EPA

United States
Environmental Protection
Agency

Industrial Waste Air Model Technical Background Document

Solid Waste and
Emergency Response
(5306W)

EPA 530-R-02-010
August 2002
www.epa.gov/industrialwaste

February 2002

Industrial Waste Air Model Technical Background Document

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Washington, DC 20460

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Acronyms and Abbreviations

ADI	Acceptable daily intake
ATSDR	Agency for Toxic Substances and Disease Registry
CAA	Clean Air Act
CAG	Carcinogen Assessment Group
CalEPA	California Environmental Protection Agency
CAS	Chemical Abstract Service
CSF	Cancer slope factor
CSTR	Continuously stirred tank reactor
EFH	*Exposure Factors Handbook*
EPA	(U.S.) Environmental Protection Agency
FR	Federal Register
HAD	Health Assessment Documents
HEA	Health Effects Assessment
HEAST	Health Effects Assessment Summary Tables
HEED	Health and Environmental Effects Document
HEEP	Health Environmental Effects Profile
HQ	Hazard quotient
HSDB	Hazardous Substance Databank
IRIS	Integrated Risk Information System
ISCST3	Industrial Source Complex, Short-Term Model, Version 3
ISMCS	International Station Meteorological Climate Summary
IWAIR	Industrial Waste Air Model
LOAEL	Lowest-observed-adverse-effect level
MLVSS	Mixed-liquor volatile suspended solids
MRL	Minimum risk level
NCEA	National Center for Environmental Assessment
NESHAP	National Emission Standards for Hazardous Air Pollutants
NOAEL	No-observed-adverse-effects level
OAQPS	Office of Air Quality Planning and Standards
ORD	Office of Research and Development
OSW	Office of Solid Waste
OW	Office of Water
RCRA	Resource Conservation and Recovery Act
REL	Reference exposure level
RfC	Reference concentration
RfD	Reference dose
SCDM	Superfund Chemical Data Matrix
SAB	Science Advisory Board
SIS	Surface Impoundment Study
SSL	Soil Screening Levels
TRI	Toxics Release Inventory
TSDF	Treatment Storage and Disposal Facility
TSS	Total suspended solids

Acronyms and Abbreviations (continued)

URF	Unit risk factor
WHO	World Health Organization
WMU	Waste management unit

1.0 Introduction

This document provides technical background information on the Industrial Waste Air (IWAIR) model. This document is a companion document to the *IWAIR User's Guide*, which provides detailed information on how to install and use the model.

1.1 Guide for Industrial Waste Management and IWAIR

The U.S. Environmental Protection Agency (EPA) and representatives from 12 state environmental agencies developed a voluntary *Guide for Industrial Waste Management* (hereafter, the *Guide*) to recommend a baseline of protective design and operating practices to manage nonhazardous industrial waste throughout the country. The guidance is designed for facility managers, regulatory agency staff, and the public, and it reflects four underlying objectives:

- Adopt a multimedia approach to protect human health and the environment.
- Tailor management practices to risk in the enormously diverse universe of waste, using the innovative, user-friendly modeling tools provided in the *Guide*.
- Reaffirm state and tribal leadership in ensuring protective industrial waste management, and use the *Guide* to complement state and tribal programs.
- Foster partnerships among facility managers, the public, and regulatory agencies.

The *Guide* recommends best management practices and key factors to consider to protect groundwater, surface water, and ambient air quality in siting, operating, and designing waste management units (WMUs); monitoring WMUs' impact on the environment; determining necessary corrective action; closing WMUs; and providing postclosure care. In particular, the guidance recommends risk-based approaches to choosing liner systems and waste application rates for groundwater protection and to evaluating the need for air controls. The CD-ROM version of the *Guide* includes user-friendly air and groundwater models to conduct these risk evaluations.

Chapter 5 of the *Guide*, entitled "Protecting Air Quality," highlights several key recommendations:

- Adopt controls to minimize particulate emissions.

- Determine whether WMUs at a facility are addressed by Clean Air Act (CAA) requirements and comply with those requirements.

- If WMUs are not specifically addressed by CAA requirements, use IWAIR to assess risks associated with volatile air emissions from units.

- Implement pollution prevention programs, treatment measures, or emissions controls to reduce volatile air emission risks.

EPA developed IWAIR and this technical background document to accompany the *Guide* to assist facility managers and regulatory agency staff in evaluating inhalation risks. Workers and residents in the vicinity of a unit may be exposed to volatile chemicals from the unit in the air they breathe. Exposure to some of these chemicals at sufficient concentrations may cause a variety of cancer and noncancer health effects (such as developmental effects in a fetus or neurological effects in an adult). With a limited amount of site-specific information, IWAIR can estimate whether specific wastes or waste management practices may pose an unacceptable risk to human health.

1.2 Model Design

IWAIR is an interactive computer program with three main components: (1) an emission model to estimate release of constituents from WMUs; (2) a dispersion model to estimate fate and transport of constituents through the atmosphere and determine ambient air concentrations at specified receptor locations; and (3) a risk model to calculate either the risk to exposed individuals or waste constituent concentrations that can be protectively managed in the unit. The program requires only a limited amount of site-specific information, including facility location, WMU characteristics, waste characteristics, and receptor information. A brief description of each component follows.

1.2.1 Emission Model

The emission model uses waste characterization, WMU, and facility information to estimate emissions for 95 constituents (identified in Table 1-1) for four types of units: land application units, landfills, waste piles, and surface impoundments. Users can add chemical properties to model additional chemicals. The emission model selected for incorporation into IWAIR is EPA's CHEMDAT8 model. This model has undergone extensive review by both EPA and industry representatives and is publicly available from EPA's Web page (http://www.epa.gov/ttn/chief/software.html).

To facilitate emission modeling with CHEMDAT8, IWAIR prompts the user to provide the required waste- and unit-specific data. Once these data are entered, the model calculates and displays chemical-specific emission rates. If users decide not to develop or use the CHEMDAT8 rates, they can enter their own site-specific emission rates.

Table 1-1. Constituents Included in IWAIR

CAS Number	Compound Name	CAS Number	Compound Name
75070	Acetaldehyde	77474	Hexachlorocyclopentadiene
67641	Acetone	67721	Hexachloroethane
75058	Acetonitrile	78591	Isophorone
107028	Acrolein	7439976	Mercury*
79061	Acrylamide	67561	Methanol
79107	Acrylic acid	110496	Methoxyethanol acetate, 2-
107131	Acrylonitrile	109864	Methoxyethanol, 2-
107051	Allyl chloride	74839	Methyl bromide
62533	Aniline	74873	Methyl chloride
71432	Benzene	78933	Methyl ethyl ketone
92875	Benzidine	108101	Methyl isobutyl ketone
50328	Benzo(a)pyrene	80626	Methyl methacrylate
75274	Bromodichloromethane	1634044	Methyl tert-butyl ether
106990	Butadiene, 1,3-	56495	Methylcholanthrene, 3-
75150	Carbon disulfide	75092	Methylene chloride
56235	Carbon tetrachloride	68122	N,N-Dimethyl formamide
108907	Chlorobenzene	91203	Naphthalene
124481	Chlorodibromomethane	110543	n-Hexane
67663	Chloroform	98953	Nitrobenzene
95578	Chlorophenol, 2-	79469	Nitropropane, 2-
126998	Chloroprene	55185	N-Nitrosodiethylamine
1319773	Cresols (total)	924163	N-Nitrosodi-n-butylamine
98828	Cumene	930552	N-Nitrosopyrrolidine
108930	Cyclohexanol	95501	o-Dichlorobenzene
96128	Dibromo-3-chloropropane, 1,2-	95534	o-Toluidine
75718	Dichlorodifluoromethane	106467	p-Dichlorobenzene
107062	Dichloroethane, 1,2-	108952	Phenol
75354	Dichloroethylene, 1,1-	85449	Phthalic anhydride
78875	Dichloropropane, 1,2 -	75569	Propylene oxide
10061015	Dichloropropylene, cis-1,3-	110861	Pyridine
10061026	Dichloropropylene, trans-1,3-	100425	Styrene
57976	Dimethylbenz[a]anthracene, 7,12-	1746016	TCDD, 2,3,7,8 -
95658	Dimethylphenol, 3,4-	630206	Tetrachloroethane, 1,1,1,2-
121142	Dinitrotoluene, 2,4-	79345	Tetrachloroethane, 1,1,2,2-
123911	Dioxane, 1,4-	127184	Tetrachloroethylene
122667	Diphenylhydrazine, 1,2-	108883	Toluene
106898	Epichlorohydrin	75252	Tribromomethane
106887	Epoxybutane, 1,2-	76131	Trichloro-1,2,2-trifluoroethane, 1,1,2-
111159	Ethoxyethanol acetate, 2-	120821	Trichlorobenzene, 1,2,4-
110805	Ethoxyethanol, 2-	71556	Trichloroethane, 1,1,1-
100414	Ethylbenzene	79005	Trichloroethane, 1,1,2-
106934	Ethylene dibromide	79016	Trichloroethylene
107211	Ethylene glycol	75694	Trichlorofluoromethane
75218	Ethylene oxide	121448	Triethylamine
50000	Formaldehyde	108054	Vinyl acetate
98011	Furfural	75014	Vinyl chloride
87683	Hexachloro-1,3-butadiene	1330207	Xylenes
118741	Hexachlorobenzene		

*Chemical properties for both elemental and divalent forms of mercury are included.

1.2.2 Dispersion Model

IWAIR's second modeling component estimates dispersion of volatilized constituents and determines air concentrations at specified receptor locations using default dispersion factors developed with EPA's Industrial Source Complex, Short-Term Model, version 3 (ISCST3). ISCST3 was run to calculate dispersion for a standardized unit emission rate (1 $\mu g/m^2$-s) to obtain a dispersion factor, which is measured in $\mu g/m^3$ per $\mu g/m^2$-s. The total air concentration estimates are then developed by IWAIR by multiplying the constituent-specific emission rates derived from CHEMDAT8 (or the rates the user specified) with a site-specific dispersion factor. Running ISCST3 to develop a new dispersion factor for each location/WMU is time consuming and requires extensive meteorological data and technical expertise. Therefore, IWAIR incorporates default dispersion factors developed using ISCST3 for many separate scenarios designed to cover a broad range of unit characteristics, including

- 60 meteorological stations, chosen to represent the different climatic and geographical regions of the contiguous 48 states, Hawaii, Puerto Rico, and parts of Alaska;

- 4 unit types;

- 17 surface areas for landfills, land application units, and surface impoundments, and 11 surface areas and 7 heights for waste piles;

- 6 receptor distances from the unit (25, 50, 75, 150, 500, 1,000 meters);

- 16 directions in relation to the edge of the unit (only the one resulting in the maximum air concentration is used).

The default dispersion factors were derived by modeling each of these scenarios, then choosing as the default the maximum dispersion factor of the 16 directions for each WMU/surface area/height/meteorological station/receptor distance combination.

Based on the size and location of a unit specified by the user, IWAIR selects an appropriate dispersion factor from the default dispersion factors in the model. If the user specifies a unit surface area or height that falls between two of the sizes already modeled, IWAIR uses an interpolation method to estimate a dispersion factor based on the two closest modeled unit sizes.

Alternatively, a user may enter a site-specific dispersion factor developed by conducting independent modeling with ISCST3 or with a different model and proceed to the next step, the risk calculation.

1.2.3 Risk Model

The third component combines the constituent's air concentration with receptor exposure factors and toxicity benchmarks to calculate either the risk from concentrations managed in the unit or the waste concentration (C_{waste}) in the unit that must not be exceeded to protect human health. In calculating either estimate, the model applies default values for exposure factors, including inhalation rate, body weight, exposure duration, and exposure frequency. These default values are based on data presented in EPA's *Exposure Factors Handbook* (U.S. EPA, 1997a) and represent average exposure conditions. IWAIR contains standard health benchmarks (cancer slope factors [CSFs] for carcinogens and reference concentrations [RfCs] for noncarcinogens) for 94 of the 95 constituents included in IWAIR.[1] These health benchmarks are obtained primarily from the Integrated Risk Information System (IRIS) and the Health Effects Assessment Summary Tables (HEAST) (U.S. EPA, 1997b, 2001a). IWAIR uses these data either to estimate risk or hazard quotients (HQs) or to estimate allowable waste concentrations. Users may override the IWAIR health benchmarks with their own values.

IWAIR only addresses risk from direct inhalation of vapor-phase emissions. Appendix A discusses the potential for risks attributable to indirect exposures.

1.3 About This Document

The remainder of this background document is organized as follows:

- Section 2, *Source Emission Estimates Using CHEMDAT8,* describes the CHEMDAT8 model used to calculate emissions.
- Section 3, *Development of Dispersion Factors Using ISCST3*, describes how dispersion factors were developed using ISCST3 and how these are used in the model.
- Section 4, *Exposure Factors,* describes the exposure factors used in the model.
- Section 5, *Inhalation Health Benchmarks,* describes the health benchmarks used in the model.
- Section 6, *Calculation of Risk or Allowable Waste Concentration*, describes the risk calculation and the allowable waste calculation.
- Section 7, *References*, lists all references cited in this document.
- Appendix A, *Considering Risks from Indirect Pathways*, describes the types of pathways by which an individual may be exposed to a constituent, explains which pathways are accounted for in IWAIR, and discusses exposures unaccounted for in IWAIR.

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[1] At the time IWAIR was released, no accepted health benchmark was available for 3,4-dimethylphenol from the hierarchy of sources used to populate the IWAIR health benchmark database, nor were data available from these sources to allow the development of a health benchmark with any confidence. In addition, IWAIR contains chemical properties for both elemental and divalent forms of mercury, but contains a health benchmark only for elemental mercury; no accepted benchmark was available for divalent mercury.

- Appendix B, *Physical-Chemical Properties for Chemicals Included in IWAIR*, presents the physical-chemical property values included in IWAIR and the sources of those values.

- Appendix C, *Sensitivity Analysis of the ISCST3 Air Dispersion Model*, describes the sensitivity analysis performed on depletion options, source shape and orientation, and receptor location and spacing.

- Appendix D, *Selection of Meteorological Stations*, discusses the approach used for selecting meteorological stations used in IWAIR and describes the region represented by each station.

2.0 Source Emission Estimates Using CHEMDAT8

This section describes the CHEMDAT8 emission model used to develop emission estimates for each WMU. Section 2.1 describes why CHEMDAT8 was chosen and provides an overview of CHEMDAT8; Section 2.2 provides scientific background on emissions modeling for aqueous- versus organic-phase wastes; Section 2.3 describes the input parameters; and Section 2.4 describes the important modeling assumptions and equations used to calculate mass emission rates.

2.1 Model Selection and Overview of CHEMDAT8

EPA's CHEMDAT8 model was selected as the model to estimate volatile emission rates from the WMUs in IWAIR. CHEMDAT8 meets the goals that were established during the model selection process. EPA sought to select a model that

- Provides emission estimates that are as accurate as possible without underestimating the constituent emissions
- Provides a relatively consistent modeling approach (in terms of model complexity and conservatism) for each of the different emission sources under consideration
- Has undergone extensive peer review and is widely accepted by both EPA and industry
- Is publicly available for use in more site-specific evaluations.

The CHEMDAT8 model was originally developed in projects funded by EPA's Office of Research and Development (ORD) and Office of Air Quality Planning and Standards (OAQPS) to support National Emission Standards for Hazardous Air Pollutants (NESHAPs) from sources such as tanks, surface impoundments, landfills, waste piles, and land application units for a variety of industry categories, including chemical manufacturers, pulp and paper manufacturing, and petroleum refining. CHEMDAT8 includes analytical models for estimating volatile compound emissions from treatment, storage, and disposal facility processes under user-specified input parameters and has been used to support the emissions standards for hazardous waste treatment, storage, and disposal facilities (U.S. EPA, 1991) regulated under Subpart CC rules of the Resource Conservation and Recovery Act (RCRA), as amended in 1984. The CHEMDAT8 model is publicly available and has undergone extensive review by both EPA and industry representatives.

CHEMDAT8 models volatile air emissions and considers most of the significant competing removal pathways that might limit those emissions (see text box). These competing removal pathways lower the potential for emission to the air as gases in various ways: adsorption limits the mass of chemical free to volatilize by binding chemical on the waste particles; biodegradation and hydrolysis reduce the mass of the chemical in the unit (although these mechanisms do generate new chemicals in the form of breakdown products); and leaching and runoff remove chemical mass from the unit by non-air pathways (i.e., to groundwater or surface water).

Competing Removal Pathways

Adsorption is the tendency of a chemical or liquid medium to attach or bind to the surface of particles in the waste.

Biodegradation is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by organisms in the waste or soil.

Hydrolysis is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by reaction with water in the waste or soil.

Leaching is the tendency of a chemical to dissolve in water in the waste or soil and follow the flow of water (e.g., due to rainfall) down through the soil to groundwater.

Runoff is the tendency of a chemical to dissolve in water in the waste or soil and follow the flow of water (e.g., due to rainfall) downhill to surface water.

For surface impoundments, CHEMDAT8 considers adsorption, biodegradation, and hydrolysis. For land application units, landfills, and waste piles, CHEMDAT8 considers biodegradation; CHEMDAT8 does not explicitly consider adsorption for these unit types, but volatilization from these unit types is limited by the relative air porosity of the soil or waste matrix. CHEMDAT8 does not consider hydrolysis in the land application unit, landfill, and waste pile, even for soil moisture or percolating rainwater. CHEMDAT8 does not consider leaching or runoff for any of the unit types, nor does it model chemical breakdown products from biodegradation or hydrolysis. As such, CHEMDAT8 is considered to provide reasonable to slightly high (environmentally conservative) estimates of air emissions from the various emission sources modeled in IWAIR.

EPA's CHEMDAT8 model is a modular component of IWAIR. The original CHEMDAT8 Lotus 1-2-3 spreadsheet was converted to Visual Basic code for use in IWAIR. In addition, the chemical-specific data in the original code were evaluated for accuracy. Some of these values have been changed to reflect newer or better information. A list of the physical-chemical property values included in IWAIR is provided in Appendix B of this document. Extensive testing was performed to ensure that the coded version produces results identical to the spreadsheet version.

This document provides information about CHEMDAT8 that is pertinent to the IWAIR program, including the CHEMDAT8 equations used in IWAIR. However, it does not attempt to reproduce the CHEMDAT8 documentation, so the equations are presented, but their derivation is not covered in any detail. For complete documentation on the CHEMDAT8 model, refer to documents available on EPA's Web page. The CHEMDAT8 spreadsheet model and model documentation may be downloaded at no charge from EPA's Web page (http://www.epa.gov/ttn/chief/software.html).

2.2 Scientific Background

A WMU contains solids, liquids (such as water), and air. Individual chemical molecules are constantly moving from one of these media to another: they may be adsorbed to solids, dissolved in liquids, or assume vapor form in air. At equilibrium, the movement into and out of each medium is equal, so that the concentration of the chemical in each medium is constant. The emissions model used in IWAIR, CHEMDAT8, assumes that equilibrium has been reached.

Partitioning refers to how a chemical tends to distribute itself among these different media. Different chemicals have differing affinities for particular phases—some chemicals tend to partition preferentially to air, while others tend to partition preferentially to water. The different tendencies of different chemicals are described by partition coefficients or equilibrium constants.

Of particular interest in modeling volatile emissions of a chemical from a liquid waste matrix is the chemical's tendency to change from a liquid form to a vapor form. As a general rule, a chemical's vapor pressure describes this tendency. The pure-component vapor pressure is a measure of this tendency for the pure chemical. A chemical in solution in another liquid (such as a waste containing multiple chemicals) will exhibit a partial vapor pressure, which is the chemical's share of the overall vapor pressure of the mixture; this partial vapor pressure is lower than the pure-component vapor pressure and is generally equal to the pure-component vapor pressure times the constituent's mole fraction (a measure of concentration reflecting the number of molecules of the chemical per unit of volume) in the solution. This general rule is known as Raoult's law.

Most chemicals do not obey Raoult's law in dilute (i.e., low concentration) aqueous solutions, but exhibit a greater tendency to partition to the vapor phase from dilute solutions than would be predicted by Raoult's law. These chemicals exhibit a higher partial vapor pressure than the direct mole fraction described above would predict.[1] This altered tendency to partition to the vapor phase in dilute solutions is referred to as Henry's law. To calculate the emissions of a constituent from a dilute solution, a partition coefficient called Henry's law constant is used. Henry's law constant relates the partial vapor pressure to the concentration in the solution.

To account for these differences in the tendency of chemicals to partition to vapor phase from different types of liquid waste matrices, CHEMDAT8 models emissions in two regimes: a dilute aqueous phase, modeled using Henry's law constant as the partition coefficient, and an organic phase, modeled using the partial vapor pressure predicted by Raoult's law as the partition coefficient. In fact, there is not a clear point at which wastes shift from dilute aqueous phase to organic phase; this is a model simplification. However, several rules of thumb are used to determine when the Raoult's law model would be more appropriate. The clearest rule is that any chemical present in excess of its solubility limit in a wastewater or its saturation concentration in soil has exceeded the bounds of "dilute aqueous" and is more appropriately modeled using

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[1] There are some exceptions to this behavior in dilute solutions. A notable exception is formaldehyde, which has lower activity in dilute aqueous solution, which means that formaldehyde will have greater emissions in a high-concentration organic-phase waste.

Raoult's law. Chemicals exceeding solubility or saturation limits will typically come out of solution and behave more like pure, organic-phase component. However, solubility and saturation limits can vary depending on site-specific parameters, such as temperature and pH of the waste. In addition, waste matrix effects[2] can cause chemicals to remain in solution at concentrations above their typical solubility or saturation limit. This scenario (an aqueous-phase waste with concentrations above typical solubility or saturation limits) is also best modeled using Raoult's law. Another rule of thumb is that a waste with a total organics concentration in excess of about 10 percent (or 100,000 ppm) is likely to behave more like an organic-phase waste than a dilute aqueous-phase waste and be more appropriately modeled using Raoult's law.

Aqueous-phase waste: a waste that is predominantly water, with low concentrations of organics. All chemicals remain in solution in the waste and are usually present at concentrations below typical solubility or saturation limits. However, it is possible for the specific components of the waste to raise the effective solubility or saturation level for a chemical, allowing it to remain in solution at concentrations above the typical solubility or saturation limit.

Organic-phase waste: a waste that is predominantly organic chemicals, with a high concentration of organics. Concentrations of some chemicals may exceed solubility or saturation limits, causing those chemicals to come out of solution and form areas of free product in the WMU. In surface impoundments, this can result in a thin organic film over the entire surface.

For land application units, landfills, and waste piles, where the waste is either a solid or mixed with a solid (such as soil), the CHEMDAT8 emissions model considers two-phase partitioning of the waste into the liquid (either aqueous or organic) phase and the air phase, using the partition coefficients described above, to estimate the equilibrium vapor composition in the pore (or air) space within the WMU. Emissions are subsequently estimated from the WMU by calculating the rate of diffusion of the vapor-phase constituent through the porous waste/soil medium.

For surface impoundments, where the waste is a liquid, the model uses a different approach that considers the resistance to mass transfer (i.e., movement of chemical mass from one phase to the other) in the liquid and gas phases at the surface of the impoundment. Emissions are calculated using an overall mass transfer coefficient, which is based on the partition coefficient (as described above), the liquid-phase mass transfer factor (which accounts for resistence to transfer in the liquid phase), and the gas-phase mass transfer factor (which accounts for resistence to transfer in the gas phase). This is referred to as the two-film model. For organic-phase wastes, the mass transfer is dominated by the gas-phase resistance and the partition coefficient; the liquid-phase mass transfer resistance is negligible and is, therefore, omitted from the calculation. This is referred to as the one-film model, or the oily film model.

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[2] "Waste matrix effects" refers to the effect that the composition of the waste has on a constituent's solubility in the waste or the tendency for the chemical to evaporate from the waste. For example, hexane has a solubility in distilled water of approximately 12 mg/L; however, its solubility in methanol is much higher (more than 100,000 mg/L) (Perry and Green, 1984). Therefore, it is likely that hexane will remain dissolved in a solution of 10 percent methanol in water at higher concentrations than the aqueous solubility limit of 12 mg/L suggests.

In the two-film model for surface impoundments, the gas-phase and liquid mass transfer coefficients are strongly affected by the turbulence of the surface impoundment's surface. Turbulence may be caused by mechanical aeration or, to a lesser extent, diffused air aeration. Therefore, whether the impoundment is aerated or not and how it is aerated are important inputs.

2.3 Emission Model Input Parameters

To model emissions using CHEMDAT8, users enter unit-specific data. Most of the inputs are used by CHEMDAT8 directly, but some are used to calculate other inputs for CHEMDAT8. The IWAIR program provides default input data for some parameters. For example, the annual average temperature and wind speed for a WMU site are automatically used as a default for a site once the site is assigned to one of the 60 meteorological stations in the IWAIR program. Users may choose to override the default data and enter their own estimates for these parameters. Thus, emissions can be modeled using CHEMDAT8 with a very limited amount of site-specific information by using the default data provided.

This section discusses the various parameters that have a significant impact on the estimated emission rates. Inputs that influence these rates include

- Input parameters specific to the physical and chemical properties of the constituent being modeled
- The characteristics of the waste material being managed
- Input parameters specific to the process and operating conditions of the WMU being modeled
- Meteorological parameters.

IWAIR checks inputs only against the limits of the model or absolute physical limits (e.g., area must be greater than zero). It does not verify that user-provided inputs are within some "typical" or "acceptable" range. However, Appendix B of the *IWAIR User's Guide* provides guidance for developing values for all input parameters.

A general discussion of the physical and chemical properties of the constituents is provided in the Section 2.3.1. Critical input parameters for the remaining sets of inputs are discussed for land application units, landfills, and waste piles in Section 2.3.2 and for surface impoundments in Section 2.3.3. The input parameters used in IWAIR differ in some respects from those needed by CHEMDAT8. When the CHEMDAT8 inputs are not readily available but can be calculated from more readily available data, IWAIR uses the more readily available input parameters. The equations used to convert these to the CHEMDAT8 inputs are documented in Section 2.4. For detailed guidance on developing input values for all parameters needed to run IWAIR, see Appendix B, "Parameter Guidance," of the *IWAIR User's Guide*.

2.3.1 Chemical-Specific Input Parameters

Chemical-specific input parameters are those parameters that relate to the physical or chemical properties of each individual chemical. The values of these parameters are different for each of the 95 chemicals included in IWAIR. Table 2-1 lists the chemical-specific input parameters needed to run IWAIR, along with minimum and maximum values, if any (a blank in the maximum column indicates that no maximum value is enforced). IWAIR comes with chemical data for 95 chemicals in its chemical properties database. Using the ADD/MODIFY CHEMICALS feature, the user can create additional entries in the chemical properties database to reflect different property values for organic chemicals included in IWAIR or to add new organic chemicals not included in IWAIR. To maintain the integrity of the original chemical data included with IWAIR, those entries cannot be edited directly; however, they may be used as the basis for new entries. Mercury is included in the IWAIR database in both divalent and elemental forms, but because of code modifications needed for mercury (to reflect differences in its behavior, since it is not an organic chemical), the user may not create additional or modified entries for mercury.

Organic Chemicals

The IWAIR model covers only organic chemicals, with the exception of mercury. Organic chemicals are those pertaining to or derived from living organisms. All organic chemicals contain carbon and most also contain hydrogen, although there are some substituted carbon compounds that do not contain hydrogen but are generally considered to be organics (e.g., carbon tetrachloride). However, elemental carbon and certain other carbon-containing compounds (e.g., carbon dioxide) are considered inorganic compounds.

Key chemical-specific input parameters that have a significant impact on modeled emissions include air-liquid equilibrium partition coefficients (vapor pressure or Henry’s law constant), liquid-solid equilibrium partition coefficients (log octanol-water partition coefficient for organics), biodegradation rate constants, and liquid and air diffusivities.

The primary data sources for the physical and chemical properties for the constituents included in IWAIR include

- EPA’s Superfund Chemical Data Matrix (SCDM) (U.S. EPA, 1997d),
- The Merck Index (Budavari, 1996),
- The National Library of Medicine’s Hazardous Substances Databank (HSDB), available on TOXNET (U.S. NLM, 2001),
- Syracuse Research Corporation’s CHEMFATE database (SRC, 1999)
- CambridgeSoft.com’s ChemFinder database (CambridgeSoft, 2001),
- EPA’s *Mercury Report to Congress* (U.S. EPA, 1997c), and
- EPA’s *Dioxin Reassessment* (U.S. EPA, 2000).

Table 2-1. Chemical-Specific Inputs

Parameter	Minimum Value	Maximum Value[a]	Comments
Chemical name			Cannot be left blank; maximum length is 60 characters
CAS number			Cannot be left blank; must be numeric; maximum length is 9 numbers
Molecular weight (g/mol)	1		
Density (g/cm^3)	>0		
Vapor pressure (mm Hg)	>0		
Henry's law constant (atm - m^3/mol)	>0		
Solubility (mg/L)	>0	1,000,000	
Diffusivity in water (cm^2/s)	>0		
Diffusivity in air (cm^2/s)	0		
Log K_{ow}	-10	10	
K_1 (L/g-h)	0		User-entered values of zero are changed to 1E−6 to prevent division by zero in IWAIR.
K_{max} (mg VO/g-h)	0		User-entered values of zero are changed to 1E−4 to prevent division by zero in IWAIR.
Soil biodegradation rate (s^{-1})	0		User-entered values of zero are changed to 1E−20 to prevent division by zero in IWAIR.
Hydrolysis constant (s^{-1})	0		
Antoine's constant A	0		
Antoine's constant B	0		
Antoine's constant C	None		
Soil saturation concentration (mg/kg)	>0		Calculated by IWAIR

[a] A blank cell indicates there is no maximum value.

These sources were used for molecular weight, density, vapor pressure, Henry's law constant, solubility, and log octanol-water partition coefficient. Liquid and air diffusivities were calculated from other properties. Antoine's coefficients (for adjusting vapor pressure to temperature) were taken from Reid et al. (1977). Soil biodegradation rate constants were taken from Howard et al. (1991). Hydrolysis rate constants were taken from Kollig (1993). Biodegradation rates for surface impoundments (K_1 and K_{max}) were taken from CHEMDAT8's chemical properties database (U.S. EPA, 1994a). The surface impoundment biodegradation rate constants in the downloaded CHEMDAT8 database file were compared with the values reported in the summary report that provided the basis for the CHEMDAT8 surface impoundment biodegradation rate values (Coburn et al., 1988). Surface impoundment biodegradation rate constants for compounds with no data were assigned biodegradation rates equal to the most similar compound in the biodegradation rate database. The specific chemical property inputs used for the emission modeling are provided in Appendix B with their chemical- and property-specific references. The following subsections briefly describe each chemical property.

Molecular Weight (g/mol). Molecular weight is used to estimate emissions. This value must be greater than or equal to 1 g/mol (the molecular weight of a single hydrogen ion).

Density (g/m^3). IWAIR uses density to determine if chemicals present in organic phase in surface impoundments are likely to float (if they are less dense than water) or sink (if they are more dense than water). Unless the value is very near 1 g/m^3 (the density of water), the model is not sensitive to variations in the value.

Vapor Pressure (mmHg). Vapor pressure and the mole fraction concentration in the liquid phase are used to calculate the constituent's partial vapor pressure. The partial vapor pressure is subsequently used as the partition coefficient for organic-phase wastes and aqueous-phase wastes with chemicals present above solubility or saturation limits. Different vapor pressures may be reported for the same chemical at different temperatures. The vapor pressures in IWAIR were chosen for temperatures as close to 25°C as possible. IWAIR corrects these to the ambient temperature (see Sections 2.4.1 and 2.4.4.1 for specific equations, and Sections 2.3.2 and 2.3.3 for a more general discussion of temperature corrections).

Henry's Law Constant (atm-m^3/mol). Henry's law constant reflects the tendency of chemicals to volatilize from dilute aqueous solutions; it is used as the partition coefficient for aqueous-phase wastes with chemicals present below solubility or saturation limits. Values can be obtained from the literature, or they can be calculated from the chemical's vapor pressure, molecular weight, and solubility using the following equation (Lyman et al., 1990):

$$H = \frac{\left(\frac{VP}{760}\right)}{\left(\left(\frac{S}{MW}\right) \times \left(\frac{1000}{1000}\right)\right)} \tag{2-1}$$

where

H = Henry's law constant (atm-m^3/mol)
VP = vapor pressure (mmHg)
S = solubility (mg/L)
MW = molecular weight (g/mol)
760 = unit conversion (mmHg/atm)
1000 = unit conversion (L/m^3)
1000 = unit conversion (mg/g).

IWAIR corrects Henry's law constant to the ambient temperature (see Sections 2.4.1 and 2.4.4.1 for specific equations, and Sections 2.3.2 and 2.3.3 for a more general discussion of temperature corrections).

Solubility (mg/L). This is the solubility of the individual chemical in water. Solubility is used for surface impoundments to identify wastes that may be supersaturated so that emissions equations may be based on the most appropriate partition coefficient (Henry's law for aqueous-phase wastes below saturation or solubility limits, and partial vapor pressure for wastes above saturation or solubility limits and organic-phase wastes).

Soil Biodegradation Rate (s^{-1}). The soil biodegradation rate is a first-order rate constant used to estimate soil biodegradation losses in land application units, landfills, and waste piles. The tendency to biodegrade in soil is often reported as half-life. Half-life is not comparable to biodegradation rate; however, the soil biodegradation rate can be calculated from the half-life as follows:

$$k_s = \frac{\ln(2)}{t_{1/2}} \qquad (2\text{-}2)$$

where

k_s = soil biodegradation rate (s^{-1})
ln(2) = natural log of 2
$t_{1/2}$ = half-life (s).

For IWAIR, the longest half-life (i.e., slowest degradation) was chosen when a range of values was reported. Observed biodegradation rates are dependent on the population of specific degrading species, microorganism acclimation, and primary versus secondary substrate utilization. In addition, there is the potential for co-metabolism and inhibition. Consequently, observed biodegradation rates for similar treatment units within the same (or similar) industry are highly variable. Order-of-magnitude variations in observed degradation rates are not unusual. This makes the development of generally applicable biodegradation rate constants a difficult task and ensures a significant level of uncertainty. As a result, users are encouraged to create new chemical entries in the IWAIR database and enter site-specific biodegradation rates if these are available.

Antoine's Constants: A, B, or C. Antoine's constants are used to adjust vapor pressure and Henry's law constant to ambient temperature.

Diffusivity in Water (cm²/s). Diffusivity in water is used to estimate emissions. Diffusivity in water can be calculated from the chemical's molecular weight and density, using the following correlation equation based on Water9 (U.S. EPA, 2001b):

$$D_w = 0.0001518 \times \left(\frac{T + 273.16}{298.16}\right) \times \left(\frac{MW}{\rho}\right)^{-0.6} \tag{2-3}$$

where

D_w = diffusivity in water (cm^2/s)
T = temperature (°C)
273.16 = unit conversion (°C to °K)
MW = molecular weight (g/mol)
ρ = density of chemical (g/cm^3).

If density is not available, diffusivity in water can be calculated using the following correlation equation based on U.S. EPA (1987b):

$$D_w = 0.00022 \times (MW)^{-\frac{2}{3}} \tag{2-4}$$

Diffusivity in Air (cm²/s). Diffusivity in air is used to estimate emissions. Diffusivity in air can be calculated from the chemical's molecular weight and density, using the following correlation equation based on Water9 (U.S. EPA, 2001b):

$$D_a = \frac{0.00229 \times (T + 273.16)^{1.5} \times \sqrt{0.034 + \left(\frac{1}{MW}\right) \times MWcor}}{\left(\left(\frac{MW}{2.5 \times \rho}\right)^{0.333} + 1.8\right)^2} \tag{2-5}$$

where

D_a = diffusivity in air (cm^2/s)
T = temperature (°C)
273.16 = unit conversion (°C to °K)
MW = molecular weight (g/mol)
ρ = density (g/cm^3)
MW_{cor} = molecular weight correlation:

$$\mathrm{MW_{cor}} = \left(1 - 0.000015 \times \mathrm{MW}^2\right) \tag{2-6}$$

If $\mathrm{MW_{cor}}$ is less than 0.4, then $\mathrm{MW_{cor}}$ is set to 0.4.

If density is not available, diffusivity is air can be calculated using the following correlation equation based on U.S. EPA (1987b):

$$\mathrm{D_a} = 1.9 \times \left(\mathrm{MW}^{-\frac{2}{3}}\right) \tag{2-7}$$

For dioxins, diffusivity in air is calculated from the molecular weight using the following equation based on EPA's *Dioxin Reassessment* (U.S. EPA, 2000):

$$\mathrm{D_a} = \left(\frac{154}{\mathrm{MW}}\right)^{0.5} \times 0.068 \tag{2-8}$$

Octanol-Water Partition Coefficient (log K_{ow}). K_{ow} is used to estimate emissions and to calculate the soil saturation concentration limit for land application units, landfills, and waste piles. Because K_{ow} can cover an extremely wide range of values, it is typically reported as the log of K_{ow}. Mercury does not have a K_{ow} because it is not an organic chemical. The soil-water partition coefficent (K_d) for mercury is used instead.

Hydrolysis Constant (s^{-1}). This value, which is used to estimate losses by hydrolysis, is the hydrolysis rate constant at neutral pH. Very few data were available on hydrolysis rates for IWAIR chemicals; therefore, only a few chemicals have them in the IWAIR database.

K_1 (L/g-h) and K_{max} (mg volatile organics/g-h). K_1 and K_{max} are used to estimate biodegradation losses in surface impoundments. IWAIR uses the CHEMDAT8 model equations for biodegradation in wastewater treatment units. These biodegradation rate equations are based on the Monod model for biodegradation (analogous to Michaelis-Menten enzyme kinetics). This biodegradation rate model is linear (first order) with constituent concentrations at low concentrations and becomes independent (zero order) at higher concentrations. Unfortunately, because of the difficulty in determining the two biodegradation rate constants (K_1 and K_{max}) needed for the Monod model, many detailed wastewater treatment source models resort to simple first-order biodegradation rate kinetics. Although inhibitory kinetics are not included in the model, by using the Monod biodegradation rate model, IWAIR provides a much better simulation of the reduced relative importance of biodegradation at high constituent concentrations than it would if it employed strictly first-order biodegradation kinetics. To include inhibitory kinetics requires a third rate constant, which is available for far fewer compounds than those used as the basis for the Monod constants.

The data sources for the biodegradation rate constants developed for the CHEMDAT8 model and used in IWAIR are fully documented in Coburn et al. (1988); a representative (although incomplete) list of the data sources includes EPA sampling at 10 different activated sludge systems and three surface impoundment units at varied industries; other full-scale sampling studies of activated sludge systems (Berglund and Whipple, 1987; Hannah et al., 1986) and surface impoundments (Demirjian et al., 1983); pilot-scale treatment studies (Petrasek, 1981; Petrasek et al., 1983; and Lesiecki et al., 1987); biodegradability flask studies (Pitter, 1976); and laboratory studies (Kincannon et al., 1982; Beltrame et al., 1980, 1982; and Beltrame, Beltrame, and Carniti, 1982). Although the biodegradation rate constants for the CHEMDAT8 model were developed in 1988, few additional data have been presented since to significantly alter these rate constants.

Biodegradation rate constants were not available for all of the IWAIR compounds. Biodegradation rate constants for compounds that did not have sufficient data were assigned the biodegradation rate constant of the most similar compound (in terms of chemical structure and biologically important functional groups) for which biodegradation rate constants could be estimated. There is some additional uncertainty for these biodegradation rate constants, but similarly structured chemicals typically have similar biodegradation rates, and the added uncertainty in the biodegradation rate constant assignments is likely not much greater than the uncertainty in the biodegradation rate constants themselves.

Soil Saturation Concentration (mg/kg). The soil saturation limit (C_{sat}) reflects the maximum concentration of a chemical that can be present in a soil matrix. C_{sat} is dependent on site-specific factors, as well as chemical properties; therefore, IWAIR calculates it from user inputs as follows:

$$C_{sat} = \frac{S}{\rho_b}(K_d \times \rho_b + \epsilon_w + H' \times \epsilon_a) \tag{2-9}$$

where

C_{sat} = soil saturation limit (mg/kg)
S = solubility (mg/L)
ρ_b = bulk density of soil/waste matrix (kg/L)
K_d = soil-water partition coefficient (L/kg), calculated as shown below for organic chemicals; this is an input for mercury
ϵ_w = water-filled porosity (unitless)
H' = dimensionless Henry's law constant (unitless = H/RT)
ϵ_a = air-filled porosity (unitless)

and

$$K_d = K_{oc} \times f_{oc} \tag{2-10}$$

where

K_{oc} = organic carbon partition coefficient (L/kg), calculated as shown below
f_{oc} = fraction organic carbon in waste (unitless).

