}} + F_{\text{lipid}} \cdot K_{\text{ow}} \quad (3.22)$$

where $K_{\text{worm-water}}$ is g/L worm/g/L water, F_{water} is the fraction of water in earthworm (dimensionless), F_{lipid} is the fraction of lipids in earthworm (dimensionless), and K_{ow} is (g-contaminant/L-octanol)/(g-contaminant/L-water). We assume that the fraction of water in the earthworm is 0.84 and lipids is 0.012 (90).

Equations 3.21 and 3.22 assume that contaminant accumulation in earthworms is governed by partitioning between soil solids, soil water, and the aqueous and lipid volumes of the earthworm's tissues (90, (45)). These equations may underestimate accumulation for chemicals for which the dietary source of exposure is significant (45). In addition, the lipid content of worms changes dramatically by season, life stage and between species and sites, which is an important consideration and a source of uncertainty that is beyond the scope of this method.

3.5.3.2 Metabolizable Organics and Metals

Unlike organics, metal uptake by earthworms is not a linear function of soil concentration. Estimating metal uptake by earthworms is problematic because first, the bioavailability of metals from the solid phase depends on metal and soil chemistry and second, uptake generally decreases with increasing soil concentrations (81). The Oak Ridge National Laboratory developed log-linear regression models for 8 metals that more appropriately characterize tissue uptake by earthworms (81) (Appendix L). For all other metals, the geometric mean of literature-derived BCFs is used.

For metabolizable organics we use the geometric mean of empirically derived values or, if unavailable, the method for non-metabolizable organics.

3.5.4 Small Birds and Mammals

3.5.4.1 Non-metabolizable and Metabolizable Organics

In response to the public's concern about the dietary transfer of contaminants from meat and dairy products to humans, B_a were developed for cow tissue and cow milk (70), (91). In human health risk assessments these B_a values are applied to swine and chickens by applying their ratio of body weight fat (70). Following this method, we used the B_a for cows as a surrogate to model contaminant uptake by small mammal prey species and small bird prey species (55). We use the deer mouse and robin to represent the small mammal and small bird prey species. Fat content values were not available for the deer mouse or robin, therefore, we assumed that the deer mouse and the robin have the same fat content as the cow (19%) and the chicken (15%).

The B_a for cows describes the transfer of contaminant concentration in feed to that in tissue is (71):

$$\log B_{acow} = -7.6 + \log K_{ow} \quad (3.23)$$

Following (71), (72) the methods to apply B_a -cow to swine and chickens, we convert the B_a to the deer mouse and robin by applying the wildlife specific intake rates and by correcting for wildlife body lipid.

$$C_{bird/mammal} = TDD_{oral} \cdot BW \cdot B_a \cdot CF \cdot UCF \quad (3.24)$$

where $C_{bird/mammal}$ is g-contaminant/g-bird/mammal body weight ww, TDD is total oral daily intake for deer mouse or robin (g-contaminant /g-bird/mammal ww body weight-day), BW is body weight of deer mouse or robin (g), B_a is cow biotransfer factor (day/kg tissue ww), CF is a lipid conversion factor, cow to small bird or cow to small mammal (dimensionless), and UCF is a unit conversion factor (1kg/1000g).

Equation 3.23 was developed using 36 chemicals with values of $\log K_{ow}$ ranging from 1.34 to 6.89 and metabolic half-lives ranging from 0.64 (Dicamba) to 12000 hours (Mirex). In order to account for contaminant metabolism, the EPA (72) recommends applying a metabolism factor. We do not recommend this post hoc approach because metabolism was implicitly accounted for in the experiments upon which Equation 3.23 is based. Thus Equation 3.23 will under- and over-estimate the B_a for contaminants that are not metabolized versus those that are rapidly metabolized, respectively. Significant uncertainties are associated with this method, notably the differences between cow and wildlife uptake, metabolism and excretion of contaminants. There is some evidence to suggest that the application of the B_a -cow to the swine and chicken may be appropriate (Summermann et al. 1978, Furst et al. 1990, Theelen et al. 1993 *in* (92)), however, there is no evidence to support this extrapolation to wildlife. It is important to note that the cow's ruminant digestion undoubtedly has implications for the uptake of contaminants. In addition, agricultural animals may behave similarly due to their high growth potential, fat content and short life spans. However, wildlife UF are not available for organic contaminants, with the exception of dioxins and furans (93), for representative omnivores, carnivores or non-ruminant herbivores, therefore, until other methods become available this method is appropriate for a screening-level risk assessment.

3.5.4.2 Metals

For metals, we use the value of B_a compiled from an extensive review of the empirical literature by Baes et al. (73).

3.5.5 Aquatic Vegetation

The organic contaminant concentration in aquatic vegetation is estimated as (54):

$$BCF = L_a \cdot K_{ow} \quad (3.25)$$

where L_a is the lipid content of the aquatic plant (kg/kg). We assume that the lipid content is 0.5% (54). Metal concentrations of aquatic plants are calculated using empirical BCF values.

3.6 Risk Calculations: the Building of MUM-Risk

MUM-Risk uses a suite of predictive model-based, risk estimation methods to assess the potential ecological risk posed by contaminants. The use of different risk “lenses” instills a greater confidence in our predictive capacity (94).

3.6.1 Risk Characterization Lenses

3.6.1.1 Lens I

The first and simplest Lens is the estimation of potential risk ascertained by comparing estimated water, sediment and soil concentrations (i.e MUM-Fate output) with national and/or state toxicological benchmarks to generate a hazard quotient. This lens is often referred to as a regulation-based approach. Since ecologically-based, air quality benchmarks are not available, air quality impacts to wildlife are considered using Lens II. Hazard Quotients are calculated as (43), (44), (56):

$$HQ = \frac{EEC}{BM} \quad (3.26)$$

where HQ is the hazard quotient (dimensionless), EEC is Expected Environmental Concentration (ug/L or mg/kg), and BM is the toxicological benchmark (ug/L or mg/kg). Values of EEC are obtained from MUM-Fate.

The values of HQ indicate a range from “Potentially Negligible” to “Potentially of Concern” (Table 3.2). Contaminants classified as COPECS are recommended for subsequent, more detailed assessment or monitoring (95)-(98). A HQ of 0.2 indicates that a contaminant is considered a COPEC. This action level of exceedence is lower than 1, the typical value chosen for ERA of contaminated waste sites or of total, not source-specific, risk (43), (44), (97), (99). This is in contrast to the situation for contaminated sites, where an action level of 1 is more appropriate since the information provided by an ERA is used to determine whether or not clean up is required. In contrast to clean-up decisions for contaminated waste sites, we suggest that COPECS be defined as a contaminant concentration that may be *approaching* a level that causes ecological risk since policy makers need time, in the order of years, to institute changes that could mitigate risks. Decision-makers typically need time to signal stakeholders that change, possibly costly change, is needed, and that alternatives and strategies to mitigate risk need to be developed. This method uses an effects-based toxicological benchmark (Lowest-Observable-Adverse-Effect-Level (LOAEL), Section 3.6.1.2); therefore, a level of conservatism is warranted. This additional conservatism allows the risk manager a level of flexibility in communicating the risk to the stakeholders, where risk managers are increasingly working

towards proactive and preventative measures to mitigate before a risk is experienced, rather than reacting to a problem.

Table 3.2: Classification for HQ for Lenses I and II

HQ/HI value	Risk Ranking	Result
HQ < 0.2	Potentially Negligible	
0.2 ≤ HQ ≤ 1	Potentially Low	Maintained as a COPEC
HQ > 1	Potentially of Concern	Maintained as a COPEC

3.6.1.2 Lens II

A Lens II assessment estimates potential risk to wildlife species by considering exposure via diet or inhalation (i.e. MUM-Exposure output). A HQ is the ratio of TDD and LOAEL for chronic exposure scenarios (97), (100), (101) (Equation 3.27)

$$HQ_{total} = \frac{TDD}{LOAEL_{reproductive}} \quad (3.27)$$

where TDD is Total Daily Intake (g-contaminant/g-bw-day) for ingestion and (g-contaminant/day) for inhalation, and LOAEL is the Lowest-Observable-Adverse-Effect-Level for reproductive effects (g-contaminant/g-bw-day) or for inhalation (g-contaminant/day).

We use a LOAEL rather than the No-Observable-Adverse-Effect-Level (NOAEL) because the magnitude of effect associated with the LOAEL can be retained and incorporated into the characterization of potential risk. It is argued that the magnitude of effect is a critical component of characterizing risk (43). In addition, a LOAEL is determined directly from experimental data and therefore has confidence intervals associated with that magnitude of effect (102). The common justification for using a NOAEL-based benchmark is the added level of conservatism and protection it introduces into the results. A NOAEL is often inappropriately applied, assuming that it indicates a safe dose, when an adverse effect may have been observed at that dose but there was not enough statistical robustness to the test to indicate a significant difference to the control (102). The main criticisms of the LOAEL are that it is limited by the doses that have been chosen for the test and that a poorly designed test will result in a higher LOAEL value due to the design and the power of the experiment (103). A low effect-concentration or dose (e.g. EC₅ or ED₁₀) that is estimated from low dose extrapolation of the contaminant's dose response curve can provide a more accurate reflection of a low effect level (103). Extrapolating to a low dose from a dose-response curve requires the slope of the curve and data in order to generate a low-dose extrapolation. Data to apply the LOAEL-based

approach is available for a large number of contaminants, while providing the information necessary for the risk manager to make ecologically-responsible decisions.

Benchmarks for chronic reproductive/developmental endpoints were chosen as sensitive benchmarks because of concern for the effects of contaminants on populations of wildlife (43), (44), (97), (99). It is assumed that population-level effects are inferred from effects on individuals in the population (44), (56), (104). Those effects are mortality in acute tests, and reproduction and growth in chronic tests (44), (56) (Mount and Stephan, 1967 *in* (105)).

We derive the benchmark values from the literature on mammalian and avian toxicity (106) and from the US Environmental Protection Agency's toxicological databases of ECOTOX and Integrated Risk Information System (IRIS), using the method derived from Sample et al. (106). They incorporate revised toxicological and allometric scaling factors (107) (Equation 3.28). The scaling factors are based on acute, oral toxicity studies, and the uncertainty associated with their application to chronic toxicity is unknown (107). The use of these allometric scaling factors is justified because of their prior use in human and ecological risk assessment (106)-(108), (109) and because they represent an improvement to the alternative use of an arbitrarily selected uncertainty factor (e.g. 10X) which is commonly applied to account for interspecies differences (109).

$$Aw = At \left(\frac{BW_t}{BW_w} \right)^{1-b} \quad (3.28)$$

where Aw is the wildlife LOAEL, At is the test species LOAEL, BW_t is the body weight of the test species, BW_w is the body weight of wildlife and b is an allometric scaling factor.

The criterion for chronic exposure for mammals was at least one year or exposure during a critical life stage and for avian studies, at least 10 weeks or exposure during a critical life stage (106).

An assessment (uncertainty) factor of 10 is applied if an endpoint other than reproduction/developmental is available and an additional factor of 10 is applied if the exposure duration was not chronic (43), (106), (109), (106). Despite the limitations of using uncertainty factors, they are a simple, transparent method of ensuring conservatism where there is uncertainty. An uncertainty factor of 10 was not used to account for inter-species differences in toxicity because the scaling factor developed by Sample and Arenal (107) (1.2 for mammals and 0.94 for birds) accounts for this extrapolation. Intra-species variation is typically not accounted for in ERA because, generally, the goal is to be protective of populations, not individuals (44), (100), (109). However, an uncertainty factor of 10 is applied to account for intra-species variation for federally or state protected species, where protection is extended to the individual (109).

To calculate a daily dose from reported food or water concentrations (dose g/g) in the toxicity study, we multiplied the media concentration by the daily intake rate for food or water (g/g day) of the test species (106) (Appendix M). For inhalation studies, we applied the daily

inhalation rate. If the test species' body weight and food intake rate were not reported, we assumed standard values (EPA, 1988a *in* (106)).

We did not extrapolate mammalian toxicity values to avian toxicity values (106), (107). Therefore, if mammalian or avian toxicity studies were not available, we did not generate benchmarks for those contaminants.

3.7 Assumptions

Many important assumptions were made in the development of MUM-Exposure and MUM-Risk. The assumptions are conservative whenever possible; however, the assumptions can result in an over-, under- or variable-estimation of risk.

Assumptions were made in order to simplify the model. They were as follows:

- Contaminants are 100% bioavailable. This results in over-estimation.
- All prey from a single trophic level are homogeneous (e.g. contaminant concentration, body weight). This results in variable-estimation.
- All wildlife are homogeneous (e.g. dose, body weight, intake rates) within each receptor class assessed (e.g. adult female, juvenile). This results in variable-estimation.
- Only chemical contaminants are contributing to the toxic risk to wildlife. This results in under-estimation.
- Wildlife do not adapt to contamination. This results in variable-estimation.
- Non-metabolizable organic contaminant uptake can be described by partitioning into the lipid content of wildlife and hence the contaminant K_{ow} . This results in variable-, mostly over-estimation.
- Protecting for reproductive and developmental toxicological endpoints are protective of populations of wildlife species. This results in variable-, mostly over-estimation.

Assumptions were made in order to fill data gaps. These assumptions were:

- Dermal exposure is negligible. This results in under-estimation.
- Contaminant uptake through water ingestion and diet have the same uptake efficiency, which is the same uptake efficiency as the test species used to develop the LOAEL value. This results in variable-, mostly over-estimation.

- Inhalation exposure has the same uptake efficiency as the test species used to develop the LOAEL value. This results in variable-, mostly over-estimation.
- Allometric scaling factors can extrapolate toxicity from test species to wildlife species. This results in variable-estimation.
- Uncertainty factors of 10 can extrapolate from acute to chronic toxicity scenarios, and non-reproductive to reproductive toxic endpoints. This results in over-estimation.
- Dose-additivity between individual contaminants. This results in variable-, mostly over-estimation.

The level of complexity of an ERA and the magnitude of uncertainty must be balanced with the overall objective of a modeling exercise, which is to simplify the system to aid in understanding and inform decision-making. Ecological conservatism governed the scientific judgments that were made to develop MUM-Exposure and MUM-Risk. The unnecessary introduction of uncertainty was avoided by excluding data that were considered ecologically irrelevant or when the level of uncertainty in the data was considered unacceptable. Probabilistic ERA methods that generate an exposure distribution would allow for improved characterization of natural variability and modeling uncertainty.

A critical issue with screening-level ERAs is the potential for chemicals or wildlife groups to be overlooked due to a lack of scientific understanding. Important lessons learned from chemicals like DDT and PCBs caution us against presuming benignity in place of our uncertainty. Therefore, when there are insufficient data to perform an exposure or toxicological assessment, the contaminant is designated a COPEC.

3.8 Summary

This research contributes to method development for ERA. Model development, particularly of models that incorporate exposure and toxicity, is an area of research that has been highlighted as critical for improving the utility of ERAs (43). The ERA method presented here advances other multi-media risk models by its relevance to the transportation sector, its applicability to non-metabolizable and metabolizable organic contaminants and metals, its generality to aquatic and terrestrial receptors, and its incorporation of inhalation and juvenile dietary exposure route. Although MUM is tailored to transportation emissions in an urban environment, this method is applicable to other scenarios that involve multiple chemical stressors present at low chronic conditions in terrestrial and aquatic environments, where all routes of exposure are relevant to wildlife exposure.

This screening-level ERA decision-support tool has been developed to inform risk managers of research needs and potential areas of concern, and to characterize the relative potential risks of contaminants. This information can be used to prioritize research, monitoring and regulatory mitigation in order to avoid costly and unnecessary monitoring and/or cleanup. Because it is a conservative assessment, contaminants that are not identified as COPECs can be

assumed to pose a negligible potential risk to the environment with a high level of confidence (55).

This ERA decision support tool can simplify environmental issues and trade-offs by translating scenarios into a consistent and coherent currency that can be used to predict and describe the outcome of different management options (110), (101), (111). In a climate of limited resources, decision-making must be informed and cost-effective, and environmental protection efforts should focus on opportunities affording the greatest potential for risk reduction.

Chapter 4 - Calibration of the Model

Multi-media fate models are based on fundamental principles chemical movement that are translated to coincide with environmental conditions through the choice of particular parameter values and their adjustment on an iterative basis. The criterion for adjustment in the calibration process is the correspondence of measured and modelled results. For multi-media models, the results used for calibration are typically measured ambient chemical concentrations in various media.

It is important to note that the model can not be validated or tested for its veracity because of the numerous unknown values and because many permutations of parameter values can lead to the same correspondence. However, because the model is based on fundamental principles and because parameter values are bounded by observed values, the range of parameter values can not be overly wide or unreasonable.

Perhaps the most important unknown in the fate module is the rate of chemical emissions. For the decision tool, we quantify chemical emissions from vehicles where these emissions are fractions of total emissions for these chemicals. The problem arises that we compare estimated media concentrations attributable to transportation-related emissions with ambient chemical concentrations attributable to total emissions. The inequality between modelled and measured concentrations limits our ability to definitively calibrate the model and to evaluate the calibrated model.

The initial set of parameter values to begin the calibration process is obtained from laboratory and field experiments. These values have an inherent uncertainty attributable to experimental and analytical errors and natural variability. In addition, values obtained from measurements of a single process may not be strictly transferable to a whole system model due to scaling issues, i.e., process values measured at single points or single times may not be reasonable within a whole system model. Thus, calibration involves adjusting parameter values known to be uncertain or highly variable within the bounds of measured values, until the closest correspondence is achieved between measured and modelled results.

The final results of the calibration process are summarized in Tables 4.1 and 4.2 for PAH and metals, respectively. These tables summarize modeled concentrations estimated by the fate module of the decision tool and those obtained from the literature. Note that the only parameter values changed to obtain chemical-specific concentrations are the physical-chemical properties of the chemical – all process rates remain constant.

The concentrations presented in Tables 4.1 and 4.2 indicate that model estimates of air and water concentrations fall within the range of measured values for PAH and metals, respectively. This is reasonable because air and water respond rapidly to changes in loadings and do not accumulate chemicals over time.

Modeled concentrations of PAH and metals in sediment and soil are generally just within or below measured concentrations. We expect this discrepancy with sediment and soil because these media accumulate chemical over time when loadings could have been higher. The steady-state version of the model does not include this time dimension, nor does the time dependent version in which loadings do not vary with time. As well, measured concentrations in fact range

over orders-of-magnitude from below detection to those reported in Tables 4.1 and 4.2. Thus, the reported range actually overestimates the range of concentrations that are found in the environment (we have summarized reported concentration ranges that are above analytical detection limits that vary amongst laboratories).

The risk assessment component of the decision tool is also based on fundamental principles of chemical exposure as judged against ecotoxicological benchmarks or reference values. Unlike the fate module, the risk assessment module can not be calibrated or evaluated. First, the literature does not contain contaminant burdens in ecological receptors that are attributable to transportation-related emissions, nor attributable to ambient urban conditions. Unless one is conducting a detailed, site-specific risk assessment that includes site-specific toxicological testing, it is not possible to determine if risk estimates are reasonable. The inability to calibrate or evaluate the model is common to most risk assessments.

Table 4.1 Modeled and measured concentrations of PAH

medium	type	phenanthrene	fluoranthene	pyrene	benzo[a]pyrene	reference
air, ng/m ³	modeled, total	3.45-60	0.9-16	0.57-10	0.0225-0.4	
	MN measured, gas-phase	5.6 (4.9-6.5)	1.2 (1.0-1.4)	0.5 (0.3-0.9)	n.d. ¹ (<DL ²)	Liu, unpublished data
	MN measured, particle- phase	0.03 (<DL-0.11)	0.08 (0.05-0.19)	0.07(0.04-0.13)	0.01 (<DL-0.14)	Liu, unpublished data
	literature range	18 (2.8-70)	7 (1.4-24)	4 (1.6-16)	0.1 (0.0016-2.9)	(112), (113), (114), (115), (116)
water, µg/L	modeled	0.000195-0.0056	0.00021-0.012	5.25E-05-0.0016	0.000024-0.018	
	literature range	0.008 (0.0021-0.034)	0.0008	0.0003	0.0002	(117), (118), (119), (120), (121)
sediment, µg/kg	modeled	0.0465-1.3	0.3-18	0.048-1.5	0.1245-94	

ww ³	literature range	1930 (350-32250)	1630 (262-5480)	2210 (219-22100)	1220 (154-10800)	(117)
soil	modeled, $\mu\text{g}/\text{kg ww}$	0.021-0.39	0.072-1.3	0.01245-0.24	0.0705-1.3	
	MN measured $\text{ng}/\text{g ww}$	49 (16-125)	56 (20-156)	37 (14-88)	11 (0.19-75)	Liu, unpublished data
	literature range $\text{ng}/\text{g ww}$	10 (22-166)	127 (37-1256)	83 (20-645)	64 (22-379)	(114), (122), (123)

¹ non-detect

² denotes below detection limit

³ wet weight

Table 4.2 Modeled and measured concentrations of metals

medium	type	cadmium	chromium	nickel	arsenic	references
air, ng/m^3	modeled	1.05-19	5.25-95	5.1-90	1.95-35	
	literature range	1.8 (0.42-4.4)	8.3 (3-20)	6.26 (1-20) ^d	(1-13)	(124), (125), (126), (127)
water, $\mu\text{g}/\text{L}$	modeled	0.15-3.7	1.2-25	0.975-22	0.0285-1.6	
	literature range	0.02 (0.01-0.041) ^a	(8-11) ^b	14		(124), (125), (126)
sediment	modeled, $\mu\text{g}/\text{kg ww}$ ^f	9.75-240	133.5-3900	45-1000	19.5-1100	
	literature range, $\text{mg}/\text{kg ww}$	14.9 (6.7-20.5)	(564-1920)	60 ^e	75-300 ^e	(124), (125), (126), (127)

soil	modeled, μg/kg ww	6.3-300	94.5-4200	31.5- 1200	13.05- 1100	
	literature range, mg/kg dw ^g	3	0.43 (0.10- 1.00) ^c	11		(124), (125), (126)

^a dissolved

^b dissolved and particulate

^c not urban specific

^d total particulate

^e dry weight to wet weight assuming water content of 80%

^f wet weight

^g dry weight

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Appendix A:
Data File Description

DATA FILE DESCRIPTION

This appendix contains the structure and content of the data files.

Input.xls

This file contains the exposure profiles, receptor specific data, toxicity values for adult and juvenile organisms, receptor and chemical specific transfer factors, and bioaccumulation factors. The table formats are slightly modified, but the information provided is the same as given in the file.

Fractions of Receptors' Diets

Receptor	Trophic Level 3 Fish	Invertebrates, Aquatic Benthos	Birds	Mammals	Invertebrates, Terrestrial	Worms
Great Blue Heron (<i>Ardea herodias</i>)	0.99	0.01	0	0	0	0
American Robin (<i>Turdus migratorius</i>)	0	0	0	0	0.56	0.15
Canada Goose (<i>Branta canadensis</i>)	0	0	0	0	0	0
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.77	0	0.16	0.07	0	0
Mallard Duck (<i>Anas platyrhynchos</i>)	0	0.75	0	0	0	0
Lesser Scaup (<i>Aythya affinis</i>)	0.063	0.84	0	0	0	0
Osprey (<i>Pandion haliaetus</i>)	1	0	0	0	0	0
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0	0	0.26	0.74	0	0
American Kestrel (<i>Falco Sparvaerius</i>)	0.019	0	0.303	0.317	0.361	0
American Woodcock (<i>Scolopax minor</i>)	0	0	0	0	0.217	0.678
Spotted Sandpiper (<i>Actitis macularia</i>)	0	1	0	0	0	0
Herring Gull (<i>Larus argentatus</i>)	0.386	0	0.035		0.421	0.017
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.73	0.05	0.005	0.005	0	0
March Wren (<i>Cistothorus palustris</i>)	0	0	0	0	1	0
Northern Bobwhite (<i>Colinus virginianus</i>)	0	0	0	0	0.18	0
Red Fox (<i>Vulpes vulpes</i>)	0	0	0.15	0.64	0.05	0
River Otter (<i>Lutra canadensis</i>)	0.88	0.12	0	0	0	0
Muskrat (<i>Ondatra zibethicus</i>)	0	0	0	0	0	0
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0	0.037	0	0.052	0.189	0.527
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0	0	0	0	0.015	0
Raccoon (<i>Procyon lotor</i>)	0.074	0.019	0.015	0.158	0.082	0.072
Mink (<i>Mustela vison</i>)	0.755	0.075	0.028	0.028	0	0
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0	0	0	0	0	0
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0	0	0	0	0.6	0

Fractions of Receptors' Diets

Receptor	Vegetation, Aquatic	Vegetation, Terrestrial	Soil	Sediment
Great Blue Heron (<i>Ardea herodias</i>)	0	0	0	0
American Robin (<i>Turdus migratorius</i>)	0	0.29	0.1	0
Canada Goose (<i>Branta Canadensis</i>)	0	1	0.08	0
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0	0	0	0
Mallard Duck (<i>Anas platyrhynchos</i>)	0.25	0	0	0.02
Lesser Scaup (<i>Aythya affinis</i>)	0.09	0	0	0.02
Osprey (<i>Pandion haliaetus</i>)	0	0	0	0
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0	0	0	0
American Kestrel (<i>Falco Sparvaerius</i>)	0	0	0	0
American Woodcock (<i>Scolopax minor</i>)	0	0.105	0.104	0
Spotted Sandpiper (<i>Actitis macularia</i>)	0	0	0	0.18
Herring Gull (<i>Larus argentatus</i>)	0	0	0	0
Belted Kingfisher (<i>Ceryle alcyon</i>)	0	0	0.05	0
March Wren (<i>Cistothorus palustris</i>)	0	0	0	0
Northern Bobwhite (<i>Colinus virginianus</i>)	0	0.82	0	0
Red Fox (<i>Vulpes vulpes</i>)	0	0.14	0.03	0
River Otter (<i>Lutra canadensis</i>)	0	0	0	0
Muskrat (<i>Ondatra zibethicus</i>)	1	0	0	0
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0	0.171	0.024	0
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0	0.985	0.024	0
Raccoon (<i>Procyon lotor</i>)	0	0.587	0.094	0
Mink (<i>Mustela vison</i>)	0.08	0	0	0
Eastern Cottontail (<i>Syvilagus floridanus</i>)	0	1	0.06	0
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0	0.38	0.02	0

Receptors' Adult Exposure Profile

Receptor	Body weight (g)	Food (gww/gww-day e, gww/a)	Water Ingestion Rate (g/g-day)	Inhalation rate (m ³ /day)
Great Blue Heron (<i>Ardea herodias</i>)	2230	1116.87	0.1010	0.7580
American Robin (<i>Turdus migratorius</i>)	80.6	66.42	0.0109	0.0588
Canada Goose (<i>Branta canadensis</i>)	3550	1658.20	0.1379	1.0843
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	5089	2252.06	0.1755	1.4308
Mallard Duck (<i>Anas platyrhynchos</i>)	1197	658.15	0.0666	0.4695
Lesser Scaup (<i>Aythya affinis</i>)	770	452.33	0.0495	0.3342
Osprey (<i>Pandion haliaetus</i>)	1925	985.62	0.0915	0.6768
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	1235	675.87	0.0680	0.4809
American Kestrel (<i>Falco Sparvaerius</i>)	124	95.80	0.0146	0.0819
American Woodcock (<i>Scolopax minor</i>)	213	151.73	0.0209	0.1243
Spotted Sandpiper (<i>Actitis macularia</i>)	47.1	42.07	0.0076	0.0389
Herring Gull (<i>Larus argentatus</i>)	951	541.25	0.0570	0.3932
Belted Kingfisher (<i>Ceryle alcyon</i>)	158	117.71	0.0171	0.0987
March Wren (<i>Cistothorus palustris</i>)	10.6	11.84	0.0028	0.0123
Northern Bobwhite (<i>Colinus virginianus</i>)	180	131.50	0.0187	0.1092
Red Fox (<i>Vulpes vulpes</i>)	3940	370.75	0.3401	1.6348
River Otter (<i>Lutra canadensis</i>)	7900	612.65	0.6361	2.8521
Muskrat (<i>Ondatra zibethicus</i>)	1350	171.09	0.1297	0.6939
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	17.4	7.39	0.0026	0.0214
Meadow Vole (<i>Microtus pennsylvanicus</i>)	22	8.76	0.0032	0.0258
Raccoon (<i>Procyon lotor</i>)	6400	526.25	0.5263	2.4099
Mink (<i>Mustela vison</i>)	974	135.17	0.0967	0.5344
Eastern Cottontail (<i>Syvilagus floridanus</i>)	1231	160.06	0.1194	0.6446
Deer Mouse (<i>Peromyscus maniculatus</i>)	20	8.17	0.0029	0.0239