Fraction organic carbon is set to a fixed value of 0.014. This value was derived from the median of a set of values for many (but not all) of the locations included in the IWAIR dispersion factor database. K_{oc} is calculated as follows (Hasset et al., 1980):

$$K_{oc} = 10^{(\log K_{ow} - 0.32)} \tag{2-11}$$

where

K_{ow} = octanol-water partition coefficent (L/kg).

2.3.2 Input Parameters for Land Application Units, Landfills, and Waste Piles

The input parameters for land-based units are presented in Tables 2-2 through 2-4.

Unit Design and Operating Parameters. The annual waste quantity, the frequency of constituent addition, and the dimensions of the unit influence a number of model input parameters. Because these are so critical and because the values of these parameters for a specific unit to be modeled should be readily available to the user, no default values are provided for these parameters. Operating life is also included here, although it does not affect emissions for waste piles. This value is used to cap the default exposure durations used by IWAIR for landfills and waste piles (30 years for residents and 7.2 years for workers) if the unit is not going to be operating that much longer, as closure of these unit types is assumed to end exposure. Postclosure exposure is assumed to occur for land application units; therefore, exposure duration is not capped at operating life.

Also in this category is the biodegradation toggle. This option lets the user choose whether to model biodegradation losses in the unit. This is set on by default for land application units, which are designed to biodegrade wastes, and off for landfills and waste piles, which often are not.

Waste Characterization. In order to generate an accurate estimate of a constituent's volatile emissions, a user of IWAIR must define the physical and chemical characteristics of the waste that will be managed in the WMU. In particular, the user must identify whether or not the waste is best described as a dilute mixture of chemical compounds (aqueous) or if the waste should be considered organic, containing high levels of organic compounds or a separate nonaqueous organic phase. These two different types of waste matrices influence the degree of partitioning that will occur from the waste to the air. Partitioning describes the affinity that a constituent has for one phase (for example, air) relative to another phase (for example, water) that drives the volatilization of organic chemicals. The choice of waste matrix will significantly affect the rate of emissions from the waste. See Section 2.2 for a more detailed discussion of

Table 2-2. Input Parameters for Landfills

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design and Operating Parameters				
Biodegradation toggle	none	off		
Operating life of landfill	yr	none	>0	Required input
Total area of landfill - all cells	m^2	none	81–8.09E+6	Required input
Average depth of landfill cell	m	none	>0	Required input
Total number of cells in landfill	unitless	none	≥1	Required input
Average annual quantity of waste disposed	Mg/yr	none	>0	Required input
Waste Characterization Information				
Dry bulk density of waste in landfill	g/cm^3	1.2	>0	ERG and Abt (1992)—uses a default of 1.4 g/cm^3 for waste sludge U.S. EPA (1989)—uses sludge density of 1.01 g/cm^3
Average molecular weight of organic-phase waste	g/mol	none	≥1	Required input for organic phase wastes
Total porosity of waste	volume fraction	0.50	>0–<1	U.S. EPA (1991)—input used for all active landfills Coburn et al. (1988)—default input for CHEMDAT8 landfill ERG and Abt (1992)—uses default of 0.40 Schroeder et al. (1994)—halogenated aliphatics used 0.46
Air-filled porosity of waste	volume fraction	0.25	>0–total porosity	U.S. EPA (1991)—input used for all active landfills Coburn et al. (1988)—default input for CHEMDAT8 landfill Schroeder et al. (1994)—halogenated aliphatics used range = 0.16 to 0.31

[a] Ranges are inclusive, except for parameters with ranges shown as “>0–x”, which must be greater than zero.

Table 2-3. Input Parameters for Land Application Units

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design and Operating Parameters				
Biodegradation toggle	none	on		
Operating life of land application unit	yr	none	>0	Required input
Tilling depth of land application unit	m	none	>0	Required input
Surface area of land application unit	m^2	none	81–8.09E+6	Required input
Average annual quantity of waste applied	Mg/yr	none	>0	Required input
Number of applications per year	yr^{-1}	none	≥1	Required input
Waste Characterization Information				
Dry bulk density of waste/soil mixture	g/cm^3	1.3	>0	Loehr et al. (1993)—reports density = 1.39 g/cm^3 for surface soil U.S. EPA (1992)—uses a default value of 1.4 g/cm^3 for sewage sludge/soil in land application unit Li and Voudrias (1994)—wet soil column density = 1.03 g/cm^3
Average molecular weight of organic-phase waste	g/mol	none	≥1	Required input for organic-phase wastes
Total porosity of waste/soil mixture	volume fraction	0.61	>0–<1	U.S. EPA (1991)—default input used for all model land application units Coburn et al. (1988)—default input for CHEMDAT8 land application units U.S. EPA (1992)—uses default of 0.4 Loehr et al. (1993)—reports porosity = 0.49 for surface soil Li and Voudrias (1994)—wet soil column porosity = 0.558
Air-filled porosity of waste/soil	volume fraction	0.5	>0–total porosity	U.S. EPA (1991)—default input used for all model land application units Coburn et al. (1988)—default input for CHEMDAT8 land application units

[a] Ranges are inclusive, except for parameters with ranges shown as “>0–x”, which must be greater than zero.

Table 2-4. Input Parameters for Waste Piles

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design and Operating Parameters				
Biodegradation toggle	none	off		
Operating life of waste pile	yr	none	>0	
Height of waste pile	m	none	1–10	Required input
Surface area of waste pile	m^2	none	20–1.3E+6	Required input
Average annual quantity of waste added to waste pile	Mg/yr	none	>0	Required input
Dry bulk density of waste	g/cm^3	1.4	>0	ERG and Abt (1992)—uses default of 1.4 g/cm^3 for waste sludge U.S. EPA (1991)—uses default of 1.8 g/cm^3 for waste pile Coburn et al. (1988)—uses “liquid in fixed waste” density of 1.16 g/cm^3 U.S. EPA (1989)—uses sludge density of 1.01 g/cm^3
Waste Characterization Information				
Average molecular weight of waste	g/mol	none	≥1	Required input for organic phase wastes
Total porosity of waste	volume fraction	0.5	>0–<1	U.S. EPA (1991)—input used for all model waste piles Coburn et al. (1988)—default input for CHEMDAT8 waste piles
Air-filled porosity of waste	volume fraction	0.25	>0–total porosity	U.S. EPA (1991)—input used for all model waste piles Coburn et al. (1988)—default input for CHEMDAT8 waste piles

[a] Ranges are inclusive, except for parameters with ranges shown as “>0–x”, which must be greater than zero.

waste matrices and partitioning. A general rule of thumb is that wastes that consist of 10 percent or more organics are best modeled as organic phase.

The molecular weight of the organic phase of the waste is a key input for modeling emissions from organic-phase wastes (this is the molecular weight of the bulk liquid, not the individual chemical). Higher waste molecular weights will result in higher emissions estimates. The range of molecular weights for common organic chemicals that might be found in Industrial D wastes spans an order of magnitude, from about 30 g/mol to about 300 g/mol. Therefore, setting this value as accurately as possible will produce the most accurate emissions estimates. In risk mode, no default value is provided; however, Appendix B of the *IWAIR User's Guide* provides an equation for estimating an appropriate molecular weight from the concentrations and molecular weights of the components of the waste. Because these components may include chemicals not being modeled in a particular IWAIR run, IWAIR cannot calculate this directly from user inputs and chemical properties. In allowable concentration mode, the molecular weight of the organic phase is set to the molecular weight of the individual chemical modeled, simulating emissions from pure component.

CHEMDAT8 is fairly sensitive to the total porosity and air porosity values that are used. Total porosity includes air porosity and the space occupied by oil and water within waste or soil. Total porosity is related to bulk density of the waste (which is also an input) as follows:

$$\epsilon_t = 1 - \frac{BD}{\rho_s} \tag{2-12}$$

where

ϵ_t = total porosity (unitless)
BD = bulk density (g/cm^3)
ρ_s = particle density (g/cm^3).

A typical value for ρ_s is 2.65 g/cm^3 (Mason and Berry, 1968). Default values are provided for waste bulk density, total porosity, and air-filled porosity, but the user is strongly encouraged to enter site-specific data, if available.

Meteorological Conditions. Two meteorological parameters are used as inputs to CHEMDAT8: annual average wind speed and annual average temperature. By default, IWAIR uses the annual average temperature and wind speed for the meteorological station identified as most representative for the site location. However, the user may override these with site-specific data.

The temperature is used for several calculations to adjust chemical properties that are dependent on temperature. These include the vapor-liquid equilibrium partition coefficient and the gas-phase diffusivity. The temperature correction adjustment for vapor-liquid equilibrium partition coefficient uses the Antoine's coefficients to calculate a ratio of the constituent's vapor pressure at the system temperature to the constituent's vapor pressure at 25°C. This ratio is used to adjust the vapor-liquid partition coefficient when either Raoult's law or Henry's law is used. The Henry's law coefficient is sometimes estimated by the constituent vapor pressure divided by solubility. Although it is more correct to consider the liquid-phase activity coefficient, it is more difficult to assess a temperature adjustment factor for the liquid-phase activity coefficient (or solubility) than for vapor pressure. In addition, solubility is generally less temperature-dependent than vapor pressure. There has been some progress in developing temperature-dependent correlations for Henry's law coefficients in recent years,[3] but these correlations were not readily available at the time of the development of CHEMDAT8, and they are still not currently available for the range of chemicals modeled by IWAIR. Therefore, the best approach for adjusting the Henry's law constants from input values determined at 25°C to the prevailing temperature of the WMU is to use the temperature correction factors developed for vapor pressure, which are based on Antoine's coefficients.

Wind speed is used to select the most appropriate empirical emission correlation equation in CHEMDAT8; there are several of these correlations, and each one applies to a specific range of wind speeds and unit sizes. The CHEMDAT8 model is insensitive to wind speeds for long-term emission estimates from land-based units.

2.3.3 Input Parameters for Surface Impoundments

The input parameters for surface impoundments are presented in Table 2-5.

Unit Design Data. The annual waste quantity (flow rate), the dimensions of the surface impoundment, and whether or not the impoundment is aerated are critical input parameters for impoundments. Because these are so critical and because the values of these parameters for a specific unit to be modeled should be readily available to the user, no default values are provided for these parameters. Operating life is also included here. This value is used to cap the default exposure durations used by IWAIR (30 years for residents and 7.2 years for workers) if the operating life is shorter than the relevant default exposure duration.

Also in this category is the biodegradation toggle. This option, in conjunction with the active biomass input, allows the user to determine what type of biodegradation is modeled. In biologically active surface impoundments, two processes occur: growth of biomass, which provides a growing matrix for chemical adsorption and loss through settling, and direct biodegradation of chemical constituents as the bacteria that form the biomass consume constituent mass. Direct biodegradation cannot occur if there is no active biomass. If an impoundment is biologically active, it may go through a transitional period during which there is active biomass (so adsorption and settling losses occur), but the biomass is not yet adapted to consume the specific chemicals present (so direct biodegradation is not occurring). This transitional period will usually end as the biomass acclimates and adapts to the chemicals present.

By default, biodegradation is set to |ON| for surface impoundments. This toggle controls direct biodegradation. Setting biodegradation to |OFF| turns off direct biodegradation, but does

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[3] e.g., the compilations of Sanders; see http://www.mpch-mainz.mpg.de/~sander/res/henry.html

Table 2-5. Input Parameters for Surface Impoundments

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design Data				
Biodegradation toggle	none	on		
Operating life	yr	none	>0	Required input
Depth of liquid in surface impoundment	m	none	>0	Required input
Surface area of surface impoundment	m^2	none	81–8.09E+6	Required input
Average annual flow rate	m^3/yr	none	>0	Required input
Aeration Data				
Fraction of surface area agitated	unitless	none	>0-1	Required input for aerated units
Submerged air flow rate	m^3/s	none	>0	Required input for diffused air aeration
Mechanical Aeration Information				
Oxygen transfer rate	lb O_2/h-hp	3	>0	U.S. EPA (1991)—range = 2.9 to 3.0 lb O_2/h-hp
Number of aerators	unitless	none	≥1	Required input for mechanically aerated impoundments
Total power input to all aerators	hp	none	>0.25	U.S. EPA (1991)—input for medium-sized, aerated surface impoundments - model units T02I and T02J
Power efficiency of aerators[b]	fraction	0.83	>0-1	U.S. EPA (1991)—range = 0.80 to 0.85
Aerator impeller diameter	cm	61	>0–100*$\sqrt{\text{WMU area}}$	U.S. EPA (1991)—input used for all model surface impoundments
Aerator impeller rotational speed	rad/s	130	>0	U.S. EPA (1991)—input used for all model surface impoundments
Waste Characteristic Data				
Average molecular weight of waste	g/mol	none	≥1	Required input for organic-phase wastes
Density of waste	g/cm^3	none	>0	Required input for organic-phase wastes

(continued)

Table 2-5. (continued)

Input Parameter	Units	Default Value	Range[a]	Basis
Active biomass concentration (as mixed-liquor volatile suspended solids (MLVSS)) in the surface impoundment	g/L	0.05	0–1,000	Coburn et al. (1988)—default value used for surface impoundments in developing biodegradation rate constants U.S. EPA (1994a)—recommended default for quiescent surface impoundments; suggests a default for aerated surface impoundments = 0.25 g/L
Total suspended solids (TSS) in surface impoundment influent	g/L	0.2	0–1,000	U.S. EPA (1994a)—range = 0.11–0.40 for surface impoundments designed for biodegradation
Total organics (total organic carbon or chemical oxygen demand) in surface impoundment influent	mg/L	200	0–1,000,000[c]	
Total biorate	mg/g biomass-h	19	≥0	U.S. EPA (1994a)—default value recommended in CHEMDAT8

[a] Ranges are inclusive, except for parameters with ranges shown as “>0–x”, which must be greater than zero.

[b] Power efficiency is a misnomer that is carried over from CHEMDAT8. This input is really the oxygen correction factor for the liquid-phase turbulent mass transfer coefficient (see Equation 2-63). The actual power efficiency, used in the equation for gas-phase turbulent mass transfer coefficient (see the equation for power number in the list of parameters for Equation 2-64), is hardwired to a value of 0.85 in CHEMDAT8. In order to maintain consistency with CHEMDAT8, IWAIR also terms this input “power efficiency” but uses it as the oxygen correction factor and hardwires the real power efficiency with a value of 0.85. The default value provided in the IWAIR model and the parameter guidance provided in Appendix B of the *IWAIR User’s Guide* for this input are consistent with its use as the oxygen correction factor.

[b] Must be greater than or equal to the sum of the concentrations of all organic chemicals specified as being in the waste by the user in risk calculation mode.

not affect adsorption loss. Setting active biomass to zero turns off biomass growth, so that adsorption losses are limited to adsorption to inlet solids. Setting active biomass to zero also turns off direct biodegradation, as biodegradation cannot occur without active biomass. IWAIR enforces this if the user sets biodegradation to |ON| and then sets active biomass to zero by automatically resetting the biodegradation option to |OFF|.

Aeration. Factors that have an impact on the relative surface area of turbulence and the intensity of that turbulence are important in determining the rate of volatilization of the chemicals in aerated surface impoundments. IWAIR can model two types of aeration, either separately or in combination: mechanical aeration and diffused air aeration.

Mechanical aeration is achieved using impellers rotating in the impoundment and agitating the liquid. Diffused air aeration is achieved through the use of diffusers that force air through the liquid, thus agitating the liquid. The extent and intensity of the turbulence are important factors in estimating emissions from aerated impoundments. For both types of aeration, the fraction of the surface area that is turbulent is an important input and no default is provided.

For mechanical aeration, the model has several input parameters that have an impact on the degree and intensity of the turbulence created by the aeration (or mixing). Total power, power per aerator (number of aerators), and impeller diameter have some impact on the emission results. A default value is provided for impeller diameter; but the user is encouraged to enter a site-specific value, if available. No default is provided for number of aerators or total power. The other parameters, such as impeller speed, power efficiency, and oxygen transfer rate have only a slight impact on the estimated emissions; default values are provided for these inputs, but the user is encouraged to enter site-specific values, if available.

For diffused air aeration, the key input is the submerged air flow. No default is provided for this parameter. The diffused air portion of CHEMDAT8 does not include correlations for calculating a turbulent mass transfer coefficient to account for increased emissions as a result of surface turbulence caused by the air flow through the liquid. However, the equations for turbulent mass transfer coefficient for mechanically aerated systems can be (and are) used to estimate this by entering inputs for a “virtual” aerator. IWAIR uses the default values for impeller diameter, impeller speed, power efficiency, and oxygen transfer rate to create a virtual aerator for diffused air systems. The total power and number of aerators are set based on the size of the unit. This is discussed in more detail in Section 2.4.4.4.

Waste Characterization Inputs. In order to generate an accurate estimate of a constituent’s volatile emissions, a user of IWAIR must define the physical and chemical characteristics of the waste that will be managed in the WMU. In particular, the user must determine if the waste is best described as a dilute mixture of chemical compounds (aqueous) or if it should be considered organic, containing high levels of organic compounds or a separate nonaqueous organic phase. These two different types of waste matrices influence the degree of partitioning that will occur from the waste to the air. Partitioning describes the affinity that a constituent has for one phase (for example, air) relative to another phase (for example, water) that drives the volatilization of organic chemicals. The choice of waste matrix will significantly affect the rate of emissions from the waste. See Section 2.2 for a more detailed discussion of waste matrices and partitioning. A general rule of thumb is that wastes that consist of 10 percent or more organics are best modeled as organic phase. CHEMDAT8 (and IWAIR) can model both aqueous- and organic-phase wastes for nonaerated (quiescent) surface impoundments, but can model only aqueous-phase wastes for aerated surface impoundments.

CHEMDAT8 includes an input for the fraction of waste that is "oily" (i.e., organic). In IWAIR, if the user models an organic waste, IWAIR assumes that this fraction is 1.

The molecular weight of the organic phase of the waste is a key input for modeling emissions from organic-phase wastes (this is the molecular weight of the bulk liquid, not the individual chemical). Higher waste molecular weights will result in higher emissions estimates. The range of molecular weights for common organic chemicals that might be found in Industrial D wastes spans an order of magnitude, from about 30 g/mol to about 300 g/mol. Therefore, setting this value as accurately as possible will produce the most accurate emissions estimates. In risk mode, no default value is provided; however, Appendix B of the *IWAIR User's Guide* provides an equation for estimating an appropriate molecular weight from the concentrations and molecular weights of the components of the waste. Because these components may include chemicals not being modeled in a particular IWAIR run, IWAIR cannot calculate this directly from user inputs and chemical properties. In allowable concentration mode, the molecular weight of the organic phase is set to the molecular weight of the individual chemical modeled, simulating emissions from pure component.

The density of the waste is also needed for modeling emissions from organic-phase wastes. In risk mode, no default value is provided; however, Appendix B of the *IWAIR User's Guide* provides an equation for estimating an appropriate density from the concentrations and densities of the components of the waste. Because these components may include chemicals not being modeled in a particular IWAIR run, IWAIR cannot calculate this directly from user inputs and chemical properties. In allowable concentration mode, the density of the organic phase is set to 1 g/cm^3, consistent with the assumption that 1,000,000 mg/L is pure component.

Factors that influence the rate of biodegradation are important in determining emissions from surface impoundments. Unlike the biodegradation rate model that is used for land application units, landfills, and waste piles, the biodegradation rate model used in CHEMDAT8 for surface impoundments is dependent on the amount of active biomass in the WMU. Therefore, the active biomass concentration is a critical parameter for impoundments (see the discussion above on biodegradation toggle and how it interacts with active biomass). A default value is provided for active biomass if the user chooses to model biodegradation, but the user is encouraged to enter a site-specific value, if available. No default value is provided if the user chooses not to model biodegradation; unless users explicitly want to model the transitional period before the biomass has adapted to the chemicals present, they should set active biomass to zero when the biodegradation toggle is set to |OFF|.

The TSS and total organics in the influent and the total biorate have an impact on the rate of biomass production and subsequently the amount of constituent that is adsorbed onto the solids. These inputs, however, have little or no impact on the estimated emission rates for most of the constituents included in IWAIR. Default values are provided, but the user is strongly encouraged to enter site-specific values, if available.

Typically, active biomass in the impoundment will be less than TSS in the influent. However, this might not be the case in all situations. The most frequent exception would be in activated sludge units where a portion of the effluent biomass is recovered and recirculated back into the unit. There may also be occasions where the biomass growth rate exceeds the solids settling rate within the unit so that the in-basin active biomass concentration is greater than the influent TSS concentration without a return activated sludge. These conditions are less frequent for surface impoundments than for tanks, which cannot be modeled using IWAIR.

Meteorological Conditions. Two meteorological parameters are used as inputs to CHEMDAT8: annual average wind speed and annual average temperature. By default, IWAIR uses the annual average temperature and wind speed for the meteorological station identified as most representative for the site location. However, the user may override these with site-specific data.

Emissions estimates for nonaerated impoundments are influenced by both temperature and wind speed. Emissions for aerated impoundments are predominantly driven by the turbulent area and associated mass transfer coefficients; therefore, the emissions from aerated impoundments are not strongly affected by the wind speed; they are affected by temperature. Wind speed is used to select the most appropriate correlation equation for calculating the liquid-phase quiescent mass transfer coefficient.

The temperature is used for several calculations to adjust chemical properties that are dependent on temperature. These include the vapor-liquid equilibrium partition coefficient and the gas-phase diffusivity; however, temperature also affects the liquid-phase diffusivity and the liquid-phase turbulent mass transfer coefficient. The temperature correction adjustment for vapor-liquid equilibrium partition coefficient uses the Antoine's coefficients to calculate a ratio of the constituent's vapor pressure at the system temperature to the constituent's vapor pressure at 25°C. This ratio is used to adjust the vapor-liquid partition coefficient when either Raoult's law or Henry's law is used. The Henry's law coefficient is sometimes estimated by the constituent vapor pressure divided by solubility. Although it is more correct to consider the liquid-phase activity coefficient, it is more difficult to assess a temperature adjustment factor for the liquid-phase activity coefficient (or solubility) than for vapor pressure. In addition, solubility is generally less temperature-dependent than vapor pressure. There has been some progress with temperature-dependent correlations for Henry's law coefficients in recent years,[4] but these were not readily available at the time of the development of CHEMDAT8, and they are still not currently available for the range of chemicals modeled by IWAIR. Therefore, the current temperature correction factor applied to the Henry's law constants based on the temperature dependence of constituent's vapor pressure as estimated using Antoine's equation remains the best approach for adjusting the Henry's law constants (input values determined at 25°C) to the prevailing temperature of the WMU. Depending on the residence time of the waste in the impoundment, the temperature of the waste is not expected to vary significantly with changing

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[4] e.g., the compilations of Sanders; see http://www.mpch-mainz.mpg.de/~sander/res/henry.html

atmospheric temperatures. Therefore, annual average temperatures are used to estimate the average waste temperature in the impoundment.

2.4 Mathematical Development of Emissions

This section describes how the inputs described in Section 2.3 are used to calculate the mass emission rate for use in subsequent risk estimates. Most of the mathematical equations used to calculate emissions were taken from the CHEMDAT8 emission model developed by EPA. The documentation of the CHEMDAT8 model can be accessed from EPA's Web site (http://www.epa.gov/ttn/chief/software.html, then select "Water8 and Chemdat8"). For convenience, the necessary equations are provided here. For a more detailed discussion or derivation of these equations, the reader is referred to the CHEMDAT8 model documentation (U.S. EPA, 1994a). Some additional equations were needed to convert the CHEMDAT8 fraction emitted to mass emission rates. Through the remainder of this section, the subsection heads indicate whether the equations in that subsection came from CHEMDAT8 or were added by IWAIR.

2.4.1 Landfills

Inputs and assumptions. The basic assumptions used for modeling landfills are as follows:

- The landfill operates for t_{life} years filling N cells of equal size sequentially.
- The active cell is modeled as being instantaneously filled at time $t = 0$, and remains open for t_{life}/N years; this is the time it takes to fill one landfill cell.
- Emissions are only calculated for one cell for t_{life}/N years (it is assumed that the cell is capped after t_{life}/N years and that the emissions from the capped landfill cells are negligible); the time of calculation is calculated as follows:

$$t_{calc} = \frac{t_{life} \times 365.25 \times 24 \times 3{,}600}{N_{cells}} \tag{2-13}$$

where

t_{calc} = time of calculation (s)
t_{life} = lifetime of unit (yr)
N_{cells} = total number of cells (unitless)
365.25 = unit conversion (d/yr)
24 = unit conversion (h/d)
3,600 = unit conversion (s/h).

- The waste is homogeneous, with an initial concentration of 1 mg/kg for the allowable concentration mode or a user-specified concentration for the risk mode; the landfill may also contain other wastes with different properties.

- Loading is calculated from the annual waste quantity and the size of the landfill, as follows:

$$L = \frac{Q_{annual} \times t_{life}}{A_{total} \times d_{total}} \tag{2-14}$$

where

L = waste loading rate ($Mg/m^3 = g/cm^3$)
Q_{annual} = annual waste quantity (Mg/yr)
A_{total} = total area of unit (m^2)
d_{total} = total depth of unit (m).

Note that if the unit is a monofill receiving only the waste modeled, the loading should equal the bulk density entered by the user. If the unit receives other wastes in addition to the waste modeled, the loading should be less than the bulk density of the waste. The loading cannot exceed the bulk density of the waste; if this condition occurs, the user will get an error message and will be required to change the inputs to eliminate this condition.

- Landfill **cell** areas and depth are used for the model run: $A_{cell} = A_{total} / N_{cells}$; $d_{cell} = d_{total}$.

- By default, biodegradation is not modeled for landfills, but the user may choose to turn biodegradation on. If the user chooses to model it, biodegradation is modeled as a first-order process based on soil half-life data.

Calculation of the equilibrium partition coefficient (CHEMDAT8). The emissions from the landfill are based primarily on the vapor-phase concentration of the pore-space gas within the landfill (in equilibrium with the disposed waste) and the diffusion rate of the constituents in this pore-space gas to the soil surface. The vapor-phase concentration is determined by the vapor-liquid equilibrium coefficient (K_{eq}). The calculation of this coefficient is dependent on the type of waste managed.

For organic-waste matrices, the vapor-liquid equilibrium coefficient is based on the constituent's partial vapor pressure (often referred to as Raoult's law), as follows:

$$K_{eq} = \frac{T_{corr}\, P_{vap}\, MW_{waste} \epsilon_a}{RTL} \tag{2-15}$$

where

K_{eq} = vapor-liquid equilibrium coefficient for constituent (g/cm^3 per g/cm^3)
T_{corr} = temperature correction factor for vapor pressure for constituent (unitless)
P_{vap} = pure component vapor pressure of constituent at 25°C (atm)
MW_{waste} = average molecular weight of the waste (g/mol)
ϵ_a = air-filled porosity (cm^3/cm^3)
R = universal gas constant = 82.1 cm^3-atm/mol-°K
T = temperature of the system (°K).

The temperature correction factor is based on the ratio of the constituent's vapor pressure, as calculated using Antoine's equation at the system's temperature, and the constituent's vapor pressure at the reference temperature for which the vapor pressure is provided, which is assumed to be 25°C in IWAIR (that is, all chemical properties in the IWAIR database correspond to the property value at 25°C). The temperature correction factor is calculated as follows:

$$T_{corr} = 10^{\left(VP_b\left(\frac{-1}{VP_c+T-273.15}+\frac{1}{VP_c+25}\right)\right)} \tag{2-16}$$

where

VP_b = Antoine's vapor pressure constant B for constituent
VP_c = Antoine's vapor pressure constant C for constituent.

The Antoine's constants used in IWAIR assume the Antoine's equation (which is $log\ P_{vap} = A - B/(C + T)$) and are developed for calculating the vapor pressure, P_{vap}, in mmHg given the temperature, T, in °C.

For aqueous matrices, the vapor-liquid equilibrium coefficient is based on the constituent's Henry's law constant, as follows:

$$K_{eq} = \frac{T_{corr}\, MW_{waste} \epsilon_a}{RTL}\left(\frac{10^6}{18}\right) \tag{2-17}$$

where

H = Henry's law constant at 25°C (atm-m^3/mol)
MW_{waste} = average molecular weight of the waste = 18 g/mol = molecular weight of water
18 = unit conversion factor for aqueous waste (cm^3/mol = 18 g/mol × 1 cm^3/g)
10^6 = unit conversion factor (cm^3/m^3).

Calculation of the effective diffusivity (CHEMDAT8). The effective diffusivity of constituent in a porous medium is calculated as follows:

$$D_{eff} = D_a \frac{\epsilon_a^{3.33} T_{C,gas}}{\epsilon_t^2} \tag{2-18}$$

where

D_{eff} = effective diffusivity of constituent in the system (cm^2/s)
D_a = diffusivity of constituent in air at 25°C (cm^2/s)
$T_{C,gas}$ = temperature correction factor for gas diffusivity (unitless)
= $(T / 298.15)^{1.75}$
ϵ_t = total porosity (cm^3/cm^3).

Calculation of the fraction emitted (CHEMDAT8). The equation used to calculate the fraction emitted is dependent on the volatilization rate constant, the biodegradation rate constant, and the time period for the calculation. The volatilization rate constant is calculated as follows:

$$K_v = \frac{K_{eq}\ D_{eff}}{d_{wmu}^{\ 2}} \tag{2-19}$$

where

K_v = volatilization rate constant for constituent (1/s)
d_{wmu} = characteristic depth of the WMU (cm) = d_{total} / 100 for a landfill.

The fraction emitted is calculated using one of the following three solution algorithms, depending on the biodegradation (b_{soil}) and volatilization rate (K_v) constants.

If $K_v / b_{soil} < 0.1089$,

$$f_{emitted} = \left(\frac{K_v}{b_{soil}}\right)^{0.5} \left[1 - e^{-t_{calc}\left(\frac{\pi^2}{4}K_v + b_{soil}\right)}\right] \tag{2-20}$$

If $K_v / b_{soil} \geq 0.1089$ *and* $K_v\ t_{calc} < 0.22$ (short-term solution),

$$f_{emitted} = 2\left(\frac{K_v t_{calc}}{\pi}\right)^{0.5} \left[1 - \frac{t_{calc} b_{soil}}{3}\right] \tag{2-21}$$

If $K_v / b_{soil} \geq 0.1089$ *and* $K_v\, t_{calc} \geq 0.22$ (first term of the Taylor series expansion solution),

$$f_{emitted} = \frac{8}{\pi^2}\left(\frac{1 - e^{-t_{calc}\left(\frac{\pi^2}{4}K_v + b_{soil}\right)}}{1 + \frac{4}{\pi^2}\left(\frac{b_{soil}}{K_v}\right)}\right) + 0.1878 \tag{2-22}$$

where

$f_{emitted}$ = fraction of constituent emitted to the atmosphere (unitless)
b_{soil} = soil biodegradation rate constant for constituent (1/s).

Calculation of the fraction biodegraded (CHEMDAT8). The fraction biodegraded and the fraction emitted are both dependent on the volatilization and biodegradation rate constants, and their values are not independent of each other. The fraction biodegraded is calculated using one of the following two equations depending on the biodegradation and volatilization rate constants, as follows:

If $K_v\, t_{calc} < 0.22$ (short-term solution),

$$f_{bio} = 1 - \left(1 - 2\left(\frac{K_v t_{calc}}{\pi}\right)^{0.5}\left[e^{-t_{calc} b_{soil}}\right]\right) - f_{emitted} \tag{2-23}$$

If $K_v\, t_{calc} \geq 0.22$ (first term of the Taylor series expansion solution),

$$f_{bio} = 1 - \left(1 - \left[\frac{8}{\pi^2}\left(1 - e^{-t_{calc}\left(\frac{\pi^2}{4}K_v\right)}\right) + 0.1878\right]\right)\left[e^{-t_{calc} b_{soil}}\right] - f_{emitted} \tag{2-24}$$

where

f_{bio} = fraction of constituent biodegraded in the WMU (unitless).

Calculation of the emission flux rate (IWAIR). The average emission flux rate for the landfill can be calculated as follows:

$$E = \frac{Q_{annual} \times C_{waste} \times L \times f_{emitted}}{A_{cell} \times \rho_b \times 365.25 \times 24 \times 3{,}600} \tag{2-25}$$

where

E = emission flux rate of constituent (g/m^2-s)
C_{waste} = concentration of constituent in waste (mg/kg = g/Mg)
A_{cell} = area of cell (m^2)
ρ_b = bulk density of waste in landfill (g/cm^3)
365.25 = unit conversion (d/yr)
24 = unit conversion (h/d)
3,600 = unit conversion (s/h).

2.4.2 Land Application Units

Inputs and assumptions. The assumptions used for modeling land application units are as follows:

- Waste application occurs N_{appl} times per year. The land application unit is modeled using time steps equal to the time between applications, as follows:

$$t_{calc} = \frac{365.25 \times 24 \times 3{,}600}{N_{appl}} \tag{2-26}$$

where

N_{appl} = number of applications per year (yr^{-1})
365.25 = unit conversion (d/yr)
24 = unit conversion (h/d)
3,600 = unit conversion (s/h).

- The land application unit operates for t_{life} years and is modeled for t_{life} plus 30 years, in order to account for up to 30 years of postclosure exposure. The total number of time steps modeled is thus

$$N_{steps} = (t_{life} + 30) \times N_{appl} \tag{2-27}$$

where

N_{steps} = total number of time steps modeled (unitless)
t_{life} = operating life of unit (yr).

This total number of time steps, N_{steps}, cannot exceed 32,766 because of code limitations for integer variables. This is unlikely to result in practical limitations, unless the operating life is very long and the number of applications per year very high. For example, daily applications (365 applications/year) for 59 years would still be within this limitation.

- The waste is homogeneous, with an initial concentration of 1 mg/kg for the allowable concentration mode or a user-specified concentration for the risk mode.
- Loading is calculated from the annual waste quantity and the size of the land application unit as follows:

$$L = \frac{Q_{annual} \times 100}{N_{appl} \times A \times d_{till}} \tag{2-28}$$

where

L = loading rate ($Mg/m^3 = g/cm^3$)
Q_{annual} = annual quantity of waste (Mg/yr)
A = area of unit (m^2)
d_{till} = tilling depth (cm)
100 = unit conversion (cm/m).

- By default, biodegradation is modeled as a first-order process based on soil half-life data. The user may choose to turn biodegradation off.
- The characteristic depth of a land application unit used in Equation 2-19 (calculation of K_v) is the tilling depth ($d_{wmu} = d_{till}$).
- The volume of the land application unit remains constant. To maintain this assumption, it is assumed that as more waste is applied, an equal volume of waste/soil mixture is buried or otherwise removed from the active tilling depth.

  The equipment used to incorporate and mix the waste with the soil in a land application unit typically does so at a fixed depth; therefore, the depth of waste incorporation is fixed. If the depth of waste added to the unit over the active life of the land application unit is significant relative to the tilling depth, subsequent applications of waste will leave the bottom-most layer of contaminated soil untilled (i.e., buried). If subsequent waste applications were added to the same fixed mass of soil, the model as constructed would perceive this as adding a fixed quantity of pure constituent to the fixed soil mass during each waste application. As such, the land application unit could eventually have higher constituent concentrations than the applied waste (for compounds that persist in the environment). Therefore, the burial loss term is needed for an accurate estimate of the maximum steady-state soil concentration (and emissions rate) according to mass balance principles.

> IWAIR further assumes that this buried waste layer does not have any significant impact on the emission estimates. There are several reasons why the buried waste is not expected to contribute significantly to the emissions. At the time of burial, the buried waste constituent concentration is less than (or at most equal to) the constituent concentration in the tilled layer of the land application unit. Secondly, experience with emission estimates of buried waste using model equations developed by Jury et al. (1990) shows that the buried waste layer contributions to emissions are typically 1 to 2 orders of magnitude less than the emissions from the surface layer (depending on the relative depths of each layer) when the initial concentrations are homogeneous (a requirement for the Jury model solution). Constituent burial tends to be a significant constituent removal mechanism only when other constituent removal mechanisms are essentially zero (i.e., chemicals that do not degrade or volatilize). Constituent loss in buried waste is a simplifying assumption with respect to volatilization, but this assumption provides a much better simulation of the land application unit constituent exposure scenarios than when waste burial is not included. Without "burial" losses, land application unit soil concentrations can exceed those in the original waste material. These "unlikely" high soil concentrations provide greater errors in the estimated long-term volatilization rates than are projected by the land application unit model with constituent burial losses.

Calculation of fraction emitted and fraction biodegraded (CHEMDAT8). The IWAIR model calculates the fraction emitted and the fraction biodegraded for each chemical in the land application unit using the CHEMDAT8 equations shown in Equations 2-15 through 2-24, as applicable, for the time interval between applications (i.e., the time of the calculation, t_{calc}, from Equation 2-26). The calculation is made for the first application given the inputs and assumptions outlined above. As the model is linear (first-order) with respect to constituent concentration, the fraction emitted and the fraction biodegraded are independent of the starting concentration. Consequently, these calculated fractions can be applied to successive waste applications assuming that the volume of the land treatment unit remains constant; this assumption is also documented above. The IWAIR model takes the fraction emitted and fraction biodegraded and calculates the long-term emissions that occur from successive use. This is an enhancement made in IWAIR and is documented in the following subsections.

Calculation of the emission rate (IWAIR). The emission rate for a land application unit is dependent on the starting concentration or mass of constituent within the land application unit for a given application. For the first application, the mass of constituent in the land application unit just after the first application is

$$M_{start,1} = M_{appl} = \frac{Q_{annual} \times C_{waste}}{N_{appl}} \tag{2-29}$$

where

$M_{start,1}$ = mass of chemical in unit at start of time step 1 (g)

M_{appl} = mass of chemical added during one application (g)
C_{waste} = concentration of chemical in waste (mg/kg = g/Mg).

The mass of constituent in the land application unit at the end of the first time of calculation (just prior to more waste being added) is

$$M_{end,1} = M_{appl} \times (1 - f_{emitted} - f_{bio}) \tag{2-30}$$

where

$M_{end,1}$ = mass of chemical in unit at end of time step 1 (g)
$f_{emitted}$ = fraction emitted (unitless).
f_{bio} = fraction biodegraded (unitless).

Note that fraction emitted and fraction biodegraded, which are calculated according to Equations 2-20 through 2-24, are not independent of each other despite their appearance as separate terms in the above equation. Fraction emitted depends on biodegradation rate and other variables, and fraction biodegraded depends on biodegradation rate and fraction emitted, among other variables.

The generalized equation for the starting mass of constituent (just after any waste application number, *n*, and taking into account the “burial” loss needed to maintain a constant land application unit volume) is

$$M_{start,n} = M_{appl} + M_{end,n-1} \times \left(1 - \frac{d_{appl}}{d_{till}}\right) \tag{2-31}$$

where

$M_{start,n}$ = mass of chemical in unit at start of time step *n* (g)
$M_{end,n-1}$ = mass of chemical in unit at end of time step *n-1* (g)
d_{appl} = depth of waste applied (cm), see Equation 2-32.

Depth of waste applied is calculated as

$$d_{appl} = \frac{Q_{annual} \times 100}{N_{appl} \times \rho_b \times A} \tag{2-32}$$

where

ρ_b = bulk density of waste ($g/cm^3 = Mg/m^3$).

Note that d_{till} must exceed d_{appl} and should probably be at least three to four times d_{appl}. The user will be warned if d_{till} does not exceed d_{appl}.

The generalized equation for the ending mass of constituent in the land application unit for any waste application number, *n*, (just prior to the *n+1* waste application) is

$$M_{end,n} = M_{start,n} \times (1 - f_{emitted} - f_{bio}) \tag{2-33}$$

where

$M_{end,n}$ = mass of chemical in unit at end of time step *n* (g).

The generalized equation for the mass of constituent emitted during any application period (time of calculation) is

$$M_{emitted,n} = M_{start,n} \times f_{emitted} \tag{2-34}$$

where

$M_{emitted,n}$ = mass of chemical emitted in time step *n* (g).

For each time period, the emission flux rate is calculated as follows:

$$E_n = \frac{M_{emitted,n}}{t_{calc} \times A} \tag{2-35}$$

where

E_n = emission flux rate in time step *n* (g/m^2-s).

The starting mass, ending mass, and emitted mass of constituent are calculated for each time step for a period equal to the life of the unit plus 30 years. This time series of emission rates for each time step must then be converted to a time-averaged emission rate for a time period corresponding to exposure assumptions. Three exposure scenarios are possible: for carcinogenic risk, IWAIR uses an average for a time period that corresponds to the exposure duration: 30 years for a resident or 7 years for a worker. For noncarcinogens, IWAIR uses a 1-year average as an indicator of the highest exposure experienced over a chronic duration.