Receptors' Juvenile Exposure Profile

Receptor	Body weight (g)	Food (gww/gww-day e, gdw/ a)	Water Ingestion Rate (g/g-day)	Inhalation rate (m ³ /day)
Great Blue Heron (<i>Ardea herodias</i>)	750	442.33	0.0487	0.3275
American Robin (<i>Turdus migratorius</i>)	5.5	6.78	0.0018	0.0074
Canada Goose (<i>Branta canadensis</i>)	1775	919.94	0.0867	0.6358
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	2500	1230.81	0.1090	0.8277
Mallard Duck (<i>Anas platyrhynchos</i>)	740	437.31	0.0482	0.3242
Lesser Scaup (<i>Aythya affinis</i>)	385	250.95	0.0311	0.1960
Osprey (<i>Pandion haliaetus</i>)	1000	564.86	0.0590	0.4088
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	600	365.91	0.0419	0.2758
American Kestrel (<i>Falco Sparvaerius</i>)	60	51.69	0.0090	0.0468
American Woodcock (<i>Scolopax minor</i>)	100	79.79	0.0126	0.0694
Spotted Sandpiper (<i>Actitis macularia</i>)	25	24.56	0.0050	0.0239
Herring Gull (<i>Larus argentatus</i>)	400	259.24	0.0319	0.2019
Belted Kingfisher (<i>Ceryle alcyon</i>)	75	62.48	0.0104	0.0556
March Wren (<i>Cistothorus palustris</i>)	5	6.25	0.0017	0.0069
Northern Bobwhite (<i>Colinus virginianus</i>)	9	10.31	0.0025	0.0109
Red Fox (<i>Vulpes vulpes</i>)	102	26.51	0.0127	0.0879
River Otter (<i>Lutra canadensis</i>)	132	31.93	0.0160	0.1080
Muskrat (<i>Ondatra zibethicus</i>)	21	8.47	0.0031	0.0248
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	1	0.94	0.0002	0.0022
Meadow Vole (<i>Microtus pennsylvanicus</i>)	2.3	1.72	0.0004	0.0042
Raccoon (<i>Procyon lotor</i>)	75	21.23	0.0096	0.0687
Mink (<i>Mustela vison</i>)	8.3	4.33	0.0013	0.0118
Eastern Cottontail (<i>Syvilagus floridanus</i>)	42.2	14.02	0.0057	0.0434
Deer Mouse (<i>Peromyscus maniculatus</i>)	1.8	1.44	0.0003	0.0035

Adult Oral Toxicity for Metals

Receptor	Arsenic	Cadmium	Chromium	Copper	Lead	Manganese	Molybdenum	Nickel	Selenium	Vanadium	Zinc
ORAL LOAEL (mg/kg day)											
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	1.78	28.26	6.62	96.87	22.81	2289.57	45.13	15.55	1.11	1.53	285.69
Great Blue Heron (<i>Ardea herodias</i>)	1.51	23.96	5.61	82.14	19.34	1941.28	38.27	13.18	0.94	1.29	242.23
American robin (<i>Turdus migratorius</i>)	0.78	12.33	2.89	42.28	9.95	999.30	19.70	6.79	0.48	0.67	124.69
Mallard Duck (<i>Anas platyrhynchos</i>)	1.28	21.16	4.96	72.53	17.07	1714.14	33.79	11.64	0.80	1.14	213.89
Canada Goose (<i>Branta canadensis</i>)	1.65	26.30	6.16	90.14	21.22	2130.46	42.00	14.47	1.03	1.42	265.84
Lesser Scaup (<i>Aythya affinis</i>)	1.22	19.37	4.54	66.40	15.63	1569.37	30.94	10.66	0.76	1.05	195.83
Osprey (<i>Pandion haliaetus</i>)	1.46	23.27	5.45	79.76	18.78	1885.01	37.16	12.80	0.91	1.26	235.21
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	1.34	21.29	4.99	72.98	17.18	1724.89	34.00	11.71	0.83	1.15	215.23
American Kestrel (<i>Falco Sparvaerius</i>)	0.85	13.44	3.15	46.09	10.85	1089.21	21.47	7.40	0.53	0.73	135.91
American Woodcock (<i>Scolopax minor</i>)	0.94	14.98	3.51	51.35	12.09	1213.68	23.92	8.24	0.59	0.81	151.44
Spotted Sandpiper (<i>Actitis macularia</i>)	0.70	11.08	2.60	37.97	8.94	897.50	17.69	6.09	0.43	0.60	111.99
Herring Gull (<i>Larus argentatus</i>)	1.27	20.21	4.73	69.27	16.31	1637.06	32.27	11.12	0.79	1.09	204.27
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.89	14.11	3.31	48.37	11.39	1143.30	22.54	7.76	0.55	0.76	142.66
March Wren (<i>Cistothorus palustris</i>)	0.52	8.22	1.93	28.18	6.63	666.02	13.13	4.52	0.32	0.44	83.11
Northern Bobwhite (<i>Colinus virginianus</i>)	0.91	14.48	3.39	49.65	11.69	1173.50	23.13	7.97	0.57	0.78	146.43
River Otter (<i>Lutra canadensis</i>)	0.79	7.16	2270.19	13.37	66.36	235.56	0.06	66.36	0.27	1.71	26.54
Muskrat (<i>Ondatra zibethicus</i>)	0.87	7.96	2524.06	14.87	73.78	261.90	0.07	73.78	0.30	1.90	29.51
Meadow Vole (<i>Microtus pennsylvanicus</i>)	1.08	9.84	3122.16	18.39	91.26	323.97	0.08	91.26	0.37	2.35	36.50
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	1.13	10.33	3277.07	19.30	95.79	340.04	0.09	95.79	0.39	2.47	38.31
Red Fox (<i>Vulpes vulpes</i>)	0.82	7.46	2366.95	13.94	69.18	245.60	0.06	69.18	0.28	1.78	27.67
Raccoon (<i>Procyon lotor</i>)	0.80	7.25	2299.05	13.54	67.20	238.56	0.06	67.20	0.28	1.73	26.88
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	1.13	10.25	3249.80	19.14	94.99	337.21	0.09	94.99	0.39	2.45	38.00
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0.88	8.00	2538.07	14.95	74.19	263.36	0.07	74.19	0.30	1.91	29.67
Mink (<i>Mustela vison</i>)	0.89	8.12	2573.98	15.16	75.24	267.08	0.07	75.24	0.31	1.94	30.09

Juvenile Oral Toxicity for Metals

Receptor	Arsenic	Cadmium	Chromium	Copper	Lead	Manganese	Molybdenum	Nickel	Selenium	Vanadium	Zinc
ORAL LOAEL (mg/kg day)											
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	1.54	24.52	5.74	84.04	19.78	1986.17	39.15	13.49	0.96	1.32	247.84
Great Blue Heron (<i>Ardea herodias</i>)	1.21	19.27	4.51	66.05	15.55	1561.13	30.77	10.60	0.76	1.04	194.80
American robin (<i>Turdus migratorius</i>)	0.45	7.21	1.69	24.71	5.82	584.12	11.51	3.97	0.28	0.39	72.89
Mallard Duck (<i>Anas platyrhynchos</i>)	1.21	19.22	4.50	65.88	15.51	1556.95	30.69	10.57	0.75	1.04	194.28
Canada Goose (<i>Branta canadensis</i>)	1.44	22.89	5.36	78.47	18.47	1854.67	36.56	12.59	0.90	1.24	231.43
Lesser Scaup (<i>Aythya affinis</i>)	1.06	16.86	3.95	57.81	13.61	1366.22	26.93	9.28	0.66	0.91	170.48
Osprey (<i>Pandion haliaetus</i>)	1.28	20.41	4.78	69.97	16.47	1653.59	32.60	11.23	0.80	1.10	206.34
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	1.16	18.43	4.32	63.17	14.87	1492.99	29.43	10.14	0.72	1.00	186.30
American Kestrel (<i>Falco Sparvaerius</i>)	0.73	11.63	2.72	39.86	9.38	942.02	18.57	6.40	0.46	0.63	117.55
American Woodcock (<i>Scolopax minor</i>)	0.81	12.88	3.02	44.15	10.39	1043.35	20.57	7.08	0.50	0.70	130.19
Spotted Sandpiper (<i>Actitis macularia</i>)	0.61	9.76	2.29	33.46	7.88	790.71	15.59	5.37	0.38	0.53	98.66
Herring Gull (<i>Larus argentatus</i>)	1.07	16.99	3.98	58.25	13.71	1376.70	27.14	9.35	0.67	0.92	171.79
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.76	12.16	2.85	41.68	9.81	985.01	19.42	6.69	0.48	0.66	122.91
March Wren (<i>Cistothorus palustris</i>)	0.44	7.07	1.66	24.25	5.71	573.09	11.30	3.89	0.28	0.38	71.51
Northern Bobwhite (<i>Colinus virginianus</i>)	0.50	7.96	1.86	27.27	6.42	644.58	12.71	4.38	0.31	0.43	80.43
River Otter (<i>Lutra canadensis</i>)	1.00	13.45	2252.04	10.10	65.83	233.68	0.11	65.83	0.27	2.19	33.93
Muskrat (<i>Ondatra zibethicus</i>)	1.12	9.31	1559.21	6.99	45.57	161.79	0.08	45.57	0.19	2.44	37.88
Meadow Vole (<i>Microtus pennsylvanicus</i>)	1.28	5.98	1001.86	4.49	29.28	103.96	0.05	29.28	0.12	2.79	43.26
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	1.35	5.06	848.13	3.80	24.79	88.00	0.04	24.79	0.10	2.93	45.48
Red Fox (<i>Vulpes vulpes</i>)	1.02	12.77	2138.85	9.59	62.52	221.93	0.11	62.52	0.26	2.22	34.46
Raccoon (<i>Procyon lotor</i>)	1.04	12.01	2011.28	9.02	58.79	208.70	0.10	58.79	0.24	2.26	35.10
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	1.30	5.70	953.93	4.28	27.88	98.98	0.05	27.88	0.11	2.83	43.90
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	1.08	10.71	1792.77	8.04	52.40	186.02	0.09	52.40	0.22	2.34	36.33
Mink (<i>Mustela vison</i>)	1.19	7.73	1295.02	5.81	37.85	134.38	0.06	37.85	0.16	2.58	40.05

Transfer Factors for Metals

Factor	Arsenic	Cadmium	Chromium	Copper	Lead	Manganese	Molybdenum	Nickel	Selenium	Vanadium	Zinc
Mammal (day/kg FW) FW=fresh weight	0.0043	0.0006	0.0070	0.0097	0.0004	0.0004	0.0025	0.0084	0.0070	0.0050	0.0242
Bird (day/kg FW)	0.2912	0.2912	1	0.5	0.2	1	0.2236	3	3.19	1.3	0.736
Milk (day/kg FW)	0.0001	0.0002	0.0015	0.0015	0.00001	0.00010	0.0016	0.004	0.0059	0.00002	0.01
Fish-water (L/kg)	29.7	215.4	55.4	200	49.0	400	10	226.8	149.7	73.7	868.0
Aq. Vegetation-water (L/kg)	200	75	80	1000	160	80	1300	50	63	2000	550
Benthic invertebrates-pore water sediment (L-water/kg- benthos)	1700	4000	4000	1000	100	4000	4000	100	2726.8	2000	40000
BCF terrestrial invertebrate	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
BCF worm-pore water	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Adult Oral Toxicity for Organics

Receptor	Acetaldehyde	Anthracene	Benzene	Benz[a] Anthracene	Benzo[b] Fluoranthene	Benzo[a] Pyrene	Benzo[e] Pyrene	Benzo[g,h,i] Perylene	Benzo[k] Fluoranthene
ORAL LOAEL (mg/kg day)									
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	9.08E-02	0.00E+00	2.39E-02	0.00E+00	9.08E-02	9.08E-02	9.08E-02	4.24E-03
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	7.70E-02	0.00E+00	2.03E-02	0.00E+00	7.70E-02	7.70E-02	7.70E-02	3.59E-03
American robin (<i>Turdus migratorius</i>)	0.00E+00	3.96E-02	0.00E+00	1.04E-02	0.00E+00	3.96E-02	3.96E-02	3.96E-02	1.85E-03
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	6.80E-02	0.00E+00	1.79E-02	0.00E+00	6.80E-02	6.80E-02	6.80E-02	3.17E-03
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	8.45E-02	0.00E+00	2.23E-02	0.00E+00	8.45E-02	8.45E-02	8.45E-02	3.94E-03
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	6.23E-02	0.00E+00	1.64E-02	0.00E+00	6.23E-02	6.23E-02	6.23E-02	2.91E-03
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	7.48E-02	0.00E+00	1.97E-02	0.00E+00	7.48E-02	7.48E-02	7.48E-02	3.49E-03
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	6.84E-02	0.00E+00	1.80E-02	0.00E+00	6.84E-02	6.84E-02	6.84E-02	3.19E-03
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	4.32E-02	0.00E+00	1.14E-02	0.00E+00	4.32E-02	4.32E-02	4.32E-02	2.02E-03
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	4.81E-02	0.00E+00	1.27E-02	0.00E+00	4.81E-02	4.81E-02	4.81E-02	2.25E-03
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	3.56E-02	0.00E+00	9.38E-03	0.00E+00	3.56E-02	3.56E-02	3.56E-02	1.66E-03
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	6.49E-02	0.00E+00	1.71E-02	0.00E+00	6.49E-02	6.49E-02	6.49E-02	3.03E-03
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	4.54E-02	0.00E+00	1.19E-02	0.00E+00	4.54E-02	4.54E-02	4.54E-02	2.12E-03
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	2.64E-02	0.00E+00	6.96E-03	0.00E+00	2.64E-02	2.64E-02	2.64E-02	1.23E-03
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	4.66E-02	0.00E+00	1.23E-02	0.00E+00	4.66E-02	4.66E-02	4.66E-02	2.17E-03
River Otter (<i>Lutra canadensis</i>)	0.00E+00	7.16E+00	1.89E+02	1.19E-02	0.00E+00	7.16E+00	0.00E+00	0.00E+00	0.00E+00
Muskrat (<i>Ondatra zibethicus</i>)	0.00E+00	7.96E+00	2.10E+02	1.33E-02	0.00E+00	7.96E+00	0.00E+00	0.00E+00	0.00E+00
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0.00E+00	9.84E+00	2.59E+02	1.64E-02	0.00E+00	9.84E+00	0.00E+00	0.00E+00	0.00E+00
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0.00E+00	1.03E+01	2.72E+02	1.72E-02	0.00E+00	1.03E+01	0.00E+00	0.00E+00	0.00E+00
Red Fox (<i>Vulpes vulpes</i>)	0.00E+00	7.46E+00	1.97E+02	1.24E-02	0.00E+00	7.46E+00	0.00E+00	0.00E+00	0.00E+00
Raccoon (<i>Procyon lotor</i>)	0.00E+00	7.25E+00	1.91E+02	1.21E-02	0.00E+00	7.25E+00	0.00E+00	0.00E+00	0.00E+00
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0.00E+00	1.02E+01	2.70E+02	1.71E-02	0.00E+00	1.02E+01	0.00E+00	0.00E+00	0.00E+00
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0.00E+00	8.00E+00	2.11E+02	1.33E-02	0.00E+00	8.00E+00	0.00E+00	0.00E+00	0.00E+00
Mink (<i>Mustela vison</i>)	0.00E+00	8.12E+00	2.14E+02	1.35E-02	0.00E+00	8.12E+00	0.00E+00	0.00E+00	0.00E+00

Adult Oral Toxicity for Organics

Receptor	Butadiene	Chrysene	Coronene	Ethylbenzene	Ethyleneglycol	Fluoranthene	Fluorene	Formaldehyde	Indeno[1,2,3-c,d] Pyrene
ORAL LOAEL (mg/kg day)									
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	3.03E-02	9.08E-02	0.00E+00	0.00E+00	9.08E-02	9.08E-02	0.00E+00	3.03E-02
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	2.57E-02	7.70E-02	0.00E+00	0.00E+00	7.70E-02	7.70E-02	0.00E+00	2.57E-02
American robin (<i>Turdus migratorius</i>)	0.00E+00	1.32E-02	3.96E-02	0.00E+00	0.00E+00	3.96E-02	3.96E-02	0.00E+00	1.32E-02
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	2.27E-02	6.80E-02	0.00E+00	0.00E+00	6.80E-02	6.80E-02	0.00E+00	2.27E-02
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	2.82E-02	8.45E-02	0.00E+00	0.00E+00	8.45E-02	8.45E-02	0.00E+00	2.82E-02
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	2.08E-02	6.23E-02	0.00E+00	0.00E+00	6.23E-02	6.23E-02	0.00E+00	2.08E-02
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	2.49E-02	7.48E-02	0.00E+00	0.00E+00	7.48E-02	7.48E-02	0.00E+00	2.49E-02
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	2.28E-02	6.84E-02	0.00E+00	0.00E+00	6.84E-02	6.84E-02	0.00E+00	2.28E-02
American Kestrel (<i>Falco Sparverius</i>)	0.00E+00	1.44E-02	4.32E-02	0.00E+00	0.00E+00	4.32E-02	4.32E-02	0.00E+00	1.44E-02
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	1.60E-02	4.81E-02	0.00E+00	0.00E+00	4.81E-02	4.81E-02	0.00E+00	1.60E-02
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	1.19E-02	3.56E-02	0.00E+00	0.00E+00	3.56E-02	3.56E-02	0.00E+00	1.19E-02
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	2.16E-02	6.49E-02	0.00E+00	0.00E+00	6.49E-02	6.49E-02	0.00E+00	2.16E-02
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	1.51E-02	4.54E-02	0.00E+00	0.00E+00	4.54E-02	4.54E-02	0.00E+00	1.51E-03
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	8.81E-03	2.64E-02	0.00E+00	0.00E+00	2.64E-02	2.64E-02	0.00E+00	8.81E-03
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	1.55E-02	4.66E-02	0.00E+00	0.00E+00	4.66E-02	4.66E-02	0.00E+00	1.55E-02
River Otter (<i>Lutra canadensis</i>)	0.00E+00	0.00E+00	0.00E+00	2.41E+00	8.29E+01	1.79E+00	2.07E+00	9.64E+00	0.00E+00
Muskrat (<i>Ondatra zibethicus</i>)	0.00E+00	0.00E+00	0.00E+00	2.68E+00	9.22E+01	1.99E+00	2.31E+00	1.07E+01	0.00E+00
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0.00E+00	0.00E+00	0.00E+00	3.32E+00	1.14E+02	2.46E+00	2.85E+00	1.33E+01	0.00E+00
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0.00E+00	0.00E+00	0.00E+00	3.48E+00	1.20E+02	2.58E+00	2.99E+00	1.39E+01	0.00E+00
Red Fox (<i>Vulpes vulpes</i>)	0.00E+00	0.00E+00	0.00E+00	2.52E+00	8.65E+01	1.87E+00	2.16E+00	1.00E+01	0.00E+00
Raccoon (<i>Procyon lotor</i>)	0.00E+00	0.00E+00	0.00E+00	2.44E+00	8.40E+01	1.81E+00	2.10E+00	9.76E+00	0.00E+00
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0.00E+00	0.00E+00	0.00E+00	3.46E+00	1.19E+02	2.56E+00	2.97E+00	1.38E+01	0.00E+00
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0.00E+00	0.00E+00	0.00E+00	2.70E+00	9.27E+01	2.00E+00	2.32E+00	1.08E+01	0.00E+00
Mink (<i>Mustela vison</i>)	0.00E+00	0.00E+00	0.00E+00	2.74E+00	9.40E+01	2.03E+00	2.35E+00	1.09E+01	0.00E+00

Adult Oral Toxicity for Organics

Receptor	MTBE	Naphthalene	n-Hexane	Phenanthrene	Pyrene	Styrene	ThiaArenes	Toluene	Xylenes	2,3,7,8-TCDD
ORAL LOAEL (mg/kg day)										
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	3.59E+00	0.00E+00	9.08E-02	9.08E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.94E-04
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	3.04E+00	0.00E+00	7.70E-02	7.70E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.64E-04
American robin (<i>Turdus migratorius</i>)	0.00E+00	1.57E+00	0.00E+00	3.96E-02	3.96E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.46E-05
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	2.69E+00	0.00E+00	6.80E-02	6.80E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.45E-04
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	3.34E+00	0.00E+00	8.45E-02	8.45E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.80E-04
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	2.46E+00	0.00E+00	6.23E-02	6.23E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.33E-04
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	2.96E+00	0.00E+00	7.48E-02	7.48E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.60E-04
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	2.70E+00	0.00E+00	6.84E-02	6.84E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.46E-04
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	1.71E+00	0.00E+00	4.32E-02	4.32E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.22E-05
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	1.90E+00	0.00E+00	4.81E-02	4.81E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E-04
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	1.41E+00	0.00E+00	3.56E-02	3.56E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.60E-05
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	2.57E+00	0.00E+00	6.49E-02	6.49E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.39E-04
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	1.79E+00	0.00E+00	4.54E-02	4.54E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.68E-05
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	1.04E+00	0.00E+00	2.64E-02	2.64E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.64E-05
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	1.84E+00	0.00E+00	4.66E-02	4.66E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.94E-05
River Otter (<i>Lutra canadensis</i>)	0.00E+00	1.18E+00	0.00E+00	0.00E+00	8.95E-01	4.10E+01	0.00E+00	1.86E+02	1.86E+00	7.22E-06
Muskrat (<i>Ondatra zibethicus</i>)	0.00E+00	1.31E+00	0.00E+00	0.00E+00	9.95E-01	4.56E+01	0.00E+00	2.07E+02	2.07E+00	8.03E-06
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0.00E+00	1.62E+00	0.00E+00	0.00E+00	1.23E+00	5.64E+01	0.00E+00	2.56E+02	2.56E+00	9.94E-06
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0.00E+00	1.70E+00	0.00E+00	0.00E+00	1.29E+00	5.92E+01	0.00E+00	2.68E+02	2.69E+00	1.04E-05
Red Fox (<i>Vulpes vulpes</i>)	0.00E+00	1.23E+00	0.00E+00	0.00E+00	9.33E-01	4.28E+01	0.00E+00	1.94E+02	1.94E+00	7.53E-06
Raccoon (<i>Procyon lotor</i>)	0.00E+00	1.19E+00	0.00E+00	0.00E+00	9.06E-01	4.15E+01	0.00E+00	1.88E+02	1.88E+00	7.32E-06
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0.00E+00	1.69E+00	0.00E+00	0.00E+00	1.28E+00	5.87E+01	0.00E+00	2.66E+02	2.66E+00	1.03E-05
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0.00E+00	1.32E+00	0.00E+00	0.00E+00	1.00E+00	4.59E+01	0.00E+00	2.08E+02	2.08E+00	8.08E-06
Mink (<i>Mustela vison</i>)	0.00E+00	1.34E+00	0.00E+00	0.00E+00	1.01E+00	4.65E+01	0.00E+00	2.11E+02	2.11E+00	8.19E-06

Juvenile Oral Toxicity for Organics

Receptor	Acetaldehyde	Anthracene	Benzene	Benz[a] Anthracene	Benzo[b] Fluoranthene	Benzo[a] Pyrene	Benzo[e] Pyrene	Benzo[g,h,i] Perylene	Benzo[k] Fluoranthene
ORAL LOAEL (mg/kg day)									
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	7.88E-02	0.00E+00	2.07E-02	0.00E+00	7.88E-02	7.88E-02	7.88E-02	3.68E-03
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	6.19E-02	0.00E+00	1.63E-02	0.00E+00	6.19E-02	6.19E-02	6.19E-02	2.89E-03
American robin (<i>Turdus migratorius</i>)	0.00E+00	2.32E-02	0.00E+00	6.10E-03	0.00E+00	2.32E-02	2.32E-02	2.32E-02	1.08E-03
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	6.18E-02	0.00E+00	1.63E-02	0.00E+00	6.18E-02	6.18E-02	6.18E-02	2.88E-03
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	7.36E-02	0.00E+00	1.94E-02	0.00E+00	7.36E-02	7.36E-02	7.36E-02	3.43E-03
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	5.42E-02	0.00E+00	1.43E-02	0.00E+00	5.42E-02	5.42E-02	5.42E-02	2.53E-03
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	6.56E-02	0.00E+00	1.73E-02	0.00E+00	6.56E-02	6.56E-02	6.56E-02	3.06E-03
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	5.92E-02	0.00E+00	1.56E-02	0.00E+00	5.92E-02	5.92E-02	5.92E-02	2.76E-03
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	3.74E-02	0.00E+00	9.84E-03	0.00E+00	3.74E-02	3.74E-02	3.74E-02	1.74E-03
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	4.14E-02	0.00E+00	1.09E-02	0.00E+00	4.14E-02	4.14E-02	4.14E-02	1.93E-03
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	3.14E-02	0.00E+00	8.26E-03	0.00E+00	3.14E-02	3.14E-02	3.14E-02	1.46E-03
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	5.46E-02	0.00E+00	1.44E-02	0.00E+00	5.46E-02	5.46E-02	5.46E-02	2.55E-03
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	3.91E-02	0.00E+00	1.03E-02	0.00E+00	3.91E-02	3.91E-02	3.91E-02	1.82E-03
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	2.27E-02	0.00E+00	5.99E-03	0.00E+00	2.27E-02	2.27E-02	2.27E-02	1.06E-03
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	2.56E-02	0.00E+00	6.73E-03	0.00E+00	2.56E-02	2.56E-02	2.56E-02	1.19E-03
River Otter (<i>Lutra canadensis</i>)	0.00E+00	9.15E+00	2.41E+02	1.52E-02	0.00E+00	9.15E+00	0.00E+00	0.00E+00	0.00E+00
Muskrat (<i>Ondatra zibethicus</i>)	0.00E+00	1.02E+01	2.69E+02	1.70E-02	0.00E+00	1.02E+01	0.00E+00	0.00E+00	0.00E+00
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0.00E+00	1.17E+01	3.08E+02	1.94E-02	0.00E+00	1.17E+01	0.00E+00	0.00E+00	0.00E+00
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0.00E+00	1.23E+01	3.23E+02	2.04E-02	0.00E+00	1.23E+01	0.00E+00	0.00E+00	0.00E+00
Red Fox (<i>Vulpes vulpes</i>)	0.00E+00	9.29E+00	2.45E+02	1.55E-02	0.00E+00	9.29E+00	0.00E+00	0.00E+00	0.00E+00
Raccoon (<i>Procyon lotor</i>)	0.00E+00	9.47E+00	2.50E+02	1.58E-02	0.00E+00	9.47E+00	0.00E+00	0.00E+00	0.00E+00
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0.00E+00	1.18E+01	3.12E+02	1.97E-02	0.00E+00	1.18E+01	0.00E+00	0.00E+00	0.00E+00
Eastern Cottontail (<i>Syvilagus floridanus</i>)	0.00E+00	9.80E+00	2.58E+02	1.63E-02	0.00E+00	9.80E+00	0.00E+00	0.00E+00	0.00E+00
Mink (<i>Mustela vison</i>)	0.00E+00	1.08E+01	2.85E+02	1.80E-02	0.00E+00	1.08E+01	0.00E+00	0.00E+00	0.00E+00

Juvenile Oral Toxicity for Organics

Receptor	Butadiene	Chrysene	Coronene	Ethylbenzene	Ethyleneglycol	Fluoranthene	Fluorene	Formaldehyde	Indeno[1,2,3-c,d] Pyrene
ORAL LOAEL (mg/kg day)									
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	2.63E-02	7.88E-08	0.00E+00	0.00E+00	7.88E-02	7.88E-02	0.00E+00	2.63E-02
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	2.06E-02	6.19E-02	0.00E+00	0.00E+00	6.19E-02	6.19E-02	0.00E+00	2.06E-02
American robin (<i>Turdus migratorius</i>)	0.00E+00	7.72E-03	2.32E-02	0.00E+00	0.00E+00	2.32E-02	2.32E-02	0.00E+00	7.72E-03
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	2.06E-02	6.18E-02	0.00E+00	0.00E+00	6.18E-02	6.18E-02	0.00E+00	2.06E-02
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	2.45E-02	7.36E-02	0.00E+00	0.00E+00	7.36E-02	7.36E-02	0.00E+00	2.45E-02
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	1.81E-02	5.42E-02	0.00E+00	0.00E+00	5.42E-02	5.42E-02	0.00E+00	1.81E-02
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	2.19E-02	6.56E-02	0.00E+00	0.00E+00	6.56E-02	6.56E-02	0.00E+00	2.19E-02
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	1.97E-02	5.92E-02	0.00E+00	0.00E+00	5.92E-02	5.92E-02	0.00E+00	1.97E-02
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	1.25E-02	3.74E-02	0.00E+00	0.00E+00	3.74E-02	3.74E-02	0.00E+00	1.25E-02
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	1.38E-02	4.14E-02	0.00E+00	0.00E+00	4.14E-02	4.14E-02	0.00E+00	1.38E-02
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	1.05E-02	3.14E-02	0.00E+00	0.00E+00	3.14E-02	3.14E-02	0.00E+00	1.05E-02
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	1.82E-02	5.46E-02	0.00E+00	0.00E+00	5.46E-02	5.46E-02	0.00E+00	1.82E-02
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	1.30E-02	3.91E-02	0.00E+00	0.00E+00	3.91E-02	3.91E-02	0.00E+00	1.30E-02
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	7.58E-03	2.27E-02	0.00E+00	0.00E+00	2.27E-02	2.27E-02	0.00E+00	7.58E-03
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	8.52E-03	2.56E-02	0.00E+00	0.00E+00	2.56E-02	2.56E-02	0.00E+00	8.52E-03
River Otter (<i>Lutra canadensis</i>)	0.00E+00	0.00E+00	0.00E+00	3.09E+00	1.06E+02	2.29E+00	2.65E+00	1.23E+01	0.00E+00
Muskrat (<i>Ondatra zibethicus</i>)	0.00E+00	0.00E+00	0.00E+00	3.45E+00	1.18E+02	2.55E+00	2.96E+00	1.38E+01	0.00E+00
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0.00E+00	0.00E+00	0.00E+00	3.93E+00	1.35E+02	2.92E+00	3.38E+00	1.57E+01	0.00E+00
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0.00E+00	0.00E+00	0.00E+00	4.14E+00	1.42E+02	3.07E+00	3.55E+00	1.65E+01	0.00E+00
Red Fox (<i>Vulpes vulpes</i>)	0.00E+00	0.00E+00	0.00E+00	3.13E+00	1.08E+02	2.32E+00	2.69E+00	1.25E+01	0.00E+00
Raccoon (<i>Procyon lotor</i>)	0.00E+00	0.00E+00	0.00E+00	3.19E+00	1.10E+02	2.37E+00	2.74E+00	1.27E+01	0.00E+00
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0.00E+00	0.00E+00	0.00E+00	3.99E+00	1.37E+02	2.96E+00	3.43E+00	1.59E+01	0.00E+00
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0.00E+00	0.00E+00	0.00E+00	3.30E+00	1.14E+02	2.45E+00	2.84E+00	1.32E+01	0.00E+00
Mink (<i>Mustela vison</i>)	0.00E+00	0.00E+00	0.00E+00	3.64E+00	1.25E+02	2.70E+00	3.13E+00	1.45E+01	0.00E+00