The additional 30 years postclosure are modeled to ensure that the period of maximum emissions is captured. For chemicals that tend to volatilize quickly, this is likely to occur during operation of the unit, as new waste additions continue to be made. For chemicals that do not tend to volatilize quickly, but build up in the unit, this is likely to occur postclosure (when waste additions stop and the maximum concentration is achieved in the unit). To capture the maximum period, IWAIR calculates all possible 30-year and 7-year averages over the life of the unit plus 30 years and chooses the maximum of these. For example, for a unit with an operating life of 10 years, eleven 30-year averages are possible, the first starting in year 1 of operation and running through 10 years of operation and 20 years postclosure, and the last starting in the first year postclosure (i.e., year 11) and running for 30 years.

The emission rate displayed on the emission screen in IWAIR and in the printed reports for all chemicals modeled is the maximum 1-year average used for noncarcinogens. However, the air concentration displayed on the RESULTS screen and in the printed reports is based on the appropriate average emission rate for the chemical and receptor. If a chemical has both a carcinogenic and a noncarcinogenic health benchmark (so that both risk and HQ are calculated), the air concentration displayed on the RESULTS screen corresponds to the carcinogenic risk calculation, not the noncarcinogenic HQ calculation. The interested user can use Equation 6-1 to convert displayed 1-year emission rates to the corresponding 1-year air concentration for such chemicals. Similarly, Equation 6-1 can be used to convert the 30- or 7-year air concentration to the corresponding emission rate (which is not displayed).

2.4.3 Waste Piles

Inputs and assumptions. The modeling assumptions used for modeling waste piles are as follows:

- The waste pile is modeled as a batch process with the waste remaining in the waste pile for one average residence time (see time of calculation equation provided in Equation 2-36). The model solution is appropriate for either of the following two scenarios:

  1. The waste pile is instantaneously filled at time $t = 0$ and remains dormant (no other waste added) for one average residence time, at which time the entire waste pile is emptied and completely filled with fresh waste.

  2. An annual quantity of waste is added to the waste pile consistently (in small quantities) throughout the year, and a corresponding quantity of the oldest waste within the waste pile is removed from the waste pile (so that the waste pile is essentially a plug-flow system).

- The waste is homogeneous, with an initial concentration of 1 mg/kg for the allowable concentration mode or a user-specified concentration for the risk mode.

- By default, biodegradation is not modeled for waste piles. Waste piles are not generally designed for biodegradation; however, if residence times of waste in the waste pile are on the order of months or years, naturally occurring microorganisms could potentially acclimate and degrade constituents within the waste pile. The wastes for which IWAIR was designed are industrial wastes, not hazardous wastes (and so presumably are not toxic enough to fail the Toxicity Characteristics

Leaching Procedure, because that would make them hazardous). Therefore, while a specific waste might not be very conducive to biomass growth, it cannot be widely assumed that the wastes for which this model was designed would be toxic to any potential biomass. Therefore, the user has the option of turning biodegradation on if site-specific conditions suggest that biodegradation is occuring. If the user chooses to model it, biodegradation is modeled as a first-order process based on soil half-life data.

- Loading is the bulk density of the waste material ($L = \rho_b$).
- The time of calculation is equal to one average residence time of waste in the waste pile. The time of calculation (or residence time) is calculated as follows:

$$t_{calc} = \frac{A \times h \times \rho_b \times 365.25 \times 24 \times 3{,}600}{Q_{annual}} \tag{2-36}$$

where

t_{calc} = time of calculation (s)
A = area of unit (m^2)
h = height of waste pile (m)
ρ_b = bulk density of waste ($g/cm^3 = Mg/m^3$)
Q_{annual} = annual waste quantity (Mg/yr)
365.25 = units conversion (d/yr)
24 = units conversion (h/d)
3,600 = units conversion (s/h).

- The waste pile geometry is modeled as a square box. The sides are assumed to be essentially vertical and are assumed to be negligible in the overall surface area of the waste. The shape of the upper surface is assumed to be square. The area and height of this box are both user inputs and are used by the emissions component.

Calculation of fraction emitted and fraction biodegraded (CHEMDAT8). The IWAIR model calculates the fraction emitted and the fraction biodegraded for each chemical in the waste pile using Equations 2-15 through 2-24, as applicable, for one residence time (i.e., the time of the calculation, t_{calc}, from Equation 2-36).

Calculation of the emission flux rate (IWAIR). The average emission flux rate for the waste pile can be calculated as follows:

$$E = \frac{Q_{annual} \times C_{waste} \times f_{emitted}}{A \times 365.25 \times 24 \times 3{,}600} \tag{2-37}$$

where

E = emission flux rate of constituent (g/m^2 - s)
C_{waste} = concentration of constituent *i* in waste (mg/kg = g/Mg)
$f_{emitted}$ = fraction of constituent *i* emitted to the atmosphere (unitless)
365.25 = units conversion (d/yr)
24 = units conversion (h/d)
3,600 = units conversion (s/h).

2.4.4 Surface Impoundments

Inputs and Assumptions. The basic modeling assumptions used for modeling surface impoundments are somewhat different for aqueous- and organic-phase wastes. For aqueous-phase wastes, assumptions include

- The impoundment operates under steady-state, well-mixed conditions (continuously stirred tank reactor (CSTR)). In a CSTR, the unit is assumed to be perfectly (or completely) mixed so that the concentration within the unit is at all times homogeneous and equal to the effluent concentration. Constituent in the influent waste stream is assumed to be instantaneously and evenly distributed within the unit. This modeling assumption is generally appropriate when aeration or mechanical mixing is present. It may also be generally applicable for certain nonaerated units whose general dimensions and orientation to prevailing winds afford significant mixing from eddy currents. An alternate model construct is the plug-flow model, which is roughly equivalent to a batch reactor. In a plug-flow system, essentially no mixing is assumed. This scenario is most appropriate for units that are quiescent and whose dimensions and orientation to prevailing winds limit wind-caused mixing (e.g., a very narrow, long, slow-moving stream). In reality, both model constructs are imperfect. Complete mixing or absolutely no mixing is never achieved. For IWAIR, it was determined that the complete mixing model construct was generally the most applicable; it was therefore used for IWAIR. Consequently, the predicted emissions for aqueous-phase wastes are most accurate for well-mixed units and are less accurate when little or no mixing (i.e., plug-flow) is present.

- Hydrolysis rate is first order with respect to constituent concentrations.

- By default, aqueous waste constituent biodegradation is modeled as first order with respect to biomass concentrations and follows Monod kinetics with respect to constituent concentrations (see discussion of the biodegradation rate constants K_1 and K_{max} in Section 2.3.1). Because the Monod kinetic model is nonlinear with respect to the constituent concentration, waste influent concentration is calculated using an iterative approach (using a Newton-Raphson routine) for the concentration calculation mode or is user-specified for the risk calculation mode. The surface area, depth, flow rate, and aeration parameters (if applicable) are all directly specified for the model unit. See Section 6.2.2 for further discussion of the Newton-Raphson method.

In addition to constituent biodegradation, growth of biomass occurs in biologically active surface impoundments, which provides a growing matrix for chemical adsorption and loss through settling. Adsorption and settling losses also occur in the absence of active biomass and biodegradation, but are limited to occurring on inlet solids. Biodegradation cannot occur if there is no active biomass. If an impoundment is biologically active, it may go through a transitional period during which there is active biomass (so biomass growth occurs, facilitating adsorption and settling losses) but the biomass is not yet adapted to consume the specific chemicals present (so biodegradation does not occur). This transitional period will usually end as the biomass acclimates and adapts to the chemicals present.

The user can control these two processes (biodegradation and adsorption losses) separately. Setting biodegradation to |OFF| turns off biodegradation, but does not affect adsorption loss. Setting active biomass to zero turns off biomass growth, so that adsorption losses are limited to adsorption to inlet solids. Because biodegradation cannot occur in the absence of active biomass, setting active biomass to zero also effectively turns off biodegradation.

For organic-phase wastes (which can be modeled only for nonaerated impoundments), assumptions include

- The impoundment is assumed to operate under steady-state, plug-flow (no mixing) conditions.
- There is no biodegradation or hydrolysis for organic-phase wastes.
- There is no adsorption modeled for organic-phase wastes.

The equations for surface impoundments are presented in the following five sections: Section 2.4.4.1, Quiescent Surface Impoundments for Aqueous-Phase Wastes; Section 2.4.4.2, Quiescent Surface Impoundments for Organic-Phase Wastes; Section 2.4.4.3, Mechanically Aerated Surface Impoundments (Aqueous-Phase Wastes Only); Section 2.4.4.4, Diffused Air Aerated Surface Impoundments (Aqueous-Phase Wastes Only); and Section 2.4.4.5, Both Mechanically and Diffused Air Aerated Surface Impoundments (Aqueous-Phase Wastes Only).

2.4.4.1 Quiescent Surface Impoundments for Aqueous-Phase Wastes

Calculation of the liquid-phase mass transfer coefficient for quiescent surface impoundments (CHEMDAT8). The appropriate correlation to use to estimate the liquid-phase mass transfer coefficient for quiescent surface impoundments is dependent on the wind speed and the fetch-to-depth ratio of the impoundment. The fetch is the linear distance across the WMU, and it is calculated from the WMU's surface area assuming a circular shape for the WMU. That is,

$$F = \left(\frac{4\ A}{\pi} \right)^{0.5} \qquad (2\text{-}38)$$

where

F = fetch of the unit (m)
A = surface area of the unit (m^2).

For wind speeds less than 3.25 m/s, the following correlation is used to calculate the liquid-phase mass transfer coefficient for quiescent surface impoundments regardless of the fetch-to-depth ratio:

$$k_{l,q} = 2.78 \times 10^{-6}\ T_{c,liq} \left(\frac{D_w}{D_{ether}} \right)^{\frac{2}{3}} \qquad (2\text{-}39)$$

where

$k_{l,q}$ = liquid-phase mass transfer coefficient for quiescent surface impoundments (m/s)
$T_{c,liq}$ = temperature correction factor for liquid-phase mass transfer coefficients (unitless) = (T / 298.15)
T = temperature of system (°K)
D_w = diffusivity of constituent in water (cm^2/s)
D_{ether} = diffusivity of ether in water (8.5E−6 cm^2/s).

For wind speeds greater than or equal to 3.25 m/s, the appropriate correlation for the liquid-phase mass transfer coefficient for quiescent surface impoundments is dependent on the fetch-to-depth ratio (F/d_{liq}) as follows:

$$For \quad \frac{F}{d_{liq}} < 14,$$

$$k_{l,q} = T_{c,\,liq}\left(1.0 \times 10^{-6} + (a \times 10^{-4})\ (U^*)^b\ Sc_{liq}^{-0.5}\right) \qquad (2\text{-}40)$$

$$For \quad 14 \leq \frac{F}{d_{liq}} \leq 51.2,$$

$$k_{l,q} = T_{c,liq} \left[2.605 \times 10^{-9} \left(\frac{F}{d_{liq}} \right) + 1.277 \times 10^{-7} \right] U_{10}^2 \left(\frac{D_w}{D_{ether}} \right)^{\frac{2}{3}} \qquad (2\text{-}41)$$

For $\frac{F}{d_{liq}} > 51.2,$

$$k_{l,q} = 2.611 \times 10^{-7}\ T_{c,liq}\ U_{10}^{2} \left(\frac{D_w}{D_{ether}} \right)^{\frac{2}{3}} \tag{2-42}$$

where

d_{liq} = depth of liquid in the surface impoundments (m)
a = equation constant, a = 34.1 for U* > 0.3 m/s; a = 144 for U* < 0.3 m/s
U^* = friction velocity (m/s) = 0.01U $(6.1 + 0.63U)^{0.5}$
U_{10} = wind speed 10 m above surface (m/s)
b = equation constant, b = 1 for U* > 0.3 m/s; b = 2.2 for U* < 0.3 m/s
Sc_{liq} = liquid-phase Schmidt number = $\mu_w/(\rho_w\ D_w)$
μ_w = viscosity of water (g/cm-s) = 9.37E−3 g/cm-s
ρ_w = density of water (g/cm^3) = 1 g/cm^3.

Calculation of gas-phase mass transfer coefficient for quiescent surface impoundments (CHEMDAT8). The gas-phase mass transfer coefficient for quiescent surface impoundments is estimated as follows:

$$k_{g,q} = (4.82 \times 10^{-3})\ T_{c,gas}\ U^{0.78}\ Sc_g^{-0.67}\ F^{-0.11} \tag{2-43}$$

where

$k_{g,q}$ = gas-phase mass transfer coefficient for quiescent surface impoundments (m/s)
$T_{c,gas}$ = temperature correction factor for gas diffusivity or gas mass transfer coefficient (unitless) = $(T / 298.15)^{1.75}$
T = temperature of system (°K)
Sc_g = gas-phase Schmidt number = $\mu_a/(\rho_a\ D_a)$
ρ_a = density of air (g/cm^3) = 1.2E−3 g/cm^3
μ_a = viscosity of gas (air) (g/cm-s) = 1.81E−4 g/cm-s
D_a = diffusivity of constituent in air (cm^2/s).

Calculation of overall mass transfer coefficient for quiescent surface impoundments for (CHEMDAT8). For aqueous wastes, the overall mass transfer coefficient that determines the rate of volatilization is determined based on a two-resistance model: a liquid-phase mass transfer resistance and a gas-phase mass transfer resistance. The overall volatilization mass transfer coefficient for quiescent surface impoundments is calculated as follows:

$$K_{OL} = K_{OL,q} = \left(\frac{1}{k_{l,q}} + \frac{1}{K_{eq}\ k_{g,q}} \right)^{-1} \tag{2-44}$$

where

K_{OL} = overall volatilization mass transfer coefficient (m/s)
$K_{OL,q}$ = overall mass transfer coefficient for quiescent surface impoundments (m/s)
K_{eq} = vapor-liquid equilibrium coefficient for constituent (g/cm^3 per g/cm^3).

Generally, Henry's law is used to estimate the vapor-liquid equilibrium coefficient for aqueous systems. The only exception to this is when the constituent is present within the surface impoundments at concentrations above the aqueous solubility. As the aqueous solubility is determined for binary systems (i.e., the constituent in pure water), a chemical's solubility in the waste matrix within the surface impoundments may be quite different than its solubility in pure water. However, Henry's law applies to dilute solutions. The aqueous solubility is used as an indication of whether or not the solution is "dilute" for a given chemical. As the steady-state concentration within the impoundment has not been calculated and cannot be calculated without first estimating the overall mass transfer coefficient, the vapor-liquid equilibrium coefficient is calculated based on Henry's law as follows:

$$K_{\mathbf{eq}} = \frac{T_{corr}\, H}{RT} \tag{2-45}$$

where

T_{corr} = temperature correction factor for vapor pressure for constituent (unitless) (see Equation 2-16)
H = Henry's law constant at 25°C (atm-m^3/mol)
R = universal gas constant = 8.21E−5 m^3-atm/mol-°K
T = temperature of the system (°K).

If the concentration within the impoundment exceeds the aqueous solubility for a given constituent based on the initial Henry's law assumption, then the vapor-liquid equilibrium partition coefficient for that chemical is recalculated using Raoult's law as follows:

$$K_{eq} = \frac{T_{corr} P_{vap}}{RT}\left(\frac{18}{10^6}\right) \tag{2-46}$$

where

P_{vap} = vapor pressure of constituent at 25°C (atm)
T = temperature of the system (°K)
18 = unit conversion factor for aqueous waste (cm^3/mol = 18 g/mol × 1 cm^3/g)
10^6 = unit conversion factor (cm^3/m^3).

Calculation of adsorption rate constant (CHEMDAT8). Sorption onto solids within the surface impoundment is a competing removal mechanism to the volatilization loss. The sorption removal rate depends on the rate at which solids enter and/or are produced within the surface impoundment and the solids-liquid partition coefficient. Solids production within the surface impoundment is dependent on either the available degradable organic matter entering the surface impoundments or the maximum overall biodegradation rate of this organic matter. The solids "wasting" rate (r_{TSS}) is the total rate at which solids enter the surface impoundment plus the rate of solids production within the surface impoundment, and it is calculated as follows:

$$r_{TSS} = 1000 TSS_{in} Q + 0.5 \times \min\left(\frac{r_{b,tot}}{3600} 1.046^{2\times(T-298)} d_{liq} AX; C_{TOC} Q \right) \tag{2-47}$$

where

r_{TSS} = total solids wasting rate (g solids/s)
1000 = unit conversion factor (L/m^3)
TSS_{in} = total suspended solids in influent (g/L)
Q = influent flow rate (m^3/s)
0.5 = assumed biomass yield coefficient (g solids/g organic consumed)
min() = function that returns the minimum value of a series of numbers separated by semicolons
$r_{b,tot}$ = biodegradation rate for total organics (mg/g-hr)
3600 = unit conversion (s/hr)
0.001 = unit conversion (g/mg)
T = temperature (°K)
X = active biomass concentration in the surface impoundment (g/L)
C_{TOC} = concentration of total organics in the surface impoundment influent (mg/L) = g/m^3.

It is assumed that the sludge is 99 percent water by weight and 1 percent solids by weight and that the sludge has a density essentially that of water (i.e., 1 g/cm^3). The sludge-liquid partition coefficient, therefore, adjusts the solid-liquid partition coefficient as follows:

$$K_s = 0.99 + 0.01 K_d \tag{2-48}$$

where

K_s = sludge-liquid partition coefficient (g/cm^3 sludge per g/cm^3 waste)
K_d = solid-liquid partition coefficient (cm^3/g solids).

For organic compounds, the following correlation is used to estimate the solid-liquid partition coefficient using the constituent's octanol-water partition coefficient as follows:

$$K_d = 10^{0.67 \log\left(K_{ow}\right)} + 0.39 \tag{2-49}$$

where

K_{ow} = octanol-water partition coefficient (unitless).

For mercury, the solid-liquid partition coefficient (K_d) is directly input in place of the octanol-water partition coefficient, and Equation 2-48 is used directly using this input value for K_d.

The adsorption rate constant is then calculated as

$$K_{ads} = \frac{100 K_s\, r_{TSS}}{10^6 d_{liq} A} \tag{2-50}$$

where

K_{ads} = adsorption rate constant (1/s)
100 = sludge solids correction factor, (100 g sludge/g solids) × (1 cm^3/g sludge)
10^6 = units correction factor (cm^3/m^3).

Calculation of effluent concentration (CHEMDAT8). All aqueous surface impoundments are modeled as well-mixed systems so that the concentration within the surface impoundment is assumed to be the same as the effluent concentration. Because of the nonlinear biodegradation rate model used for aqueous surface impoundments, the steady-state solution for the effluent concentration (and concentration within the surface impoundment) requires the solution of a quadratic equation, as follows:

$$C_{liq} = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \tag{2-51}$$

where

C_{liq} = constituent concentration in the surface impoundment and in the effluent (mg/L = g/m^3)
a,b,c = quadratic equation terms, which are defined in the following equations:

Quadratic term *a*:

$$a = \frac{1}{t_{res}} + \frac{K_{OL}}{d_{liq}} + K_{hyd} + K_{ads} \tag{2-52}$$

where

t_{res} = hydraulic residence time (s) = d_{liq} × A/Q
K_{hyd} = hydrolysis rate constant (1/s).

Quadratic term *b*:

$$b = a\left(\frac{K_{max}}{K_1}\right) + 1.046^{(T-298)}\left(\frac{K_{max} X}{3600}\right) - \frac{C_{in}}{t_{res}} \tag{2-53}$$

where

K_{max} = maximum biodegradation rate constant (mg/g-hr)
K_1 = first-order biodegradation rate constant (g/L-hr)
T = temperature (°K)
3600 = units conversion factor (s/hr)
C_{in} = constituent concentration in surface impoundment influent (mg/L = g/m^3)

Quadratic term *c*:

$$c = -\left(\frac{K_{max}}{K_1}\right)\left(\frac{C_{in}}{t_{res}}\right) \tag{2-54}$$

Calculation of fraction emitted (CHEMDAT8). The fraction emitted is the mass of constituent volatilized per mass of constituent influent to the surface impoundment:

$$f_{emitted} = \frac{A K_{OL} C_{liq}}{Q C_{in}} \tag{2-55}$$

where

$f_{emitted}$ = fraction of constituent emitted to the atmosphere (unitless).

Calculation of fraction adsorbed (CHEMDAT8). The fraction adsorbed is the mass of constituent adsorbed per mass of constituent influent to the surface impoundment:

$$f_{adsorbed} = \frac{A\ d_{liq}\ K_{ads}\ C_{liq}}{Q\ C_{in}} \tag{2-56}$$

where

$f_{adsorbed}$ = fraction of constituent adsorbed (unitless).

Calculation of emission flux rate (IWAIR). The emission flux rate is calculated as follows:

$$E = \frac{f_{emitted} Q C_{in}}{A} = K_{OL} C_{liq} \tag{2-57}$$

where

E = emission flux rate of constituent (g/m^2-s).

2.4.4.2 Quiescent Surface Impoundments for Organic-Phase Wastes.

Biodegradation, hydrolysis, and adsorption are not modeled for organic-phase wastes.

Calculation of gas-phase mass transfer coefficient for quiescent surface impoundments (CHEMDAT8). The gas-phase mass transfer coefficient for quiescent surface impoundments is estimated as follows:

$$k_{g,q} = (4.82 \times 10^{-3})\ T_{c,gas}^{0.67}\ U^{0.78}\ Sc_g^{-0.67}\ F^{-0.11} \qquad (2\text{-}58)$$

where

T = temperature of system (°K).

Calculation of overall mass transfer coefficient for organic systems (CHEMDAT8). For organic wastes, the liquid-phase mass transfer coefficient is assumed to be noncontrolling. The liquid-phase mass transfer correlations presented previously for aqueous surface impoundments assume the liquid is water, and these are not applicable to an impoundment containing organic (i.e., nonaqueous) wastes. Consequently, the overall mass transfer coefficient for organic systems is calculated based on the gas-phase mass transfer coefficient and the equilibrium partition coefficient as follows:

$$K_{OL,org} = K_{eq}\ k_{g,q} \qquad (2\text{-}59)$$

where

$K_{OL,org}$ = overall mass transfer coefficient for organic waste (m/s).

The vapor-liquid equilibrium coefficient is calculated using Raoult's law similarly to the vapor-liquid equilibrium coefficient for aqueous systems when Raoult's law is used (Equation 2-46), except the unit conversion factor for aqueous waste is now calculated based on the organic waste properties as follows:

$$K_{eq} = \frac{T_{corr} P_{vap}}{RT} \left(\frac{MW}{\rho_{liq} 10^6} \right) \qquad (2\text{-}60)$$

where

T = temperature of the system (°K)
MW = molecular weight of the organic waste (g/mol)
ρ_{liq} = density of organic waste (g/cm^3)
10^6 = unit conversion factor (cm^3/m^3).

Calculation of fraction emitted (CHEMDAT8). There are no other loss mechanisms for organic systems besides volatilization and the surface impoundment effluent. The fraction emitted is calculated based on a plug-flow model solution as follows:

$$f_{emitted} = 1 - e^{\left(\frac{-AK_{OL,org}}{Q}\right)} \tag{2-61}$$

Calculation of emission flux rate (IWAIR). The emission flux rate is calculated as follows:

$$E = \frac{f_{emitted} QC_{in}}{A} = K_{OL} C_{liq} \tag{2-62}$$

2.4.4.3 Mechanically Aerated Surface Impoundments (Aqueous-Phase Wastes Only). Mechanical aeration is effected by impellers or mixers that agitate the surface of impoundment. Correlations are available to estimate the turbulent mass transfer coefficients for these agitated surfaces based on the power input to the aerators, the impeller size, the rotation speed, and so forth. These correlations are presented below. Although the agitated surface area may extend well beyond the diameter of the aerator impeller, there is usually some portion of the surface impoundment surface area that is not affected by the aerators and that remains quiescent. The overall quiescent mass transfer coefficient for these areas is calculated exactly as it is for quiescent impoundments (Equation 2-38 through Equation 2-46).

Note that organic-phase wastes cannot be modeled for aerated impoundments; the CHEMDAT8 oily film model used to model organic-phase wastes in nonaerated surface impoundments is not applicable to aerated impoundments, as the aeration breaks up the organic film modeled.

Calculation of the liquid-phase mass transfer coefficient for turbulent surface impoundments (CHEMDAT8). The liquid-phase mass transfer coefficient for turbulent surface impoundments is calculated as

$$k_{l,t} = T_{c,liq} \left(\frac{8.22 \times 10^{-3} \; J \; P_{tot} \; 1.024^{(T-20)} \; O_{cf} \; MW_w}{10.76 \; A_t \; \rho_l} \right) \left(\frac{D_w}{D_{O_2,w}} \right)^{0.5} \tag{2-63}$$

where

$k_{l,t}$ = liquid-phase mass transfer coefficient for turbulent surface impoundments (m/s)
J = oxygen transfer rate (lb O_2/h-hp)
P_{tot} = total power to the impellers (hp)
T = liquid temperature in WMU (°C)

O_{cf} = oxygen correction factor[5] (unitless)
MW_w = molecular weight of water (g/mol) = 18 g/mol
A_t = surface area for affected by the aeration (i.e., turbulent) (m^2) = $A \times f_{aer}$
A = surface area of surface impoundment (m^2)
f_{aer} = fraction of total surface impoundment surface area affected by aeration (unitless)
$D_{O2,w}$ = diffusivity of oxygen in water (cm^2/s) = 2.4E−5 cm^2/s.

Calculation of the gas-phase mass transfer coefficient for turbulent surface impoundments (CHEMDAT8). The gas-phase mass transfer coefficient for turbulent surface impoundments is calculated as

$$k_{g,t} = 1.35 \times 10^{-7}\ T_{c,gas}\ Re_g^{1.42}\ p^{0.4}\ Sc_g^{0.5}\ Fr^{-0.21}\ D_a MW_a\ d_{imp}^{-1} \tag{2-64}$$

where

$k_{g,t}$ = gas-phase mass transfer coefficient for turbulent surface areas (m/s)
Re_g = gas-phase Reynolds number = $(d_{imp}^2\ w\ \rho_a)/\mu_g$
p = power number = $0.85\ (550\ P_{tot}/N_{aer})\ g_c\ /\ [(62.428\rho_w)w^3\ (d_{imp}/30.48)^5]$
g_c = gravitational constant = 32.17 lb_m-ft/s^2-lb_f
N_{aer} = number of aerators
w = rotational speed (rad/s)
Fr = Froud number = $[w^2\ (d_{imp}/30.48)]/\ g_c$
MW_a = molecular weight of air (g/mol) = 29 g/mol
d_{imp} = impeller diameter (cm).

Calculation of the overall turbulent surface mass transfer coefficient (CHEMDAT8). The overall turbulent surface mass transfer coefficient is calculated based on the two-resistance module as follows:

$$K_{OL,t} = \left(\frac{1}{k_{l,t}} + \frac{1}{K_{eq}\ k_{g,t}} \right)^{-1} \tag{2-65}$$

where

$K_{OL,t}$ = overall turbulent surface mass transfer coefficient (m/s).

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[5] CHEMDAT8 misnames this input power efficiency. The actual power efficiency, used in the equation for gas-phase turbulent mass transfer coefficient, is hardwired to a value of 0.85 in CHEMDAT8 (see the equation for power number in the list of parameters for Equation 2-64). In order to maintain consistency with CHEMDAT8, IWAIR also terms this input power efficiency and hardwires the real "power efficiency" with a value of 0.85. The default value provided in the IWAIR model and the parameter guidance provided in Appendix B of the *IWAIR User's Guide* for this input are consistent with its use as the oxygen correction factor.

The vapor-liquid partition coefficient is calculated using Equation 2-45 (based on Henry's law) for the initial calculation of the constituent concentration within the surface impoundment. If the constituent concentration within the surface impoundment exceeds the aqueous solubility limit, then the overall mass transfer coefficients are re-calculated using Equation 2-46 for the vapor-liquid partition coefficient (based on Raoult's law).

Calculation of the overall volatilization mass transfer coefficient (CHEMDAT8). The overall volatilization mass transfer coefficient is calculated based on an area-weighted average as follows:

$$K_{OL} = \frac{K_{OL,t}\ A_t + K_{OL,q}\ A_q}{A} \tag{2-66}$$

where

$K_{OL,q}$ = overall mass transfer coefficient for quiescent surface areas (m/s)
A_q = quiescent surface area = $(1-f_{aer})$ A (m^2) (Note: $A_t + A_q$ must equal A).

Calculation of emission flux rates (IWAIR). Once the overall mass transfer coefficient is calculated, the calculations of the adsorption rate coefficient, effluent constituent concentration, fraction emitted, fraction adsorbed, and emission flux rates follow the equations presented for quiescent, aqueous surface impoundments (Equations 2-47 through Equation 2-57).

2.4.4.4 Diffused Air Aerated Surface Impoundments (Aqueous-Phase Wastes Only). Diffused air aeration is effected by blowing air through diffusers or spargers located below the liquid surface (typically near the bottom of the impoundment) and allowing the air bubbles to rise through the liquid to the liquid surface. The rising air bubbles are assumed to come into equilibrium with the liquid so that the diffused air acts to "strip" volatiles from the impoundment. Additionally, the rising bubbles tend to agitate and mix the air-liquid interface, increasing the mass transfer (or creating turbulence) between the air and liquid. No correlations have been developed to estimate the "turbulent" mass transfer coefficients when the turbulence is caused by diffused air aeration; therefore, IWAIR assigns "virtual mechanical aerators" to use as inputs for calculating the overall mass transfer coefficient for the turbulent surfaces following the procedures described for mechanically aerated surface impoundments. Again, there is usually some portion of the surface impoundment surface area that is not affected by the aeration and that remains quiescent. The overall quiescent mass transfer coefficient for these areas is calculated exactly as it is for quiescent, aqueous impoundments (Equation 2-38 through Equation 2-46).

Organic-phase wastes cannot be modeled for aerated impoundments; the CHEMDAT8 oily film model used to model organic-phase wastes in nonaerated surface impoundments is not applicable to aerated impoundments, as the aeration breaks up the organic film modeled.

Calculation of emission rate constant for diffused air (CHEMDAT8). The emission rate caused by the "stripping" action of the bubbles rising through the wastewater is calculated assuming that all of the diffused air comes into equilibrium with the wastewater. An effective first-order emission rate constant is calculated for the diffused air constituent loss as

$$K_{diff} = \frac{K_{eq}\ Q_{air}}{d_{liq}\ A} \tag{2-67}$$

where

K_{diff} = emission rate constant for diffused air (1/s)
Q_{air} = diffused air flow rate (m^3/s).

Again, the vapor-liquid equilibrium partition coefficient is calculated using Equation 2-45 (based on Henry's law) for the initial calculation of the constituent concentration within the surface impoundment. If the constituent concentration within the surface impoundment exceeds the aqueous solubility limit, then the overall mass transfer coefficients are re-calculated using Equation 2-46 for the vapor-liquid partition coefficient (based on Raoult's law).

Calculation of "virtual mechanical aerator" parameters (IWAIR). Diffused air agitates the liquid surface, causing an increased emission rate. This effect is modeled by selecting "virtual mechanical aerator" parameter inputs to be used in calculating the overall turbulent surface area mass transfer coefficient. The algorithms used to calculate the "virtual mechanical aerator" parameters for the diffused-air-only surface impoundments are designed to model a "low" degree of surface turbulence caused by the diffused aeration. If the diffused air system creates a high degree of surface turbulence, the user could develop alternative mechanical aerator inputs and model the unit using the BOTH (DIFFUSED AIR & MECHANICAL) option.

The factor that controls the parameters selected for the virtual mechanical aerator is the turbulent surface area (total surface impoundment area × fraction agitated). Thus, the fraction-agitated parameter for diffused-air-only surface impoundments has a direct impact on the fraction of the surface area to which the overall turbulent mass transfer coefficient is applied, and to a lesser degree, the actual value of the turbulent mass transfer coefficient.

It is assumed that 10 m^2 of surface turbulence is generated per horsepower of a typical aerator. The Treatment Storage and Disposal Facility (TSDF) survey (U.S. EPA, 1991) provides data on several model units with mechanical aerators, including total aerator power and turbulent surface area. The values for turbulent surface area per hp for these model units ranges from 3 to 8.4 m^2/hp. These units reflect real mechanical aerators; diffused air aerators would typically produce less turbulence over a greater area, so a greater turbulent area per hp is desired for the virtual aerators. Thibodeux (1976) provides a range of 0.11 to 20.1 m^2/hp that is typical for mechanically aerated systems. Therefore, a value of 10 m^2/hp was selected as greater than the TSDF reported values and roughly the midpoint of the Thibodeux range. The total power input for the virtual mechanical aerator is then calculated as

$$P_{tot} = \frac{A f_{aer}}{10} \tag{2-68}$$

where

P_{tot} = total power to the impellers (hp)
10 = assumed area of agitation per horsepower applied to aerator (m^2/hp).

It is also assumed that the horsepower of a single aerator is not to exceed 15 hp, and the number of aerators should be a whole number. Consequently, the number of aerators is calculated as follows:

$$N_{aer} = \mathrm{round}\left(\frac{P_{tot}}{15} + 0.5\right) \tag{2-69}$$

where

round() = function that rounds the value to the nearest integer
15 = assumed maximum horsepower of an aerator (hp/aerator)
0.5 = value used to make the round() function round up to the next highest integer.

All other aerator parameters (impeller diameter, impeller speed, oxygen transfer rate, and power efficiency) are selected based on the IWAIR default values for these parameters.

Calculation of the overall volatilization mass transfer coefficient (CHEMDAT8). The overall volatilization mass transfer coefficient is calculated as an area-weighted average of the overall quiescent surface area and turbulent surface area mass transfer coefficients (Equation 2-66). These quiescent surface and turbulent surface mass transfer coefficients are calculated as described in Sections 2.4.4.1 and 2.4.4.3, respectively.

Calculation of effluent concentration (CHEMDAT8). The effluent concentration (and the concentration within the surface impoundment) is calculated using Equation 2-51, but the quadratic term *a* includes the emission rate constant for diffused air as follows:

Quadratic term *a* for systems with diffused air:

$$a = \frac{1}{t_{res}} + \frac{K_{OL}}{d_{liq}} + K_{hyd} + K_{ads} + K_{diff} \tag{2-70}$$

The equation for the quadratic term *b* remains unchanged, but it includes the quadratic term *a* within its equation, so that the value of the quadratic term *b* term is dependent on the diffused air rate constant (K_{diff}).

Calculation of emission flux rates (IWAIR). The remainder of the calculations (fraction emitted, fraction adsorbed, and emission flux rates) follow the equations presented for quiescent, aqueous surface impoundments (Equations 2-55 through Equation 2-57).

2.4.4.5 Both Mechanically and Diffused Air Aerated Surface Impoundments (Aqueous-Phase Wastes Only). Some surface impoundments operate both mechanical aerators and diffused air aeration. These aerators may be used in separate areas of the surface impoundment, or the mechanical aerators may operate above the diffused air aeration (i.e., mechanically agitating the area where the diffused air bubbles are reaching the liquid surface). This system is modeled exactly like the diffused aeration system, except that the mechanical aerator inputs provided by the user are used rather than the values imputed for the "virtual mechanical aerator." As such, the IWAIR solution is most applicable for surface impoundments with mechanical aerators placed above the diffused air aeration or for surface impoundments where the degree of turbulence and or the area affected by the diffused air aeration is small in comparison to the mechanically agitated surface. In these cases, the area affected by the mechanical aeration can be used directly to estimate the fraction agitated input parameter (f_{aer}).

The equations used to calculate the emissions from the both mechanical and diffused air aerated surface impoundments follow the method used for diffused-air-only surface impoundments presented in Section 2.4.4.4 (without the need to calculate "virtual mechanical aerator" parameters).

Note that organic-phase wastes cannot be modeled for aerated impoundments; the CHEMDAT8 oily film model used to model organic-phase wastes in nonaerated surface impoundments is not applicable to aerated impoundments, as the aeration breaks up the organic film modeled.

3.0 Development of Dispersion Factors Using ISCST3

In assessing the potential risk from an emissions source, one of the properties that must be evaluated is the ability of the atmosphere in the local area to disperse the chemicals emitted. When a chemical is emitted, the resulting plume moves away from the source and begins to spread both horizontally and vertically at a rate that is dependant on local atmospheric conditions. The more the plume spreads (i.e., disperses), the lower the concentration of the emitted chemicals will be in the ambient air. Dispersion models are designed to integrate meteorological information into a series of mathematical equations to determine where the material travels after release and how fast the material is ultimately removed from the atmosphere.

IWAIR uses dispersion factors to relate an emission rate to an air concentration at some specified location. A dispersion factor is essentially a measure of the amount of dispersion that occurs from a unit of emission. Dispersion modeling is complex and requires an extensive data set; therefore, the IWAIR model has incorporated a database of dispersion factors. For IWAIR, dispersion was modeled using a standardized unit emission rate (1 $\mu g/m^2$-s) to obtain the air concentration (referred to as a dispersion factor) at a specific point away from the emission source. The unit of measure of the dispersion factor is $\mu g/m^3$ per $\mu g/m^2$-s. The most important inputs to dispersion modeling are the emission rate, meteorological data, the area of the WMU, the height of the WMU relative to the surrounding terrain, and the location of the receptor relative to the WMU. The default dispersion factors in IWAIR were developed for many separate scenarios designed to cover a broad range of unit characteristics, including

- 60 meteorological stations, chosen to represent the different climatic and geographical regions of the contiguous 48 states, Hawaii, Puerto Rico, and parts of Alaska;
- 4 unit types;
- 17 surface areas for landfills, land application units, and surface impoundments, and 11 surface areas and 7 heights for waste piles;
- 6 receptor distances from the unit (25, 50, 75, 150, 500, 1,000 meters); and
- 16 directions in relation to the edge of the unit (only the maximum direction is used).

The default dispersion factors were derived by modeling many scenarios with various combinations of parameters, then choosing as the default the maximum dispersion factor for each WMU/surface area/height/meteorological station/receptor distance combination.

Based on the size and location of a unit, as specified by the user, IWAIR selects an appropriate dispersion factor from the default dispersion factors in the model. If the user specifies a unit surface area or height that falls between two of the sizes already modeled, IWAIR used an interpolation method to estimate a dispersion factor based on the two closest model unit sizes.

The ISCST3 dispersion model (U.S. EPA, 1995) was selected to develop the dispersion factors in IWAIR. ISCST3 was chosen because it can provide reasonably accurate dispersion estimates for both ground-level and elevated area sources. Section 3.1 describes the development of the dispersion factor database used in IWAIR. Section 3.2 describes the interpolation method.

3.1 Development of Dispersion Factor Database

Figure 3-1 summarizes the process by which the dispersion factor database was developed. Each step is described in the following subsections.

3.1.1 Identify WMU Areas and Heights for Dispersion Modeling (Step 1)

Area and height aboveground of a WMU are two of the most sensitive parameters in dispersion modeling. To construct a database that contains benchmark dispersion coefficients, an appropriate set of “model” units to run had to be determined. This set of areas and heights was chosen to cover a range of realistic unit areas and heights and to have a high probability of achieving interpolation errors less than about 5 percent.

Land application units, landfills, and surface impoundments are all ground-level sources and are modeled the same way using ISCST3. However, waste piles are elevated sources and must be modeled separately in ISCST3. Therefore, two sets of areas were developed, one for ground-level sources (land application units, landfills, and surface impoundments), and one for waste piles. In addition, a set of heights was developed for waste piles.[1]

The primary source of data used in the analysis for determining the appropriate range of WMU areas to model was the Industrial D Screening Survey responses (Schroeder et al., 1987). These survey data provide information on the distribution of areas of nonhazardous WMUs across the contiguous 48 states. As a starting point to determine how many and what areas might be needed to adequately cover the reported range, EPA used a statistical method called the Dalenius-Hodges procedure to develop area strata from the Industrial D survey data. This method attempts to break down the distribution of a known variable (in this case, area) that is assumed to be highly correlated with the model output (in this case, dispersion factor) into a

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[1] This important distinction in the dispersion modeling between ground-level sources and elevated sources makes the use of the IWAIR surface impoundment component inappropriate to modeling tanks, which are usually elevated.