Juvenile Oral Toxicity for Organics

Receptor	MTBE	Naphthalene	n-Hexane	Phenanthrene	Pyrene	Styrene	ThiaArenes	Toluene	Xylenes	2,3,7,8-TCDD
ORAL LOAEL (mg/kg day)										
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	3.11E+00	0.00E+00	7.88E-02	7.88E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.68E-04
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	2.45E+00	0.00E+00	6.19E-02	6.19E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.32E-04
American robin (<i>Turdus migratorius</i>)	0.00E+00	9.16E-01	0.00E+00	2.32E-02	2.32E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.95E-05
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	2.44E+00	0.00E+00	6.18E-02	6.18E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.32E-04
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	2.91E+00	0.00E+00	7.36E-02	7.36E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.57E-04
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	2.14E+00	0.00E+00	5.42E-02	5.42E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.16E-04
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	2.59E+00	0.00E+00	6.56E-02	6.56E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E-04
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	2.34E+00	0.00E+00	5.92E-02	5.92E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.26E-04
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	1.48E+00	0.00E+00	3.74E-02	3.74E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.98E-05
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	1.64E+00	0.00E+00	4.14E-02	4.14E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.83E-05
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	1.24E+00	0.00E+00	3.14E-02	3.14E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.69E-05
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	2.16E+00	0.00E+00	5.46E-02	5.46E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.17E-04
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	1.54E+00	0.00E+00	3.91E-02	3.91E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.34E-05
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	8.99E-01	0.00E+00	2.27E-02	2.27E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.85E-05
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	1.01E+00	0.00E+00	2.56E-02	2.56E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.46E-05
River Otter (<i>Lutra canadensis</i>)	0.00E+00	1.51E+00	0.00E+00	0.00E+00	1.14E+00	5.24E+01	0.00E+00	2.38E+02	2.38E+00	9.34E-05
Muskrat (<i>Ondatra zibethicus</i>)	0.00E+00	1.68E+00	0.00E+00	0.00E+00	1.28E+00	5.85E+01	0.00E+00	2.65E+02	2.66E+00	6.47E-05
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0.00E+00	1.92E+00	0.00E+00	0.00E+00	1.46E+00	6.69E+01	0.00E+00	3.03E+02	3.03E+00	4.15E-05
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0.00E+00	2.02E+00	0.00E+00	0.00E+00	1.53E+00	7.03E+01	0.00E+00	3.19E+02	3.19E+00	3.52E-05
Red Fox (<i>Vulpes vulpes</i>)	0.00E+00	1.53E+00	0.00E+00	0.00E+00	1.16E+00	5.32E+01	0.00E+00	2.41E+02	2.42E+00	8.87E-05
Raccoon (<i>Procyon lotor</i>)	0.00E+00	1.56E+00	0.00E+00	0.00E+00	1.18E+00	5.42E+01	0.00E+00	2.46E+02	2.46E+00	8.34E-05
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	0.00E+00	1.95E+00	0.00E+00	0.00E+00	1.48E+00	6.78E+01	0.00E+00	3.08E+02	3.08E+00	3.96E-05
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0.00E+00	1.61E+00	0.00E+00	0.00E+00	1.22E+00	5.61E+01	0.00E+00	2.55E+02	2.55E+00	7.43E-05
Mink (<i>Mustela vison</i>)	0.00E+00	1.78E+00	0.00E+00	0.00E+00	1.35E+00	6.19E+01	0.00E+00	2.81E+02	2.81E+00	5.37E-05

Adult Inhalation Toxicity for Organics

Receptor	Acetaldehyde	Anthracene	Benzene	Benz[a] Anthracene	Benzo[b] Fluoranthene	Benzo[a] Pyrene	Benzo[e] Pyrene	Benzo[g,h,i] Perylene	Benzo[k] Fluoranthene
INHALATION (mg/day)									
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American robin (<i>Turdus migratorius</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
River Otter (<i>Lutra canadensis</i>)	2.06E+01	0.00E+00	7.89E-02	0.00E+00	0.00E+00	1.31E-01	0.00E+00	0.00E+00	0.00E+00
Muskrat (<i>Ondatra zibethicus</i>)	1.86E+01	0.00E+00	7.10E-02	0.00E+00	0.00E+00	1.18E-01	0.00E+00	0.00E+00	0.00E+00
Meadow Vole (<i>Microtus pennsylvanicus</i>)	1.50E+01	0.00E+00	5.74E-02	0.00E+00	0.00E+00	9.55E-02	0.00E+00	0.00E+00	0.00E+00
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	1.43E+01	0.00E+00	5.46E-02	0.00E+00	0.00E+00	9.10E-02	0.00E+00	0.00E+00	0.00E+00
Red Fox (<i>Vulpes vulpes</i>)	1.98E+01	0.00E+00	7.57E-02	0.00E+00	0.00E+00	1.26E-01	0.00E+00	0.00E+00	0.00E+00
Raccoon (<i>Procyon lotor</i>)	2.04E+01	0.00E+00	7.79E-02	0.00E+00	0.00E+00	1.30E-01	0.00E+00	0.00E+00	0.00E+00
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	1.44E+01	0.00E+00	5.51E-02	0.00E+00	0.00E+00	9.18E-02	0.00E+00	0.00E+00	0.00E+00
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	1.85E+01	0.00E+00	7.06E-02	0.00E+00	0.00E+00	1.18E-01	0.00E+00	0.00E+00	0.00E+00
Mink (<i>Mustela vison</i>)	1.82E+01	0.00E+00	6.96E-02	0.00E+00	0.00E+00	1.16E-01	0.00E+00	0.00E+00	0.00E+00

Adult Inhalation Toxicity for Organics

Receptor	Butadiene	Chrysene	Coronene	Ethylbenzene	Ethyleneglycol	Fluoranthene	Fluorene	Formaldehyde	Indeno[1,2,3-c,d] Pyrene
INHALATION (mg/day)									
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American robin (<i>Turdus migratorius</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
River Otter (<i>Lutra canadensis</i>)	3.46E-01	0.00E+00	0.00E+00	3.72E+03	0.00E+00	0.00E+00	0.00E+00	7.18E-02	0.00E+00
Muskrat (<i>Ondatra zibethicus</i>)	3.11E-01	0.00E+00	0.00E+00	3.34E+03	0.00E+00	0.00E+00	0.00E+00	4.97E-02	0.00E+00
Meadow Vole (<i>Microtus pennsylvanicus</i>)	2.51E-01	0.00E+00	0.00E+00	2.70E+03	0.00E+00	0.00E+00	0.00E+00	3.19E-02	0.00E+00
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	2.40E-01	0.00E+00	0.00E+00	2.57E+03	0.00E+00	0.00E+00	0.00E+00	2.70E-02	0.00E+00
Red Fox (<i>Vulpes vulpes</i>)	3.32E-01	0.00E+00	0.00E+00	3.56E+03	0.00E+00	0.00E+00	0.00E+00	6.81E-02	0.00E+00
Raccoon (<i>Procyon lotor</i>)	3.41E-01	0.00E+00	0.00E+00	3.67E+03	0.00E+00	0.00E+00	0.00E+00	6.41E-02	0.00E+00
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	2.42E-01	0.00E+00	0.00E+00	2.60E+03	0.00E+00	0.00E+00	0.00E+00	3.04E-02	0.00E+00
Eastern Cottontail (<i>Syvilagus floridanus</i>)	3.09E-01	0.00E+00	0.00E+00	3.32E+03	0.00E+00	0.00E+00	0.00E+00	5.71E-02	0.00E+00
Mink (<i>Mustela vison</i>)	3.05E-01	0.00E+00	0.00E+00	3.28E+03	0.00E+00	0.00E+00	0.00E+00	4.13E-02	0.00E+00

Adult Inhalation Toxicity for Organics

Receptor	MTBE	Naphthalene	n-Hexane	Phenanthrene	Pyrene	Styrene	ThiaArenes	Toluene	Xylenes	2,3,7,8-TCDD
INHALATION (mg/day)										
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Great Blue Heron (<i>Ardea herodias</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American robin (<i>Turdus migratorius</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Mallard Duck (<i>Anas platyrhynchos</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Canada Goose (<i>Branta canadensis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Lesser Scaup (<i>Aythya affinis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Osprey (<i>Pandion haliaetus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American Kestrel (<i>Falco Sparvaerius</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
American Woodcock (<i>Scolopax minor</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Spotted Sandpiper (<i>Actitis macularia</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Herring Gull (<i>Larus argentatus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
March Wren (<i>Cistothorus palustris</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Northern Bobwhite (<i>Colinus virginianus</i>)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
River Otter (<i>Lutra canadensis</i>)	1.67E+02	2.81E-01	8.79E+00	0.00E+00	0.00E+00	3.65E+02	0.00E+00	3.74E+01	6.68E-01	0.00E+00
Muskrat (<i>Ondatra zibethicus</i>)	1.50E+02	1.97E-01	7.90E+00	0.00E+00	0.00E+00	3.28E+02	0.00E+00	3.36E+01	6.01E-01	0.00E+00
Meadow Vole (<i>Microtus pennsylvanicus</i>)	1.21E+02	9.70E-02	6.39E+00	0.00E+00	0.00E+00	2.65E+02	0.00E+00	2.72E+01	4.85E-01	0.00E+00
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	1.15E+02	8.26E-02	6.09E+00	0.00E+00	0.00E+00	2.53E+02	0.00E+00	2.59E+01	4.63E-01	0.00E+00
Red Fox (<i>Vulpes vulpes</i>)	1.60E+02	2.44E-01	8.43E+00	0.00E+00	0.00E+00	3.50E+02	0.00E+00	3.59E+01	6.40E-01	0.00E+00
Raccoon (<i>Procyon lotor</i>)	1.65E+02	2.69E-01	8.68E+00	0.00E+00	0.00E+00	3.60E+02	0.00E+00	3.69E+01	6.59E-01	0.00E+00
Prairie Deer Mouse (<i>Peromyscus maniculatus</i>)	1.16E+02	8.49E-02	6.14E+00	0.00E+00	0.00E+00	2.55E+02	0.00E+00	2.61E+01	4.66E-01	0.00E+00
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	1.49E+02	1.94E-01	7.86E+00	0.00E+00	0.00E+00	3.26E+02	0.00E+00	3.35E+01	5.97E-01	0.00E+00
Mink (<i>Mustela vison</i>)	1.47E+02	1.85E-01	7.75E+00	0.00E+00	0.00E+00	3.22E+02	0.00E+00	3.30E+01	5.89E-01	0.00E+00

Transfer Factors for Organics

Receptor	Acetaldehyde	Anthracene	Benzene	Benz[a]Anthracene	Benzo[b]Fluoranthene	Benzo[a]Pyrene	Benzo[e]Pyrene	Benzo[g,h,i]Perylene	Benzo[k]Fluoranthene
EMPIRICAL									
Fish-water (L/kg)	4.00E-01	1.14E+03	1.10E+01	4.81E+02	1.58E+04	1.09E+03			2.94E+04
Aq. Vegetation-water (L/kg)		7.10E+03	3.39E+01	3.16E+03		3.31E+03			
Benthic invertebrates-pore water sediment (L-water/kg-benthos)		1.66E+04			3.93E+00	1.75E+04			5.04E+00
BCF terrestrial invertebrates									
BCF worm-pore water									
Mammal (day/kg FW) FW=fresh weight	1.39E-08	2.34E-04	3.27E-06	1.25E-02	3.52E-02	1.07E-02			7.98E-02
Bird (day/kg FW)	1.19E-08	5.85E-04	2.72E-06	9.46E-03	3.16E-02	2.67E-02			3.14E-02
Milk (day/kg FW)	4.79E-09	2.16E-04	1.04E-06	3.89E-03	1.12E-02	1.03E-02			2.45E-02
NON-EMPIRICAL									
LogK _{ow}	4.30E-01	4.45E+00	2.18E+00	5.70E+00	6.12E+00	6.04E+00	6.90E+00	6.58E+00	6.84E+00
K _{ow}	2.69E+00	2.82E+04	1.51E+02	5.01E+05	1.32E+06	1.10E+06	7.94E+06	3.80E+06	6.92E+06
Fish-water (L/kg)	1.35E-01	1.41E+03	7.57E+00	2.51E+04	6.59E+04	5.48E+04	3.97E+05	1.90E+05	3.46E+05
Aq. Vegetation-water (L/kg)	1.35E-02	1.41E+02	7.57E-01	2.51E+03	6.59E+03	5.48E+03	3.97E+04	1.90E+04	3.46E+04
Benthic invertebrates-sediment (kg-sediment DW/kg-benthos) DW= dry weight	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00
BCF terrestrial invertebrates	1.61E-01	3.15E+02	4.36E+00	3.33E+03	7.35E+03	2.11E+02	3.20E+04	1.75E+04	2.86E+04
K _{worm-water}	8.72E-01	3.39E+02	2.66E+00	6.02E+03	1.58E+04	3.26E+03	9.53E+04	4.56E+04	8.30E+04

Transfer Factors for Organics

Receptor	Butadiene	Chrysene	Coronene	Ethylbenzene	Ethyleneglycol	Fluoranthene	Fluorene	Formaldehyde	Indeno[1,2,3-c,d]Pyrene
EMPIRICAL									
Fish-water (L/kg)	1.90E+01	2.80E+04		6.32E+01	4.58E-01	3.14E+03	2.66E+01	4.96E-01	3.96E+02
Aq. Vegetation-water (L/kg)				2.04E+02	1.91E+02				
Benthic invertebrates-pore water sediment (L-water/kg-benthos)		1.23E+02				1.76E+02			
BCF terrestrial invertebrates									
BCF worm-pore water									
Mammal (day/kg FW) FW=fresh weight	2.50E-06	1.34E-02			3.10E-10	1.39E-03	5.68E-03	7.20E-09	1.30E-06
Bird (day/kg FW)		1.09E-02		2.63E-05					
Milk (day/kg FW)	7.9E-07	4.18E-03			9.9E-11	2.00E-04	7.90E-09	2.3E-09	0.0000004
NON-EMPIRICAL									
LogK _{ow}	1.99E+00	5.75E+00	6.75E+00	3.12E+00	1.93E+00	5.22E+00	4.18E+00	3.40E-01	7.24E+00
K _{ow}	9.77E+01	5.62E+05	5.62E+06	1.32E+03	1.17E-02	1.66E+05	1.51E+04	2.19E+00	1.74E+07
Fish-water (L/kg)	4.89E+00	2.81E+04	2.81E+05	6.59E+01	5.87E-04	8.30E+03	7.57E+02	1.09E-01	8.69E+05
Aq. Vegetation-water (L/kg)	4.89E-01	2.81E+03	2.81E+04	6.59E+00	5.87E-05	8.30E+02	7.57E+01	1.09E-02	8.69E+04
Benthic invertebrates-sediment (kg-sediment DW/kg-benthos) DW= dry weight	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00
BCF terrestrial invertebrates	3.05E+00	3.66E+03	2.41E+04	2.57E+01	1.88E-03	1.35E+03	1.89E+02	1.36E-01	6.08E+04
K _{worm-water}	2.01E+00	6.75E+03	6.75E+04	1.67E+01	8.40E-01	1.99E+03	1.82E+02	8.66E-01	2.09E+05

Transfer Factors for Organics

Receptor	MTBE	Naphthalene	n-Hexane	Phenanthrene	Pyrene	Styrene	ThiaArenes	Toluene	Xylenes	2,3,7,8-TCDD
EMPIRICAL										
Fish-water (L/kg)	3.10E+00	1.68E+02	5.40E+02	2.66E+03	2.60E+03	1.67E+02		2.38E+01	6.85E+01	1.64E+04
Aq. Vegetation-water (L/kg)		1.16E+04		1.14E+04	3.24E+04			2.42E+02	2.54E+02	
Benthic invertebrates-pore water sediment (L-water/kg-benthos)		3.67E+01		3.08E+02	3.64E+02			2.79E+00	1.18E+01	
BCF terrestrial invertebrates										
BCF worm-pore water										
Mammal (day/kg FW) FW=fresh weight	2.20E-07	1.60E-06	2.00E-04	2.00E-02	2.00E-03	1.60E-02		5.10E-07	5.00E-05	6.49E-01
Bird (day/kg FW)										
milk (day/kg FW)	0.000000069	9.99E-06	0.000063	6.30E-03	6.30E-04	5.00E-02		1.60E-07	1.60E-05	9.32E-04
NON-EMPIRICAL										
LogK _{ow}	1.30E+00	3.37E+00	3.90E+00	4.57E+00	5.00E+00	2.95E+00		2.68E+00	3.11E+00	6.64E+00
K _{ow}	2.00E+01	2.34E+03	7.94E+03	3.72E+04	1.00E+05	8.91E+02	1.00E+00	4.79E+02	1.29E+03	4.37E+06
Fish-water (L/kg)	9.98E-01	1.17E+02	3.97E+02	1.86E+03	5.00E+03	4.46E+01	5.00E-02	2.39E+01	6.44E+01	2.95E+06
Aq. Vegetation-water (L/kg)	9.98E-02	1.17E+01	3.97E+01	1.86E+02	5.00E+02	4.46E+00	5.00E-03	2.39E+00	6.44E+00	2.18E+04
Benthic invertebrates-sediment (kg-sediment DW/kg-benthos)	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00	3.00E+00
BCF terrestrial invertebrates	8.29E-01	4.11E+01	1.12E+02	3.95E+02	8.89E+02	1.86E+01	7.14E-02	1.12E+01	2.52E+01	1.96E+04
K _{worm-water}	1.08E+00	2.90E+01	9.62E+01	4.47E+02	1.20E+03	1.15E+01	8.52E-01	6.58E+00	1.63E+01	5.24E+04

Media.dim

This file contains the land use coverage data as well as the thickness and the interfacial area of each environmental compartment for each box. The data file is too long to be included in this appendix. The data in the file are in a sequential format. The first 27 numbers are for box 1, the next 27 numbers are for box 2 and so on. The 27 numbers represent the areas of air, lake, river, lake sediments, river sediments, soil, vegetation, snow, and organic film; the thicknesses of air, lake, river, lake sediments, river sediments, soil, vegetation, snow, and organic film; and the interfacial surface areas between air-lake, air-river, lake-sediments, river-sediments, air-soil, air-snow, air-vegetation, soil-snow, and air-organic film.

Trans_data.inp

This file contains the mass transfer coefficients for transport processes. The data as they appear represent: the mass transfer coefficients, in m/s, for air-to-water, air-to-organic film, air-to-soil, air-to-vegetation, lake water-to-sediments, river water-to-sediments, lake water-to-air, and river water-to-air; the aerosol deposition velocity in m/s; the rates, in m/s, of lake sediments deposition, lake sediments resuspension, lake sediments burial, river sediments deposition, river sediments resuspension, and river sediments burial; the precipitation rate (m/year); the scavenging ratio; the mechanical removal factor; the soil diffusive characteristic path and sediments diffusive characteristic path in m; the precipitation intercept factor and the rain splash factor; and the soil resuspension rate in m/y.

3
2
2
3
0.03
0.06
0.03
0.07
100
9e-8
1e-8
4e-8
7e-8
2e-8
1e-8
0.9
200000
1e-10
0.05
0.005
0.6
0.01
1e-8

Roads.inp

This file contains the traffic volume and road length information that is used to calculate the emissions for each box. Each row of information represents the data for one box, starting from box 1 and ending at box 81. Each row of data gives road length in km, average daily traffic for light duty vehicles, and average daily traffic for heavy duty vehicles, respectively.

Box	Road Length (Km)	Avg. Daily Traffic Light Duty Vehicles	Avg. Daily Traffic Heavy Duty Vehicles
1	52	53278	1066
2	63	83818	1676
3	81	46176	924
4	88	27340	547
5	58	47048	941
6	62	60247	1205
7	43	36061	721
8	80	20871	417
9	56	78203	1564
10	51	53013	1060
11	51	43066	861
12	71	42021	840
13	89	31620	632
14	93	19331	387
15	48	72341	1447
16	89	29554	591
17	43	22998	460
18	89	41550	831
19	79	27338	547
20	100	30537	611
21	75	21371	427
22	118	19482	390
23	136	15977	320
24	144	38660	773
25	51	68466	1369
26	79	50300	1006
27	80	68345	1367
28	40	51389	1028
29	81	55867	1117
30	86	71480	1430
31	227	36845	737
32	110	19399	388
33	127	45903	918
34	65	75463	1509
35	96	25490	510
36	46	81847	1637

Box	Road Length (Km)	Avg. Daily Traffic Light Duty Vehicles	Avg. Daily Traffic Heavy Duty Vehicles
37	37	75508	1510
38	81	47732	955
39	90	51604	1032
40	206	67960	1359
41	256	48017	960
42	195	46471	929
43	150	59121	1182
44	67	43268	865
45	68	30949	619
46	64	70370	1407
47	83	53783	1076
48	68	44641	893
49	171	77082	1542
50	284	41730	835
51	245	48644	973
52	65	48860	977
53	71	69834	1397
54	37	40182	804
55	51	28542	571
56	68	24048	481
57	86	64104	1282
58	134	52542	1051
59	222	40841	817
60	257	67025	1341
61	221	33023	660
62	79	73157	1463
63	61	61471	1229
64	37	17193	344
65	54	75579	1512
66	89	47508	950
67	144	62331	1447
68	112	68970	1379
69	125	62966	1459
70	82	76701	1534
71	83	74212	1484
72	36	60534	1211
73	62	62200	1244
74	48	38488	770
75	82	57099	1142
76	62	66341	1327
77	76	40315	806
78	75	81956	1639
79	59	21587	432
80	71	37830	757
81	34	30159	603

Appendix B:
Land Use Coverage

The following table gives box-specific land use coverage.

Box	Land Use Cover, m ²							
	Air	Lake	River	Lake sediments	River sediments	Soil	Vegetation	Impervious surfaces
1	24866100	906895	57205	906895	57205	22888350	22888350	1033650
2	24949800	1153990	70210	1153990	70210	22511133	22511133	1234467
3	25100100	158950	1350550	158950	1350550	17005554	17005554	6605046
4	25100100	40915	597385	40915	597385	16588242	16588242	7893558
5	24949800	10000	10000	10000	10000	18814194	18814194	6135606
6	25100100	61300	12700	61300	12700	21927753	21927753	3118347
7	25100100	5413600	294400	5413600	294400	16875495	16875495	2536605
8	24949800	3360745	186355	3360745	186355	19697607	19697607	1725093
9	25100100	2073115	118585	2073115	118585	21903417	21903417	1024983
10	24744600	2191960	124840	2191960	124840	20288403	20288403	2159397
11	24800400	244270	22330	244270	22330	14957334	14957334	9596466
12	24949800	10000	10000	10000	10000	21412665	21412665	3537135
13	24949800	147520	1247680	147520	1247680	18158985	18158985	5415615
14	24800400	444340	32860	444340	32860	14255163	14255163	10088037
15	24949800	634510	79390	634510	79390	17837721	17837721	6418179
16	24949800	2631430	147970	2631430	147970	19369134	19369134	2821266
17	24800400	4506445	246655	4506445	246655	18140571	18140571	1926729
18	24949800	1997875	114625	1997875	114625	21026304	21026304	1830996
19	24966900	1284805	77095	1284805	77095	22179870	22179870	1445130
20	24949800	2382625	134875	2382625	134875	13859928	13859928	8592372
21	25100100	238285	22015	238285	22015	13645116	13645116	11214684

Box	Land Use Cover, m ²							
	Air	Lake	River	Lake sediments	River sediments	Soil	Vegetation	Impervious surfaces
22	25100100	262180	1018720	262180	1018720	13627701	13627701	10211499
23	24949800	1019755	63145	1019755	63145	13685499	13685499	10201401
24	25100100	1746505	101395	1746505	101395	14053023	14053023	9219177
25	25100100	4444885	243415	4444885	243415	15769404	15769404	4662396
26	24949800	1423315	84385	1423315	84385	17923878	17923878	5538222
27	25100100	9681760	519040	9681760	519040	10491651	10491651	4427649
28	24957000	229735	21565	229735	21565	20752416	20752416	3973284
29	24949800	2115865	120835	2115865	120835	15847695	15847695	6885405
30	25100100	775450	95050	775450	95050	13764411	13764411	10485189
31	25100100	515260	948340	515260	948340	12813228	12813228	10843272
32	24949800	413560	31240	413560	31240	13879746	13879746	10645254
33	25100100	1913230	110170	1913230	110170	11972466	11972466	11124234
34	25100100	4018240	220960	4018240	220960	13545846	13545846	7335054
35	24949800	1593460	93340	1593460	93340	15952662	15952662	7330338
36	25100100	1388260	82540	1388260	82540	16800579	16800579	6848721
37	24524100	2271475	129025	2271475	129025	13124106	13124106	9019494
38	24800400	2650240	148960	2650240	148960	12378159	12378159	9643041
39	24949800	552070	38530	552070	38530	13997790	13997790	10381410
40	24949800	374680	557020	374680	557020	12306663	12306663	11731437
41	24800400	58780	936820	58780	936820	9522252	9522252	14302548
42	24949800	203230	20170	203230	20170	14458473	14458473	10287927
43	24949800	529840	37360	529840	37360	14141502	14141502	10261098
44	24800400	1218115	73585	1218115	73585	14743134	14743134	8785566
45	24949800	498205	35695	498205	35695	17747163	17747163	6688737

Box	Land Use Cover, m ²							
	Air	Lake	River	Lake sediments	River sediments	Soil	Vegetation	Impervious surfaces
46	24946200	2742130	313570	2742130	313570	15033924	15033924	6876576
47	24949800	183565	19135	183565	19135	15210441	15210441	9556659
48	25100100	359695	28405	359695	28405	13920318	13920318	10811682
49	25100100	3650590	201610	3650590	201610	11191383	11191383	10076517
50	24949800	197650	447850	197650	447850	13022010	13022010	11302290
51	25100100	59545	951355	59545	951355	12562569	12562569	11546631
52	25092000	134650	1131850	134650	1131850	11665188	11665188	12180312
53	24949800	866080	1294120	866080	1294120	13060458	13060458	9749142
54	25100100	676900	45100	676900	45100	16913151	16913151	7484949
55	24584400	741880	48520	741880	48520	16756569	16756569	7057431
56	24949800	1325845	79255	1325845	79255	14052267	14052267	9512433
57	25100100	788905	50995	788905	50995	15308487	15308487	8971713
58	25100100	1053100	64900	1053100	64900	13027923	13027923	10974177
59	24949800	934255	58645	934255	58645	14537619	14537619	9439281
60	25100100	1355050	1355050	1355050	1355050	13749993	13749993	8660007
61	25100100	801280	349120	801280	349120	16315731	16315731	7653969
62	24949800	2157850	2157850	2157850	2157850	13740408	13740408	6913692
63	25100100	404560	108640	404560	108640	19758852	19758852	4848048
64	24786900	1898695	109405	1898695	109405	18587493	18587493	4211307
65	24800400	1867060	107740	1867060	107740	15668973	15668973	7176627
66	24949800	1258300	75700	1258300	75700	16349346	16349346	7286454
67	24949800	509320	36280	509320	36280	12636945	12636945	11787255
68	24800400	2012725	677575	2012725	677575	13674393	13674393	8455707
69	24949800	2109160	909640	2109160	909640	14647680	14647680	7303320

Box	Land Use Cover, m ²							
	Air	Lake	River	Lake sediments	River sediments	Soil	Vegetation	Impervious surfaces
70	24949800	1013770	62830	1013770	62830	19499508	19499508	4393692
71	24800400	517600	348400	517600	348400	17446680	17446680	6507720
72	24949800	184870	1583830	184870	1583830	18391905	18391905	4809195
73	24981300	2027440	514360	2027440	514360	17611092	17611092	4848408
74	24949800	2116000	536500	2116000	536500	17707608	17707608	4609692
75	25100100	1400410	605890	1400410	605890	16530399	16530399	6583401
76	25100100	668800	668800	668800	668800	16881939	16881939	6900561
77	24949800	2257210	973090	2257210	973090	15254856	15254856	6484644
78	25100100	1024885	63415	1024885	63415	17385813	17385813	6645987
79	25100100	681175	45325	681175	45325	21251115	21251115	3142485
80	24949800	196210	1685890	196210	1685890	20451978	20451978	2635722
81	25100100	1573120	2354680	1573120	2354680	18342423	18342423	2849877