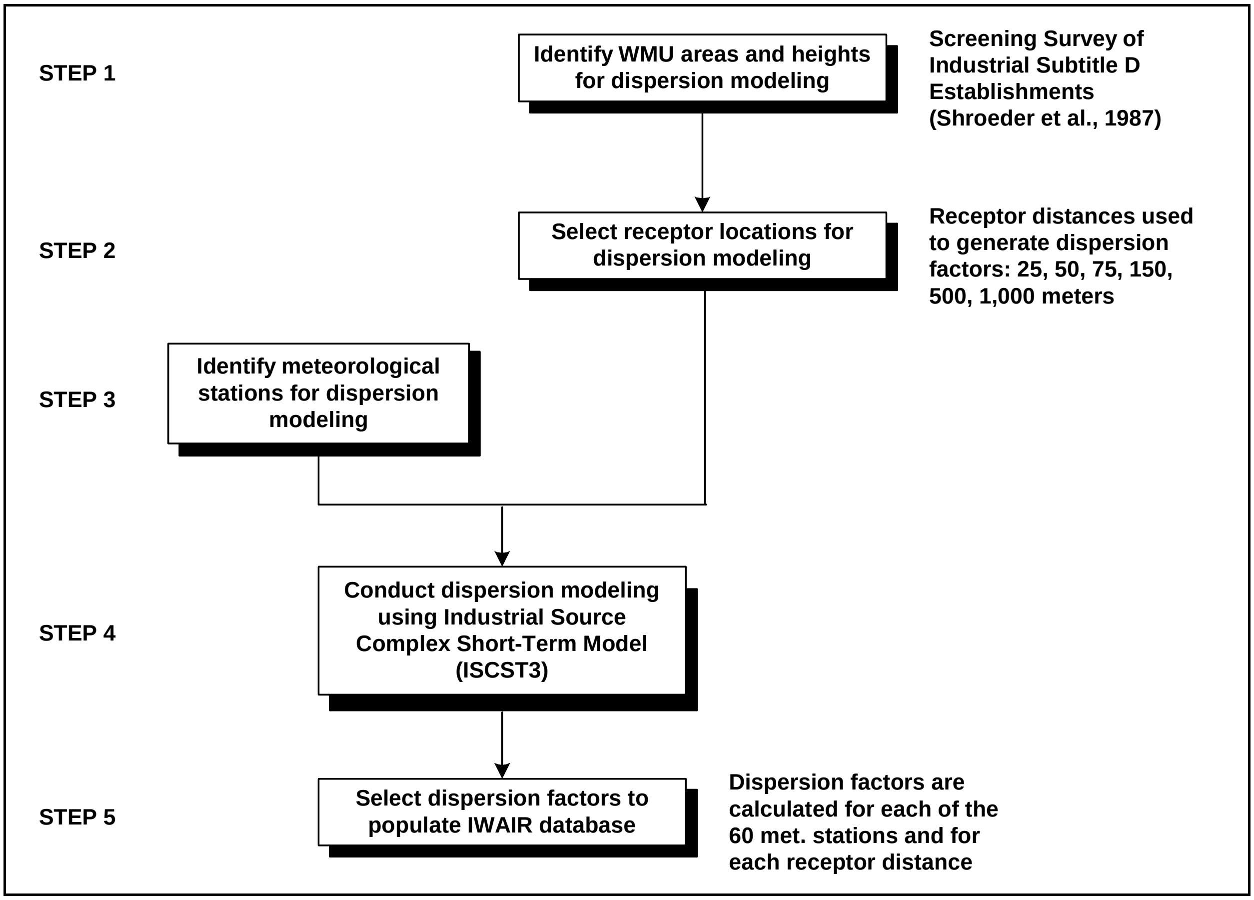

Figure 3-1. Development of dispersion factor database.

fixed number of strata in an optimal way. An area near the midpoint (in this case, the median) for each stratum is then used to represent that stratum.

No data were available on waste pile height. Best professional judgement suggested a realistic range from 1 to 10 m. (For comparison, 10 m is about the height of a 3-story building.) Within this range, seven heights were selected at 1 to 2 m intervals, with smaller intervals at lower heights.

To determine the adequacy of this initial set of areas and heights in achieving the goal of less than 5 percent interpolation error, EPA examined graphical plots of interpolation errors using one- or two-dimensional linear interpolation. These interpolation error plots were generated for three meteorological stations: Fresno, California; Minneapolis, Minnesota; and Salt Lake City, Utah. These stations were chosen to include a range of different wind roses and climate regimes to determine whether the interpolation errors differed significantly based on these factors. Very similar data patterns were seen for these three stations; therefore, EPA felt that further investigation of potential variations by meteorological station was not needed. The steps taken to generate the error plots were as follows:

1. For each of the three sample meteorological stations, run ISCST3 to generate outputs at a set of areas (for ground-level sources) or areas/heights (for waste piles) that represent midpoints between the initial sets of areas and heights. (The midpoints are the points at which error should be the largest.) These ISCST3 outputs represent the "true" outputs for purposes of calculating interpolation errors.

2. For each of the area or area/height midpoints, apply the interpolation algorithm (the interpolation algorithm is discussed in Section 3.2) to estimate the ISCST3 output value.

3. Compute the percentage interpolation error, defined as

$$\frac{(\text{“true” value} - \text{interpolated value})}{(\text{“true” value})} \times 100 \,. \tag{3-1}$$

The error plots using the initial set of areas and heights suggested that additional areas were needed in specific parts of the distribution. Therefore, three areas were added to the set for ground-level sources, and four areas were added to the set for waste piles. A new error plot indicated that this succeeded in reducing the interpolation errors for ground-level sources to within the 5 percent goal using linear interpolation. Errors for waste piles were still as high as about 15 percent, exceeding the 5 percent goal. However, generating data for additional surface areas and heights is only one technique for reducing interpolation errors. Another way to reduce interpolation errors is to choose a more sophisticated interpolation method. This approach was taken for waste piles (and is discussed in Section 3.2), and no further additional areas were added for waste piles.

Table 3-1 shows the final set of surface areas and heights selected for the IWAIR dispersion database. Seventeen areas were modeled for ground-level sources, and 77 combinations of 11 areas and 7 heights were modeled for waste piles.

3.1.2 Select Receptor Locations for Dispersion Modeling (Step 2)

The ISCST3 model allows the user to specify receptors with a Cartesian receptor grid or a polar receptor grid. In general, Cartesian receptor grids are used for near-source receptors and polar receptor grids for more distant receptors. Because it takes a substantial amount of time for the ISCST3 model to execute with a large number of receptor points, it was necessary to reduce the number of receptors without missing representative outputs. Therefore, a sensitivity analysis was conducted on area sources to determine the receptor locations and spacings (see Appendix C for details).

The results of the sensitivity analysis of area sources show that the maximum impacts are generally higher for a dense receptor grid (i.e., 64 or 32 receptors on each square) than for a scattered receptor grid (i.e., 16 receptors on each square). For this application, however, the differences in maximum receptor impacts are not significant between a dense and a scattered

Table 3-1. Final Surface Areas and Heights Used for ISCST3 Model Runs

Ground-Level Sources	Waste Piles	
Areas (m^2)	Areas (m^2)	Heights (m)
81	20	1
324	162	2
567	486	4
1551	2100	5
4047	6,100	6
12,546	10,100	8
40,500	55,550	10
78,957	101,000	
161,880	500,667	
243,000	900,333	
376,776	1,300,000	
607,000		
906,528		
1,157,442		
1,408,356		
4,749,178		
8,090,000		

receptor grid. Therefore, 16 evenly spaced receptor points on each square were used in the modeling. The sensitivity analysis also shows that the maximum downwind concentrations decrease sharply from the edge of the area source to about 1,000 meters from the source. Therefore, receptor points were placed at 25, 50, 75, 150, 500, and 1,000 meters so that a user could examine the areas most likely to have risks of concern.

Because the flat terrain option is used in the dispersion modeling, receptor elevations were not considered.

3.1.3 Identify Meteorological Stations for Dispersion Modeling (Step 3)

Meteorological data at more than 200 meteorological stations in the United States are available on the SCRAM Bulletin Board (http://www.epa.gov/scram001) and from a number of other sources. Because of the time required to develop dispersion factors, it was not feasible to include dispersion factors in IWAIR for all of these stations. Therefore, EPA developed an approach to select a subset of these stations for use in IWAIR. This approach considers the factors most important for the inhalation pathway risk modeling done by IWAIR.

The approach used involved two main steps:

1. Identify contiguous areas that are sufficiently similar with regard to the parameters that affect dispersion that they can be reasonably represented by one meteorological station. The parameters used were

    - Surface-level meteorological data (e.g., wind patterns and atmospheric stability)
    - Physiographic features (e.g., mountains, plains)
    - Bailey's ecoregions and subregions
    - Land cover (e.g., forest, urban areas).

2. For each contiguous area, select one meteorological station to represent the area. The station selection step considered the following parameters:

    - Industrial activity
    - Population density
    - Location within the area
    - Years of meteorological data available
    - Average wind speed.

Appendix D describes the selection process in detail. Table 3-2 lists the 60 stations chosen; Figure 3-2 shows the selected stations and their assigned regions for the contiguous 48 states. Appendix D provides additional maps showing regions of the 48 states on a larger scale, as well as Alaska and Hawaii.

Zip codes were overlaid on the regions, and a database matching zip codes to meteorological stations was generated for use in IWAIR. In addition, latitudinal/longitudinal coordinates of the polygons are used in IWAIR to select a meteorological station based on a facility's latitudinal/longitudinal coordinates.

Table 3-2. Surface-Level Meteorological Stations in IWAIR, by State

Station Number	Station Name	State
26451	Anchorage/WSMO Airport	AK
25309	Juneau/International Airport	AK
13963	Little Rock/Adams Field	AR
23183	Phoenix/Sky Harbor International Airport	AZ
93193	Fresno/Air Terminal	CA
23174	Los Angeles/International Airport	CA
24257	Redding/AAF	CA
23234	San Francisco/International Airport	CA
23062	Denver/Stapleton International Airport	CO
14740	Hartford/Bradley International Airport	CT
12839	Miami/International Airport	FL
12842	Tampa/International Airport	FL
13874	Atlanta/Atlanta-Hartsfield International	GA
03813	Macon/Lewis B Wilson Airport	GA
22521	Honolulu/International Airport	HI
94910	Waterloo/Municipal Airport	IA
24131	Boise/Air Terminal	ID
94846	Chicago/O’Hare International Airport	IL
03937	Lake Charles/Municipal Airport	LA
12916	New Orleans/International Airport	LA
13957	Shreveport/Regional Airport	LA
14764	Portland/International Jetport	ME
94847	Detroit/Metropolitan Airport	MI
14840	Muskegon/County Airport	MI
14922	Minneapolis-St Paul/International Airport	MN
13994	St. Louis/Lambert International Airport	MO
13865	Meridian/Key Field	MS
24033	Billings/Logan International Airport	MT
03812	Asheville/Regional Airport	NC
13722	Raleigh/Raleigh-Durham Airport	NC

(continued)

Table 3-2. (continued)

Station Number	Station Name	State
24011	Bismarck/Municipal Airport	ND
14935	Grand Island/Airport	NE
23050	Albuquerque/International Airport	NM
23169	Las Vegas/McCarran International Airport	NV
24128	Winnemucca/WSO Airport	NV
14820	Cleveland/Hopkins International Airport	OH
93815	Dayton/International Airport	OH
13968	Tulsa/International Airport	OK
94224	Astoria/Clatsop County Airport	OR
24232	Salem/McNary Field	OR
14751	Harrisburg/Capital City Airport	PA
13739	Philadelphia/International Airport	PA
14778	Williamsport-Lycoming/County	PA
11641	San Juan/Isla Verde International Airport	PR
13880	Charleston/International Airport	SC
13877	Bristol/Tri City Airport	TN
13897	Nashville/Metro Airport	TN
23047	Amarillo/International Airport	TX
13958	Austin/Municipal Airport	TX
12924	Corpus Christi/International Airport	TX
03927	Dallas/Fort Worth/Regional Airport	TX
12960	Houston/Intercontinental Airport	TX
23023	Midland/Regional Air Terminal	TX
24127	Salt Lake City/International Airport	UT
13737	Norfolk/International Airport	VA
14742	Burlington/International Airport	VT
24233	Seattle/Seattle-Tacoma International	WA
24157	Spokane/International Airport	WA
03860	Huntington/Tri-State Airport	WV
24089	Casper/Natrona Co International Airport	WY

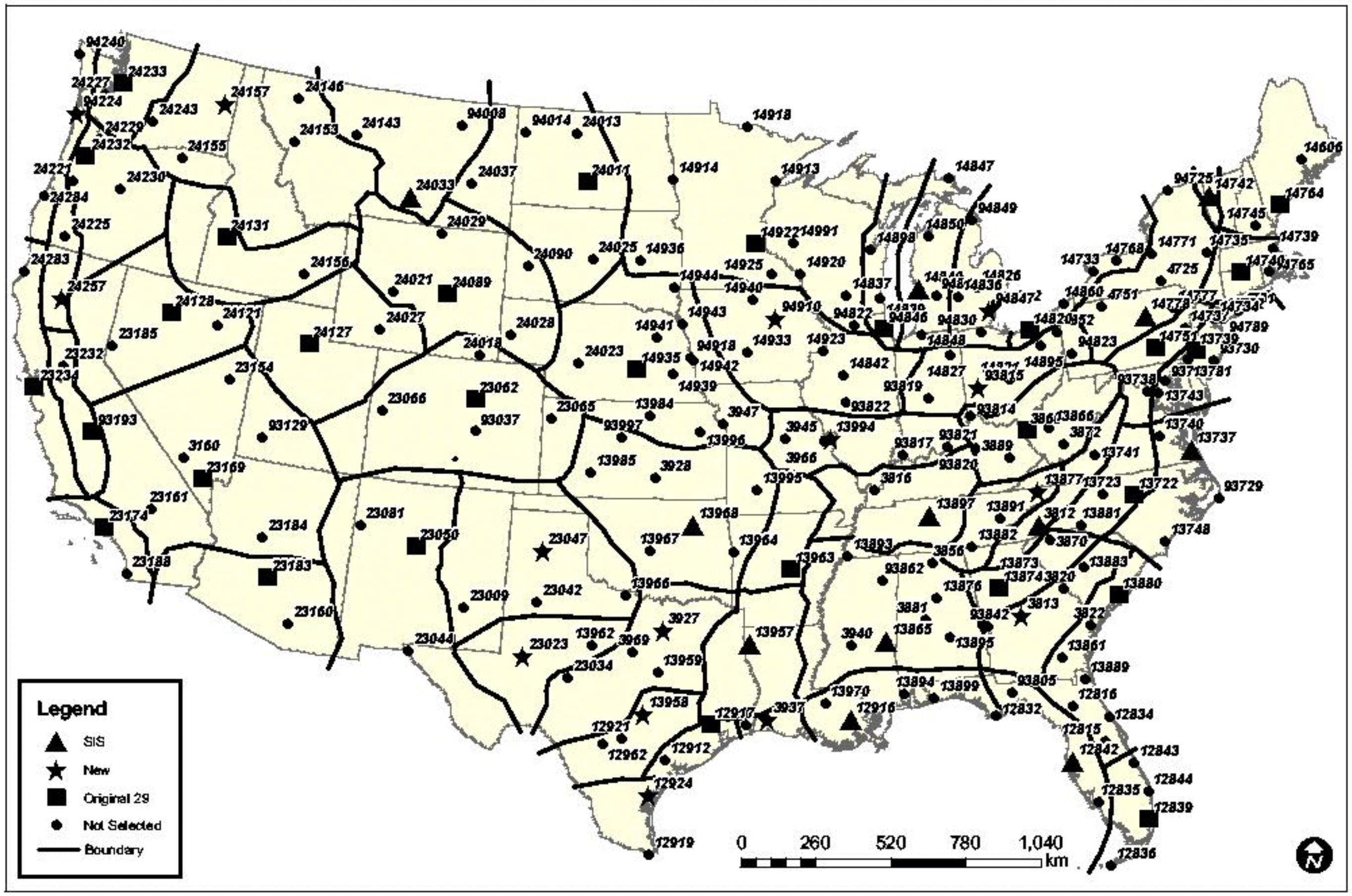

Figure 3-2. Meteorological stations and region boundaries for the contiguous 48 states.

The modeling analysis was conducted using 5 years of representative meteorological data from each of the 60 meteorological stations. Five-year wind roses representing the frequency of wind directions and wind speeds for the 60 meteorological stations were analyzed. These show that the 60 meteorological stations represent a variety of wind patterns.

Shape of Wind Rose for 60 Meteorological Stations

Shape of Wind Rose	No. of Stations
Strongly directional (>20% in 1 direction)	10
Moderately directional (15–20% in 1 direction)	14
Mildly directional (10–14% in 1 direction)	26
Weakly directional (<10% in 1 direction)	10

Wind direction and wind speed are typically the most important meteorological inputs for dispersion modeling analysis. Wind direction determines the direction of the greatest impacts (usually in the prevailing wind direction). For IWAIR, however, wind direction is not important because only the direction of maximum air concentration is used. IWAIR determines air concentration in 16 directions, and uses only the maximum of these; the actual direction associated with that maximum is not retained. Wind speed is inversely proportional to ground-level air concentrations, so that the lower the wind speed, the higher the air concentration.

Mixing height determines the heights to which pollutants can be diffused vertically. Stability class is also an important factor in determining the rate of lateral and vertical diffusion. The more unstable the air, the greater the diffusion.

3.1.4 Conduct Dispersion Modeling Using Industrial Source Complex Short-Term Model, Version 3 (Step 4)

This section discusses the critical parameters of the selected model, ISCST3; the results of sensitivity analyses performed to investigate several of the model parameters; and the receptor locations. Results of the sensitivity analyses are presented in Appendix C.

Key Meteorological Data for the ISCST3 Model without Depletion

Wind direction determines the direction of the greatest impacts.

Wind speed is inversely proportional to ground-level air concentration, so the lower the wind speed, the higher the concentration.

Stability class influences rate of lateral and vertical diffusion. The more unstable the air, the lower the concentration.

Mixing height determines the maximum height to which emissions can disperse vertically. The lower the mixing height, the higher the concentration.

It is impossible to make a general statement about whether IWAIR over- or underestimates actual dispersion coefficients, as this would depend completely on site-specific factors. For some sites, it will overestimate, and for others, underestimate. Because the dispersion assumptions built into IWAIR may not be applicable to all sites, IWAIR was programmed to accommodate user-entered dispersion factors that are a more accurate reflection of the site-specific conditions prevailing at the user's site, if these are available.

3.1.4.1 General Assumptions. This section discusses depletion, rural versus urban mode, and terrain assumptions.

Depletion. ISCST3 can calculate vapor air concentrations with or without wet and dry depletion of vapors. Modeled concentrations without depletion are higher than those with depletion. The dispersion factors for IWAIR were modeled without wet or dry depletion of vapors.

ISCST3 can model dry depletion of vapors only as a chemical-specific process. By contrast, ISCST3 can model wet depletion of vapors as non-chemical-specific process. Thus, vapor air concentrations modeled without depletion or with only wet depletion of vapors can be used for any chemical; vapor air concentrations modeled with dry depletion of vapors are chemical-specific and must be modeled separately for each chemical of interest.

Assumptions Made for Dispersion Modeling

- Dry and wet depletion options were not activated in the dispersion modeling.
- The rural option was used in the dispersion modeling because the types of WMUs being assessed are typically in nonurban areas.
- Flat terrain was assumed.
- An area source was modeled for all WMUs.
- To minimize error due to site orientation, a square area source with sides parallel to *x*- and *y*-axes was modeled.
- Receptor points were placed on 25, 50, 75, 150, 500, and 1,000 m receptor squares starting from the edge of the source, with 16 receptor points on each square.
- Modeling was conducted using a unit emission rate of 1 $\mu g/m^2$-s.

Generating chemical-specific dispersion factors that included dry depletion of vapors would have significantly limited the number of meteorological stations and WMU areas and heights that could be included in IWAIR. Dry depletion of vapors is expected to have a relatively small impact on vapor air concentration; by contrast, the differences in air concentration between different areas and different meteorological stations are considerably greater. Thus, dry depletion of vapors was not modeled, in order to include a greater number of more generally applicable dispersion factors.

A sensitivity analysis showed that the differences in the maximum concentrations with wet depletion and without wet depletion are very small, even for a wet location (less than 0.4 percent). The sensitivity analysis also shows that the run time for calculating concentrations using the ISCST3 model with wet depletion is 15 to 30 times longer than the run time without wet depletion for the 5th and 95th percentile of the sizes of land application units. (The difference is greater for larger sources.) Therefore, concentrations were calculated without wet depletion in this analysis so that a greater number of meteorological locations could be modeled and included in IWAIR.

Rural versus Urban Mode. ISCST3 may be run in rural or urban mode, depending on land use within a 3 km radius from the source. These modes differ with respect to wind profile exponent and potential temperature gradients. Unless the site is located in a heavily metropolitan area, the rural option is generally more appropriate. Because the types of WMUs being assessed are typically in nonurban areas, the rural option was used to develop dispersion factors for IWAIR.

Terrain. Flat terrain for both the source and the surrounding area was assumed in the modeling analysis for two reasons: (1) ISCST3 can only model flat terrain for area sources,[2] and (2) complex terrain simulations in the surrounding area result in air concentrations that are highly dependent on site-specific topography. A specific WMU's location in relation to a hill or valley produces results that would not be applicable to other locations. Complex terrain applications are extremely site-specific; therefore, model calculations from one particular complex terrain location cannot be applied to another. Conversely, simulations from flat terrain produce values that are more universally applicable.

3.1.4.2 Source Release Parameters. This section describes the source parameters and assumptions used in the dispersion modeling, including source type and elevation, and source shape and orientation.

Source Type and Elevation. ISCST3 can model three different types of sources: point, area, and volume. All WMU types modeled in this analysis were modeled as area sources. Landfills, land application units, and surface impoundments were modeled as ground-level sources, and waste piles were modeled as elevated sources.

Source Shape and Orientation. The shape of WMUs facilities and their orientation to the wind affect dispersion. However, in developing generally applicable dispersion factors for use in a screening model, it was necessary to make some assumptions about shape and orientation. A square shape was chosen for the general dispersion factors in IWAIR to minimize the errors caused by source shape and orientation.

A sensitivity analysis was conducted to compare the air concentrations from a square area source, a rectangular area source oriented east to west, and a rectangular area source oriented north to south to determine what role source shape and orientation play in determining dispersion coefficients of air pollutants. The results show that the differences in dispersion factors between the square area source and the two rectangular area sources are smaller than the differences between the two rectangular sources. In addition, a square area source has the least amount of impact on orientation. Because information on source shapes or orientations is not available, a square source was chosen to minimize the errors caused by source shapes and orientations (see the sensitivity analysis in Appendix C for details).

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[2] ISCST3 can model three types of terrain for point sources: flat, simple, and complex (in simple terrain, the terrain features are all below the centerline of the plume; in complex terrain, some terrain features are at or above the centerline of the plume). However, for area sources, only flat terrain can be modeled. Typically, terrain considerations are only important for buoyant emissions from stacks, where the plume is above ground level. In that situation, terrain can affect where the plume reaches ground level, and it can significantly affect predicted ground-level air concentrations. With area sources, the plume is already at ground level, so terrain (either simple or complex) does not significantly affect ground-level air concentrations regardless of receptor distance.

3.1.5 Select Dispersion Factors to Populate IWAIR Database (Step 5)

Dispersion factors were calculated by running ISCST3 with a unit emission rate (i.e., 1 μg/m^2-s). The selected areas for each type of WMU were modeled with 60 representative meteorological locations in the United States using 5 years of meteorological data to estimate dispersion factors. Annual average dispersion factors at all receptor points were calculated.

Typically, the location of maximum impacts with respect to the source is determined by the prevailing wind direction. For each distance, the maximum dispersion factor of the 16 directions was used in the IWAIR database. For ground-level area sources (i.e., landfills, land application units, and surface impoundments), maximum annual-average dispersion factors are always located on the first receptor square (i.e., 25 m receptors). For elevated area sources (i.e., waste piles), the maximum annual-average dispersion factors are usually located on the first receptor square and occasionally located on the second or third receptor square. However, dispersion factors for all six distances are included in the IWAIR database. The annual-average dispersion factors increase with the increasing area of the sources.

Maximum dispersion factors vary with meteorological location. For landfills, land application units, and surface impoundments, the maximum dispersion factors at some meteorological locations can be twice as high as those at other locations. For waste piles, the maximum dispersion factors at some meteorological locations are more than twice those at other meteorological locations.

3.2 Interpolation of Dispersion Factor

As described in Section 3.1, a set of areas and heights were identified for modeling ground-level sources (land application units, landfills, and surface impoundments) and elevated sources (waste piles), and these were modeled for 60 meteorological locations to produce a set of dispersion factors at six receptor distances for use in IWAIR. Each dispersion factor is specific to an area, height, meteorological location, and receptor distance.

This set of dispersion factors may not include a dispersion factor that exactly matches the user’s conditions. The user may be at a different meteorological location, have receptors located at different distances, or have a unit of a different area and height. For meteorological location and receptor distance, users must use one of IWAIR’s 60 meteorological locations or six distances (unless they enter their own dispersion factors); there will be some error associated with this that cannot be reduced. The error associated with differences in the area and height of a unit, however, may be reduced by interpolating between the dispersion factors contained in IWAIR.

The simplest form of interpolation is a one-dimensional linear interpolation. A one-dimensional linear interpolation would estimate a dispersion factor by adjusting for a single variable (in this case, area) and assuming that dispersion factor is linear with that variable. This is done as follows:

$$DF = \left(\frac{A - A_i}{A_j - A_i} \right) \times (DF_j - DF_i) + DF_i \tag{3-2}$$

where

DF = dispersion factor for specific WMU ([µg/m^3]/[µg/m^2-s])
A = area of specific WMU (m^2)
A_i = area modeled in dispersion modeling immediately below area of specific WMU (m^2)
A_j = area modeled in dispersion modeling immediately above area of specific WMU (m^2)
DF_i = dispersion factor developed for area *i* ([µg/m^3]/[µg/m^2-s])
DF_j = dispersion factor developed for area *j* ([µg/m^3]/[µg/m^2-s]).

Linear interpolation can also be two-dimensional to adjust for two variables (in this case, area and height).[3] Finally, nonlinear interpolation (both one- and two-dimensional) may be performed if the output variable (dispersion factor) is not linear with the input variables (area and height).

For ground-level sources, EPA analyzed interpolation error using a one-dimensional linear interpolation (see Section 3.1.1). This analysis indicated that interpolation errors of 5 percent or less could be achieved using linear interpolation on the areas identified in Table 3-1.

For waste piles, a similar analysis of interpolation errors using two-dimensional linear interpolation indicated that a very large number of areas would have to be modeled to reduce interpolation error to 5 percent using linear interpolation techniques. Therefore, EPA chose to implement a two-dimensional spline approach instead. A spline is a nonlinear interpolation technique that takes into account other points near the point of interest rather than just the two adjacent ones (as in linear interpolation). A cubic spline was used in IWAIR. The equations for implementing a spline are standard but complex; see, for example, Mathews (1992), Section 5.3, for details. This approach tends to be more accurate because it accounts for the nonlinear nature of the relationship between area or height and dispersion factor. However, it may behave unpredictably, producing inaccurate results, especially near the edge of the surface (where it has fewer nearby data points to work from) or where the gradient of the surface is steep (i.e., relatively large changes in dispersion factor occur for relatively small changes in area or height). Repeating the error analysis using a two-dimensional spline indicated that interpolation errors of 5 percent or less could be achieved using the areas identified in Table 3-1.

However, as noted above, a spline can occasionally produce inaccurate results. As a check on the spline method, EPA also included the two-dimensional linear interpolation

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[3] For a given area, *A*, and height, *h*, the algorithm first performs a one-dimensional linear interpolation on height for the two available areas adjacent to *A*. From these two interpolated dispersion factors, another one-dimensional linear interpolation is then performed in the area domain.

algorithm in the IWAIR code. The linear interpolation is known to underestimate dispersion factors at all times; therefore, it provides a useful check on the spline. Thus, at an interpolated point, both a spline interpolation and a two-dimensional linear interpolation are performed. In general, the spline's estimate is preferred and used, but some tests (e.g., negative splined concentration) and comparisons against the linearly interpolated value, as well as the values at the surrounding four grid points, are made first. The linear interpolation value is used, and the user notified of that fact, if the splined air concentration is

- less than or equal to zero,
- less than the linear interpolated value,
- less than the minimum of the four nearest points in the database, or
- greater than the maximum of the four nearest points in the database.

4.0 Exposure Factors

This section describes the development of the exposure factors used in IWAIR. These factors are used in the risk equations documented in Section 6. All data in this section are from the *Exposure Factors Handbook* (U.S. EPA, 1997a; hereafter, the EFH). These exposure factors are used only for carcinogenic chemicals (see box below for carcinogens included in IWAIR; the user may add additional carcinogens). For noncarcinogens, the HQ is a ratio of air concentration to the health benchmark (an RfC), and no exposure factors are used.

All exposure factors were developed for the following subpopulations:

- Children aged <1 year
- Children aged 1–5 years
- Children aged 6–11 years
- Children aged 12–18 years
- Adult residents (aged 19 and older)
- Workers.

The age ranges for children were selected for consistency with the data on inhalation rate in the EFH. Most exposure factors were selected to represent typical or central tendency values, not high-end values.

Carcinogens Included in IWAIR

Acetaldehyde
Acrylamide
Acrylonitrile
Allyl chloride
Aniline
Benzene
Benzidine
Benzo(*a*)pyrene
Bromodichloromethane
Butadiene, 1,3-
Carbon tetrachloride
Chlorodibromomethane
Dibromo-3-chloropropane, 1,2-
Dichlorobenzene, p-
Dichloroethane, 1,2-
Dichloroethylene, 1,1-
Dichloropropylene, cis-1,3-
Dichloropropylene, trans-1,3-
Dimethylbenz[*a*]anthracene, 7,12-
Dinitrotoluene, 2,4-
Dioxane, 1,4-
Diphenylhydrazine, 1,2-
Epichlorohydrin
Ethylbenzene
Ethylene dibromide
Ethylene oxide
Formaldehyde
Hexachloro-1,3-butadiene
Hexachlorobenzene
Hexachloroethane
Methyl chloride (chloromethane)
Methylcholanthrene, 3-
Methylene chloride
Nitropropane, 2-
N-Nitrosodiethylamine
N-Nitrosodi-*n*-butylamine
N-Nitrosopyrrolidine
Propylene oxide
TCDD, 2,3,7,8-
Tetrachloroethane, 1,1,1,2-
Tetrachloroethane, 1,1,2,2-
Tetrachloroethylene
Toluidine, o-
Tribromomethane
Trichloroethane, 1,1,2-
Trichloroethylene
Vinyl chloride

Table 4-1 summarizes the exposure factors used in IWAIR. Sections 4.1 through 4.4 describe how the values for inhalation rate, body weight, exposure duration, and exposure frequency, respectively, were determined.

Table 4-1. Summary of Exposure Factors Used in IWAIR

Receptor	Inhalation Rate (m^3/d)	Body Weight (kg)	Exposure Duration (yr)	Exposure Frequency (d/yr)
Child <1	4.5	9.1	1	350
Child 1–5	7.55	15.4	5	350
Child 6–11	11.75	30.8	6	350
Child 12–18	14.0	57.2	7	350
Adult Resident	13.3	69.1	11	350
Worker	10.4	71.8	7.2	250

4.1 Inhalation Rate

To assess chronic exposures, an average daily inhalation rate is needed. Such a rate is based on inhalation values for a variety of activities averaged together.

Table 4-2 summarizes the inhalation rates for long-term exposure recommended in the EFH. The values for adult females (11.3 m^3/d) and adult males (15.2 m^3/d) were averaged and used in IWAIR. For children, the values for males and females were first averaged for each age group if they were not presented as combined male/female. These combined male/female rates for each age group were averaged to form the age groups used in IWAIR. For example, the combined values for ages 1–2 and 3–5 were averaged to obtain a value for ages 1–5.

Table 4-2. Recommended Inhalation Rates for Residents

	Inhalation Rate (m^3/d)		
Age (yr)	**Males**	**Females**	**Males and Females**
<1	NA	NA	4.5
1–2	NA	NA	6.8
3–5	NA	NA	8.3
6–8	NA	NA	10
9–11	14	13	NA
12–14	15	12	NA
15–18	17	12	NA
Adults (19–65+)	15.2	11.3	NA

NA = Not available.
Source: U.S. EPA, 1997a, Table 5-23.

Table 4-3 summarizes the values for inhalation rate for workers presented in the EFH. The recommended hourly average of 1.3 m^3/h was used in IWAIR. To convert this to a daily value, an 8 h workday was assumed, yielding a daily inhalation rate for workers of 10.4 m^3/d. This rate is lower than the adult resident average because it only accounts for 8 h/d instead of 24 h/d.

Table 4-3. Recommended Inhalation Rates for Workers

Activity Type	Mean (m^3/h)	Upper Percentile (m^3/h)
Slow activities	1.1	NA
Moderate activities	1.5	NA
Heavy activities	2.3	NA
Hourly average	1.3	3.5

NA = Not available.
Source: U.S. EPA, 1997a, Table 5-23.

4.2 Body Weight

Body weights were needed that were consistent with the inhalation rates used. Therefore, body weights were needed for children aged <1, 1–5, 6–11, and 12–18 years; adult residents aged 19–29 years; and workers of all ages.

The EFH presents summary data on body weight for adults in EFH Table 7-2. The data for males and females combined are summarized here in Table 4-4. Because an adult resident aged 19–29 was desired, the weighted average of the values for adults aged 18–24 and 25–34 was used, weighting each by the number of years in that age range (six in the 18–24 range and five in the 25–34 range).

Table 4-4. Body Weights for Adults, Males and Females Combined, by Age

Age (yr)	Body Weight (kg)
18–24	67.2
25–34	71.5
35–44	74.0
45–54	74.5
55–65	73.4
65–74	70.7
All (18–74)	71.8

Source: U.S. EPA (1997a), Table 7-2.

For children, the EFH contains mean body weights for 1-year age intervals (e.g., 1 year, 2 years). These values, summarized in Table 4-5 were averaged across the age ranges used in IWAIR.

Table 4-5. Body Weights for Male and Female Children Combined, Aged 6 Months to 18 Years

Age (yr)	Mean (kg)	Age (yr)	Mean (kg)
6–11 months	9.1	10	36.3
1	11.3	11	41.1
2	13.3	12	45.3
3	15.3	13	50.4
4	17.4	14	56.0
5	19.7	15	58.1
6	22.6	16	62.6
7	24.9	17	63.2
8	28.1	18	65.1
9	31.5		

Source: U.S. EPA (1997a), Table 7-3.

4.3 Exposure Duration

For residents, exposure duration was based on data on population mobility reported in the EFH. An overall exposure duration of 30 years, which represents the 75th to 90th percentile for all ages and genders (EFH, Table 15-167), was selected as a high-end value for residents. The 30-year exposure duration was then allocated to the various age ranges modeled, based on the number of years in each age bracket.

For workers, the typical default exposure values used in the past were an 8 h shift, 250 d/yr, for 40 years. The EFH presents data on occupational mobility that are in stark contrast to the assumed value of 40 years at a single place of employment. As presented in the EFH, the median occupational tenure of the working population (109.1 million people) aged 16 years and older in January 1987 was 6.6 years. This value includes full- and part-time workers. The worker modeled in IWAIR is assumed to be a full-time worker. Therefore, a value of 7.2 years, from EFH Table 15-160 and reflecting the median for full-time male and female workers of all ages, was used.

For most unit types, exposure is expected to end when the unit is closed. If this is the case, then exposure duration should not exceed the specified operating life of the unit. In IWAIR, the surface impoundment, landfill, and waste pile are assumed to conform to this expectation. Thus, for those unit types, if the user specifies an operating life of the unit less than the above exposure duration for the selected receptor type, then the operating life is used instead. Land application units are an exception to this assumption. Exposure to constituents applied to land application units is expected to continue after closure. Therefore, in IWAIR, the exposure duration for land application units is not capped using the operating life specified, but is always 30 years for residents and 7.2 years for workers.

4.4 Exposure Frequency

Exposure frequency is the number of days per year that a receptor is exposed. A value of 350 d/yr was used for residents, and a value of 250 d/yr was used for workers. These are based, respectively, on 7 d/wk and 5 d/wk for 50 wk/yr and account for the receptor being elsewhere on vacation for 2 wk/yr.

5.0 Inhalation Health Benchmarks

Chronic inhalation health benchmarks used in IWAIR include RfCs to evaluate noncancer risk from inhalation exposures, and inhalation CSFs to evaluate risk for carcinogens. Inhalation CSFs are used in the model for carcinogenic constituents, regardless of the availability of an RfC. A majority of inhalation health benchmarks were identified in IRIS and HEAST (U.S. EPA, 1997b, 2001a). IRIS and HEAST are maintained by EPA, and values from IRIS and HEAST were used in the model whenever available. Benchmarks from Superfund Risk Assessment Issue Papers, provisional EPA benchmarks, and benchmarks derived by the Agency for Toxic Substances and Disease Registry (ATSDR) and the California Environmental Protection Agency (CalEPA) were also used.

This section presents the noncancer and cancer inhalation benchmarks used in IWAIR. Section 5.1 describes the different types of human health benchmarks used in IWAIR; Sections 5.2 and 5.3 discuss data sources and the hierarchy used to select benchmarks for inclusion in IWAIR; and Section 5.4 provides the inhalation health benchmarks included in IWAIR for each constituent.

IWAIR provides at least one health benchmark for all chemicals included in its database except 3,4-dimethylphenol and divalent mercury. Users may override the IWAIR values with their own values. In this way, users can include new information that becomes available on health benchmarks after IWAIR is released.

5.1 Background

A chemical’s ability to cause an adverse health effect depends on the toxicity of the chemical, the chemical’s route of exposure to an individual (either through inhalation or ingestion), the duration of exposure, and the dose received (the amount that a human inhales or ingests). The toxicity of a constituent is defined by a human health benchmark for each route of exposure. Essentially, a benchmark is a quantitative value used to predict a chemical’s possible toxicity and ability to induce a health effect at certain levels of exposure. These health benchmarks are derived from toxicity data based on animal studies or human epidemiological studies. Each benchmark represents a dose-response estimate that relates the likelihood and severity of adverse health effects to exposure and dose. Because individual chemicals cause different health effects at different doses, benchmarks are chemical-specific.

The RfC is an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is unlikely to pose an appreciable risk of deleterious noncancer effects during an individual’s lifetime. It is not a direct estimator of risk but rather a reference point to gauge the potential effects. At exposures increasingly greater than the RfC, the potential for adverse health effects increases. Lifetime exposure above the RfC does not imply that an adverse health effect would necessarily occur (U.S. EPA, 2001a).

The RfC is the primary benchmark used to evaluate noncarcinogenic hazards posed by inhalation exposures to chemicals. It is based on the "threshold" approach, which is the theory that there is a "safe" exposure level (i.e., a threshold) that must be exceeded before an adverse noncancer effect occurs. RfCs do not provide true dose-response information in that they are estimates of an exposure level or concentration that is believed to be below the threshold level or no-observed-adverse-effects level (NOAEL). The degree of uncertainty and confidence levels in RfCs vary and are based on different toxic effects.

The CSF is an upper-bound estimate (approximating a 95 percent confidence limit) of the increased human cancer risk from a lifetime exposure to an agent. This estimate is usually expressed in units of proportion (of a population) affected per mg of agent per kg body weight per day $(\text{mg/kg-d})^{-1}$. The unit risk factor (URF), which is calculated from the slope factor, is the upper-bound excess lifetime cancer risk estimated to result from continuous exposure to an agent at a concentration of 1 $\mu g/m^3$ in air. That is, if the unit risk factor equals 1.5E–6 $(\mu g/m^3)^{-1}$, then 1.5 excess tumors are expected to develop per 1,000,000 people if they are exposed to 1 µg of the chemical in 1 m^3 of air daily for a lifetime (U.S. EPA, 2001a). Unlike RfCs, CSFs and URFs do not represent "safe" exposure levels; rather, they describe the relationship between level of exposure and probability of effect or risk.

5.2 Data Sources

Human health benchmarks were obtained primarily from IRIS, EPA's electronic database containing information on human health effects (U.S. EPA, 2001a), and from HEAST, a comprehensive listing of provisional noncarcinogenic and carcinogenic health toxicity values derived by EPA (U.S. EPA, 1997b). These sources and others used are described below. Inhalation CSFs are not available from IRIS (with the exception of benzidene) and are often not available from other sources, so they were calculated from inhalation URFs (which are available from IRIS), using the following equation (U.S. EPA, 1997b):

$$CSF_{inh} = \frac{URF_{inh} \times BW \times 1000}{IR} \tag{5-1}$$

where

CSF_{inh} = inhalation cancer slope factor $(\text{mg/kg-d})^{-1}$
URF_{inh} = inhalation unit risk factor $(\mu g/m^3)^{-1}$
BW = body weight (kg) = 70 kg
1000 = unit conversion (µg/mg)
IR = inhalation rate (m^3/day) = 20 m^3/day

The body weight and inhalation rate used in this equation are averages; because these standard estimates of body weight and inhalation rate are used by EPA in the calculation of URFs, these values are needed to convert inhalation URFs to inhalation CSFs.

The following sections describe each of the data sources used.

5.2.1 IRIS

Benchmarks in IRIS are prepared and maintained by EPA, and values from IRIS were used in IWAIR whenever available. Each chemical file in IRIS contains descriptive and quantitative information on potential health effects. Health benchmarks for chronic noncarcinogenic health effects include reference doses (RfDs) and RfCs. Cancer classification, oral CSFs, and inhalation URFs are included for carcinogenic effects. IRIS is the official repository of Agency-wide consensus information on human health toxicity benchmarks for use in risk assessments.