Appendix C:
List of Files - Complete Model

LIST OF FILES

The following files comprise the complete model

data_exch.bas	grid26.min
em_data.inp	grid27.min
Form1.frm	grid28.min
Form2.frm	grid29.min
Form2.frx	grid3.min
FrmBackground.frm	grid30.min
FrmDataIn.frm	grid31.min
FrmDataIn.frx	grid32.min
FrmMain.frm	grid33.min
FrmMain.frx	grid34.min
FrmMapMain.frm	grid35.min
FrmMapSec.frm	grid36.min
FrmMeasured.frm	grid37.min
FrmMedia.frm	grid38.min
FrmOutGraphic.frm	grid39.min
FrmOutGraphic.frx	grid4.min
FrmOutIntermedia.frm	grid40.min
FrmOutMassConc.frm	grid41.min
FrmOutSpatial.frm	grid42.min
FrmSplash.frm	grid43.min
FrmSplash.frx	grid44.min
FrmSteady.frm	grid45.min
FrmWildDose.frm	grid46.min
FrmWildIntake.frm	grid47.min
FrmWildRisk.frm	grid48.min
grid1.min	grid49.min
grid10.min	grid5.min
grid11.min	grid50.min
grid12.min	grid51.min
grid13.min	grid52.min
grid14.min	grid53.min
grid15.min	grid54.min
grid16.min	grid55.min
grid17.min	grid56.min
grid18.min	grid57.min
grid19.min	grid58.min
grid2.min	grid59.min
grid20.min	grid6.min
grid21.min	grid60.min
grid22.min	grid61.min
grid23.min	grid62.min
grid24.min	grid63.min
grid25.min	grid64.min

grid65.min
grid66.min
grid67.min
grid68.min
grid69.min
grid7.min
grid70.min
grid71.min
grid72.min
grid73.min
grid74.min
grid75.min
grid76.min
grid77.min
grid78.min
grid79.min
grid8.min
grid80.min
grid81.min
grid9.min
input.xls
interbox.inp
main.bas

media.dim
media.pcp
met_data.inp
metals- check.xls
metals.pcp
Minn1.Inp
Minn2.Inp
Minn3.Inp
Minn4.Inp
Minn5.Inp
Module3.bas
Organics.pcp
orig.min
Risk_Exposurebas.bas
roads.inp
sewer_sys.min
trans_data.inp
Varibales.bas
version_1.PDM
version_1.vbp

Appendix D:

Wildlife Parameters Database

Wildlife Parameters Database

Receptors	Exposure Scenario	Exposure Factor	Body Weights		Intake Rates			
			Adult Female (g)	Juvenile (g)	Free-living metabolic (kcal/g-d)	Food Ingestion gww/gww-d ^a gdw/gww d ^b	Water Ingestion (g/g-day)	Inhalation (m ³ /day)
BIRDS								
Great Blue Heron, (<i>Ardea herodias</i>)	6.5 months	0.54	2230	750	AE	0.18	AE	AE
Migrate: leave October, arrive mid-march		0				0.18		
American Robin (<i>Turdus migratorius</i>)	7 months	0.58	80.6	5.5	AE	1.52	AE	AE
Migrate Early November to March		0						
Canada Goose (<i>Branta canadensis</i>)	7 months	0.58	3550	1775	AE	0.031	AE	AE
No winter scenario/ Migrate		0						
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	7 months	0.58	5089	2500	AE	0.12	AE	AE
No winter scenario/ fall Migration October back early March		0						
Mallard Duck (<i>Anas platyrhynchos</i>)	7 months	0.58	1197	740	AE	AE	AE	AE
No winter scenario/fall migration mid-October to mid-March		0						
Lesser Scaup (<i>Aythya affinis</i>)	6 months	0.5	770	385	AE	AE	AE	AE
Migrate mid October to mid April		0						

^a AE=Allometric Equation

^b EP=Empirical

Receptors	Fraction of item in diet													
	Forage Fish	Piscivorous Fish	Aquatic Invertebrates	Birds	Mammals	Invertebrates Terrestrial	Worms	Vegetation Aquatic	Vegetation Terrestrial	Soil	Sediment (Lake Water)	Sediment (River Water)	Lake Water	River Water
Great Blue Heron (<i>Ardea herodias</i>)	0.98	0	0.01	0	0	0	0	0	0	0	0	0	0.5	0.5
Migrate from October to mid-March														
American Robin (<i>Turdus migratorius</i>)	0	0	0	0	0	0.56	0.15	0	0.29	0.1	0	0	0.5	0.5
Migrate Early November to March														
Canada Goose (<i>Branta canadensis</i>)	0	0	0	0	0	0	0	0	1	0.082	0	0	0.5	0.5
No winter scenario/ Migrate														
Bald Eagle (<i>Haliaeetus leucocephalus</i>)	0.77	0	0	0.16	0.07	0	0	0	0	0	0	0	0.5	0.5
No winter scenario/ fall migration October back early March														
Mallard Duck (<i>Anas platyrhynchos</i>)	0	0	0.75	0	0	0	0	0.25	0	0	0.01	0.01	0.5	0.5
No winter scenario/fall migration mid-October to mid-March														
Lesser Scaup (<i>Aythya affinis</i>)	0.063	0	0.84	0	0	0	0	0.09	0	0	0.01	0.01	0.5	0.5
Migrate mid October to mid April														

Receptors	Exposure Scenario	Exposure Factor	Body Weights		Intake Rates			
			Adult Female (g)	Juvenile (g)	Free-living metabolic (kcal/g-d)	Food Ingestion gww/gww-d ^a gdw/gww d ^b	Water Ingestion (g/g-day)	Inhalation (m ³ /day)
BIRDS								
Osprey (<i>Pandion haliaetus</i>)	5 months	0.42	1925	1000	AE	AE	AE	AE
Migrate late August to early April		0						
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	9 months	0.75	1235	600	AE	AE	AE	AE
Migrate late November to early March		0						
American Kestrel (<i>Falco Sparvaerius</i>)	6 months	0.5	124	60	AE	AE	AE	AE
Migrate early September to early March		0						
American Woodcock (<i>Scolopax minor</i>)	6 months	0.5	213	100	0.315	AE	AE	AE
Migrate late September return April		0						
Spotted Sandpiper (<i>Actitis macularia</i>)	9 months	0.75	47.1	25	AE	AE	AE	AE
Migrate November to March		0						
Herring Gull (<i>Larus argentatus</i>)	6 months	0.5	951	400	AE	0.18	AE	AE
Migrate from September to April		0						
Belted Kingfisher (<i>Ceryle alcyon</i>)	8 months	0.67	158	75	AE	0.5/nestlings 1.5	AE	AE
Migrate mid-November to mid-March		0						
March Wren (<i>Cistothorus palustris</i>)	6 months	0.5	10.6	5	0.88	0.99	AE	AE
Migrate September to April		0						
Northern Bobwhite (<i>Colinus virginianus</i>)	8 months	0.67	180	9	AE	0.073	0.13	AE
Active all year round	4 months	0.33	183			0.093		
Red Fox (<i>Vulpes vulpes</i>)	12 months	0.67	3940	102	AE	adult 0.075/ juv. 0.16	AE	AE
Active all year round		0.33	3940					

^a AE=Allometric Equation

^b EP=Empirical

Receptors	Fraction of item in diet													
	Forage Fish	Piscivorous Fish	Aquatic Invertebrates	Birds	Mammals	Invertebrates Terrestrial	Worms	Vegetation Aquatic	Vegetation Terrestrial	Soil	Sediment (Lake Water)	Sediment (River Water)	Lake Water	River Water
Osprey (<i>Pandion haliaetus</i>)	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0.5
Migrate late August to early April														
Red-tailed Hawk (<i>Buteo jamaicensis</i>)	0	0	0	0.26	0.74	0	0	0	0	0	0	0	0.5	0.5
Migrate late November to early March														
American Kestrel (<i>Falco Sparvaerius</i>)	0	0	0	0.303	0.317	0.361	0	0	0	0	0	0	0.5	0.5
Migrate early September to early March														
American Woodcock (<i>Scolopax minor</i>)	0	0	0	0	0	0.217	0.678	0	0.105	0.104	0	0	0.5	0.5
Migrate late September return April														
Spotted Sandpiper (<i>Actitis macularia</i>)	0	0	1	0	0	0	0	0	0	0	0.09	0.09	0.5	0.5
Migrate November to March														
Herring Gull (<i>Larus argentatus</i>)	0.386	0	0	0.035		0.421	0.017	0	0	0	0	0	0.5	0.5
Migrate from September to April														
Belted Kingfisher (<i>Ceryle alcyon</i>)	0.46	0	0.05	0.005	0.005	0	0	0	0	0.05	0	0	0.5	0.5
Migrate mid-November to mid-March														
March Wren (<i>Cistothorus palustris</i>)	0	0	0	0	0	1	0	0	0	0	0	0	0.5	0.5
Migrate September to April														
Northern Bobwhite (<i>Colinus virginianus</i>)	0	0	0	0	0	0.18	0	0	0.82	0	0	0	0.5	0.5
Active all year round	0	0	0	0	0	0.03	0	0	0.97	0	0	0	0	0
Red Fox (<i>Vulpes vulpes</i>)	0	0	0	0.15	0.64	0.05	0	0	0.14	0.028	0	0	0.5	0.5
Active all year round				0.9	0.65	0.001			0.26	0.028			0	0

Receptors	Exposure Scenario	Exposure Factor	Body Weights		Intake Rates			
			Adult Female (g)	Juvenile (g)	Free-living metabolic (kcal/g-d)	Food Ingestion gww/gww-d ^a gdw/gww d ^b	Water Ingestion (g/g-day)	Inhalation (m ³ /day)
MAMMALS								
River Otter (<i>Lutra canadensis</i>)	12 months	0.67	7900	132	AE	AE	AE	AE
Active all year round		0.33	7900					
Muskrat (<i>Ondatra zibethicus</i>)	12 months	0.67	1350	21	AE	0.34	AE	AE
Active all year round		0.33	1350					
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	12 months	0.67	17.4	1	0.68	0.49	0.223	AE
Active all year round		0.33	17.4					
Meadow Vole (<i>Microtus pennsylvanicus</i>)	12 months	0.67	22	2.3	AE	0.325	0.21	AE
Active all year round		0.33	18					
Raccoon (<i>Procyon lotor</i>)	9 months	0.75	6400	75	AE	AE	AE	AE
Hibernate Late November to March/April		0						
Mink (<i>Mustela vison</i>)	12 months	0.67	974	8.3	AE	0.16	0.028	AE
Active all year round		0.33	974					
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	12 months	0.67	1231	42.2	AE	AE	AE	AE
Active all year round		0.33	1231					
Deer Mouse (<i>Peromyscus maniculatus</i>)	12 months	0.67	20	1.8	592	0.45	AE	AE
Active all year round		0.33	20					

^a AE=Allometric Equation

^b EP=Empirical

Receptors	Fraction of item in diet													
	Forage Fish	Piscivorous Fish	Aquatic Invertebrates	Birds	Mammals	Invertebrates Terrestrial	Worms	Vegetation Aquatic	Vegetation Terrestrial	Soil	Sediment (Lake Water)	Sediment (River Water)	Lake Water	River Water
River Otter (<i>Lutra canadensis</i>)	0.7	0.18	0.12	0	0	0	0	0	0	0	0	0	0.5	0.5
Active all year round	0.99	0	0.01	0	0	0	0	0	0	0	0	0	0	0
Muskrat (<i>Ondatra zibethicus</i>)	0	0	0	0	0	0	0	1	0	0	0	0	0.5	0.5
Active all year round	0	0	0	0	0	0	0	1	0	0	0	0	0	0
Short-Tailed Shrew (<i>Blarina brevicauda</i>)	0	0	0.037	0	0.052	0.189	0.527	0	0.171	0.024	0	0	0.5	0.5
Active all year round	0	0	0.037	0	0.052	0.189	0.527	0	0.171	0.024	0	0	0	0
Meadow Vole (<i>Microtus pennsylvanicus</i>)	0	0	0	0	0	0.015	0	0	0.985	0.024	0	0	0.5	0.5
Active all year round	0	0	0	0	0	0.01	0	0	0.99	0.024	0	0	0	0
Raccoon (<i>Procyon lotor</i>)	0	0	0.019	0.015	0.158	0.082	0.072	0	0.587	0.094	0	0	0.5	0.5
Hibernate Late November to March/April														
Mink (<i>Mustela vison</i>)	0.73	0	0.075	0.0275	0.0275	0	0	0.08	0	0	0	0	0.5	0.5
Active all year round	0.73	0	0.075	0.0275	0.0275	0	0	0.08	0	0	0	0	0	0
Eastern Cottontail (<i>Sylvilagus floridanus</i>)	0	0	0	0	0	0	0	0	1	0.062	0	0	0.5	0.5
Active all year round	0	0	0	0	0	0	0	0	1	0.062	0	0	0	0
Deer Mouse (<i>Peromyscus maniculatus</i>)	0	0	0	0	0	0.6	0	0	0.38	0.02	0	0	0.5	0.5
Active all year round						0.55	0	0	0.43	0.02	0	0	0	0

Appendix E:

Percentage Water Content Values for Select Media and Biota.

Percentage Water Content Values for Select Media and Biota.

<i>Media</i>	<i>Percentage Water Content</i>	<i>Reference</i>
Fish (general)	80%	(128)
Bony fishes	75%	(47)
Pacific herring	68%	(47)
Aquatic invertebrates (general)	83.3%	(129)
Crabs (w/shell)	74%	(47)
Isopods, amphipods	71%-80%	(47)
Cladocerans	79%-87%	(47)
Earth worms	83.3%	(129)
	84% (depurated)	(47)
Grasshoppers, crickets	69%	(47)
Beetles (adult)	61%	(47)
Terrestrial vegetation	80%	(72)
Seeds (dicots)	9.3%	(47)
Fruit (pulp, skin)	77%	(47)
Algae	84%	(47)
Aquatic macrophytes	87%	(47)
River sediments	80%	(130)

<i>Media</i>	<i>Percentage Water Content</i>	<i>Reference</i>
Lake sediments	95%	(130)
Soil	30%	(130)
Milk	87%	(72)
Beef	70%	(72)
Chicken	75%	(72)
Mammals (mice, voles, rabbits)	68%	(47)
Bird (passerine)	68%	(47)
Snakes, lizards	66%	(47)
Frogs, toads	85%	(47)

Appendix F:

Unit Conversion Factors used in MUM-Exposure and MUM-Risk.