5.2.2 Superfund Technical Support Center

The Superfund Technical Support Center (EPA's National Center for Environmental Assessment (NCEA)) derives provisional RfCs, RfDs, and CSFs for certain chemicals. These provisional health benchmarks can be found in Risk Assessment Issue Papers. Some of the provisional values have been externally peer reviewed. The provisional health benchmarks have not undergone EPA's formal review process for finalizing benchmarks and do not represent Agency-wide consensus information.

A health benchmark developed by EPA is considered "provisional" if the value has had some form of Agency review but does not represent Agency-wide consensus (i.e., it does not appear on IRIS). At the time each provisional health benchmark was derived, all available toxicological information was evaluated, the value was calculated using the most current methodology, and a consensus was reached on the value by an individual EPA program office (but not Agency-wide) (U.S. EPA, 1997b). All health benchmarks not identified from IRIS, including minimum risk levels (MRLs) and CalEPA cancer potency factors and reference exposure levels (RELs), were treated as provisional health benchmarks.

5.2.3 HEAST

HEAST is a comprehensive listing of provisional noncarcinogenic and carcinogenic health toxicity values (RfDs, RfCs, URFs, and CSFs) derived by EPA (U.S. EPA, 1997b). HEAST benchmarks are considered secondary to those contained in IRIS. Although the health toxicity values in HEAST have undergone review and have the concurrence of individual EPA program offices, either they have not been reviewed as extensively as those in IRIS or their data set is not complete enough for the values to be listed in IRIS. HEAST benchmarks have not been updated in several years and do not represent Agency-wide consensus information.

5.2.4 Other EPA Documents

EPA has also derived health benchmark values that are reported in other risk assessment documents, such as Health Assessment Documents (HADs), Health Effect Assessments (HEAs), Health and Environmental Effects Profiles (HEEPs), Health and Environmental Effects Documents (HEEDs), Drinking Water Criteria Documents, and Ambient Water Quality Criteria Documents. Evaluations of potential carcinogenicity of chemicals in support of reportable quantity adjustments were published by EPA's Carcinogen Assessment Group (CAG) and may include cancer potency factor estimates. Health toxicity values identified in these EPA documents are usually dated and are not recognized as Agency-wide consensus information or verified benchmarks.

5.2.5 ATSDR

ATSDR calculates MRLs that are substance-specific health guidance levels for noncarcinogenic endpoints. An MRL is an estimate of the daily human exposure to a hazardous substance that is unlikely to pose an appreciable risk of adverse noncancer health effects over a specified exposure duration. MRLs are based on noncancer health effects only and are not based on a consideration of cancer effects. MRLs are derived for acute, intermediate, and chronic exposure durations for oral and inhalation routes of exposure. Inhalation and oral MRLs are derived in a manner similar to EPA's RfCs and RfDs, respectively (i.e., ATSDR uses the NOAEL/uncertainty factor (UF) approach); however, MRLs are intended to serve as screening levels and are exposure-duration-specific. Also, ATSDR uses EPA's 1994 inhalation dosimetry methodology (U.S. EPA, 1994b) in the derivation of inhalation MRLs.

5.2.6 CalEPA

CalEPA has developed cancer potency factors for chemicals regulated under California's Hot Spots Air Toxics Program (CalEPA, 1999a). The cancer potency factors are analogous to EPA's oral and inhalation CSFs. CalEPA has also developed chronic inhalation RELs, analogous to EPA's RfC, for 120 substances (CalEPA, 1999b, 2000). CalEPA used EPA's 1994 inhalation dosimetry methodology in the derivation of inhalation RELs. The cancer potency factors and inhalation RELs have undergone internal peer review by various California agencies and have been the subject of public comment.

5.3 Hierarchy Used

Different benchmarks from more than one of the above sources may be available for some chemicals. EPA established a hierarchy for the data sources to determine which benchmark would be used when more than one was available. In establishing this hierarchy, EPA sources were preferred over non-EPA sources, and among EPA sources, those reflecting greater consensus and review were preferred.

Because IRIS is EPA's official repository of Agency-wide consensus human health risk information, benchmarks from IRIS were used whenever available. Benchmarks from the Superfund Technical Support Center and HEAST were used if none were available from IRIS. If health benchmarks were not available from IRIS, the Superfund Technical Support Center, or HEAST, benchmarks from alternative sources were sought. Benchmarks were selected from sources in the following order of preference:

- IRIS
- Superfund Technical Support Center Provisional Benchmarks
- HEAST
- ATSDR MRLs
- CalEPA chronic inhalation RELs and cancer potency factors
- EPA health assessment documents
- Various other EPA health benchmark sources.

5.4 Chronic Inhalation Health Benchmarks Included in IWAIR

The chronic inhalation health benchmarks used in IWAIR are summarized in Table 5-1. The CAS number, constituent name, RfC (in units of mg/m^3), noncancer target organs, inhalation CSF $(mg/kg\text{-}d)^{-1}$, inhalation URF $(\mu g/m^3)^{-1}$, and reference for each benchmark are provided in this table. "RfC target organ or critical effect" refers to the target organ (e.g., kidney, liver) or critical effect used as the basis for the RfC. The critical effect for a few benchmarks is listed as "no effect" and refers to the fact that no adverse effects were observed in the principal study. For acetonitrile, the RfC was based on increased mortality at higher dosage levels; therefore, the target organ was classified as "death." A key to the references cited and abbreviations used is provided at the end of the table.

For a majority of IWAIR constituents, human health benchmarks were available from IRIS (U.S. EPA, 2001a), Superfund Risk Issue Papers, or HEAST (U.S. EPA, 1997b). Benchmarks also were obtained from ATSDR (2001) or CalEPA (1999a, 1999b, 2000). In most cases, the benchmarks were taken directly from the cited source. This section describes the exceptions, in which benchmarks were adapted from the cited source.

- The cancer risk estimates for **benzene** are provided as ranges in IRIS. The inhalation URF for benzene is 2.2E−6 to 7.8E−6 $(\mu g/m^3)^{-1}$ (U.S. EPA, 2001a). For IWAIR, the upper-range estimate was used (i.e., 7.8E−6 $(\mu g/m^3)^{-1}$ for the inhalation URF).

- Based on use of the linearized multistage model, an inhalation URF of 4.4E−6 per $\mu g/m^3$ was recommended for **vinyl chloride** in IRIS and was used for IWAIR to account for continuous, lifetime exposure during adulthood; an inhalation CSF of 1.5E−2 per mg/kg-d was calculated from the URF.

- The benchmarks for 1,3-dichloropropene were used as surrogate data for **cis-1,3-dichloropropylene** and **trans-1,3-dichloropropylene**. The studies cited in the IRIS file for 1,3-dichloropropene used a technical-grade chemical that contained about a 50/50 mixture of the cis- and trans-isomers. The RfC is 2E−2 mg/m^3. The inhalation URF for 1,3-dichloropropene is 4E−6 $(\mu g/m^3)^{-1}$ (U.S. EPA, 2001a).

Table 5-1. Chronic Inhalation Health Benchmarks Used in IWAIR

Name	CAS No.	RfC (mg/m^3)	RfC Ref	RfC Target Organ or Critical Effect	URF (µg/m3)$^{-1}$	URF Ref	CSFi (mg/kg-d)$^{-1}$	CSFi Ref
Acetaldehyde	75-07-0	9.0E-03	I	Respiratory	2.2E-06	I	7.7E-03	calc
Acetone	67-64-1	3.1E+01	A	Neurological				
Acetonitrile	75-05-8	6.0E-02	I	Death				
Acrolein	107-02-8	2.0E-05	I	Respiratory				
Acrylamide	79-06-1				1.3E-03	I	4.6E+00	calc
Acrylic acid	79-10-7	1.0E-03	I	Respiratory				
Acrylonitrile	107-13-1	2.0E-03	I	Respiratory	6.8E-05	I	2.4E-01	calc
Allyl chloride	107-05-1	1.0E-03	I	Neurotoxicity	6.0E-06	C99a	2.1E-02	calc
Aniline	62-53-3	1.0E-03	I	Spleen	1.6E-06	C99a	5.6E-03	calc
Benzene	71-43-2	6.0E-02	C00	Hematological, developmental, neurological	7.8E-06	I	2.7E-02	calc
Benzidine	92-87-5				6.7E-02	I	2.3E+02	I
Benzo(a)pyrene	50-32-8				1.1E-03	C99a	3.9E+00	calc
Bromodichloromethane	75-27-4				1.8E-05	AC	6.2E-02	AC
Butadiene, 1,3-	106-99-0	2.0E-02	C00	Reproductive	2.8E-04	I	9.8E-01	calc
Carbon disulfide	75-15-0	7.0E-01	I	Neurological				
Carbon tetrachloride	56-23-5	7.0E-03	SF	Liver	1.5E-05	I	5.3E-02	calc
Chlorobenzene	108-90-7	6.0E-02	SF	Liver				
Chlorodibromomethane	124-48-1				2.4E-05	AC	8.4E-02	AC
Chloroform	67-66-3	1.0E-01	A	Liver				
Chlorophenol, 2-	95-57-8	1.4E-03	AC	Reproductive, developmental				
Chloroprene	126-99-8	7.0E-03	H	Respiratory				
Cresols (total)	1319-77-3	6.0E-01	C00	Neurological				
Cumene	98-82-8	4.0E-01	I	Adrenal, kidney				
Cyclohexanol	108-93-0	2.0E-05	solv	NA				
Dibromo-3-chloropropane, 1,2-	96-12-8	2.0E-04	I	Reproductive	6.9E-07	H	2.4E-03	calc
Dichlorodifluoromethane	75-71-8	2.0E-01	H	Liver				
Dichloroethane, 1,2-	107-06-2	2.4E+00	A	Liver	2.6E-05	I	9.1E-02	calc
Dichloroethylene, 1,1-	75-35-4	7.0E-02	C00	Liver	5.0E-05	I	1.8E-01	calc

(continued)

Table 5-1. (continued)

Name	CAS No.	RfC (mg/m^3)	RfC Ref	RfC Target Organ or Critical Effect	URF (µg/m3)$^{-1}$	URF Ref	CSFi (mg/kg-d)$^{-1}$	CSFi Ref
Dichloropropane, 1,2-	78-87-5	4.0E-03	I	Respiratory				
Dichloropropylene, cis-1,3-	10061-01-5	2.0E-02	surr	Respiratory	4.0E-06	surr	1.4E-02	calc
Dichloropropylene, trans-1,3-	10061-02-6	2.0E-02	surr	Respiratory	4.0E-06	surr	1.4E-02	calc
Dimethylbenz[a]anthracene, 7,12-	57-97-6				7.1E-02	C99a	2.5E+02	calc
Dimethylphenol, 3,4-	95-65-8							
Dinitrotoluene, 2,4-	121-14-2				8.9E-05	C99a	3.1E-01	calc
Dioxane, 1,4-	123-91-1	3.0E+00	C00	Liver, kidney, hematological	7.7E-06	C99a	2.7E-02	calc
Diphenylhydrazine, 1,2-	122-66-7				2.2E-04	I	7.7E-01	calc
Epichlorohydrin	106-89-8	1.0E-03	I	Respiratory	1.2E-06	I	4.2E-03	calc
Epoxybutane, 1,2-	106-88-7	2.0E-02	I	Respiratory				
Ethoxyethanol acetate, 2-	111-15-9	3.0E-01	C00	Developmental				
Ethoxyethanol, 2-	110-80-5	2.0E-01	I	Hematological, reproductive				
Ethylbenzene	100-41-4	1.0E+00	I	Developmental	1.1E-06	SF	3.9E-03	calc
Ethylene dibromide	106-93-4	2.0E-04	H	Reproductive	2.2E-04	I	7.7E-01	calc
Ethylene glycol	107-21-1	4.0E-01	C00	Respiratory, kidney, developmental				
Ethylene oxide	75-21-8	3.0E-02	C00	Neurological	1.0E-04	H	3.5E-01	calc
Formaldehyde	50-00-0	9.8E-03	A	Respiratory	1.3E-05	I	4.6E-02	calc
Furfural	98-01-1	5.0E-02	H	Respiratory				
Hexachloro-1,3-butadiene	87-68-3				2.2E-05	I	7.7E-02	calc
Hexachlorobenzene	118-74-1				4.6E-04	I	1.6E+00	calc
Hexachlorocyclopentadiene	77-47-4	2.0E-04	I	Respiratory				
Hexachloroethane	67-72-1				4.0E-06	I	1.4E-02	calc
Isophorone	78-59-1	2.0E+00	C99b	Developmental, kidney, liver				
Mercury (elemental)	7439-97-6	3.0E-04	I	Neurotoxicity				
Methanol	67-56-1	4.0E+00	C00	Developmental				
Methoxyethanol acetate, 2-	110-49-6	9.0E-02	C00	Reproductive				
Methoxyethanol, 2-	109-86-4	2.0E-02	I	Reproductive				

(continued)

Table 5-1. (continued)

Name	CAS No.	RfC (mg/m^3)	RfC Ref	RfC Target Organ or Critical Effect	URF (µg/m3)$^{-1}$	URF Ref	CSFi (mg/kg-d)$^{-1}$	CSFi Ref
Methyl bromide	74-83-9	5.0E-03	I	Respiratory				
Methyl chloride	74-87-3	9.0E-02	I	Neurological	1.8E-06	H	6.3E-03	calc
Methyl ethyl ketone	78-93-3	1.0E+00	I	Developmental				
Methyl isobutyl ketone	108-10-1	8.0E-02	H	Liver, kidney				
Methyl methacrylate	80-62-6	7.0E-01	I	Respiratory				
Methyl tert-butyl ether	1634-04-4	3.0E+00	I	Kidney, liver, eye				
Methylcholanthrene, 3-	56-49-5				6.3E-03	C99a	2.2E+01	calc
Methylene chloride	75-09-2	3.0E+00	H	Liver	4.7E-07	I	1.6E-03	calc
N,N-Dimethyl formamide	68-12-2	3.0E-02	I	Liver				
Naphthalene	91-20-3	3.0E-03	I	Respiratory				
n-Hexane	110-54-3	2.0E-01	I	Neurotoxicity, respiratory				
Nitrobenzene	98-95-3	2.0E-03	H	Adrenal, hematological, kidney, liver				
Nitropropane, 2-	79-46-9	2.0E-02	I	Liver	2.7E-03	H	9.5E+00	calc
N-Nitrosodiethylamine	55-18-5				4.3E-02	I	1.5E+02	calc
N-Nitrosodi-n-butylamine	924-16-3				1.6E-03	I	5.6E+00	calc
N-Nitrosopyrrolidine	930-55-2				6.1E-04	I	2.1E+00	calc
o-Dichlorobenzene	95-50-1	2.0E-01	H	Body weight				
o-Toluidine	95-53-4				6.9E-05	AC	2.4E-01	AC
p-Dichlorobenzene	106-46-7	8.0E-01	I	Liver	1.1E-05	C99a	3.9E-02	calc
Phenol	108-95-2	2.0E-01	C00	Liver, cardiovascular, kidney, neurological				
Phthalic anhydride	85-44-9	1.2E-01	H	Respiratory				
Propylene oxide	75-56-9	3.0E-02	I	Respiratory	3.7E-06	I	1.3E-02	calc
Pyridine	110-86-1	7.0E-03	EPA86	Liver				
Styrene	100-42-5	1.0E+00	I	Neurotoxicity				
TCDD, 2,3,7,8-	1746-01-6				3.3E+01	H	1.5E+05	H
Tetrachloroethane, 1,1,1,2-	630-20-6				7.4E-06	I	2.6E-02	calc

(continued)

Table 5-1. (continued)

Name	CAS No.	RfC (mg/m^3)	RfC Ref	RfC Target Organ or Critical Effect	URF (μg/m3)$^{-1}$	URF Ref	CSFi (mg/kg-d)$^{-1}$	CSFi Ref
Tetrachloroethane, 1,1,2,2-	79-34-5				5.8E-05	I	2.0E-01	calc
Tetrachloroethylene	127-18-4	3.0E-01	A	Neurological	5.8E-07	HAD	2.0E-03	HAD
Toluene	108-88-3	4.0E-01	I	Neurological, respiratory				
Tribromomethane	75-25-2				1.1E-06	I	3.9E-03	calc
Trichloro-1,2,2-trifluoroethane, 1,1,2-	76-13-1	3.0E+01	H	Body weight				
Trichlorobenzene, 1,2,4-	120-82-1	2.0E-01	H	Liver				
Trichloroethane, 1,1,1-	71-55-6	2.2E+00	SF	Neurological				
Trichloroethane, 1,1,2-	79-00-5				1.6E-05	I	5.6E-02	calc
Trichloroethylene	79-01-6	6.0E-01	C00	Neurological, eyes	1.7E-06	HAD	6.0E-03	HAD
Trichlorofluoromethane	75-69-4	7.0E-01	H	Kidney, respiratory				
Triethylamine	121-44-8	7.0E-03	I	Respiratory				
Vinyl acetate	108-05-4	2.0E-01	I	Respiratory				
Vinyl chloride	75-01-4	1.0E-01	I	Liver	4.4E-06	I	1.5E-02	calc
Xylenes	1330-20-7	4.0E-01	A	Neurological				

[a] Sources:
A = ATSDR MRLs (ATSDR, 2001)
AC = Developed for the Air Characteristic Study (U.S. EPA, 1999d)
C99a = CalEPA cancer potency factor (CalEPA, 1999a)
C99b = CalEPA chronic RELs (CalEPA, 1999b)
C00 = CalEPA chronic RELs (CalEPA, 2000)
I = IRIS (U.S. EPA, 2001a)
H = HEAST (U.S. EPA, 1997b)
HAD = Health Assessment Document (U.S. EPA, 1986a, 1987a)
SF = Superfund Risk Issue Paper (U.S. EPA, 1998a, 1999a,b,c)
solv = 63 FR 64371-0402 (U.S. EPA, 1998b)
surr = surrogate

[b] RfC and URF are for 1,3-dichloropropylene (U.S. EPA, 2001a)

[c] RfC is for total xylenes (ATSDR, 2001).

- A provisional subchronic RfC of 2E‑2 mg/m^3 was developed by the Superfund Technical Support Center (U.S. EPA, 1999a) for **carbon tetrachloride**. A provisional chronic RfC of 7E‑3 was derived by applying an uncertainty factor of 3 to account for the use of a subchronic study.

- An inhalation acceptable daily intake (ADI) of 2E‑3 mg/kg-d based on an inhalation study was identified for **pyridine** (U.S. EPA, 1986b). An ADI is defined as "the amount of chemical to which humans can be exposed on a daily basis over an extended period of time (usually a lifetime) without suffering a deleterious effect." The units of an ADI (mg/kg-d) differ from those of an RfC (mg/m^3), illustrating that the inhalation ADI represents an internal dose, while an RfC represents an air concentration. In the U.S. EPA (1986b), EPA calculated the inhalation ADI by

  1. Using a lowest-observed-adverse-effect level (LOAEL) of 32.35 mg/m^3 (for increased liver weights observed in rats exposed to pyridine via inhalation)

  2. Assuming a rat breathes 0.223 m^3/day, absorbs 50 percent of the inhaled pyridine, and weighs 0.35 kg

  3. Converting from intermittent to continuous exposure by multiplying by 7/24 and 5/7.[1] (A "transformed dose" of 2.15 mg/kg-d results from these first three steps).

  4. Dividing the "transformed dose" of 2.15 mg/kg-d by an uncertainty factor of 1,000 (10 for interspecies extrapolation, 10 for human variability, and 10 for use of a LOAEL) (U.S. EPA, 1986b).

  The equation used in U.S. EPA (1986b) to calculate the inhalation ADI is as follows:

$$\text{inhalation ADI} = \frac{\text{LOAEL} \times \text{IR} \times 0.50 \times 5/7 \times 7/24}{\text{BW} \times 1000}$$

  where

  LOAEL = lowest-observed-adverse-effect level (mg/m^3) = 32.35
  IR = inhalation rate of rat (m^3/d) = 0.233
  BW = body weight of rat (kg) = 0.35.

---

[1] Rats were exposed to pyridine for 7 hours per day (instead of 24), 5 days per week (instead of 7).

For IWAIR, the inhalation ADI was converted to a provisional RfC of 7E−3 mg/m^3 by eliminating the parameters that were used to estimate an internal dose: rat inhalation rate, percent absorption, and rat body weight, thereby resulting in an air concentration suitable for use as a provisional RfC. The calculation is as follows:

$$\text{provisional RfC} = \frac{\text{LOAEL} \times 5/7 \times 7/24}{1000}$$

where

LOAEL = lowest-observed-adverse-effect level (mg/m^3) = 32.35.

Provisional inhalation health benchmarks were developed in the Air Characteristic Study (U.S. EPA, 1999d) for several constituents lacking IRIS, HEAST, alternative EPA, or ATSDR values. Those used for IWAIR are summarized in Table 5-2 below. Additional details on the derivation of these inhalation benchmarks can be found in the *Revised Risk Assessment for the Air Characteristic Study* (U.S. EPA, 1999d).

- A provisional RfC was developed in the Air Characteristic Study for **2-chlorophenol** using route-to-route extrapolation of the oral RfD.
- Based on oral CSFs from IRIS and HEAST, provisional inhalation URFs and inhalation CSFs were developed for **bromodichloromethane**, **chlorodibromomethane**, and **o-toluidine**.

Table 5-2. Provisional Inhalation Benchmarks Developed in the Air Characteristic Study

CAS No.	Chemical Name	RfC (mg/m^3)	RfC Target	Inh URF (µg/m^3)$^{-1}$	Inh CSF (mg/kg-d)$^{-1}$
75-27-4	Bromodichloromethane (dichlorobromomethane)			1.8E−5	6.2E−2
124-48-1	Chlorodibromomethane (dibromochloromethane)			2.4E−5	8.4E−2
95-57-8	2-Chlorophenol (o-)	1.4E−3	Reproductive, developmental		
95-53-4	o-Toluidine (2-methylaniline)			6.9E−5	2.4E−1

Finally, **chloroform** presents an unusual case. EPA has classified chloroform as a Group B2, Probable Human Carcinogen, based on an increased incidence of several tumor types in rats and mice (U.S. EPA, 2001a). However, based on an evaluation initiated by EPA's Office of Water (OW), the Office of Solid Waste (OSW) now believes the weight of evidence for the carcinogenic mode of action for chloroform does not support a mutagenic mode of action; therefore, a nonlinear low-dose extrapolation is more appropriate for assessing risk from exposure to chloroform. EPA's Science Advisory Board (SAB), the World Health Organization (WHO), the Society of Toxicology, and EPA all strongly endorse the nonlinear approach for assessing risks from chloroform. Although OW conducted its evaluation of chloroform carcinogenicity for oral exposure, a nonlinear approach for low-dose extrapolation would apply to inhalation exposure to chloroform as well, because chloroform's mode of action is understood to be the same for both ingestion and inhalation exposures. Specifically, tumorigenesis for both ingestion and inhalation exposures is induced through cytotoxicity (cell death) produced by the oxidative generation of highly reactive metabolites (phosgene and hydrochloric acid), followed by regenerative cell proliferation (U.S. EPA, 1998c). Chloroform-induced liver tumors in mice have only been seen after bolus corn oil dosing and have not been observed following administration by other routes (i.e., drinking water and inhalation). As explained in EPA OW's March 31, 1998, and December 16, 1998, *Federal Register* notices pertaining to chloroform (U.S. EPA 1998c and 1998d, respectively), EPA now believes that "based on the current evidence for the mode of action by which chloroform may cause tumorigenesis, ... a nonlinear approach is more appropriate for extrapolating low dose cancer risk rather than the low dose linear approach..." (U.S. EPA 1998c). OW determined that, given chloroform's mode of carcinogenic action, liver toxicity (a noncancer health effect) actually "is a more sensitive effect of chloroform than the induction of tumors" and that protecting against liver toxicity "should be protective against carcinogenicity given that the putative mode of action ... for chloroform involves cytotoxicity as a key event preceding tumor development" (U.S. EPA 1998c).

The recent evaluations conducted by OW concluded that protecting against chloroform's noncancer health effects protects against excess cancer risk. EPA now believes that the noncancer health effects resulting from inhalation of chloroform would precede the development of cancer and would occur at lower doses than tumor development. Although EPA has not finalized a noncancer health benchmark for inhalation exposure (i.e., an RfC), ATSDR has developed an inhalation MRL for chloroform. Therefore, ATSDR's chronic inhalation MRL for chloroform (0.1 mg/m^3) was used in IWAIR.

6.0 Calculation of Risk or Allowable Waste Concentration

This section describes how IWAIR calculates risk or allowable waste concentration using the emission rate, dispersion factor, exposure factors, and health benchmarks described in previous sections.

6.1 Calculation of Risk or Hazard Quotient

IWAIR calculates risk for carcinogens and HQ for noncarcinogens. To calculate risk from a specified chemical to a specified receptor, IWAIR uses the following steps:

1. Calculate emission rates from user inputs or user-specified emission rates; the emission rates are chemical-specific and, if calculated by IWAIR, depend on user-specified waste concentrations.

2. Calculate dispersion factors from user inputs or user-specified dispersion factors; the dispersion factors are receptor-specific.

3. Calculate air concentrations from emission rates and dispersion factors; the air concentrations are chemical- and receptor-specific.

4. Calculate risks or HQs from air concentrations and, for carcinogens, exposure factors.

Calculation of emission rates and dispersion factors (Steps 1 and 2) is discussed in Sections 2 and 3 of this document. For Step 3, IWAIR calculates air concentration from WMU emission rates and dispersion factors, as follows:

$$C_{air,j} = (E_j \times 10^6) \times DF \tag{6-1}$$

where

$C_{air,j}$ = air concentration of chemical *j* ($\mu g/m^3$)
E_j = volatile emission rate of chemical *j* (g/m^2-s)
10^6 = unit conversion ($\mu g/g$)
DF = dispersion factor ($[\mu g/m^3]/[\mu g/m^2$-s]).

For Step 4, IWAIR then uses this calculated air concentration, the exposure factors described in Section 4, and the health benchmarks described in Section 5 to calculate risk or HQ. The following subsections describe this calculation for carcinogens and noncarcinogens.

6.1.1 Calculation of Risk for Carcinogens

Risk for carcinogens is calculated as follows:

$$\mathrm{Risk}_j = \frac{C_{air,j} \times 10^{-3} \times \mathrm{CSF}_j \times \mathrm{EF}}{\mathrm{AT} \times 365} \times \sum_{i=1}^{5} \frac{\mathrm{IR}_i \times \mathrm{ED}_i}{\mathrm{BW}_i} \tag{6-2}$$

where

10^{-3} = unit conversion (mg/µg)
Risk_j = individual risk for chemical *j* (unitless)
CSF_j = cancer slope factor for chemical *j* (per mg/kg-d)
i = index on age group (e.g., <1 yr, 1–5 yrs, 6–11 yrs, 12–19 yrs, Adult)
IR_i = inhalation rate for age group *i* (m^3/d)
ED_i = exposure duration for age group *i* (yr)
EF = exposure frequency (d/yr)
AT = averaging time (yr) = 70
365 = unit conversion (d/yr)
BW_i = body weight for age group *i* (kg).

Averaging time corresponds to a typical lifetime and is a fixed input to this equation because it must be consistent with the 70-year averaging time used to develop the CSF. This averaging time reflects the lifetime over which cancer risks are averaged. It is not related to the exposure duration (which is the length of time a receptor is exposed to a chemical) or the averaging period used for emission rates (which is the length of time over which emission rates are averaged; this is set to correspond to the exposure duration).

Equation 6-2 reflects calculation of carcinogenic risk for residents and must be modified slightly to calculate risk for workers. Exposure factors for adult workers are used in place of age-specific exposure factors for residents. Thus, the summation over age group, *i*, is not needed for workers.

IWAIR also calculates the cumulative risk for all carcinogens modeled in a run. This is a simple sum of the chemical-specific risks already calculated, as follows:

$$\mathrm{CumRisk} = \sum_{j=1}^{n} \mathrm{Risk}_j \tag{6-3}$$

where

CumRisk = cumulative individual risk for all carcinogens modeled (unitless)
j = index on chemical
n = number of carcinogens modeled.

6.1.2 Calculation of HQ for Noncarcinogens

The HQ for noncarcinogens, which is not dependent on exposure factors, is calculated as follows:

$$HQ_j = \frac{C_{air,j} \times 10^{-3}}{RfC_j} \tag{6-4}$$

where

HQ_j = hazard quotient for chemical *j* (unitless)
10^{-3} = unit conversion (mg/µg)
RfC_j = reference concentration for chemical *j* (mg/m^3).

No cumulative HQ is calculated for noncarcinogens. Such summing of HQs is appropriate only when the chemicals involved have the same target organ.

6.2 Calculation of Allowable Waste Concentration

The calculation of the allowable waste concentration from a target risk or HQ is somewhat more complex than the risk calculation for several reasons.

First, emission rates depend on whether the waste modeled is aqueous-phase or organic-phase. In risk calculation mode, the user establishes the waste type as an input, and IWAIR calculates emission rates and the ensuing risk or HQ for that waste type. In allowable concentration mode, IWAIR must determine whether to base the allowable concentration on an emission rate for an aqueous-phase waste or an organic-phase waste.

Second, if risk is linear with waste concentration, then emission rates may be calculated for a unit waste concentration, and air concentration and risk and HQ equations may be solved for waste concentration. This is the case for land application units, landfills, and waste piles. However, emission rates are not linear with waste concentration for aqueous-phase wastes in surface impoundments because of nonlinearities in biodegradation processes. In surface impoundments, biodegradation is first order at low concentrations and eventually becomes zero order at higher concentrations. The concentration at which this shift occurs is chemical-specific. This is not the case with organic-phase emissions from surface impoundments, because biodegradation is not modeled in that scenario because of model limitations. Therefore, for aqueous-phase wastes in surface impoundments, an iterative risk calculation approach must be used to calculate allowable waste concentration.

Finally, when solving the risk and HQ equations for waste concentration (or when iteratively solving the risk equations for increasing concentrations), care must be taken to ensure that the resulting concentration is within physical limits for the associated waste type.

The following subsections describe how allowable waste concentrations are calculated for land application units, landfills, and waste piles; how allowable waste concentrations are calculated for surface impoundments; and how IWAIR sets an allowable waste concentration that observes physical limitations.

6.2.1 Calculating Allowable Waste Concentrations for Land Application Units, Landfills, and Waste Piles

To calculate an allowable concentration, IWAIR uses the following steps:

1. Calculate unitized emission rates from user inputs or user-specified unitized emission rates; the emission rates are chemical-specific and correspond to a waste concentration of 1 mg/kg or mg/L; if calculated by IWAIR, unitized emission rates are also specific to waste type (i.e., aqueous- or organic-phase).

2. Calculate dispersion factors from user inputs or user-specified dispersion factors; the dispersion factors are receptor-specific.

3. Calculate target air concentrations from target risk or HQ, health benchmarks, and, for carcinogens, exposure factors; the air concentrations are chemical- and receptor-specific.

4. Calculate waste concentrations from air concentrations, dispersion factors, and unitized emission rates, for aqueous- and organic-phase wastes.

5. Choose an allowable concentration from the waste concentrations calculated for aqueous- and organic-phase wastes.

Calculation of emission rates and dispersion factors (Steps 1 and 2) is discussed in Sections 2 and 3 of this document. For Step 3, IWAIR uses the same underlying risk and HQ equations presented in Section 6.1 to calculate allowable concentration for land application units, landfills, and waste piles. Equations 6-2 (for risk) and 6-4 (for HQ) may be solved for air concentration. The risk or HQ in those equations becomes the target risk or HQ selected by the user.

For Step 4, IWAIR then uses an equation comparable to Equation 6-1 to relate air concentration to waste concentration. However, this equation must be adapted to reflect the use of a unitized emission rate associated with a waste concentration of 1 mg/kg. This new equation assumes that emissions are linear with waste concentration. The adapted equation is as follows:

$$C_{air} = (C_{waste} \times E_{unit} \times 10^6) \times DF \qquad (6\text{-}5)$$

where

C_{air} = air concentration (µg/m^3)
C_{waste} = waste concentration (mg/kg or mg/L)
E_{unit} = normalized volatile emission rate of constituent ([g/m^2-s]/[mg/kg] or [g/m^2-s]/[mg/L])
10^6 = unit conversion (µg/g)
DF = dispersion factor ([µg/m^3]/[µg/m^2-s]).

Equation 6-5 may be solved for waste concentration to calculate waste concentration from air concentration. This equation is then used with both an aqueous-phase emission rate and an organic-phase emission rate, to get an aqueous-phase waste concentration and an organic-phase waste concentration. Section 6.2.3 describes how IWAIR uses those two concentrations to set an allowable waste concentration (Step 5).

6.2.2 Calculating Allowable Waste Concentrations for Surface Impoundments

For organic-phase wastes in surface impoundments, emissions are linear with waste concentration, so waste concentration is calculated following Steps 1 to 4, as described in Section 6.2.1.

For aqueous-phase wastes in surface impoundments, emissions are not linear with waste concentration. Therefore, an iterative method adapted from the Newton-Raphson method was used in IWAIR.

The Newton-Raphson method is a commonly used formula for locating the root of an equation, i.e., the value of *x* at which f(*x*) is zero (Chapra and Canale, 1985). The method is based on the geometrical argument that the intersection of a tangent to a function at an initial guess, x_i, with the *x*-axis is a better approximation of the root than x_i. As illustrated in Figure 6-1, the method can be adapted to a nonzero target value of f(*x*), α; in this case, the intersection of the tangent with the line corresponding to $y = \alpha$ is used as the next approximation.

Mathematically, the slope of this tangent, $f'(x_i)$ is given as follows:

$$f'(x_i) = \frac{f(x_i) - \alpha}{x_i - x_{i+1}} \tag{6-6}$$

where

$f'(x_i)$ = the slope of f(*x*) at x_i
$f(x_i)$ = the value of f(*x*) at x_i
α = the target value for f(*x*)
x_i = the initial guess for *x*
x_{i+1} = the next approximation of *x*.

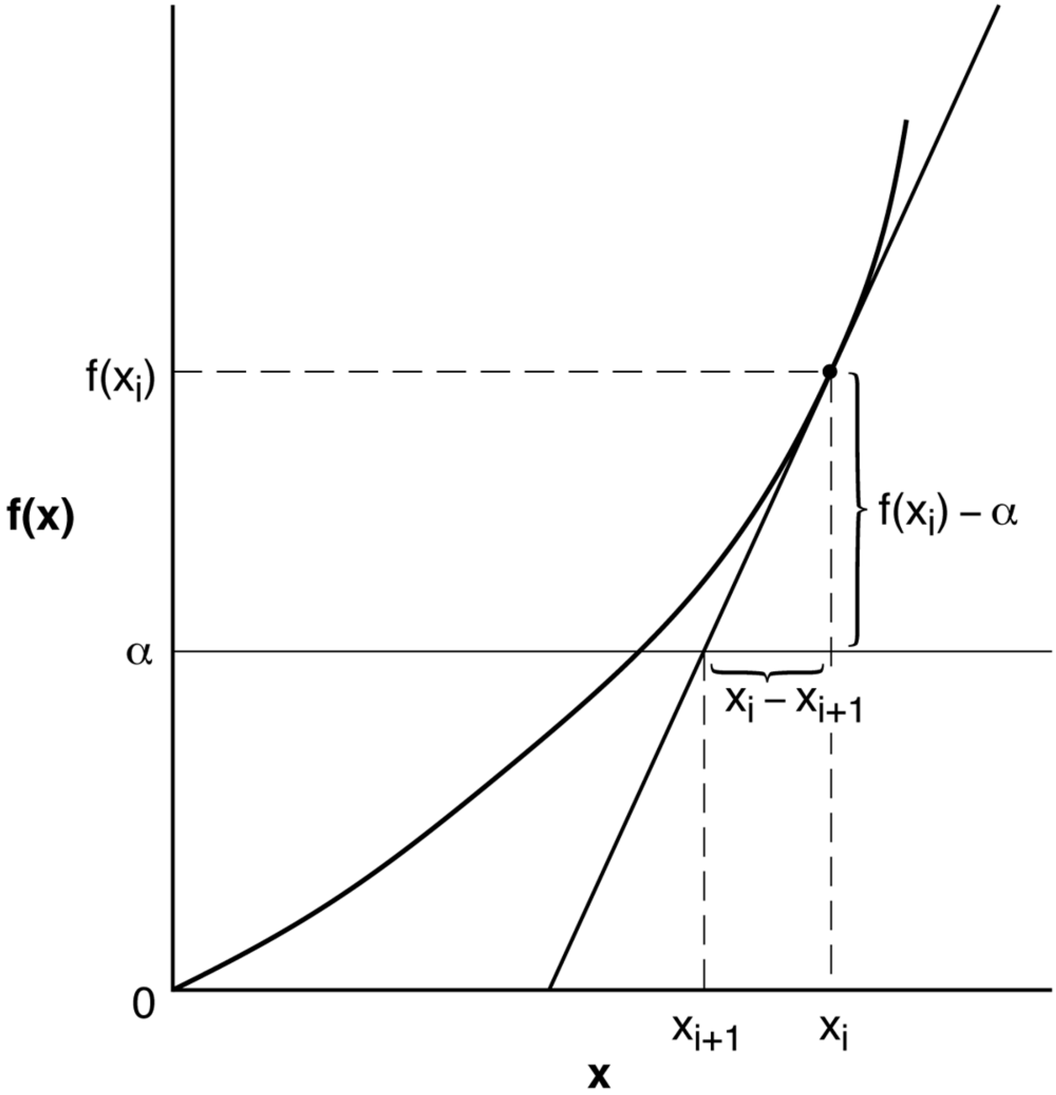

Figure 6-1. Graphical interpretation of the Newton-Raphson method.

This can be rearranged as follows to solve for x_{i+1}:

$$x_{i+1} = x_i - \frac{f(x_i) - \alpha}{f'(x_i)} \quad . \tag{6-7}$$

Equation 6-7 gives an improved value of x for the next iteration; however, to use it, $f'(x_i)$ must first be estimated. This is done using finite difference methods:

$$f'(x_i) = \frac{f(x_i + \epsilon) - f(x_i)}{\epsilon} \tag{6-8}$$

where

$f(x_i + \epsilon)$ = the value of f(*x*) at $x_i + \epsilon$
ϵ = a small value relative to x_i.

For IWAIR, ϵ was set to $0.1x_i$.

This method can be applied iteratively until f(*x*) is within a predefined tolerance of the target, α. For IWAIR, the stopping criteria was set to $f(x) = \alpha \pm 1\%$.

For IWAIR, the variable *x* in the general Newton-Raphson method is waste concentration, and the function f(*x*) is the calculation of either risk or HQ based on waste concentration following the Steps 1 through 4 laid out in Section 6.1 for risk mode.

As for the other units, where risk is linear with waste concentration, both an aqueous-phase waste concentration (using the Newton-Raphsm method) and an organic-phase waste concentration (using the approach described in Section 6.2.1) are developed. Section 6.2.3 describes how IWAIR uses those concentrations to set an allowable waste concentration (Step 5).

6.2.3 Setting an Allowable Waste Concentration

The final step, Step 5, to setting an allowable waste concentration is to choose between the waste concentrations based on aqueous-phase emissions and organic-phase emissions and to ensure that the resulting concentration does not exceed physical limitations.

As discussed in Section 2, wastes are typically assumed to be aqueous phase (i.e., dilute wastes that partition primarily to water). However, aqueous-phase wastes are likely to occur in land application units, landfills, and waste piles only up to the soil saturation limit, and in surface impoundments up to the solubility of the chemical in water. At concentrations above the soil saturation or solubility limit, wastes are more likely to occur in organic phase, unless waste matrix effects allow supersaturated conditions to occur. Although it is possible for aqueous-phase wastes to exist with chemicals present above the saturation or solubility limit, this is an unusual occurrence. Therefore, IWAIR limits calculated allowable waste concentrations based on aqueous-phase emission rates to the soil saturation or solubility limit or lower. The solubility limit is a chemical-specific property and is included in the IWAIR chemical properties database. The soil saturation limit is dependent on site-specific factors, as well as chemical properties; therefore, IWAIR calculates it from user inputs as follows:

$$C_{sat} = \frac{S}{\rho_b} (K_d \times \rho_b + \epsilon_w + H' \times \epsilon_a) \tag{6-9}$$

where

C_{sat} = soil saturation limit (mg/kg)
S = solubility limit (mg/L)

ρ_b = bulk density of soil/waste matrix (kg/L)
K_d = soil-water partition coefficient (L/kg), calculated as shown below in Equation 6-10 for organic chemicals; this is an input for mercury
ϵ_w = water-filled soil porosity (unitless)
H' = dimensionless Henry's law constant (unitless = H/RT)
ϵ_a = air-filled soil porosity (unitless).

and

$$K_d = K_{oc} \times f_{oc} \tag{6-10}$$

where

K_d = soil-water partition coefficient (L/kg)
K_{oc} = organic carbon partition coefficient (L/kg), calculated as shown below in Equation 6-11
f_{oc} = fraction organic carbon in waste (unitless).