Unit Conversion Factors used in MUM-Exposure and MUM-Risk

Variable	Equation	Explanation/ References
Lake Water River Water Volume to mass	$C_{water} \left(\frac{g}{g} \right) = \frac{g}{m^3} \cdot \frac{m^3}{1000kg} \cdot \frac{1kg}{1000g}$	
Lake Sediment Volume to mass	$C_{sed} \left(\frac{g}{g} dw \right) = \frac{g}{m^3_{ww}} \cdot \frac{m^3}{1 \times 10^6 cm^3} \cdot \frac{cm^3}{2.4g}$	
River Sediment Volume to mass	$C_{sed} \left(\frac{g}{g} dw \right) = \frac{g}{m^3_{ww}} \cdot \frac{m^3}{1 \times 10^6 cm^3} \cdot \frac{cm^3}{2.4g}$	
Soil Pore Water Volume to mass	$C_{porewater_{soil}} \left(\frac{g}{g} \right) = \frac{g}{m^3} \cdot \frac{m^3}{1000kg} \cdot \frac{1kg}{1000g}$	
Soil Volume to mass	$C_{soil} \left(\frac{g}{g} dw \right) = \frac{g}{m^3_{ww}} \cdot \frac{m^3}{1 \times 10^6 cm^3} \cdot \frac{cm^3}{2.4g}$	
Vegetation Volume to mass	$C_{vegetation_{terrestrial}} \left(\frac{g}{g} \right) = \frac{g}{m^3} \cdot \frac{m^3}{850kg} \cdot \frac{1kg}{1000g}$	

Variable	Equation	Explanation/ References
Dry weight to Wet weight	$WW = \frac{DW}{\left[\frac{(100 - WC)}{100} \right]}$	WW = wet weight DW = dry weight WC = water content
Wet weight to Dry weight	$DW = WW \cdot \left[\frac{(100 - WC)}{100} \right]$	WW = wet weight DW = dry weight WC = water content
MUM-Risk Sediment for Organics (units in ug/kg dw)	$C_{sediment} \left(\frac{ug}{kg} dw \right) = \frac{g}{m^3 ww} \cdot \frac{m^3}{1 \times 10^6 cm^3} \cdot \frac{cm^3}{2.4g} \cdot \frac{1000g}{1kg} \cdot \frac{1 \times 10^6 ug}{1g} \div CF$	
MUM-Risk Sediment for Metals (units in mg/kg dw)	$C_{sediment} \left(\frac{mg}{kg} dw \right) = \frac{g}{m^3 ww} \cdot \frac{m^3}{1 \times 10^6 cm^3} \cdot \frac{cm^3}{2.4g} \cdot \frac{1000g}{1kg} \cdot \frac{1000mg}{1g} \div CF$	
MUM-Risk Water (units in ug/L)	$C_{water\ lake} \left(\frac{ug}{L} \right) = \frac{g}{m^3} \cdot \frac{m^3}{1000L} \cdot \frac{1 \times 10^6 ug}{1g}$	
Fish BCF	$BCF = \frac{L}{kg}$ $BCF(g/g) = \frac{L}{kg} \cdot \frac{kg}{1000g} \cdot \frac{kg}{1L} \cdot \frac{1000g}{1kg}$	

Appendix G:

Allometric Equations used in MUM-Exposure

Allometric Equations used in MUM-Exposure

Variable	Equation	Explanation/References
Bird inhalation rate	$IR = (0.002002 \cdot BW^{0.77}) \cdot 3 \text{ (g)}$	IR = inhalation rate (m ³ /day) BW = Body weight (g) Lasiewski and Calder (59)
Mammal inhalation rate	$IR = (0.002173 \cdot BW^{0.80}) \cdot 3 \text{ (g)}$	IR = inhalation rate (m ³ /day) BW = Body weight (g) Stahl (78)
Total Daily Water Intake	$NIR_{water} = \frac{IR_{water} \cdot UCF_a}{BW \cdot UCF_b} \text{ (kg)}$	NIR _{water} = g contaminant/g body weight normalized-day BW = body weight (kg) IR _{water} = L/day UCF _{a(L to g)} = unit conversion factor, $UCF = \frac{1kg \cdot 1000g}{1L \cdot 1kg}$ UCF _{b(kg to g)} = unit conversion factor, $UCF = \frac{1000g}{1kg}$
Bird drinking water intake rate	$IR_{water} = 0.059 \cdot BW^{0.67} \text{ (L / day)}$	Based on 21 species, Calder and Braun (61) BW = body weight (kg)
Mammals drinking water intake rate	$IR_{water} = 0.099 \cdot BW^{0.90} \text{ (L / day)}$	Calder and Braun (61) BW = body weight (kg)
All bird food intake rate	$IR_{food} = 0.648BW^{0.651}$	Nagy (52) (g dw/g ww day)
Passerine birds food intake rate	$IR_{food} = 0.398 \cdot BW^{0.850}$	Nagy (52) (g dw/g ww day)
Non-Passerine birds food intake rate	$IR_{food} = 0.301 \cdot BW^{0.751}$	Nagy (52) (g dw/g ww day)
All mammals food intake rate	$IR_{food} = 0.235 \cdot BW^{0.822}$	Nagy (52) (g dw/g ww day)

Variable	Equation	Explanation/References
Rodents food intake rate	$IR_{food} = 0.621 \cdot BW^{0.564}$	Nagy (52) (g dw/g ww day)
Herbivores & Non-Herbivores food intake rate	$IR_{food} = 0.577 \cdot BW^{0.727}$	Nagy (52) (g dw/g ww day)
All birds Free-living metabolic rate	$NFMR = \frac{3.12 \cdot BW^{0.605}}{BW}$	(52)
Passerine birds Free-living metabolic rate	$NFMR = \frac{2.123 \cdot BW^{0.749}}{BW}$	(52)
Non-passerine birds Free-living metabolic rate	$NFMR = \frac{1.146 \cdot BW^{0.749}}{BW}$	(52)
All mammals Free-living metabolic rate	$NFMR = \frac{0.8 \cdot BW^{0.813}}{BW}$	(52)
Rodent Free-living metabolic rate	$NFMR = \frac{2.514 \cdot BW^{0.507}}{BW}$	(52)
Non-herbivore mammal Free-living metabolic rate	$NFMR = \frac{0.6167 \cdot BW^{0.862}}{BW}$	(52)
Herbivore mammal Free-living metabolic rate	$NFMR = \frac{1.419 \cdot BW^{0.727}}{BW}$	(52)

Appendix H:

Estimated Soil/Sediment proportion (%) in select species' diets.

Estimated Soil/Sediment proportion (%) in select species' diets.

Species	Estimated Percent Soil in Diet (dry weight)	References
Canada Goose (representative herbivorous geese, feeding on open fields)	8.2	(63)
Mallard (representative surface feeding or dabbling duck, mostly herbivorous, although sometimes consuming aquatic invertebrates)	2	(63)
American widgeon (dabbling duck, feeding on stems and leaves)	3	(131)
Green-winged teal (dabbling duck, feeding on seeds)	1	(131)
Northern pintail (dabbling duck, feeding on seeds)	1	(131)
American black duck (dabbling duck, feeding on seeds)	1	(131)
Wood duck (herbivorous and insectivorous)	11	(63)
Blue-winged teal	2	(63)
Ring-necked duck (representative bay (diving) duck: omnivorous, primarily invertebrates, snails, clams, insects)	2	(63)
American woodcock (representative of woodcock and snipe, primarily soil invertebrate diet)	10.4	(63)
Semipalmated sandpiper (probe mud or soil for invertebrates)	30	(63)
Western sandpiper	18	(63)
Stilt Sandpiper	17	(63)
Least sandpiper	7.3	(63)

Species	Estimated Percent Soil in Diet (dry weight)	References
Cattle (terrestrial herbivore mammal)	2.9 Geometric mean of 12 sampling periods from two studies.	(132), (133)
Pronghorn (terrestrial herbivore)	5.4	(134)
Mule deer (terrestrial herbivore)	2.1 Spring value; ranged between 2.1 spring to 0.6 summer.	(64)
Red fox (terrestrial carnivore/omnivore)	2.8	(63)
Raccoon (terrestrial omnivore)	9.4	(63)
White-footed mouse (representative of deer and white-footed mouse; primarily granivorous/omnivorous)	2	(63)
Meadow vole (representative of burrowing herbivore rodent)	2.4	(63)
Black-tailed prairie dog	7.7	(63)
White-tailed prairie dog	2.7	(63)
White-tailed deer	2	(63)
Bison	6.8	(63)
Elk	2	(63)
Moose	2	(63)
Jackrabbit (terrestrial grazing herbivore)	6.3	(134)
Hispid Cotton Rats (herbivorous rodent)	2.8	(134)

Appendix I:

Assimilative Efficiencies for Consumer/Prey Relationships (as cited in (47)).

Assimilative Efficiencies for Consumer/Prey Relationships (as cited in (47)).

Consumer	Food item	Assimilative Efficiency (AE)
Birds		
Birds of prey	birds, small mammals	0.78
Eagles, seabirds	fish	0.79
Waterfowl	aquatic invertebrates	0.77
Birds	terrestrial insects	0.72
Birds ^a	terrestrial plants	0.49
Waterfowl ^b	aquatic plants	0.39
Mammals		
Mammals	small birds, mammals	0.84
Mammals	fish	0.91
Small mammals	insects	0.87
Small mammals ^c	terrestrial vegetation	0.69

a Average calculated from 7 studies (wild seeds, cultivated seeds, fruit pulp, skin, seeds, grasses, leaves, stems, twigs, pine needles)

b Average calculated from 3 studies (emergents, aquatic vegetation and bulbs, rhizomes)

c Average calculated from 4 studies (voles, mice; lemmings, voles; rabbits, voles, mice; rabbits, voles, rats)

Appendix J:

Gross Energy for prey species (as reported in (47)) and the derived arithmetic means for food items categories used in MUM-Exposure

Gross Energy for prey species (as reported in (47)) and the derived arithmetic means for food items categories used in MUM-Exposure.

Food Item	Gross Energy of Food Source (GE) kcal/g wet weight
Bivalves (without shell)	0.8
Crabs (with shell)	1
Shrimp	1.1
Isopods, amphipods	1.1
Cladocerans	0.74
Aquatic invertebrates Average	0.95
Bony fishes	1.2
Pacific herring	2
Fish Average	1.6
Aquatic Vegetation Average	0.51
Earthworms	0.78
Grasshoppers, crickets	1.7
Beetles (adult)	1.5
Terrestrial Invertebrates Average	1.3
Mammals average (mice, voles, rabbits)	1.7
Passerines with typical fat reserves	1.9
Mallard (flesh only)	2
Gulls, terns	1.9
Birds Average	1.9
Young grasses	1.3
fruit (pulp, skin)	1.1
Terrestrial Vegetation Average	1.2

Appendix K:

Food Chain Multipliers (87) used to calculate BAFs.

Food Chain Multipliers (87) used to calculate BAFs.

Log K_{ow}	Forage Fish	Piscivorous Fish	Log K_{ow}	Forage Fish	Piscivorous Fish
4.0	1.253	1.072	6.6	13.980	25.645
4.1	1.315	1.096	6.7	14.223	26.363
4.2	1.380	1.130	6.8	14.355	26.669
4.3	1.491	1.178	6.9	14.388	26.669
4.4	1.614	1.242	7.0	14.305	26.242
4.5	1.766	1.334	7.1	14.142	25.468
4.6	1.950	1.459	7.2	13.852	24.322
4.7	2.175	1.633	7.3	13.474	22.856
4.8	2.452	1.871	7.4	12.987	21.038
4.9	2.780	2.193	7.5	12.517	18.967
5.0	3.181	2.612	7.6	11.708	16.749
5.1	3.643	3.162	7.7	10.914	14.388
5.2	4.188	3.873	7.8	10.069	12.050
5.3	4.803	4.742	7.9	9.162	9.840
5.4	5.502	5.821	8.0	8.222	7.798
5.5	6.266	7.079	8.1	7.278	6.012
5.6	7.096	8.551	8.2	6.361	4.519
5.7	7.962	10.209	8.3	5.489	3.311
5.8	8.841	12.050	8.4	4.683	2.371
5.9	9.716	13.964	8.5	3.949	1.663
6.0	10.556	15.996	8.6	3.296	1.146
6.1	11.337	17.783	8.7	2.732	0.778
6.2	12.064	19.907	8.8	2.246	0.521
6.3	12.691	21.677	8.9	1.837	0.345
6.4	13.228	23.281	9.0	1.493	0.226
6.5	13.662	24.604			

Appendix L:

Worm uptake models (81) used in MUM-Exposure.

Worm uptake models (81)used in MUM-Exposure

Analyte	Model	Reference
As	$\ln C_{earthworm} = -0.185 + 0.993 \ln C_{soil} - 0.291(pH)$	(81)
Cd	$\log C_{earthworm} = 0.66 \log C_{soil} + 1.21$	(135)
Cu	$\ln C_{earthworm} = 1.675 + 0.264 \ln C_{soil}$	(81)
Hg	$\ln C_{earthworm} = 0.0781 + 0.3369 \ln C_{soil}$	(81)
Mn	$\ln C_{earthworm} = -0.809 + 0.682 \ln C_{soil}$	(81)
Pb	$\ln C_{earthworm} = -0.218 + 0.807 \ln C_{soil}$	(81)
Se	$\ln C_{earthworm} = -0.075 + 0.0.733 \ln C_{soil}$	(81)
Zn	$\ln C_{earthworm} = 4.449 + 0.328 \ln C_{soil}$	(81)

Appendix M:

Oral toxicological benchmarks (mg/kg-day) developed based on (106) and (107).

Oral toxicological benchmarks (mg/kg-day) developed based on (106)and (107).

Wildlife	B[a]P	Cd
Great Blue Heron	7.7 X10 ⁻²	24.0
Robin	4.0 X10 ⁻²	12.3
Mallard	6.8 X10 ⁻²	21.2
Red Fox	7.5	7.5
Prairie Deer Mouse	10.2	10.3
Eastern cottontail	8.0	8.0
Mink	8.1	8.2

e.g. Derivation of Great Blue Heron Oral toxicological benchmark for Cadmium (mg/kg-day)

$$DD_{ts} = Dose \cdot IR_{food}$$

$$DD_{ts} \left(\frac{g_{cont}}{g_{bw} \cdot day} \right) = 0.00021 \left(\frac{g_{cont}}{g_{food}} \right) \cdot 0.1 \left(\frac{g_{food}}{g_{bw} \cdot day} \right)$$

$$DD_{ts} = 0.000021$$

$$BM_{gbh} = DD_{ts} \cdot \left(\frac{BW_{ts}}{BW_{gbh}} \right)^{sf} \cdot \frac{1000g}{1kg} \cdot \frac{1000mg}{1g}$$

$$BM_{gbh} \left(\frac{mg_{cont}}{kg_{bw} \cdot day} \right) = 0.000021 \left(\frac{g_{cont}}{g_{bw} \cdot day} \right) \cdot \left(\frac{1153g}{2230g} \right)^{-0.2} \cdot \frac{1000g}{1kg} \cdot \frac{1000mg}{1g}$$

$$BM_{gbh} = 24.0 \left(\frac{mg_{cont}}{kg_{bw} \cdot day} \right)$$

where DD_{ts} is daily dose for the test species (g-cont/g-bw-day), Dose is experimental dose expressed as the food concentration (g-cont/g-food), IR_{food} is Daily Food Intake Rate for the test species normalized to body weight (g-food/g-bw-day), BM_{gbh} is the toxicological benchmark for great blue heron (mg-contaminant/kg-bw-day), BW is body weight for the test species or the great blue heron (g-bw), and sf is a scaling factor (dimensionless).