Fraction organic carbon is set to a fixed value of 0.014. This value was derived from the median of a set of values for many (but not all) of the locations included in the IWAIR dispersion factor database.

$$K_{oc} = 10^{(\log K_{ow} - 0.32)} \tag{6-11}$$

where

K_{ow} = octanol-water partition coefficient (L/kg).

Wastes can occur in the organic phase at concentrations below the soil saturation or solubility limit, as well as up to 1,000,000 mg/kg or mg/L (ppm). Regardless of whether the chemical is in the aqueous or organic phase, the concentration cannot exceed 1,000,000 mg/kg or mg/L (ppm) by definition. Therefore, IWAIR limits calculated allowable waste concentrations based on organic-phase emission rates to 1,000,000 ppm or lower.

As described in Sections 6.2.1 and 6.2.2, IWAIR calculates waste concentrations for both aqueous- and organic-phase emission rates. It then chooses between them using the following decision rules:

- If one of the two concentrations is physically impossible (greater than saturation or solubility limits for aqueous phase, or greater than 1,000,000 ppm for organic phase), it is discarded and the other is used.

- If both concentrations are impossible, then the allowable concentration is set to the saturation or solubility limit or 1,000,000 ppm, depending on which produces the higher risk. That risk is reported as the maximum achievable risk.

- If both concentrations are physically possible, IWAIR selects the lower of the two. This is the lowest concentration that could produce the target risk. The underlying waste type (aqueous or organic) is reported. For most chemicals, this will be the concentration based on aqueous-phase emissions, as these are greater than the organic-phase emissions for the same concentration and, therefore, produce greater risk. Formaldehyde is a notable exception and has greater emissions (and therefore greater risk) from an organic-phase waste than an aqueous-phase waste.

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Appendix A

Considering Risks from Indirect Pathways

Appendix A

Considering Risks from Indirect Pathways

A.1 What are "Indirect Risks"?

<u>Direct Pathways</u>: An individual is directly exposed to the contaminated medium, such as air or groundwater, into which the chemical was released.

<u>Indirect Pathways</u>: An individual is indirectly exposed when a chemical that is released into one medium (for example, air), is subsequently transported to other media, such as water, soil, or food, to which the individual comes in contact.

IWAIR assesses exposures by direct inhalation of a chemical. It is possible, however, that environmental contaminants can be transferred to other media resulting in an indirect exposure to the pollutant. The purpose of this section is to provide risk assessors with information on health risks that may result from volatile emissions other than from the inhalation pathway. An indirect pathway of exposure is when a chemical that is released into one medium (for example, air) is subsequently transported to other media, such as water, soil, or food, to which a receptor is exposed. For example, chemical vapors that are released from a WMU and transported to an adjacent agricultural field may diffuse into vegetation, deposit on vegetation, or may be taken up by vegetation from the soil. Individuals who subsequently eat the produce from that field may be exposed to contaminants in their diet. Additional indirect exposures can occur through the ingestion of contaminated fish, or animal products, such as milk, beef, pork, poultry, and eggs.

Figure A-1 shows these pathways graphically. The arrows indicate the flow of pollutants through the pathways. Pollutants are released from a source, dispersed through the air, and deposited on crops, pastures, soil, and surface water. From there, they may be taken up into plants or animal tissues. Humans may then be exposed by ingesting soil (through hand-to-mouth contact), ingesting plant products, or ingesting animal products (including fish). Although not shown in Figure A-1, humans may also ingest groundwater and surface water as drinking water sources. Groundwater exposures are modeled by the Industrial Waste Management Evaluation Model (IWEM), and surface water sources of drinking water are presumed to be treated to remove contaminants.

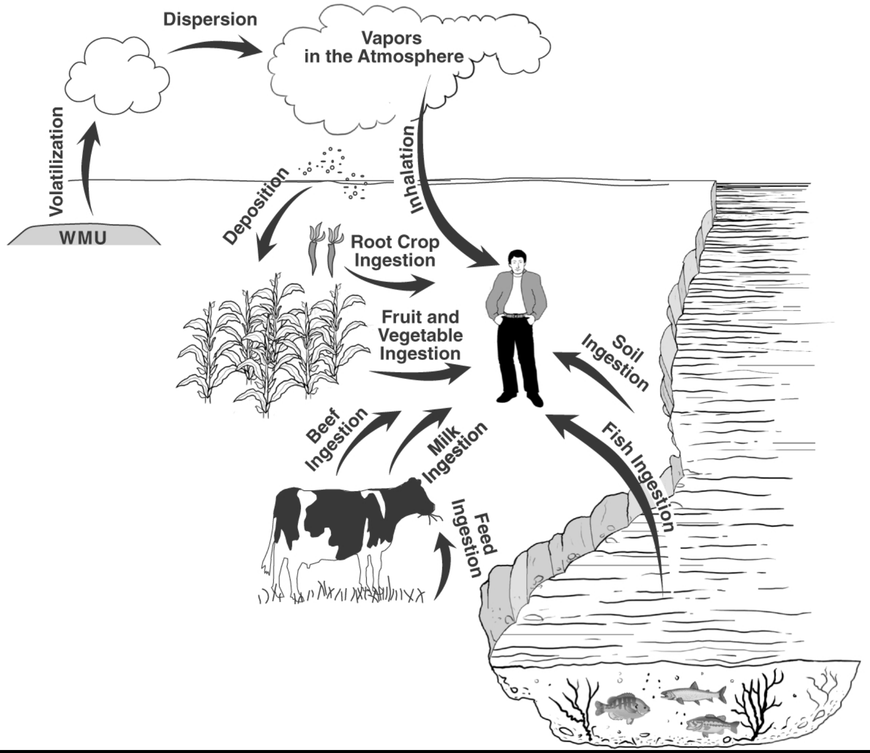

Figure A-1. Indirect exposure pathways.

A.2 Determining When Indirect Pathways May Be Important

There are two key factors a facility manager should consider when determining the need to assess the human health risk from indirect pathways of exposure. First, only certain land uses near a WMU may pose potential risks through indirect exposure pathways. Second, only certain chemicals may have properties that favor indirect pathways. These two criteria are explained in the following paragraphs.

A.2.1 Land Use

As described above, indirect exposures can occur when a vapor-phase constituent in the air is transported into surface water or taken up by produce or by animal products (via feed plants or surface water). However, these pathways are unlikely to be of concern unless the land use near the site includes one or more of the following:

- Residential home-gardening
- Agriculture (including production of produce and animal products for human consumption)
- Farms that grow feed for animals

- Recreational fishing
- Recreational hunting areas.

A.2.2 Chemical Properties

In addition to land use, the chemical properties of the constituents in the waste are important in determining whether indirect pathways are of potential concern. Some chemicals exhibit properties that tend to favor indirect pathways, while others do not, or do so to a lesser extent. The chemical properties of interest are those that reflect the tendency for a chemical to be persistent in the environment, bioaccumulate in plants or animals, or be toxic when ingested.[1] A facility manager should consider these properties when determining whether an assessment of indirect pathways may be necessary for the WMU. The following subsections provide a brief description of some of the chemical properties that can be used to predict a constituent's persistence, bioaccumulation potential, and toxicity.

Persistence

A chemical's persistence refers to how long the chemical remains in the environment without being chemically or biologically broken down or altered. A chemical considered to be highly persistent remains in the environment for a relatively long period of time, although it may move through different media (e.g., from soil to water to sediment). Because persistent chemicals remain in the environment, they can accumulate in environmental media and/or plant and animal tissue. As a result, the temporal window for exposure through both direct and indirect pathways may be extended, and the likelihood of exposure will increase. Persistence is frequently expressed in terms of half-life. For example, if a chemical has a half-life of 2 days, it will take 2 days for a given quantity of the chemical to be reduced by one-half due to chemical and biological processes. The longer the half-life, the more persistent the chemical. A related chemical property is degradation rate, which is inversely related to half-life. Thus, the lower the degradation rate, the more persistent the chemical. Data on soil biodegradation rates are presented for the IWAIR chemicals in Appendix B; this property may be used as a general indicator of persistence potential.

Bioaccumulation Potential

Bioaccumulation potential refers to a chemical's tendency to accumulate in plants and animals. For example, plants may accumulate chemicals from the soil through their roots. Some of these chemicals are transformed or combined with others and used by the plant; others are simply eliminated; and others accumulate in the plant roots, leaves, or edible parts of the plant. Animals also bioaccumulate certain chemicals in different tissues or organs. For chemicals that

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[1] The tendency of chemical constituents to be persistent and bioaccumulate are a function of both the chemical/physical attributes of the chemical (e.g., K_{ow}) and the environmental setting (such as the physical characteristics of the system, e.g., dissolved organic carbon, soil pH; or the biology of organisms that inhabit the system, e.g., crops, fish species); however, it is convenient to think of persistence and bioaccumulation potential as intrinsic properties when considering indirect exposure pathways.

bioaccumulate, the concentration in the plants and animals can be higher than the concentration in the environment. As a result, a human who eats the plant or animal may be exposed to a higher concentration in the food than in the contaminated medium.[2] Bioaccumulation potential may be expressed as a bioaccumulation factor (BAF) or a bioconcentration factor (BCF); these factors express the relationship between the concentration in biota and the concentration in the environmental medium. Bioaccumulation potential may also be expressed as a biotransfer factor for animal products, representing the relationship between the exposure concentration and the mass of contaminated plants ingested daily.

Chemicals that tend to accumulate in plants and animal tissues often have a characteristically high affinity for lipids (fats). This tendency is reflected by the octanol-water partition coefficient (K_{ow}),[3] a laboratory measurement of the attraction of a chemical to water versus its attraction to lipids (fats). In these experiments, octanol is used as a surrogate for lipids. Because chemicals with higher K_{ow} values have been shown to have a greater tendency to accumulate in the fatty tissue of animals, the BAF and BCF are generally accepted as useful predictors of bioaccumulation potential (see text box for definitions and examples of other parameters that are often used to evaluate indirect exposures through the ingestion of produce and animal products). Some chemicals with high K_{ow} values, such as polycyclic aromatic hydrocarbons (PAHs), do not accumulate appreciably in animals that have the capacity to metabolize the chemical and eliminate it from their systems. Moreover, this strong affinity for lipids also means that the chemical has a strong affinity for organic carbon in soil and surface water. Chemicals that are strongly sorbed to the organic component in soil may not be readily taken up by plants. For example, dioxin is poorly taken up from the soil by virtually all species of plants that have been tested.

Parameters Used to Evaluate Indirect Exposures

BCF: Bioconcentration Factor for Fish. Defined as the ratio of chemical concentration in the fish to the concentration in the surface water. Fish are exposed only to contaminated water.

BAF: Bioaccumulation Factor for Fish. Defined as the ratio of the chemical concentration in fish to the concentration in the surface water. Fish are exposed to contaminated water and plants/prey.

BSAF: Biota-Sediment Accumulation Factor for Fish. Generally applied only to highly hydrophobic organic chemicals, and defined as the ratio of the lipid-normalized concentration in fish to the organic carbon-normalized concentration in surface sediment. Fish are exposed to contaminated pore water, sediment, and plants/prey.

Br: Plant-Soil Bioconcentration Factor. Defined as the ratio between the chemical concentration in the plant and the concentration in soil. It varies by plant group (e.g., root vegetables, aboveground vegetables).

Bv: Air-Plant Bioconcentration Factor. Defined as the mass-based ratio between the chemical concentration in the plant and the vapor-phase chemical concentration in the air. It is varies by plant group (e.g., leafy vegetables, forage).

Ba: Plant-Animal Biotransfer Factor. Defined as the ratio between the chemical concentration in the animal tissue and the amount of chemical ingested per day. It varies by type of animal tissue (e.g., beef, milk).

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[2] Even though the concentration in food may not be significantly higher than in the environmental media, the consumption rate of produce and meat/dairy products may lead to a substantial exposure to contaminants.

[3] Because octanol-water coefficients can span many orders of magnitude, they are normally discussed in terms of their log values (log K_{ow}).

Consequently, the use of chemical properties should be supplemented with information from field studies to determine whether the chemical is of potential concern through indirect exposure pathways. Data on log K_{ow} are presented for the IWAIR chemicals in Appendix B; they may be used as a first-cut indicator of bioaccumulation potential. As a general rule, chemicals with relatively high K_{ow} values tend to accumulate in plants and animals to a greater extent than chemicals with relatively low K_{ow} values.

Toxicity

The toxicity of chemicals to humans depends on the route of exposure—inhalation or ingestion. IWAIR contains health benchmarks for inhalation exposures. However, the indirect pathways discussed here refer to ingestion exposures. Therefore, even if a chemical is released into the air and tends to bioaccumulate in plant or animal products, if it is not very toxic by the ingestion pathway, then indirect pathways will be of less concern. Two benchmarks are used to predict the toxicity of a chemical that is ingested: the cancer slope factor (CSF, which measures the tendency of a chemical to cause cancer) and the reference dose (RfD, which provides a threshold below which a chemical is unlikely to result in adverse, noncancer health effects). The CSF is a measure of carcinogenic potency; consequently, a *larger* value indicates greater toxicity. However, the RfD is a threshold at which adverse effects are not expected; therefore, a *smaller* value indicates greater toxicity.

Oral toxicity benchmarks are not used in IWAIR; therefore, for convenience, the oral toxicity benchmarks (oral CSF and RfD) are presented for the IWAIR chemicals in Table A-1.

A.3 Additional Information

Indirect risk assessments are often site-specific, require a significant amount of information about the area surrounding the WMU, and can be complex depending on the chemicals of concern. However, indirect pathways should not be overlooked as a potential source of risk if the chemical properties and surrounding land uses suggest potential risks through indirect exposures.

If it appears that indirect pathways may be of concern, *Methodology for Assessing Health Risks Associated with Multiple Pathways of Exposure to Combustor Emissions* (U.S. EPA, 1998b) presents guidance developed by the Agency for conducting indirect risk assessments for most chemicals. This document can be used to determine whether further assessment of indirect pathways is needed, and, if so, how to conduct such an assessment. For dioxin-like compounds, indirect pathways are evaluated somewhat differently; see U.S. EPA (2000a), *Exposure and Human Health Reassessment of 2,3,7,8-Tetrachlorodibenzo-p-Dioxin (TCDD) and Related Compounds. Part I: Estimating Exposure to Dioxin-Like Compounds.*

Table A-1. Oral Health Benchmarks for IWAIR Chemicals

IWAIR Constituent Name	CASRN	RfD (mg/kg-d)	RfD Source	CSFo (per mg/kg-d)	CSFo Source	Comment
1,1,1,2-Tetrachloroethane	630-20-6	3.0E-02	IRIS	2.6E-02	IRIS	
1,1,1-Trichloroethane	71-55-6	2.8E-01	SF			
1,1,2,2-Tetrachloroethane	79-34-5	6.0E-02	SF	2.0E-01	IRIS	
1,1,2-Trichloro-1,2,2-trifluoroethane	76-13-1	3.0E+01	IRIS			
1,1,2-Trichloroethane	79-00-5	4.0E-03	IRIS	5.7E-02	IRIS	
1,1-Dichloroethylene	75-35-4	9.0E-03	IRIS	6.0E-01	IRIS	
1,2,4-Trichlorobenzene	120-82-1	1.0E-02	IRIS			
1,2-Dibromo-3-chloropropane	96-12-8			1.4E+00	HEAST	intermediate MRL available
1,2-Dichloroethane	107-06-2			9.1E-02	IRIS	intermediate MRL available
1,2-Dichloropropane	78-87-5	9.0E-02	ATSDR	6.8E-02	HEAST	
1,2-Diphenylhydrazine	122-66-7			8.0E-01	IRIS	
1,2-Epoxybutane	106-88-7					
1,3-Butadiene	106-99-0					
1,4-Dioxane	123-91-1			1.1E-02	IRIS	
2,3,7,8-TCDD	1746-01-6	1.0E-09	ATSDR	1.5E+05	HEAST	
2,4-Dinitrotoluene	121-14-2	2.0E-03	IRIS	6.8E-01	IRIS	CSFo is for 2,4-/2,6-mixture
2-Chlorophenol	95-57-8	5.0E-03	IRIS			
2-Ethoxyethanol	110-80-5	4.0E-01	HEAST			
2-Ethoxyethanol acetate	111-15-9	3.0E-01	HEAST			
2-Methoxyethanol	109-86-4	1.0E-03	HEAST			
2-Methoxyethanol acetate	110-49-6	2.0E-03	HEAST			
2-Nitropropane	79-46-9					
3,4-Dimethylphenol	95-65-8	1.0E-03	IRIS			
3-Methylcholanthrene	56-49-5					
7,12-Dimethylbenz[a]anthracene	57-97-6					

(continued)

Table A-1. (continued)

IWAIR Constituent Name	CASRN	RfD (mg/kg-d)	RfD Source	CSFo (per mg/kg-d)	CSFo Source	Comment
Acetaldehyde	75-07-0					
Acetone	67-64-1	1.0E-01	IRIS			
Acetonitrile	75-05-8					
Acrolein	107-02-8	2.0E-02	HEAST			
Acrylamide	79-06-1	2.0E-04	IRIS	4.5E+00	IRIS	
Acrylic acid	79-10-7	5.0E-01	IRIS			
Acrylonitrile	107-13-1	1.0E-03	HEAST	5.4E-01	IRIS	
Allyl chloride	107-05-1					
Aniline	62-53-3			5.7E-03	IRIS	
Benzene	71-43-2			5.5E-02	IRIS	upper range estimate used for CSFo
Benzidine	92-87-5	3.0E-03	IRIS	2.3E+02	IRIS	
Benzo(a)pyrene	50-32-8			7.3E+00	IRIS	
Bromodichloromethane	75-27-4	2.0E-02	IRIS	6.2E-02	IRIS	
Carbon disulfide	75-15-0	1.0E-01	IRIS			
Carbon tetrachloride	56-23-5	7.0E-04	IRIS	1.3E-01	IRIS	
Chlorobenzene	108-90-7	2.0E-02	IRIS			
Chlorodibromomethane	124-48-1	2.0E-02	IRIS	8.4E-02	IRIS	
Chloroform	67-66-3	1.0E-02	IRIS			
Chloroprene	126-99-8	2.0E-02	HEAST			
cis-1,3-Dichloropropylene	10061-01-5	3.0E-02	IRIS	1.0E-01	IRIS	RfD & CSFo are for 1,3-dichloropropene
Cresols (total)	1319-77-3	5.0E-02	surr			RfD is for m-cresol
Cumene	98-82-8	1.0E-01	IRIS			
Cyclohexanol	108-93-0	1.7E-05	solvents			
Dichlorodifluoromethane	75-71-8	2.0E-01	IRIS			
Epichlorohydrin	106-89-8	2.0E-03	HEAST	9.9E-03	IRIS	

(continued)

Table A-1. (continued)

IWAIR Constituent Name	CASRN	RfD (mg/kg-d)	RfD Source	CSFo (per mg/kg-d)	CSFo Source	Comment
Ethylbenzene	100-41-4	1.0E-01	IRIS			
Ethylene dibromide	106-93-4			8.5E+01	IRIS	
Ethylene glycol	107-21-1	2.0E+00	IRIS			
Ethylene oxide	75-21-8			1.0E+00	HEAST	
Formaldehyde	50-00-0	2.0E-01	IRIS			
Furfural	98-01-1	3.0E-03	IRIS			
Hexachloro-1,3-butadiene	87-68-3	3.0E-04	SF	7.8E-02	IRIS	
Hexachlorobenzene	118-74-1	8.0E-04	IRIS	1.6E+00	IRIS	
Hexachlorocyclopentadiene	77-47-4	6.0E-03	IRIS			
Hexachloroethane	67-72-1	1.0E-03	IRIS	1.4E-02	IRIS	
Isophorone	78-59-1	2.0E-01	IRIS	9.5E-04	IRIS	
Mercury	7439-97-6	1.0E-04	surr			RfD is for methyl mercury
Methanol	67-56-1	5.0E-01	IRIS			
Methyl bromide	74-83-9	1.4E-03	IRIS			
Methyl chloride	74-87-3			1.3E-02	HEAST	
Methyl ethyl ketone	78-93-3	6.0E-01	IRIS			
Methyl isobutyl ketone	108-10-1	8.0E-02	HEAST			
Methyl methacrylate	80-62-6	1.4E+00	IRIS			
Methyl tert-butyl ether	1634-04-4					intermediate MRL available
Methylene chloride	75-09-2	6.0E-02	IRIS	7.5E-03	IRIS	
N,N-Dimethyl formamide	68-12-2	1.0E-01	HEAST			
Naphthalene	91-20-3	2.0E-02	IRIS			
n-Hexane	110-54-3	1.1E+01	SF			
Nitrobenzene	98-95-3	5.0E-04	IRIS			
N-Nitrosodiethylamine	55-18-5			1.5E+02	IRIS	
N-Nitrosodi-n-butylamine	924-16-3			5.4E+00	IRIS	

(continued)

Table A-1. (continued)

IWAIR Constituent Name	CASRN	RfD (mg/kg-d)	RfD Source	CSFo (per mg/kg-d)	CSFo Source	Comment
N-Nitrosopyrrolidine	930-55-2			2.1E+00	IRIS	
o-Dichlorobenzene	95-50-1	9.0E-02	IRIS			
o-Toluidine	95-53-4			2.4E-01	HEAST	
p-Dichlorobenzene	106-46-7			2.4E-02	HEAST	intermediate MRL available
Phenol	108-95-2	6.0E-01	IRIS			
Phthalic anhydride	85-44-9	2.0E+00	IRIS			
Propylene oxide	75-56-9			2.4E-01	IRIS	
Pyridine	110-86-1	1.0E-03	IRIS			
Styrene	100-42-5	2.0E-01	IRIS			
Tetrachloroethylene	127-18-4	1.0E-02	IRIS	5.2E-02	HAD	
Toluene	108-88-3	2.0E-01	IRIS			
trans-1,3-Dichloropropylene	10061-02-6	3.0E-02	IRIS	1.0E-01	IRIS	RfD & CSFo are for 1,3-dichloropropene
Tribromomethane	75-25-2	2.0E-02	IRIS	7.9E-03	IRIS	
Trichloroethylene	79-01-6			1.1E-02	HAD	
Trichlorofluoromethane	75-69-4	3.0E-01	IRIS			
Triethylamine	121-44-8					
Vinyl acetate	108-05-4	1.0E+00	HEAST			
Vinyl chloride	75-01-4	3.0E-03	IRIS	7.2E-01	IRIS	CSFo is for continuous adult exposure
Xylenes	1330-20-7	2.0E+00	IRIS			

[a] Sources:
ATSDR = ATSDR oral minimal risk levels (ATSDR, 2001)
IRIS = Integrated Risk Information System (U.S. EPA, 2001)
HEAST = Health Effects Assessment Summary Tables (U.S. EPA, 1997a)
HAD = Health Assessment Document (U.S. EPA, 1986, 1987)
SF = Superfund Risk Issue Paper (U.S. EPA, 1998c, 1999a, 1999b, 2000b)
solvents = 63 FR 64371-0402 (U.S. EPA, 1998a)
surr = surrogate

Finally, as noted above, various chemical properties indicative of the potential for indirect pathway concern are presented in Appendix B for IWAIR chemicals. For other chemicals, the following sources may be useful:

log K_{ow}

- EPA's Superfund Chemical Data Matrix (SCDM) (U.S. EPA, 1997b)
- The Merck Index (Budavari, 1996)
- The National Library of Medicine's Hazardous Substances Databank (HSDB), available on TOXNET (U.S. NLM, 2001)
- Syracuse Research Corporation's CHEMFATE database (SRC, 1999)
- CambridgeSoft.com's ChemFinder database (CambridgeSoft, 2001)
- Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles (ATSDR, 2001)
- EPA's *Dioxin Reassessment* (U.S. EPA, 2000a)—for dioxins only

Half-life

- Howard et al. (1991)

Toxicity (in order of preference)

- Integrated Risk Information System (IRIS) (U.S. EPA, 2001)
- Superfund Technical Support Center Provisional Benchmarks (U.S. EPA, 1998c, 1999a, 1999b, 2000b)
- Health Effects Assessment Summary Tables (HEAST) (U.S. EPA, 1997a)
- Agency for Toxic Substances and Disease Registry oral minimal risk levels (MRLs) (ATSDR, 2001)
- California Environmental Protection Agency (CalEPA) cancer potency factors (CalEPA, 1999)
- EPA health assessment documents (U.S. EPA, 1986, 1987, 1998a).

A.4 References

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Appendix B

Physical-Chemical Properties for Chemicals Included in IWAIR

Appendix B

Physical-Chemical Properties for Chemicals Included in IWAIR

This appendix presents the physical-chemical property values included in IWAIR and the sources of those values. Each table provides the data for one chemical; the chemicals are shown in CAS-number order. The following source references are used throughout:

Calculated based on EPA (1987)	U.S. EPA (1987)
Calculated based on Lyman (1990)	Lyman et al. (1990)
Calculated based on WATER9 (2001)	U.S. EPA (2001)
Calculated based on EPA's Dioxin Reassessment (2000)	U.S. EPA (2000)
CHEMDAT8	U.S. EPA (1994)
Chemfate	SRC (2000)
ChemFinder	CambridgeSoft (2001)
Dioxin Reassessment	U.S. EPA (2000)
Hansch et al. (1995) (unpub)	Hansch et al. (1995)
Howard et al. (1991)	Howard et al. (1991)
HSDB	U.S. NLM (2001)
Kollig (1993)	Kollig (1993)
KowWIN	SRC (2001)
Mackay et al. (1992)	Mackay et al. (1992)
Merck	Budavari (1996)
MRTC	U.S. EPA (1997a)
SCDM	U.S. EPA (1997b)

Table B-1. Chemical-Specific Inputs for Formaldehyde (50-00-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.1E-01	g/cm3	SCDM
HLC	Henry's law constant	3.4E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-5.0E-02	unitless	SCDM
MW	Molecular Weight	3.0E+01	g/mol	SCDM
Sol	Solubility	5.5E+05	mg/L	SCDM
VP	Vapor pressure	5.2E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	5.0E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.7E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.7E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.7E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-2. Chemical-Specific Inputs for Benzo(a)pyrene (50-32-8)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	1.1E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.1E+00	unitless	SCDM
MW	Molecular Weight	2.5E+02	g/mol	SCDM
Sol	Solubility	1.6E-03	mg/L	SCDM
VP	Vapor pressure	5.5E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	1.4E+00	g/cm3	HSDB
Ksg	Soil degradation rate	1.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	9.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	6.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-3. Chemical-Specific Inputs for N-Nitrosodiethylamine (55-18-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.4E-01	g/cm3	SCDM
HLC	Henry's law constant	3.6E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.8E-01	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	9.3E+04	mg/L	SCDM
VP	Vapor pressure	8.6E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.4E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-4. Chemical-Specific Inputs for Carbon tetrachloride (56-23-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	3.0E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.7E+00	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	7.9E+02	mg/L	SCDM
VP	Vapor pressure	1.2E+02	mmHg	SCDM
Kh	Hydrolysis rate	5.4E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.5E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-5. Chemical-Specific Inputs for 3-Methylcholanthrene (56-49-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	9.4E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.4E+00	unitless	SCDM
MW	Molecular Weight	2.7E+02	g/mol	SCDM
Sol	Solubility	3.2E-03	mg/L	SCDM
VP	Vapor pressure	7.7E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.7E-09	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	6.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-6. Chemical-Specific Inputs for 7,12-Dimethylbenz[a]anthracene (57-97-6)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.1E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.6E+00	unitless	SCDM
MW	Molecular Weight	2.6E+02	g/mol	SCDM
Sol	Solubility	2.5E-02	mg/L	SCDM
VP	Vapor pressure	5.6E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.7E-02	cm2/s	Calculated based on EPA, 1987.
Dw	Diffusion coefficient in water	5.5E-06	cm2/s	Calculated based on EPA, 1987.
Density	Density of the chemical	1.0E+00	g/cm3	-

Table B-7. Chemical-Specific Inputs for Aniline (62-53-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	1.9E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	9.8E-01	unitless	SCDM
MW	Molecular Weight	9.3E+01	g/mol	SCDM
Sol	Solubility	3.6E+04	mg/L	SCDM
VP	Vapor pressure	4.9E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.6E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.1E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	7.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-8. Chemical-Specific Inputs for Methanol (67-56-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.9E-01	g/cm3	SCDM
HLC	Henry's law constant	4.5E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-7.1E-01	unitless	SCDM
MW	Molecular Weight	3.2E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	1.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.6E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.7E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-9. Chemical-Specific Inputs for Acetone (67-64-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.9E-01	g/cm3	SCDM
HLC	Henry's law constant	3.9E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-2.4E-01	unitless	SCDM
MW	Molecular Weight	5.8E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	2.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.1E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.3E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-10. Chemical-Specific Inputs for Chloroform (67-66-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	3.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.9E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	7.9E+03	mg/L	SCDM
VP	Vapor pressure	2.0E+02	mmHg	SCDM
Kh	Hydrolysis rate	3.2E-12	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.3E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-11. Chemical-Specific Inputs for Hexachloroethane (67-72-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.1E+00	g/cm3	SCDM
HLC	Henry's law constant	3.9E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.0E+00	unitless	SCDM
MW	Molecular Weight	2.4E+02	g/mol	SCDM
Sol	Solubility	5.0E+01	mg/L	SCDM
VP	Vapor pressure	2.1E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-12. Chemical-Specific Inputs for N,N-Dimethyl formamide (68-12-2)

Parameter	Definition	Value	Units	Reference
Ksg	Soil degradation rate	1.0E-20	sec-1	no value for Ksg in existing hierarchy
Density	Density of the chemical	9.4E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
HLC	Henry's law constant	7.4E-08	atm-m3/mol	HSDB
Sol	Solubility	1.0E+06	mg/L	HSDB
VP	Vapor pressure	3.7E+00	mmHg	HSDB
LogKow	Octanol-water partition coeficient	-1.0E+00	unitless	Hansch et al., 1995
MW	Molecular Weight	7.3E+01	g/mol	Chemfate
K1	Aqueous degradation rate (low)	1.3E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-13. Chemical-Specific Inputs for Benzene (71-43-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.8E-01	g/cm3	SCDM
HLC	Henry's law constant	5.6E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	7.8E+01	g/mol	SCDM
Sol	Solubility	1.8E+03	mg/L	SCDM
VP	Vapor pressure	9.5E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.9E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-14. Chemical-Specific Inputs for 1,1,1-Trichloroethane (71-55-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	1.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	1.3E+03	mg/L	SCDM
VP	Vapor pressure	1.2E+02	mmHg	SCDM
Kh	Hydrolysis rate	2.0E-08	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-15. Chemical-Specific Inputs for Methyl bromide (74-83-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.7E+00	g/cm3	SCDM
HLC	Henry's law constant	6.2E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.2E+00	unitless	SCDM
MW	Molecular Weight	9.5E+01	g/mol	SCDM
Sol	Solubility	1.5E+04	mg/L	SCDM
VP	Vapor pressure	1.6E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-16. Chemical-Specific Inputs for Methyl chloride (74-87-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.1E-01	g/cm3	SCDM
HLC	Henry's law constant	8.8E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	9.1E-01	unitless	SCDM
MW	Molecular Weight	5.0E+01	g/mol	SCDM
Sol	Solubility	5.3E+03	mg/L	SCDM
VP	Vapor pressure	4.3E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.2E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.5E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.2E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.4E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-17. Chemical-Specific Inputs for Vinyl chloride (75-01-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.1E-01	g/cm3	SCDM
HLC	Henry's law constant	2.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	6.3E+01	g/mol	SCDM
Sol	Solubility	2.8E+03	mg/L	SCDM
VP	Vapor pressure	3.0E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.7E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-18. Chemical-Specific Inputs for Acetonitrile (75-05-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.9E-01	g/cm3	SCDM
HLC	Henry's law constant	3.5E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-3.4E-01	unitless	SCDM
MW	Molecular Weight	4.1E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.1E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.3E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.4E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-19. Chemical-Specific Inputs for Acetaldehyde (75-07-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.8E-01	g/cm3	SCDM
HLC	Henry's law constant	7.9E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-4.7E-01	unitless	SCDM
MW	Molecular Weight	4.4E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.0E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	8.2E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.6E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.3E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-20. Chemical-Specific Inputs for Methylene chloride (75-09-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	2.2E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.3E+00	unitless	SCDM
MW	Molecular Weight	8.5E+01	g/mol	SCDM
Sol	Solubility	1.3E+04	mg/L	SCDM
VP	Vapor pressure	4.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-21. Chemical-Specific Inputs for Carbon disulfide (75-15-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	3.0E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	7.6E+01	g/mol	SCDM
Sol	Solubility	1.2E+03	mg/L	SCDM
VP	Vapor pressure	3.6E+02	mmHg	SCDM
Ksg	Soil degradation rate	1.0E-20	sec-1	no value for Ksg in existing hierarchy
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
K1	Aqueous degradation rate (low)	8.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-22. Chemical-Specific Inputs for Ethylene oxide (75-21-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.9E-01	g/cm3	Merck
Kh	Hydrolysis rate	6.7E-07	sec-1	Kollig, 1993
Sol	Solubility	1.0E+06	mg/L	HSDB
Ksg	Soil degradation rate	6.8E-07	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	-3.0E-01	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.5E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	4.4E+01	g/mol	Chemfate
VP	Vapor pressure	1.3E+03	mmHg	Chemfate
K1	Aqueous degradation rate (low)	9.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.3E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.5E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-23. Chemical-Specific Inputs for Tribromomethane (75-25-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.9E+00	g/cm3	SCDM
HLC	Henry's law constant	5.3E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.4E+00	unitless	SCDM
MW	Molecular Weight	2.5E+02	g/mol	SCDM
Sol	Solubility	3.1E+03	mg/L	SCDM
VP	Vapor pressure	5.5E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-24. Chemical-Specific Inputs for Bromodichloromethane (75-27-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.0E+00	g/cm3	SCDM
HLC	Henry's law constant	1.6E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	1.6E+02	g/mol	SCDM
Sol	Solubility	6.7E+03	mg/L	SCDM
VP	Vapor pressure	5.0E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-25. Chemical-Specific Inputs for 1,1-Dichloroethylene (75-35-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.6E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	9.7E+01	g/mol	SCDM
Sol	Solubility	2.3E+03	mg/L	SCDM
VP	Vapor pressure	6.0E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	9.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-26. Chemical-Specific Inputs for Propylene oxide (75-56-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.6E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
VP	Vapor pressure	5.4E+02	mmHg	HSDB
Ksg	Soil degradation rate	6.5E-07	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	3.0E-02	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.2E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	5.8E+01	g/mol	Chemfate
Sol	Solubility	4.1E+05	mg/L	Chemfate
K1	Aqueous degradation rate (low)	1.7E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-27. Chemical-Specific Inputs for Trichlorofluoromethane (75-69-4)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	9.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E+00	unitless	SCDM
MW	Molecular Weight	1.4E+02	g/mol	SCDM
Sol	Solubility	1.1E+03	mg/L	SCDM
VP	Vapor pressure	8.0E+02	mmHg	SCDM
Density	Density of the chemical	1.5E+00	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.2E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-28. Chemical-Specific Inputs for Dichlorodifluoromethane (75-71-8)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.4E-01	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.2E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	2.8E+02	mg/L	SCDM
VP	Vapor pressure	4.8E+03	mmHg	SCDM
Density	Density of the chemical	1.5E+00	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.7E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-29. Chemical-Specific Inputs for 1,1,2-Trichloro-1,2,2-trifluoroethane (76-13-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	4.8E-01	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.2E+00	unitless	SCDM
MW	Molecular Weight	1.9E+02	g/mol	SCDM
Sol	Solubility	1.7E+02	mg/L	SCDM
VP	Vapor pressure	3.3E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-30. Chemical-Specific Inputs for Hexachlorocyclopentadiene (77-47-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.7E+00	g/cm3	SCDM
HLC	Henry's law constant	2.7E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	5.4E+00	unitless	SCDM
MW	Molecular Weight	2.7E+02	g/mol	SCDM
Sol	Solubility	1.8E+00	mg/L	SCDM
VP	Vapor pressure	6.0E-02	mmHg	SCDM
Kh	Hydrolysis rate	7.9E-07	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.4E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-31. Chemical-Specific Inputs for Isophorone (78-59-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.3E-01	g/cm3	SCDM
HLC	Henry's law constant	6.6E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.7E+00	unitless	SCDM
MW	Molecular Weight	1.4E+02	g/mol	SCDM
Sol	Solubility	1.2E+04	mg/L	SCDM
VP	Vapor pressure	4.4E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-32. Chemical-Specific Inputs for 1,2-Dichloropropane (78-87-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.8E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.8E+03	mg/L	SCDM
VP	Vapor pressure	5.2E+01	mmHg	SCDM
Kh	Hydrolysis rate	1.5E-09	sec-1	Kollig, 1993
Ksg	Soil degradation rate	6.2E-09	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.7E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.7E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-33. Chemical-Specific Inputs for Methyl ethyl ketone (78-93-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.1E-01	g/cm3	SCDM
HLC	Henry's law constant	5.6E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.8E-01	unitless	SCDM
MW	Molecular Weight	7.2E+01	g/mol	SCDM
Sol	Solubility	2.2E+05	mg/L	SCDM
VP	Vapor pressure	9.5E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.0E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-34. Chemical-Specific Inputs for 1,1,2-Trichloroethane (79-00-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.4E+00	g/cm3	SCDM
HLC	Henry's law constant	9.1E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	4.4E+03	mg/L	SCDM
VP	Vapor pressure	2.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	8.7E-13	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-35. Chemical-Specific Inputs for Trichloroethylene (79-01-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	1.0E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.7E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	1.1E+03	mg/L	SCDM
VP	Vapor pressure	7.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	8.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.9E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-36. Chemical-Specific Inputs for Acrylamide (79-06-1)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	1.0E-09	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-9.6E-01	unitless	SCDM
MW	Molecular Weight	7.1E+01	g/mol	SCDM
Sol	Solubility	6.4E+05	mg/L	SCDM
VP	Vapor pressure	7.0E-03	mmHg	SCDM
Density	Density of the chemical	1.1E+00	g/cm3	Merck
Kh	Hydrolysis rate	5.7E-10	sec-1	Kollig, 1993
K1	Aqueous degradation rate (low)	2.7E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	1.1E+01	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.3E-05	cm2/s	Calculated based on WATER9, 2001.
Ksg	Soil degradation rate	2.0E-06	sec-1	Calculated based on data in Howard, 1989

Table B-37. Chemical-Specific Inputs for Acrylic acid (79-10-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	1.2E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.5E-01	unitless	SCDM
MW	Molecular Weight	7.2E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	4.0E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	5.7E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	6.5E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-38. Chemical-Specific Inputs for 1,1,2,2-Tetrachloroethane (79-34-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	3.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.4E+00	unitless	SCDM
MW	Molecular Weight	1.7E+02	g/mol	SCDM
Sol	Solubility	3.0E+03	mg/L	SCDM
VP	Vapor pressure	4.6E+00	mmHg	SCDM
Kh	Hydrolysis rate	1.6E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.8E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.3E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-39. Chemical-Specific Inputs for 2-Nitropropane (79-46-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.8E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	8.7E-01	unitless	SCDM
MW	Molecular Weight	8.9E+01	g/mol	SCDM
Sol	Solubility	1.7E+04	mg/L	SCDM
VP	Vapor pressure	1.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-40. Chemical-Specific Inputs for Methyl methacrylate (80-62-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.4E-01	g/cm3	SCDM
HLC	Henry's law constant	3.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.4E+00	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	1.5E+04	mg/L	SCDM
VP	Vapor pressure	3.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.3E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-41. Chemical-Specific Inputs for Phthalic anhydride (85-44-9)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	1.6E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-6.2E-01	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	6.2E+03	mg/L	SCDM
VP	Vapor pressure	5.2E-04	mmHg	SCDM
Kh	Hydrolysis rate	1.6E-12	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.3E-04	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.8E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.7E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-42. Chemical-Specific Inputs for Hexachloro-1,3-butadiene (87-68-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	8.1E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.8E+00	unitless	SCDM
MW	Molecular Weight	2.6E+02	g/mol	SCDM
Sol	Solubility	3.2E+00	mg/L	SCDM
VP	Vapor pressure	2.2E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.0E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-43. Chemical-Specific Inputs for Naphthalene (91-20-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	4.8E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.4E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	3.1E+01	mg/L	SCDM
VP	Vapor pressure	8.5E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.7E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.3E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.4E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.0E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-44. Chemical-Specific Inputs for Benzidine (92-87-5)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.9E-11	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.7E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	5.0E+02	mg/L	SCDM
VP	Vapor pressure	8.0E-09	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	1.3E+00	g/cm3	HSDB
Ksg	Soil degradation rate	1.0E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.6E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-45. Chemical-Specific Inputs for o-Dichlorobenzene (95-50-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	1.9E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.4E+00	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	1.6E+02	mg/L	SCDM
VP	Vapor pressure	1.4E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	5.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-46. Chemical-Specific Inputs for o-Toluidine (95-53-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	2.7E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.3E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	1.7E+04	mg/L	SCDM
VP	Vapor pressure	3.2E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	8.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-47. Chemical-Specific Inputs for 2-Chlorophenol (95-57-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	3.9E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	1.3E+02	g/mol	SCDM
Sol	Solubility	2.2E+04	mg/L	SCDM
VP	Vapor pressure	2.3E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.4E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	8.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-48. Chemical-Specific Inputs for 3,4-Dimethylphenol (95-65-8)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.8E-01	g/cm3	HSDB
MW	Molecular Weight	1.2E+02	g/mol	HSDB
Sol	Solubility	4.8E+03	mg/L	HSDB
VP	Vapor pressure	3.6E-02	mmHg	HSDB
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	2.2E+00	unitless	Hansch et al., 1995
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	5.5E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.5E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.9E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.
HLC	Henry's law constant	1.2E-06	atm-m3/mol	Calculated Based on Lyman, 1990.

Table B-49. Chemical-Specific Inputs for 1,2-Dibromo-3-chloropropane (96-12-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.1E+00	g/cm3	SCDM
HLC	Henry's law constant	1.5E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.3E+00	unitless	SCDM
MW	Molecular Weight	2.4E+02	g/mol	SCDM
Sol	Solubility	1.2E+03	mg/L	SCDM
VP	Vapor pressure	5.8E-01	mmHg	SCDM
Kh	Hydrolysis rate	1.3E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-50. Chemical-Specific Inputs for Furfural (98-01-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	4.0E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.1E-01	unitless	SCDM
MW	Molecular Weight	9.6E+01	g/mol	SCDM
Sol	Solubility	1.1E+05	mg/L	SCDM
VP	Vapor pressure	2.2E+00	mmHg	SCDM
Ksg	Soil degradation rate	1.0E-20	sec-1	no value for Ksg in existing hierarchy
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
K1	Aqueous degradation rate (low)	5.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-51. Chemical-Specific Inputs for Cumene (98-82-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.6E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E+00	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.6E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	6.1E+01	mg/L	SCDM
VP	Vapor pressure	4.5E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.0E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.9E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-52. Chemical-Specific Inputs for Nitrobenzene (98-95-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.4E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.8E+00	unitless	SCDM
MW	Molecular Weight	1.2E+02	g/mol	SCDM
Sol	Solubility	2.1E+03	mg/L	SCDM
VP	Vapor pressure	2.5E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.1E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.3E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-53. Chemical-Specific Inputs for Ethylbenzene (100-41-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.7E-01	g/cm3	SCDM
HLC	Henry's law constant	7.9E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.1E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	1.7E+02	mg/L	SCDM
VP	Vapor pressure	9.6E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	8.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.1E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.8E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-54. Chemical-Specific Inputs for Styrene (100-42-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.1E-01	g/cm3	SCDM
HLC	Henry's law constant	2.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.9E+00	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	3.1E+02	mg/L	SCDM
VP	Vapor pressure	6.1E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.1E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-55. Chemical-Specific Inputs for p-Dichlorobenzene (106-46-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	2.4E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.4E+00	unitless	SCDM
MW	Molecular Weight	1.5E+02	g/mol	SCDM
Sol	Solubility	7.4E+01	mg/L	SCDM
VP	Vapor pressure	1.0E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.3E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.4E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.7E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-56. Chemical-Specific Inputs for 1,2-Epoxybutane (106-88-7)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	8.4E-01	g/cm3	HSDB
VP	Vapor pressure	1.8E+02	mmHg	HSDB
Ksg	Soil degradation rate	6.2E-07	sec-1	Howard et al, 1991
HLC	Henry's law constant	1.8E-04	atm-m3/mol	Chemfate
LogKow	Octanol-water partition coeficient	2.6E-01	unitless	Chemfate
MW	Molecular Weight	7.2E+01	g/mol	Chemfate
Sol	Solubility	9.5E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	4.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-57. Chemical-Specific Inputs for Epichlorohydrin (106-89-8)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.0E-05	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E-01	unitless	SCDM
MW	Molecular Weight	9.3E+01	g/mol	SCDM
Sol	Solubility	6.6E+04	mg/L	SCDM
VP	Vapor pressure	1.6E+01	mmHg	SCDM
Density	Density of the chemical	1.2E+00	g/cm3	Merck
Kh	Hydrolysis rate	9.8E-07	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-58. Chemical-Specific Inputs for Ethylene dibromide (106-93-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.2E+00	g/cm3	SCDM
HLC	Henry's law constant	7.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.9E+02	g/mol	SCDM
Sol	Solubility	4.2E+03	mg/L	SCDM
VP	Vapor pressure	1.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	2.0E-08	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	5.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.7E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-59. Chemical-Specific Inputs for 1,3-Butadiene (106-99-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	6.1E-01	g/cm3	SCDM
HLC	Henry's law constant	7.4E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	5.4E+01	g/mol	SCDM
Sol	Solubility	7.4E+02	mg/L	SCDM
VP	Vapor pressure	2.1E+03	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.0E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-60. Chemical-Specific Inputs for Acrolein (107-02-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.4E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.0E-02	unitless	SCDM
MW	Molecular Weight	5.6E+01	g/mol	SCDM
Sol	Solubility	2.1E+05	mg/L	SCDM
VP	Vapor pressure	2.7E+02	mmHg	SCDM
Kh	Hydrolysis rate	2.1E+01	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	7.8E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-61. Chemical-Specific Inputs for Allyl chloride (107-05-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.4E-01	g/cm3	SCDM
HLC	Henry's law constant	1.1E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	7.7E+01	g/mol	SCDM
Sol	Solubility	3.4E+03	mg/L	SCDM
VP	Vapor pressure	3.7E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.8E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-62. Chemical-Specific Inputs for 1,2-Dichloroethane (107-06-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	9.8E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	9.9E+01	g/mol	SCDM
Sol	Solubility	8.5E+03	mg/L	SCDM
VP	Vapor pressure	7.9E+01	mmHg	SCDM
Kh	Hydrolysis rate	3.0E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	9.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-63. Chemical-Specific Inputs for Acrylonitrile (107-13-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.1E-01	g/cm3	SCDM
HLC	Henry's law constant	1.0E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.5E-01	unitless	SCDM
MW	Molecular Weight	5.3E+01	g/mol	SCDM
Sol	Solubility	7.4E+04	mg/L	SCDM
VP	Vapor pressure	1.1E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.5E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.1E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.2E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-64. Chemical-Specific Inputs for Ethylene glycol (107-21-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	6.0E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.4E+00	unitless	SCDM
MW	Molecular Weight	6.2E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.2E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	6.7E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	1.2E-01	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.4E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-65. Chemical-Specific Inputs for Vinyl acetate (108-05-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.3E-01	g/cm3	SCDM
HLC	Henry's law constant	5.1E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	7.3E-01	unitless	SCDM
MW	Molecular Weight	8.6E+01	g/mol	SCDM
Sol	Solubility	2.0E+04	mg/L	SCDM
VP	Vapor pressure	9.0E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-66. Chemical-Specific Inputs for Methyl isobutyl ketone (108-10-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.0E-01	g/cm3	SCDM
HLC	Henry's law constant	1.4E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.2E+00	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	1.9E+04	mg/L	SCDM
VP	Vapor pressure	2.0E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.5E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	7.4E-01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.7E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-67. Chemical-Specific Inputs for Toluene (108-88-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	8.7E-01	g/cm3	SCDM
HLC	Henry's law constant	6.6E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.8E+00	unitless	SCDM
MW	Molecular Weight	9.2E+01	g/mol	SCDM
Sol	Solubility	5.3E+02	mg/L	SCDM
VP	Vapor pressure	2.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.6E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.4E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.2E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-68. Chemical-Specific Inputs for Chlorobenzene (108-90-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	3.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.9E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	4.7E+02	mg/L	SCDM
VP	Vapor pressure	1.2E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.4E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.9E-01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-69. Chemical-Specific Inputs for Cyclohexanol (108-93-0)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.6E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
VP	Vapor pressure	8.0E-01	mmHg	HSDB
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	1.2E+00	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.0E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	1.0E+02	g/mol	Chemfate
Sol	Solubility	4.3E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	5.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	9.1E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.1E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-70. Chemical-Specific Inputs for Phenol (108-95-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	4.0E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	SCDM
MW	Molecular Weight	9.4E+01	g/mol	SCDM
Sol	Solubility	8.3E+04	mg/L	SCDM
VP	Vapor pressure	2.8E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	8.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.3E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.1E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-71. Chemical-Specific Inputs for 2-Methoxyethanol (109-86-4)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.6E-01	g/cm3	HSDB
Sol	Solubility	1.0E+06	mg/L	HSDB
VP	Vapor pressure	6.2E+00	mmHg	HSDB
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	-7.7E-01	unitless	Hansch et al., 1995
HLC	Henry's law constant	8.1E-08	atm-m3/mol	Chemfate
MW	Molecular Weight	7.6E+01	g/mol	Chemfate
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-72. Chemical-Specific Inputs for 2-Methoxyethanol acetate (110-49-6)

Parameter	Definition	Value	Units	Reference
LogKow	Octanol-water partition coeficient	1.0E-01	unitless	KowWIN
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	1.0E+00	g/cm3	HSDB
MW	Molecular Weight	1.2E+02	g/mol	HSDB
Sol	Solubility	1.0E+06	mg/L	HSDB
VP	Vapor pressure	2.0E+00	mmHg	HSDB
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.7E-06	cm2/s	Calculated based on WATER9, 2001.
HLC	Henry's law constant	3.1E-07	atm-m3/mol	Calculated Based on Lyman, 1990.

Table B-73. Chemical-Specific Inputs for n-Hexane (110-54-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	6.5E-01	g/cm3	SCDM
HLC	Henry's law constant	1.4E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.0E+00	unitless	SCDM
MW	Molecular Weight	8.6E+01	g/mol	SCDM
Sol	Solubility	1.2E+01	mg/L	SCDM
VP	Vapor pressure	1.5E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	5.0E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.5E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-74. Chemical-Specific Inputs for 2-Ethoxyethanol (110-80-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.3E-01	g/cm3	SCDM
HLC	Henry's law constant	1.2E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.0E-01	unitless	SCDM
MW	Molecular Weight	9.0E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	5.3E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-75. Chemical-Specific Inputs for Pyridine (110-86-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.8E-01	g/cm3	SCDM
HLC	Henry's law constant	8.9E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	6.7E-01	unitless	SCDM
MW	Molecular Weight	7.9E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	2.1E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.1E-06	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	2.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	3.5E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	9.3E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-76. Chemical-Specific Inputs for 2-Ethoxyethanol acetate (111-15-9)

Parameter	Definition	Value	Units	Reference
LogKow	Octanol-water partition coeficient	5.9E-01	unitless	KowWIN
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.7E-01	g/cm3	HSDB
HLC	Henry's law constant	1.8E-06	atm-m3/mol	HSDB
Sol	Solubility	2.3E+05	mg/L	HSDB
VP	Vapor pressure	2.3E+00	mmHg	HSDB
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
MW	Molecular Weight	1.3E+02	g/mol	Chemfate
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.0E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.0E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-77. Chemical-Specific Inputs for Hexachlorobenzene (118-74-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.0E+00	g/cm3	SCDM
HLC	Henry's law constant	1.3E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	5.9E+00	unitless	SCDM
MW	Molecular Weight	2.8E+02	g/mol	SCDM
Sol	Solubility	5.0E-03	mg/L	SCDM
VP	Vapor pressure	1.8E-05	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	3.8E-09	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	9.6E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.0E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	2.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-78. Chemical-Specific Inputs for 1,2,4-Trichlorobenzene (120-82-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	1.4E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	4.0E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	3.5E+01	mg/L	SCDM
VP	Vapor pressure	4.3E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	4.4E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.7E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.2E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.5E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-79. Chemical-Specific Inputs for 2,4-Dinitrotoluene (121-14-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.3E+00	g/cm3	SCDM
HLC	Henry's law constant	9.3E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	2.7E+02	mg/L	SCDM
VP	Vapor pressure	1.5E-04	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	3.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.9E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-80. Chemical-Specific Inputs for Triethylamine (121-44-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	7.3E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	0.0E+00	sec-1	HSDB
VP	Vapor pressure	5.7E+01	mmHg	HSDB
LogKow	Octanol-water partition coeficient	1.5E+00	unitless	Hansch et al., 1995
HLC	Henry's law constant	1.4E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	1.0E+02	g/mol	Chemfate
Sol	Solubility	5.5E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	1.1E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	9.7E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-81. Chemical-Specific Inputs for 1,2-Diphenylhydrazine (122-66-7)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
HLC	Henry's law constant	1.5E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.9E+00	unitless	SCDM
MW	Molecular Weight	1.8E+02	g/mol	SCDM
Sol	Solubility	6.8E+01	mg/L	SCDM
VP	Vapor pressure	4.3E-04	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.9E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.9E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	1.4E+01	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	5.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	7.3E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-82. Chemical-Specific Inputs for 1,4-Dioxane (123-91-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.0E+00	g/cm3	SCDM
HLC	Henry's law constant	4.8E-06	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-3.9E-01	unitless	SCDM
MW	Molecular Weight	8.8E+01	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	3.8E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.9E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.3E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.5E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.4E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-83. Chemical-Specific Inputs for Chlorodibromomethane (124-48-1)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	2.5E+00	g/cm3	SCDM
HLC	Henry's law constant	7.8E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.2E+00	unitless	SCDM
MW	Molecular Weight	2.1E+02	g/mol	SCDM
Sol	Solubility	2.6E+03	mg/L	SCDM
VP	Vapor pressure	4.9E+00	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	3.5E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	3.7E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.1E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-84. Chemical-Specific Inputs for Chloroprene (126-99-8)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	9.6E-01	g/cm3	SCDM
LogKow	Octanol-water partition coeficient	2.1E+00	unitless	SCDM
MW	Molecular Weight	8.9E+01	g/mol	SCDM
Sol	Solubility	1.7E+03	mg/L	SCDM
VP	Vapor pressure	2.1E+02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
HLC	Henry's law constant	1.2E-02	atm-m3/mol	Chemfate
K1	Aqueous degradation rate (low)	2.2E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.2E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	7.8E+02	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.8E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-85. Chemical-Specific Inputs for Tetrachloroethylene (127-18-4)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.6E+00	g/cm3	SCDM
HLC	Henry's law constant	1.8E-02	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.7E+00	unitless	SCDM
MW	Molecular Weight	1.7E+02	g/mol	SCDM
Sol	Solubility	2.0E+02	mg/L	SCDM
VP	Vapor pressure	1.9E+01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.2E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	5.1E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.4E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-86. Chemical-Specific Inputs for 1,1,1,2-Tetrachloroethane (630-20-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.5E+00	g/cm3	SCDM
HLC	Henry's law constant	2.4E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.6E+00	unitless	SCDM
MW	Molecular Weight	1.7E+02	g/mol	SCDM
Sol	Solubility	1.1E+03	mg/L	SCDM
VP	Vapor pressure	1.2E+01	mmHg	SCDM
Kh	Hydrolysis rate	4.3E-10	sec-1	Kollig, 1993
Ksg	Soil degradation rate	1.2E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	6.8E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	6.2E+00	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.9E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.8E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.1E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-87. Chemical-Specific Inputs for N-Nitrosodi-n-butylamine (924-16-3)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	3.2E-04	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.4E+00	unitless	SCDM
MW	Molecular Weight	1.6E+02	g/mol	SCDM
Sol	Solubility	1.3E+03	mg/L	SCDM
VP	Vapor pressure	3.0E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	9.0E-01	g/cm3	HSDB
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-04	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	4.2E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	6.8E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-88. Chemical-Specific Inputs for N-Nitrosopyrrolidine (930-55-2)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	1.2E-08	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	-1.9E-01	unitless	SCDM
MW	Molecular Weight	1.0E+02	g/mol	SCDM
Sol	Solubility	1.0E+06	mg/L	SCDM
VP	Vapor pressure	9.2E-02	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-04	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	8.0E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-89. Chemical-Specific Inputs for Cresols (total) (1319-77-3)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.1E+00	g/cm3	SCDM
HLC	Henry's law constant	9.5E-07	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.3E+04	mg/L	SCDM
VP	Vapor pressure	1.8E-01	mmHg	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.8E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.7E+01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	2.3E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	8.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.8E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.4E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	9.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-90. Chemical-Specific Inputs for Xylenes (1330-20-7)

Parameter	Definition	Value	Units	Reference
HLC	Henry's law constant	6.7E-03	atm-m3/mol	SCDM
LogKow	Octanol-water partition coeficient	3.2E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	1.8E+02	mg/L	SCDM
VP	Vapor pressure	8.0E+00	mmHg	SCDM
Density	Density of the chemical	8.7E-01	g/cm3	Merck
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Ksg	Soil degradation rate	2.9E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	1.8E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	4.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.9E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	6.9E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.5E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-91. Chemical-Specific Inputs for Methyl tert-butyl ether (1634-04-4)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	Kollig, 1993
Density	Density of the chemical	7.4E-01	g/cm3	HSDB
VP	Vapor pressure	2.5E+02	mmHg	HSDB
Ksg	Soil degradation rate	4.5E-08	sec-1	Howard et al, 1991
LogKow	Octanol-water partition coeficient	9.4E-01	unitless	Hansch et al., 1995
HLC	Henry's law constant	5.9E-04	atm-m3/mol	Chemfate
MW	Molecular Weight	8.8E+01	g/mol	Chemfate
Sol	Solubility	5.1E+04	mg/L	Chemfate
K1	Aqueous degradation rate (low)	7.1E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.8E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.1E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.2E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.5E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	8.6E-06	cm2/s	Calculated based on WATER9, 2001.

Table B-92. Chemical-Specific Inputs for 2,3,7,8-TCDD (1746-01-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.8E+00	g/cm3	Mackay et al, 1992
Ksg	Soil degradation rate	1.4E-08	sec-1	Howard et al, 1991
HLC	Henry's law constant	3.3E-05	atm-m3/mol	Dioxin Reassessment
Kh	Hydrolysis rate	0.0E+00	sec-1	Dioxin Reassessment
LogKow	Octanol-water partition coeficient	6.8E+00	unitless	Dioxin Reassessment
MW	Molecular Weight	3.2E+02	g/mol	Dioxin Reassessment
Sol	Solubility	1.9E-05	mg/L	Dioxin Reassessment
VP	Vapor pressure	1.5E-09	mmHg	Dioxin Reassessment
K1	Aqueous degradation rate (low)	3.1E-02	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-03	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	7.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	2.4E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	1.6E+02	K	CHEMDAT8
Dw	Diffusion coefficient in water	6.8E-06	cm2/s	Calculated based on WATER9, 2001.
Da	Diffusivity of chemical in air	4.7E-02	cm2/s	Calculated based on EPA's Dioxin Reassessment, 2000.

Table B-93. Chemical-Specific Inputs for Mercury (7439-97-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.4E+01	g/cm3	SCDM
Kh	Hydrolysis rate	0.0E+00	sec-1	not applicable for metallic species
Ksg	Soil degradation rate	0.0E+00	sec-1	not applicable for metallic species
HLC	Henry's law constant	7.1E-03	atm-m3/mol	MRTC
LogKd	soil-water partition coeficient	3.0E+00	unitless	MRTC
MW	Molecular Weight	2.0E+02	g/mol	MRTC
Sol	Solubility	5.6E-02	mg/L	Merck
VP	Vapor pressure	2.0E-03	mmHg	Merck
K1	Aqueous degradation rate (low)	1.0E+00	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.0E-04	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	0.0E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	0.0E+00	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.7E+02	K	CHEMDAT8
Dw	Diffusion coefficient in water	3.0E-05	cm2/s	Calculated based on WATER9, 2001.
Da	Diffusivity of chemical in air	5.5E-02	cm2/s	Calculated based on EPA, 1987.

Table B-94. Chemical-Specific Inputs for Divalent mercury (7439-97-7)

Parameter	Definition	Value	Units	Reference
Kh	Hydrolysis rate	0.0E+00	sec-1	not applicable for metallic species
Ksg	Soil degradation rate	0.0E+00	sec-1	not applicable for metallic species
HLC	Henry's law constant	7.1E-10	atm-m3/mol	MRTC
LogKd	soil-water partition coeficient	4.8E+00	unitless	MRTC
MW	Molecular Weight	2.0E+02	g/mol	MRTC
Sol	Solubility	7.4E+04	mg/L	Merck
Density	Density of the chemical	5.6E+00	g/cm3	HSDB
VP	Vapor pressure	1.0E+00	mmHg	HSDB
Dw	Diffusion coefficient in water	1.8E-05	cm2/s	Calculated based on WATER9, 2001.
Da	Diffusivity of chemical in air	5.5E-02	cm2/s	Calculated based on EPA, 1987.
K1	Aqueous degradation rate (low)			
Kmax	Aqueous degradation rate (max)			
VP Coeff A	Antoine's coefficient A			
VP Coeff B	Antoine's coefficient B			
VP Coeff C	Antoine's coefficient C			

Table B-95. Chemical-Specific Inputs for cis-1,3-Dichloropropylene (10061-01-5)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.7E+03	mg/L	SCDM
VP	Vapor pressure	3.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	1.3E-06	sec-1	Kollig, 1993
HLC	Henry's law constant	2.4E-03	atm-m3/mol	HSDB
Ksg	Soil degradation rate	7.1E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

Table B-96. Chemical-Specific Inputs for trans-1,3-Dichloropropylene (10061-02-6)

Parameter	Definition	Value	Units	Reference
Density	Density of the chemical	1.2E+00	g/cm3	SCDM
LogKow	Octanol-water partition coeficient	2.0E+00	unitless	SCDM
MW	Molecular Weight	1.1E+02	g/mol	SCDM
Sol	Solubility	2.7E+03	mg/L	SCDM
VP	Vapor pressure	2.3E+01	mmHg	SCDM
Kh	Hydrolysis rate	1.3E-06	sec-1	Kollig, 1993
HLC	Henry's law constant	1.8E-03	atm-m3/mol	HSDB
Ksg	Soil degradation rate	7.1E-07	sec-1	Howard et al, 1991
K1	Aqueous degradation rate (low)	7.6E-01	L/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
Kmax	Aqueous degradation rate (max)	1.1E+01	mg VO/g-hr	CHEMDAT8 or degradation database for CHEMDAT6
VP Coeff A	Antoine's coefficient A	6.8E+00	K	CHEMDAT8
VP Coeff B	Antoine's coefficient B	1.3E+03	K	CHEMDAT8
VP Coeff C	Antoine's coefficient C	2.3E+02	K	CHEMDAT8
Da	Diffusivity of chemical in air	7.6E-02	cm2/s	Calculated based on WATER9, 2001.
Dw	Diffusion coefficient in water	1.0E-05	cm2/s	Calculated based on WATER9, 2001.

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Appendix C

Sensitivity Analysis of ISCST3 Air Dispersion Model

Appendix C

Sensitivity Analysis of ISCST3 Air Dispersion Model

This appendix describes the sensitivity analysis performed on depletion options, source shape and orientation, and receptor location and spacing.

C.1 Options with and without Depletion

A sensitivity analysis was conducted using the ISCST3 model to determine whether the wet depletion option should be used when developing dispersion factors for IWAIR. A discussion of the analysis follows.

The wet depletion option may be used when estimating air concentrations with ISCST3. The concentrations modeled without depletion are higher than those modeled with depletion. Because it takes much longer to run the ISCST3 model with wet depletion than without wet depletion, a sensitivity analysis was performed to investigate the differences in estimated air concentrations with and without selecting wet depletion.

In this investigation, the 5th and the 95th percentile of sizes of land application units were used to determine the relationship between concentrations with depletions and sizes of units; those areas are 1,200 m^2 and 1,700,000 m^2, respectively.

Two meteorological stations representing a wet location and a dry location were selected for the sensitivity analysis: Atlanta, Georgia, with 49.8 inches precipitation per year (a relatively high annual precipitation rate), and Winnemucca, Nevada, with 8.1 inches precipitation per year (a relatively low annual precipitation rate). The reason for selecting a wet site and a dry site was to examine (1) whether wet depletion has a more significant impact for a wet site than a dry site; and (2) the differences in ambient concentrations that a very wet site can make with and without selecting wet depletion.

Annual average concentrations with and without wet depletion also were calculated using 5 years of meteorological data from Atlanta and Winnemucca for the 5th and 95th percentile of areas of land application units. The results show that the differences in the maximum concentrations with and without wet depletion are small for both locations. However, the differences in the maximum concentrations between those calculated with wet depletion and those calculated without wet depletion are about 5 to 10 times greater for the wet site (Atlanta) than the dry site (Winnemuca). Tables C-1a and C-1b show that for the 95th percentile unit size, at 50 meters from the edge of the unit, the differences in the maximum concentrations are only 0.03 percent and 0.37 percent for Winnemucca and Atlanta, respectively. This means that model concentrations with and without wet depletion are about the same.

Table C-1a. Differences in Values of Vapor Air Concentration Calculated with Wet Depletion and without Wet Depletion

(Atlanta, GA Site)

5th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
19.3 (1)	7.40752	7.40716	0.00036	0.005%
47.3 (1)	0.93175	0.93159	0.00016	0.017%
75.2 (1)	0.38178	0.38168	0.00010	0.026%
100	0.25129	0.25121	0.00008	0.032%
103.2 (1)	0.21003	0.20996	0.00007	0.033%
187.0 (1)	0.06886	0.06882	0.00004	0.058%
200	0.07091	0.07086	0.00005	0.071%
300	0.03390	0.03387	0.00003	0.088%
400	0.02026	0.02024	0.00002	0.099%
500	0.01359	0.01357	0.00002	0.147%
600	0.00981	0.00979	0.00002	0.204%
800	0.00590	0.00589	0.00001	0.169%
1000	0.00400	0.00399	0.00001	0.250%
1500	0.00205	0.00205	0.00000	0.000%
2000	0.00128	0.00128	0.00000	0.000%
3000	0.00068	0.00067	0.00001	1.471%
4000	0.00044	0.00043	0.00001	2.273%
5000	0.00031	0.00031	0.00000	0.000%
10000	0.00011	0.00011	0.00000	0.000%

95th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
651.9 (1)	0.00614	0.00612	0.00002	0.33%
676.9 (1)	0.00574	0.00573	0.00001	0.17%
701.9 (1)	0.00539	0.00537	0.00002	0.37%
726.9 (1)	0.00507	0.00505	0.00002	0.39%
801.9 (1)	0.00427	0.00426	0.00001	0.23%
1000	0.00400	0.00399	0.00001	0.25%
1100	0.00342	0.00341	0.00001	0.29%
1200	0.00296	0.00295	0.00001	0.34%
1300	0.00260	0.00259	0.00001	0.38%
1400	0.00230	0.00229	0.00001	0.43%
1500	0.00205	0.00205	0.00000	0.00%
1600	0.00185	0.00184	0.00001	0.54%
1800	0.00152	0.00152	0.00000	0.00%
2000	0.00128	0.00128	0.00000	0.00%
3000	0.00068	0.00067	0.00001	1.47%
4000	0.00044	0.00043	0.00001	2.27%
5000	0.00031	0.00031	0.00000	0.00%
10000	0.00011	0.00011	0.00000	0.00%

(1) These refer to the distances from the center of emission source to the maximum concentration points along 0, 25, 50, 75, and 150 meter receptor squares, respectively.

Table C-1b. Differences in Values of Vapor Air Concentration Calculated with Wet Depletion and without Wet Depletion

(Winnemucca, NV Site)

5th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
17.3 (1)	7.79132	7.79125	0.00007	0.001%
42.3 (1)	1.08468	1.08464	0.00004	0.004%
67.3 (1)	0.48369	0.48367	0.00002	0.004%
92.3 (1)	0.27965	0.27963	0.00002	0.007%
100	0.24315	0.24313	0.00002	0.008%
167.3 (1)	0.09949	0.09948	0.00001	0.010%
200	0.07296	0.07295	0.00001	0.014%
300	0.03600	0.03599	0.00001	0.028%
400	0.02181	0.02180	0.00001	0.046%
500	0.01475	0.01474	0.00001	0.068%
600	0.01070	0.01070	0.00000	0.000%
800	0.00649	0.00648	0.00001	0.154%
1000	0.00443	0.00443	0.00000	0.000%
1500	0.00229	0.00229	0.00000	0.000%
2000	0.00144	0.00144	0.00000	0.000%
3000	0.00077	0.00077	0.00000	0.000%
4000	0.00050	0.00050	0.00000	0.000%
5000	0.00036	0.00036	0.00000	0.000%
10000	0.00013	0.00013	0.00000	0.000%

95th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
651.9 (1)	23.14326	23.13885	0.00441	0.02%
676.9 (1)	13.86979	13.86551	0.00428	0.03%
701.9 (1)	11.62889	11.62486	0.00403	0.03%
726.9 (1)	10.25373	10.24985	0.00388	0.04%
801.9 (1)	7.84900	7.84548	0.00352	0.04%
1000	5.85241	5.84988	0.00253	0.04%
1100	4.69239	4.68991	0.00248	0.05%
1200	3.98357	3.98130	0.00227	0.06%
1300	3.43255	3.43045	0.00210	0.06%
1400	2.99083	2.98887	0.00196	0.07%
1500	2.63019	2.62837	0.00182	0.07%
1600	2.33211	2.33042	0.00169	0.07%
1800	1.93762	1.93554	0.00208	0.11%
2000	1.65686	1.65487	0.00199	0.12%
3000	0.91889	0.91727	0.00162	0.18%
4000	0.61160	0.61020	0.00140	0.23%
5000	0.45013	0.44890	0.00123	0.27%
10000	0.17843	0.17767	0.00076	0.43%

(1) These refer to the distances from the center of emission source to the maximum concentration points along 0, 25, 50, 75, and 150 meter receptor squares, respectively.

C.2 Source Shape and Orientation

A sensitivity analysis was conducted using the ISCST3 air model to determine what role source shape and orientation play in determining dispersion coefficients of air pollutants. A discussion of this analysis follows.

Three different sources were chosen for this analysis. The sources were a square (Source No. 1), a rectangle oriented east to west (Source No. 2), and a rectangle oriented north to south (Source No. 3). All three sources had an area of 400 m^2 in order to ensure that equal emission rates were compared. The rectangles were selected to be exactly two times longer and half as wide as the square (see Figure C-1).

Two meteorological stations. Little Rock, Arkansas, and Los Angeles, California, were selected for this modeling analysis in order to compare two different meteorological regimes. Little Rock was selected because of its evenly distributed wind directions, and Los Angeles was selected because it has a predominantly southwest wind direction (see Figure C-2). Five years of meteorological data were used for this analysis.

Each area source was modeled with similar receptor grids to ensure consistency. Sixteen receptors were placed on the edge of each of the area sources, and another 16 were placed 25 m out from the edge. Each of these two receptor groups were modeled as a Cartesian receptor grid. Two receptor rings were also placed at 50 and 100 m out from the center of the source. This polar receptor grid consisted of 16 receptors with a 22.5° interval between receptors. See Figures C-3a through C-3c for receptor locations.

The ISCST3 model was run using the meteorological data from Little Rock, Arkansas, and Los Angeles, California, and the results are shown in Tables C-2a and C-2b. The results indicated that the standard deviation of the differences in air concentrations is greatest between the two rectangular source shapes (source No. 2 and source No. 3). This difference is due to the orientation of the source. This occurs for both the Cartesian receptor grid and the polar receptor grid at both meteorological locations. This shows that the model is sensitive to the orientation of the rectangular area source.

Standard deviations are significantly smaller when the square source (Source No. 1) is compared with either rectangular source (Source No. 2 or 3). This shows that the differences in dispersion factors between the square source and the two rectangular sources are less than the differences between the two rectangular sources. A square area source also contributes the least amount of impact of orientation. Because the dispersion factors in IWAIR must applicable to a variety of source shapes and orientations, a square source will minimize the errors caused by different source shapes and orientations.

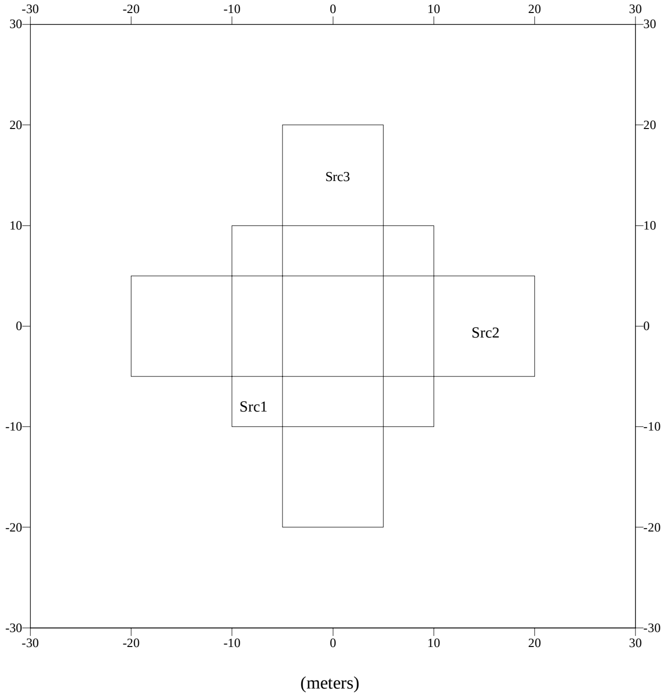
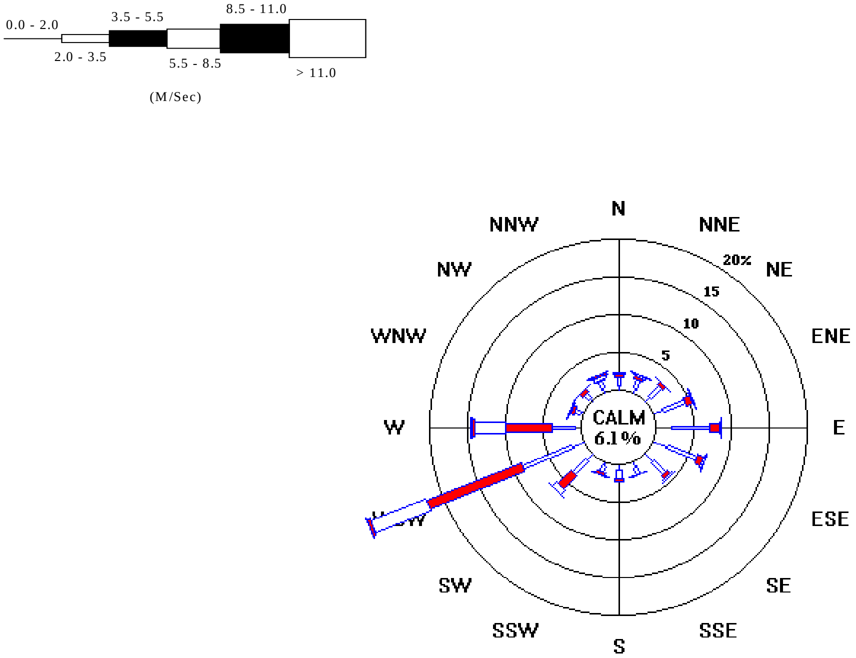


Figure C-1. Source shapes and orientations.

Los Angeles, California



Little Rock, Arkansas

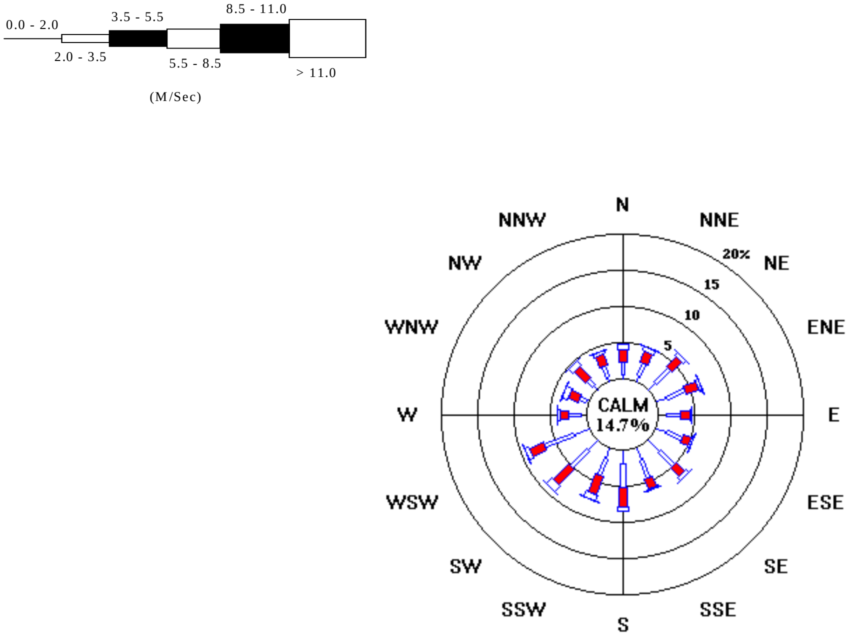


Figure C-2. Wind roses.

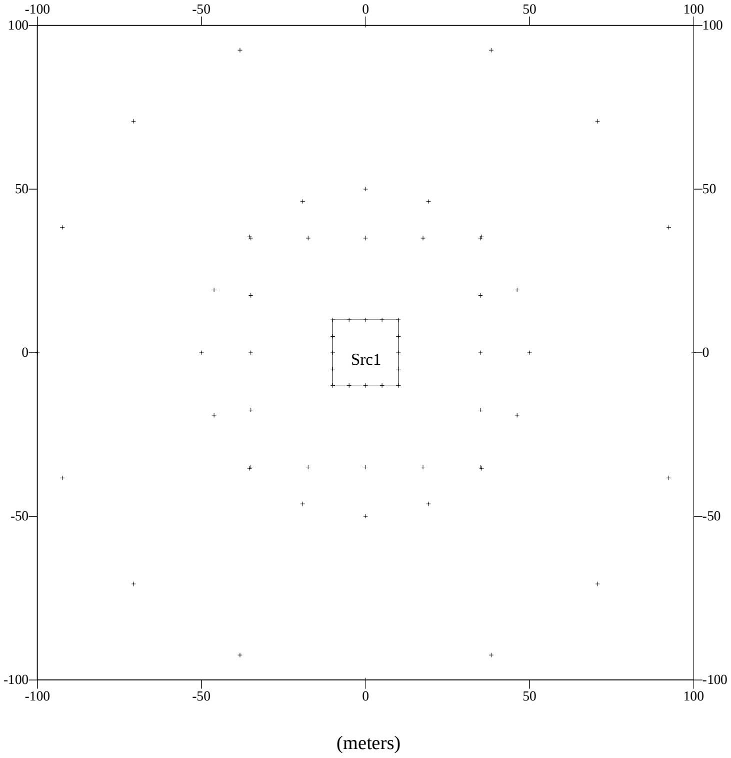


Figure C-3a. Receptor locations (Source No. 1).

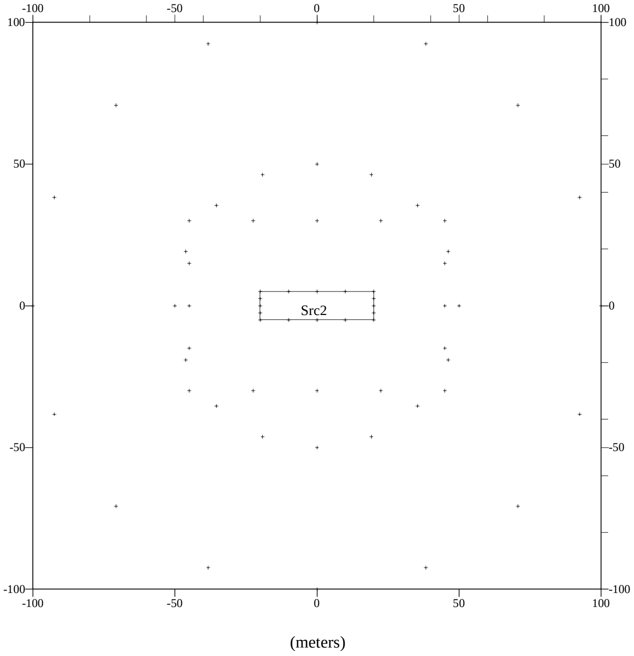


Figure C-3b. Receptor locations (Source No. 2).

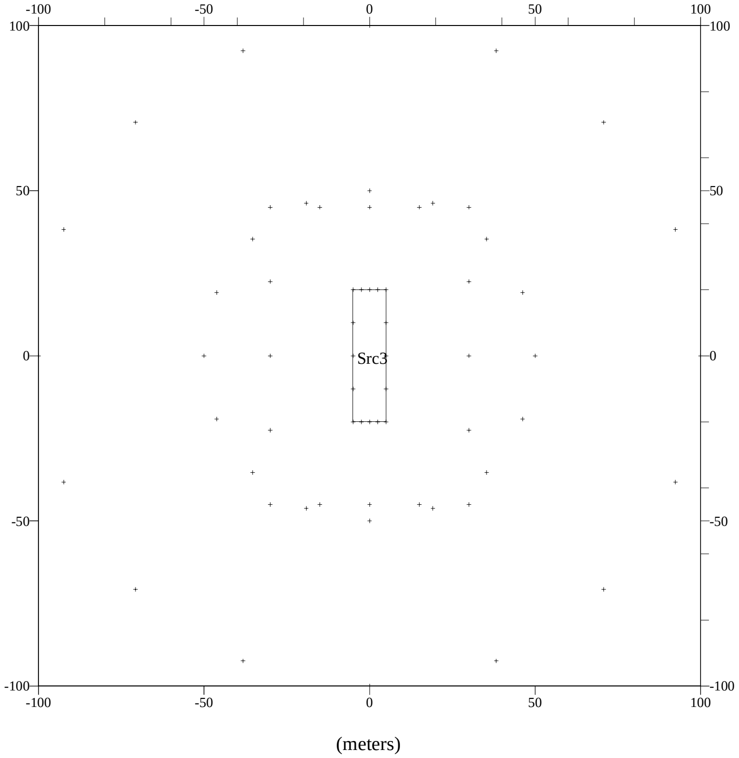


Figure C-3c. Receptor locations (Source No. 3).

Table C-2a. Comparisons of Dispersion Factors (ug/m^3 / $ug/s\text{-}m^2$) for Different Source Shapes and Orientations (Little Rock, Arkansas)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Polar Receptor Grid														
X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.
19	46	0.190	19	46	0.199	19	46	0.211	0.010	5%	0.021	11%	0.012	6%
38	92	0.050	38	92	0.051	38	92	0.051	0.001	1%	0.001	2%	0.000	1%
35	35	0.249	35	35	0.243	35	35	0.278	-0.007	-3%	0.028	11%	0.035	14%
71	71	0.067	71	71	0.067	71	71	0.069	-0.001	-1%	0.001	2%	0.002	3%
46	19	0.321	46	19	0.361	46	19	0.256	0.041	13%	-0.065	-20%	-0.105	-29%
92	38	0.095	92	38	0.098	92	38	0.088	0.003	3%	-0.007	-7%	-0.010	-10%
50	0	0.124	50	0	0.128	50	0	0.147	0.004	3%	0.023	19%	0.020	15%
100	0	0.030	100	0	0.030	100	0	0.033	0.000	-1%	0.003	9%	0.003	11%
46	-19	0.085	46	-19	0.096	46	-19	0.084	0.011	12%	-0.001	-1%	-0.011	-12%
92	-38	0.023	92	-38	0.024	92	-38	0.023	0.001	2%	-0.001	-2%	-0.001	-5%
35	-35	0.106	35	-35	0.109	35	-35	0.103	0.003	3%	-0.003	-3%	-0.006	-6%
71	-71	0.030	71	-71	0.030	71	-71	0.029	0.000	0%	0.000	-1%	-0.001	-2%
19	-46	0.117	19	-46	0.113	19	-46	0.128	-0.005	-4%	0.011	9%	0.016	14%
38	-92	0.033	38	-92	0.032	38	-92	0.034	-0.001	-4%	0.001	2%	0.002	7%
0	-50	0.122	0	-50	0.117	0	-50	0.143	-0.005	-4%	0.021	17%	0.026	22%
0	-100	0.035	0	-100	0.033	0	-100	0.037	-0.002	-5%	0.002	5%	0.004	11%
-19	-46	0.134	-19	-46	0.128	-19	-46	0.150	-0.006	-4%	0.016	12%	0.022	17%
-38	-92	0.038	-38	-92	0.036	-38	-92	0.038	-0.002	-4%	0.001	2%	0.002	6%
-35	-35	0.161	-35	-35	0.158	-35	-35	0.170	-0.003	-2%	0.009	6%	0.012	8%
-71	-71	0.043	-71	-71	0.043	-71	-71	0.045	0.000	1%	0.001	3%	0.001	3%
-46	-19	0.159	-46	-19	0.185	-46	-19	0.140	0.026	16%	-0.019	-12%	-0.045	-24%
-92	-38	0.044	-92	-38	0.046	-92	-38	0.043	0.002	4%	-0.002	-4%	-0.004	-8%
-50	0	0.103	-50	0	0.114	-50	0	0.107	0.011	11%	0.004	4%	-0.007	-6%
-100	0	0.027	-100	0	0.027	-100	0	0.027	0.000	2%	0.000	1%	0.000	0%
-46	19	0.126	-46	19	0.145	-46	19	0.118	0.019	15%	-0.008	-6%	-0.027	-18%
-92	38	0.035	-92	38	0.036	-92	38	0.034	0.001	4%	-0.001	-4%	-0.003	-7%
-35	35	0.152	-35	35	0.160	-35	35	0.153	0.008	5%	0.001	0%	-0.007	-5%
-71	71	0.041	-71	71	0.042	-71	71	0.041	0.001	3%	0.001	2%	-0.001	-2%
-19	46	0.173	-19	46	0.179	-19	46	0.187	0.007	4%	0.014	8%	0.008	4%
-38	92	0.047	-38	92	0.047	-38	92	0.048	0.000	0%	0.001	3%	0.001	3%
0	50	0.224	0	50	0.191	0	50	0.276	-0.032	-14%	0.052	23%	0.085	44%
0	100	0.068	0	100	0.061	0	100	0.074	-0.008	-11%	0.006	9%	0.014	22%
								Standard Deviation:	**0.012**	**7%**	**0.018**	**9%**	**0.028**	**14%**

(continued)

Table C-2a. (continued)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Cartesion Receptor Grid														
X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.
-10	-10	3.014	-20	-5	2.675	-5	-20	2.673	-0.339	-11%	-0.341	-11%	-0.002	0%
-5	-10	4.266	-10	-5	4.219	-2.5	-20	3.451	-0.047	-1%	-0.815	-19%	-0.769	-18%
0	-10	4.354	0	-5	4.307	0	-20	3.526	-0.047	-1%	-0.827	-19%	-0.781	-18%
5	-10	3.961	10	-5	4.069	2.5	-20	3.152	0.109	3%	-0.809	-20%	-0.918	-23%
10	-10	2.175	20	-5	1.899	5	-20	2.011	-0.276	-13%	-0.164	-8%	0.112	6%
10	-5	5.211	20	-2.5	3.875	5	-10	5.567	-1.337	-26%	0.355	7%	1.692	44%
10	0	5.968	20	0	4.704	5	0	5.913	-1.264	-21%	-0.055	-1%	1.209	26%
10	5	6.012	20	2.5	4.918	5	10	5.834	-1.094	-18%	-0.178	-3%	0.916	19%
10	10	4.946	20	5	4.468	5	20	4.344	-0.477	-10%	-0.602	-12%	-0.125	-3%
5	10	6.804	10	5	6.758	2.5	20	5.550	-0.047	-1%	-1.254	-18%	-1.208	-18%
0	10	6.846	0	5	6.830	0	20	5.604	-0.016	0%	-1.242	-18%	-1.226	-18%
-5	10	6.157	-10	5	6.353	-2.5	20	4.954	0.196	3%	-1.203	-20%	-1.399	-22%
-10	10	3.245	-20	5	2.793	-5	20	3.052	-0.451	-14%	-0.193	-6%	0.259	9%
-10	5	4.923	-20	2.5	3.801	-5	10	5.166	-1.121	-23%	0.244	5%	1.365	36%
-10	0	5.169	-20	0	4.032	-5	0	5.287	-1.137	-22%	0.118	2%	1.255	31%
-10	-5	4.809	-20	-2.5	3.727	-5	-10	4.991	-1.081	-22%	0.182	4%	1.264	34%
-35	-35	0.164	-45	-30	0.158	-30	-45	0.132	-0.006	-4%	-0.032	-19%	-0.026	-16%
-17.5	-35	0.219	-22.5	-30	0.247	-15	-45	0.167	0.027	12%	-0.052	-24%	-0.079	-32%
0	-35	0.243	0	-30	0.284	0	-45	0.179	0.041	17%	-0.063	-26%	-0.104	-37%
17.5	-35	0.186	22.5	-30	0.192	15	-45	0.147	0.006	3%	-0.039	-21%	-0.045	-23%
35	-35	0.108	45	-30	0.088	30	-45	0.100	-0.020	-19%	-0.008	-7%	0.012	14%
35	-17.5	0.141	45	-15	0.105	30	-22.5	0.160	-0.036	-25%	0.019	14%	0.055	52%
35	0	0.277	45	0	0.164	30	0	0.401	-0.113	-41%	0.124	45%	0.236	144%
35	17.5	0.503	45	15	0.396	30	22.5	0.466	-0.107	-21%	-0.037	-7%	0.070	18%
35	35	0.254	45	30	0.263	30	45	0.200	0.009	3%	-0.054	-21%	-0.063	-24%
17.5	35	0.315	22.5	30	0.373	15	45	0.234	0.058	18%	-0.081	-26%	-0.139	-37%
0	35	0.417	0	30	0.445	0	45	0.341	0.028	7%	-0.076	-18%	-0.104	-23%
-17.5	35	0.272	-22.5	30	0.286	-15	45	0.214	0.014	5%	-0.057	-21%	-0.071	-25%
-35	35	0.155	-45	30	0.131	-30	45	0.146	-0.024	-15%	-0.009	-6%	0.015	11%
-35	17.5	0.211	-45	15	0.155	-30	22.5	0.232	-0.056	-27%	0.022	10%	0.078	50%
-35	0	0.213	-45	0	0.145	-30	0	0.298	-0.068	-32%	0.084	40%	0.153	106%
-35	-17.5	0.265	-45	-15	0.193	-30	-22.5	0.264	-0.073	-27%	-0.002	-1%	0.071	37%
								Standard Deviation:	**0.463**	**15%**	**0.435**	**17%**	**0.747**	**41%**

(continued)

Table C-2b. Comparisons of Dispersion Factors (ug/m^3 / $ug/s\text{-}m^2$) for Different Source Shapes and Orientations (Los Angeles, California)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Polar Receptor Grid														
X (m)	**Y (m)**	**UAC**	**X (m)**	**Y (m)**	**UAC**	**X (m)**	**Y (m)**	**UAC**	**Diff. In UAC**	**% of Diff.**	**Diff. In UAC**	**% of Diff.**	**Diff. In UAC**	**% of Diff.**
19	46	0.059	19	46	0.065	19	46	0.069	0.006	9%	0.010	17%	0.005	7%
38	92	0.016	38	92	0.016	38	92	0.016	0.000	-1%	0.000	3%	0.001	4%
35	35	0.188	35	35	0.168	35	35	0.284	-0.020	-11%	0.096	51%	0.116	69%
71	71	0.046	71	71	0.045	71	71	0.052	-0.001	-3%	0.006	13%	0.007	16%
46	19	0.582	46	19	0.607	46	19	0.461	0.025	4%	-0.121	-21%	-0.146	-24%
92	38	0.172	92	38	0.174	92	38	0.161	0.003	2%	-0.011	-6%	-0.014	-8%
50	0	0.278	50	0	0.293	50	0	0.293	0.014	5%	0.015	5%	0.001	0%
100	0	0.068	100	0	0.067	100	0	0.074	-0.001	-2%	0.005	8%	0.007	10%
46	-19	0.061	46	-19	0.062	46	-19	0.087	0.002	3%	0.026	43%	0.025	40%
92	-38	0.015	92	-38	0.015	92	-38	0.016	0.000	0%	0.002	10%	0.002	11%
35	-35	0.062	35	-35	0.068	35	-35	0.062	0.006	10%	0.000	0%	-0.006	-9%
71	-71	0.016	71	-71	0.017	71	-71	0.017	0.001	4%	0.001	3%	0.000	-1%
19	-46	0.080	19	-46	0.076	19	-46	0.087	-0.004	-4%	0.007	9%	0.011	14%
38	-92	0.023	38	-92	0.022	38	-92	0.024	-0.001	-5%	0.001	3%	0.002	8%
0	-50	0.086	0	-50	0.084	0	-50	0.096	-0.003	-3%	0.009	11%	0.012	15%
0	-100	0.023	0	-100	0.024	0	-100	0.024	0.000	1%	0.001	3%	0.000	2%
-19	-46	0.099	-19	-46	0.092	-19	-46	0.108	-0.006	-7%	0.009	9%	0.016	17%
-38	-92	0.028	-38	-92	0.027	-38	-92	0.028	-0.001	-2%	0.000	1%	0.001	3%
-35	-35	0.122	-35	-35	0.119	-35	-35	0.143	-0.003	-2%	0.021	18%	0.024	20%
-71	-71	0.033	-71	-71	0.032	-71	-71	0.034	0.000	-1%	0.001	4%	0.002	5%
-46	-19	0.218	-46	-19	0.223	-46	-19	0.226	0.005	2%	0.008	4%	0.003	2%
-92	-38	0.060	-92	-38	0.061	-92	-38	0.061	0.001	1%	0.001	1%	0.000	0%
-50	0	0.320	-50	0	0.378	-50	0	0.278	0.057	18%	-0.042	-13%	-0.099	-26%
-100	0	0.093	-100	0	0.098	-100	0	0.087	0.005	6%	-0.006	-6%	-0.011	-11%
-46	19	0.264	-46	19	0.273	-46	19	0.260	0.009	3%	-0.005	-2%	-0.013	-5%
-92	38	0.074	-92	38	0.075	-92	38	0.073	0.001	1%	-0.001	-2%	-0.002	-2%
-35	35	0.137	-35	35	0.123	-35	35	0.164	-0.014	-10%	0.027	20%	0.041	33%
-71	71	0.037	-71	71	0.035	-71	71	0.039	-0.002	-5%	0.002	4%	0.003	9%
-19	46	0.063	-19	46	0.066	-19	46	0.073	0.003	4%	0.010	15%	0.007	11%
-38	92	0.017	-38	92	0.017	-38	92	0.018	0.000	-2%	0.001	3%	0.001	5%
0	50	0.067	0	50	0.058	0	50	0.080	-0.008	-12%	0.014	21%	0.022	37%
0	100	0.020	0	100	0.018	0	100	0.021	-0.002	-9%	0.001	6%	0.003	15%
								Standard Deviation:	**0.013**	**6%**	**0.030**	**14%**	**0.040**	**18%**

(continued)

Table C-2b. (continued)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Cartesion Receptor Grid														
X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.
-10	-10	3.225	-20	-5	3.241	-5	-20	2.674	0.016	1%	-0.551	-17%	-0.567	-17%
-5	-10	4.025	-10	-5	4.333	-2.5	-20	3.119	0.308	8%	-0.906	-23%	-1.214	-28%
0	-10	3.952	0	-5	4.297	0	-20	3.050	0.345	9%	-0.902	-23%	-1.247	-29%
5	-10	3.431	10	-5	3.871	2.5	-20	2.564	0.440	13%	-0.867	-25%	-1.307	-34%
10	-10	1.683	20	-5	1.592	5	-20	1.511	-0.091	-5%	-0.172	-10%	-0.081	-5%
10	-5	5.931	20	-2.5	4.787	5	-10	5.570	-1.143	-19%	-0.360	-6%	0.783	16%
10	0	6.636	20	0	5.882	5	0	5.644	-0.754	-11%	-0.992	-15%	-0.238	-4%
10	5	6.640	20	2.5	6.294	5	10	5.524	-0.346	-5%	-1.116	-17%	-0.770	-12%
10	10	5.600	20	5	5.866	5	20	4.325	0.266	5%	-1.275	-23%	-1.541	-26%
5	10	6.893	10	5	8.126	2.5	20	4.939	1.232	18%	-1.955	-28%	-3.187	-39%
0	10	6.860	0	5	8.285	0	20	4.913	1.424	21%	-1.947	-28%	-3.371	-41%
-5	10	6.031	-10	5	7.442	-2.5	20	4.156	1.411	23%	-1.875	-31%	-3.286	-44%
-10	10	3.393	-20	5	3.497	-5	20	2.702	0.103	3%	-0.691	-20%	-0.794	-23%
-10	5	5.649	-20	2.5	5.102	-5	10	5.015	-0.547	-10%	-0.634	-11%	-0.088	-2%
-10	0	5.944	-20	0	5.373	-5	0	5.167	-0.572	-10%	-0.777	-13%	-0.205	-4%
-10	-5	5.663	-20	-2.5	5.028	-5	-10	5.104	-0.635	-11%	-0.559	-10%	0.076	2%
-35	-35	0.124	-45	-30	0.139	-30	-45	0.095	0.014	11%	-0.029	-23%	-0.043	-31%
-17.5	-35	0.158	-22.5	-30	0.183	-15	-45	0.123	0.025	16%	-0.035	-22%	-0.060	-33%
0	-35	0.172	0	-30	0.199	0	-45	0.121	0.028	16%	-0.050	-29%	-0.078	-39%
17.5	-35	0.123	22.5	-30	0.124	15	-45	0.100	0.001	0%	-0.024	-19%	-0.024	-20%
35	-35	0.064	45	-30	0.053	30	-45	0.063	-0.011	-17%	-0.001	-2%	0.010	19%
35	-17.5	0.095	45	-15	0.076	30	-22.5	0.119	-0.019	-20%	0.024	25%	0.043	57%
35	0	0.592	45	0	0.377	30	0	0.696	-0.215	-36%	0.104	18%	0.319	85%
35	17.5	0.829	45	15	0.739	30	22.5	0.683	-0.090	-11%	-0.146	-18%	-0.055	-7%
35	35	0.192	45	30	0.304	30	45	0.101	0.112	58%	-0.091	-47%	-0.203	-67%
17.5	35	0.109	22.5	30	0.195	15	45	0.072	0.086	78%	-0.037	-34%	-0.122	-63%
0	35	0.125	0	30	0.144	0	45	0.100	0.019	15%	-0.025	-20%	-0.044	-31%
-17.5	35	0.113	-22.5	30	0.160	-15	45	0.077	0.047	42%	-0.035	-31%	-0.082	-52%
-35	35	0.139	-45	30	0.166	-30	45	0.089	0.026	19%	-0.050	-36%	-0.077	-46%
-35	17.5	0.387	-45	15	0.335	-30	22.5	0.370	-0.053	-14%	-0.017	-4%	0.036	11%
-35	0	0.603	-45	0	0.472	-30	0	0.603	-0.131	-22%	0.000	0%	0.131	28%
-35	-17.5	0.318	-45	-15	0.275	-30	-22.5	0.316	-0.043	-13%	-0.002	-1%	0.041	15%
								Standard Deviation:	**0.542**	**24%**	**0.614**	**15%**	**1.026**	**33%**

C.3 Receptor Locations and Spacings

A sensitivity analysis was conducted using the ISCST3 model to determine the impact of receptor locations and spacings on estimated air concentrations. A discussion of the analysis follows.

Because it takes a substantial amount of time for the ISCST3 model to execute, it was necessary to choose a limited number of receptors to be represented in the dispersion factor database in IWAIR. The larger the number of receptor points, the longer the run time. However, modeling fewer receptors may result in the omission of the maximum point for assessing exposure impacts. Therefore, a sensitivity analysis was conducted to determine the number of receptors needed to adequately capture maximum air concentrations and to locate ideal receptor placements.

A wind rose was plotted for each of the 60 meteorological stations to be included in IWAIR for a 5-year time period in order to choose two meteorological stations for this sensitivity analysis. The stations at Little Rock, Arkansas, and Los Angeles, California, were selected. The wind roses show that Little Rock has very evenly distributed wind directions, and Los Angeles has a predominant southwest to west wind (Figure C-2). Little Rock and Los Angeles were chosen to determine if a higher density of receptors should be placed downwind of a site near Los Angeles, as compared to a site near Little Rock. Similarly, the 5th, 50th, and 95th percentile of areas of land application units were used in the sensitivity analysis to determine the extent of which the area of the unit affects receptor locations and spacings. The areas of the 5th, 50th, and 95th percentile of sizes of land application units are 1,200 m^2, 100,000 m^2, and 1,700,000 m^2, respectively.

The dispersion modeling was conducted using two sets of receptor grids. The first set of receptor points (Cartesian receptor grid) was placed around the modeled source with distances of 0, 25, 50, 75, and 150 m from the edge of the unit. Square-shaped, ground-level area sources were used in the modeling. Therefore, these receptors are located on five squares surrounding the source. The second set of receptor points (polar receptor grid) was placed outside of the first set of receptors to 10 km from the center of the source. Because the ISCST3 model's area source algorithm does not consider elevated terrain, receptor elevations were not entered in the modeling.

In this sensitivity analysis, both downwind and lateral receptor spacings were investigated for the three unit sizes using 5 years of meteorological data from Little Rock and Los Angeles. For the first set of receptor points (i.e., Cartesian receptor grid), five downwind distances of 0, 25, 50, 75, and 150 m from the edge of the source were used. For lateral receptor spacing, choices of 64, 32, and 16 equally spaced receptor points for each square were used in the modeling to identify the number of receptors needed to adequately characterize the maximum impacts (see Figures C-4a through C-4c for Cartesian receptor locations and spacings ((50th percentile)). For the second set of receptor points (i.e., polar receptor grid), about 20 downwind distances (i.e., receptor rings) were used. Receptor lateral intervals of 22.5° and 10° were used to determine whether 22.5° spacing can adequately characterize the maximum impacts. With a

22.5° interval, there are 16 receptors on each ring. There are 36 receptors on each ring for the 10° interval. See Figures E-5a and C-5b for polar receptor locations (5th percentile).

The results (Figures C-6a through C-6f) show that the maximum downwind concentrations decrease sharply from the edge of the area source to 150 m from the source. The maximum concentrations decrease more sharply for a smaller area source than for a larger one. This means that more close-to-source receptors are generally needed for a small area source than for a large one.

The results also show that the maximum impacts are generally higher for a dense receptor grid (i.e., 64 or 32 receptors on each square) than for a scattered receptor grid (i.e., 16 receptors on each square). However, the differences of the maximum receptor impacts are not significant between a dense and a scattered receptor grid (Figures C-6a through C-6f). The above conclusions apply to both Little Rock and Los Angeles. This means that the distribution of wind directions does not play an important role in determining receptor lateral spacings.

Figures C-7a through C-7f compare the maximum concentrations at each ring for 22.5° and 10° intervals. The results show that the differences of the maximum concentrations are greater for close-to-source receptors than for more distant receptors, and the differences are greater for larger area sources than for smaller area sources. The differences of the maximum concentrations for 22.5° and 10° intervals are generally small, and the concentrations tend to be the same at 10 km. The conclusions were drawn from both Little Rock and Los Angeles meteorological data.

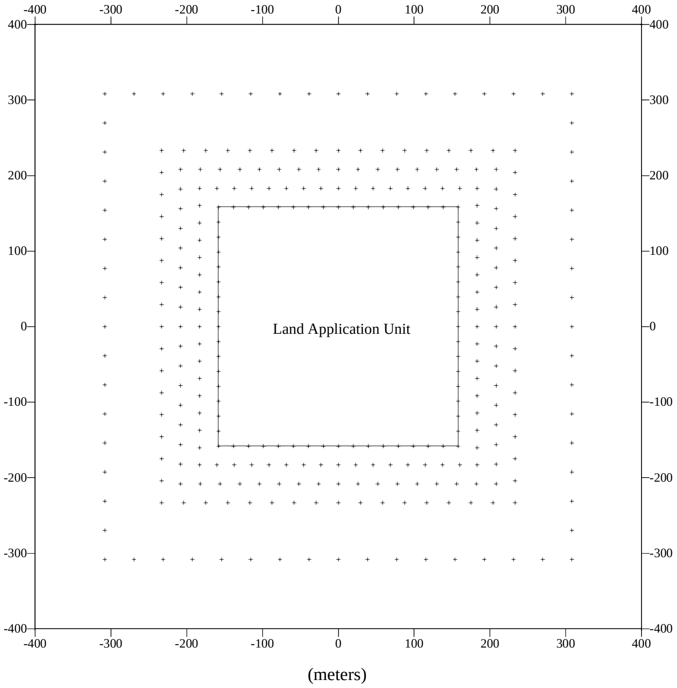


Figure C-4a. Cartesian receptor grid (64 receptors each square).

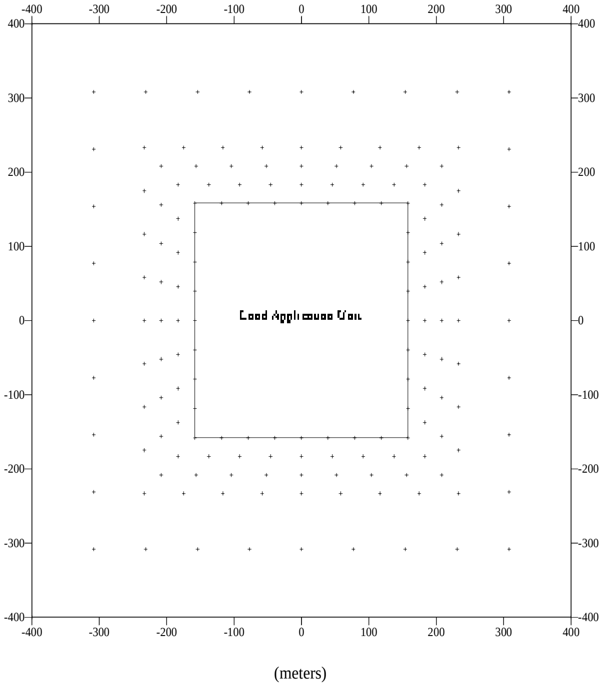


Figure C-4b. Cartesian receptor grid (32 receptors each square).

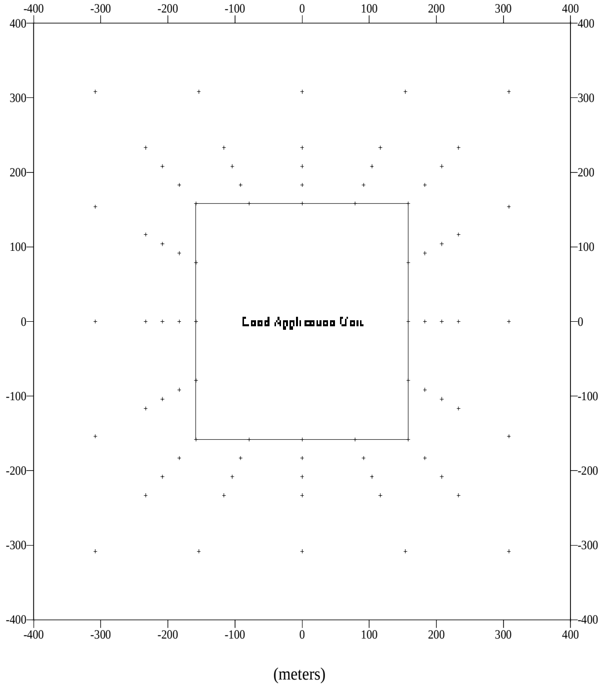


Figure C-4c. Cartesian receptor grid (16 receptors each square).

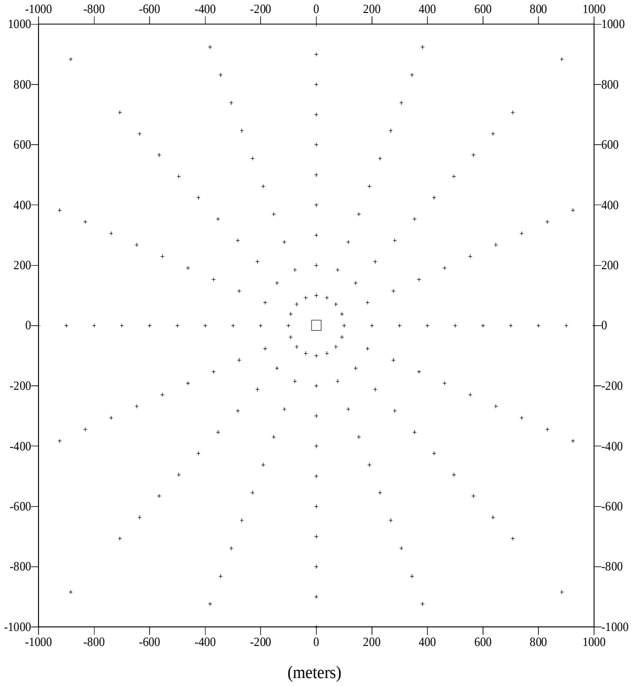


Figure C-5a. Polar receptor grid (22.5 degree).

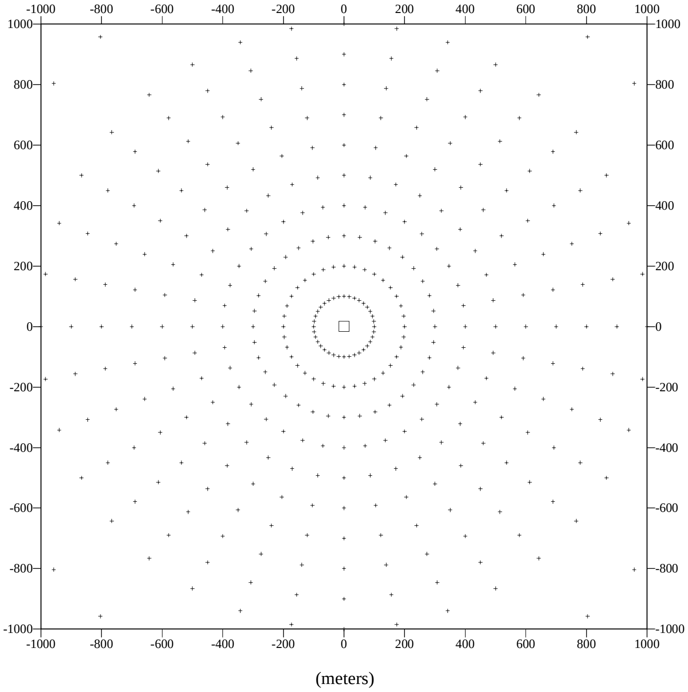


Figure C-5b. Polar receptor grid (10 degree).

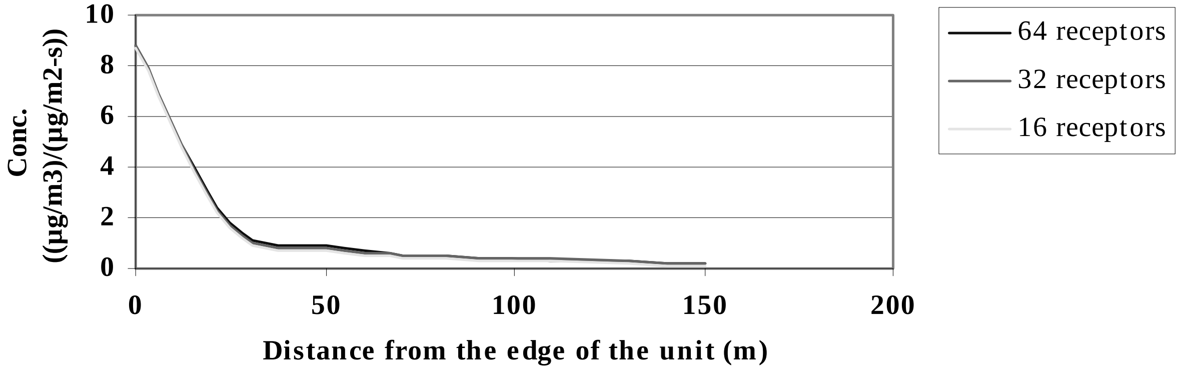


Figure C-6a. Maximum concentrations, Cartesian grid (5th percentile area, land application unit, Los Angeles, CA).

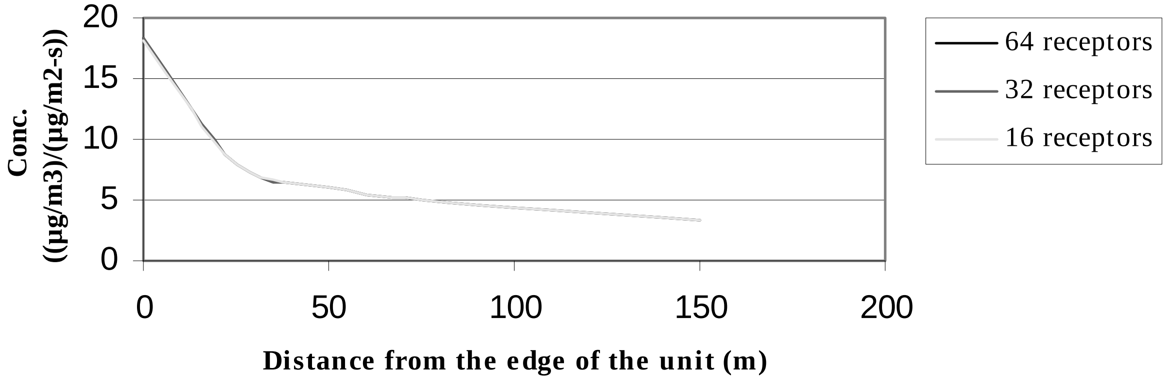


Figure C-6b. Maximum concentrations, Cartesian grid (50th percentile area, land application unit, Los Angeles, CA).

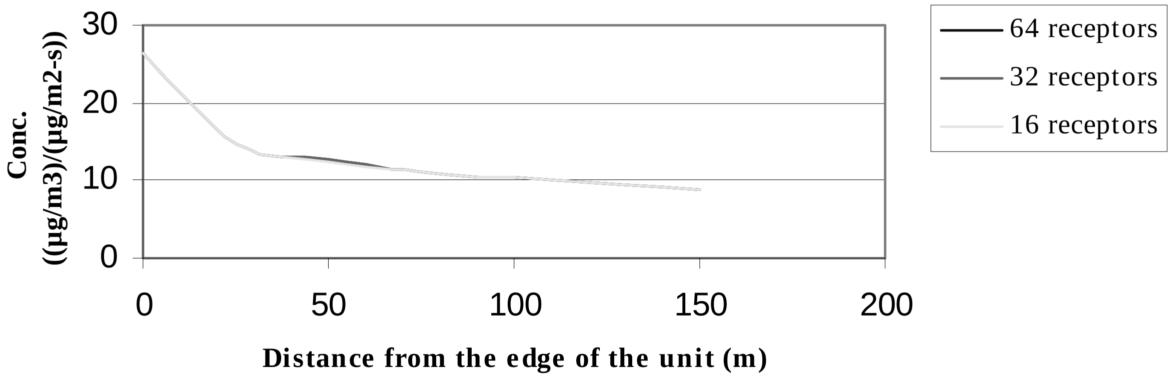


Figure C-6c. Maximum concentrations, Cartesian grid (95th percentile area, land application unit, Los Angeles, CA).

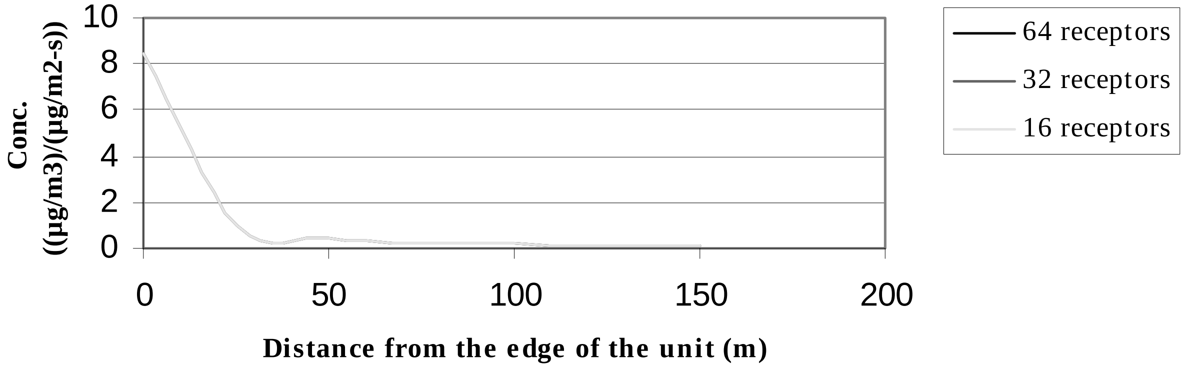


Figure C-6d. Maximum concentrations, Cartesian grid (5th percentile area, land application unit, Little Rock, AR).

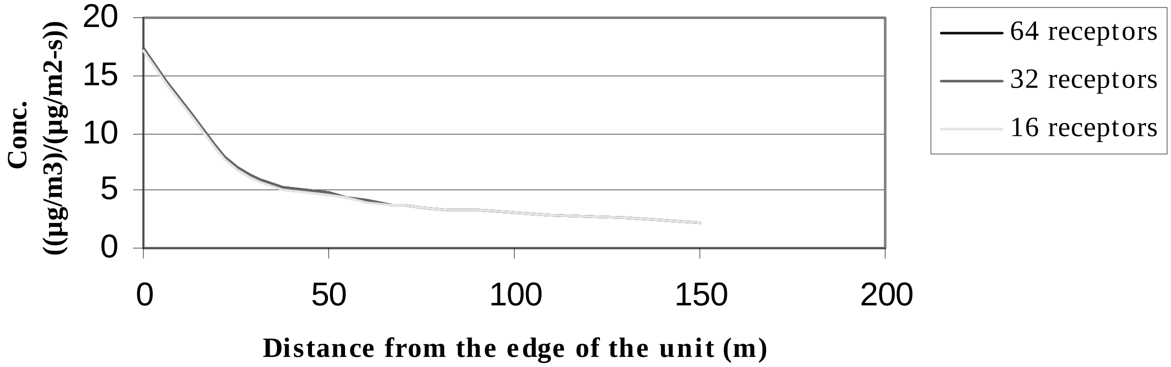


Figure C-6e. Maximum moncentrations, Cartesian grid (50th percentile area, land application unit, Little Rock, AR).

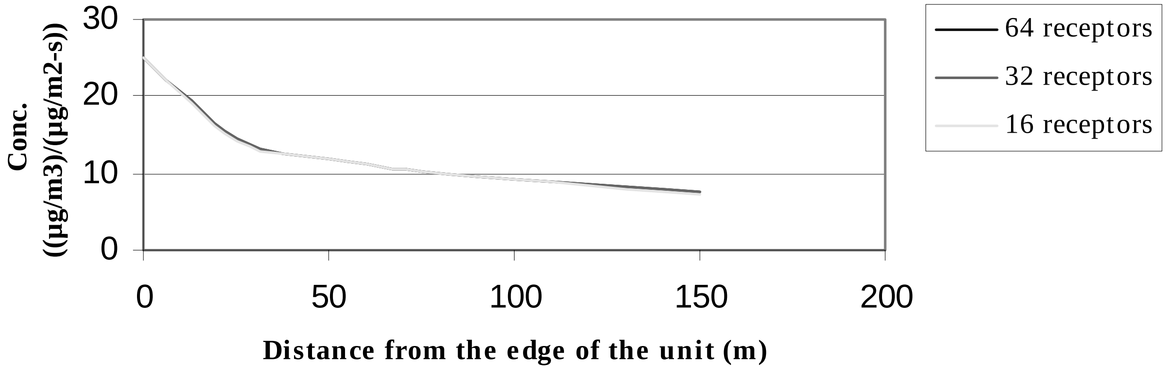


Figure C-6f. Maximum concentrations, Cartesian grid (95th percentile area, land application unit, Little Rock, AR).

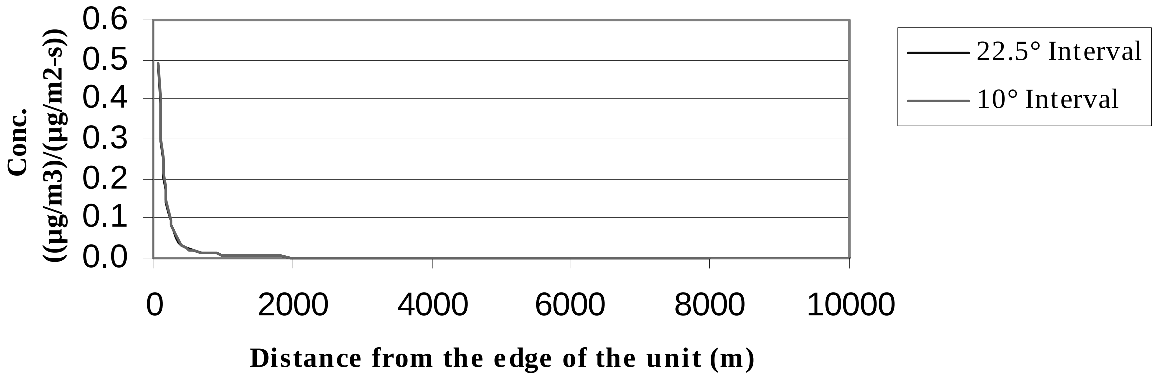


Figure C-7a. Maximum concentrations, polar grid (5th percentile area, land application unit, Los Angeles, CA).

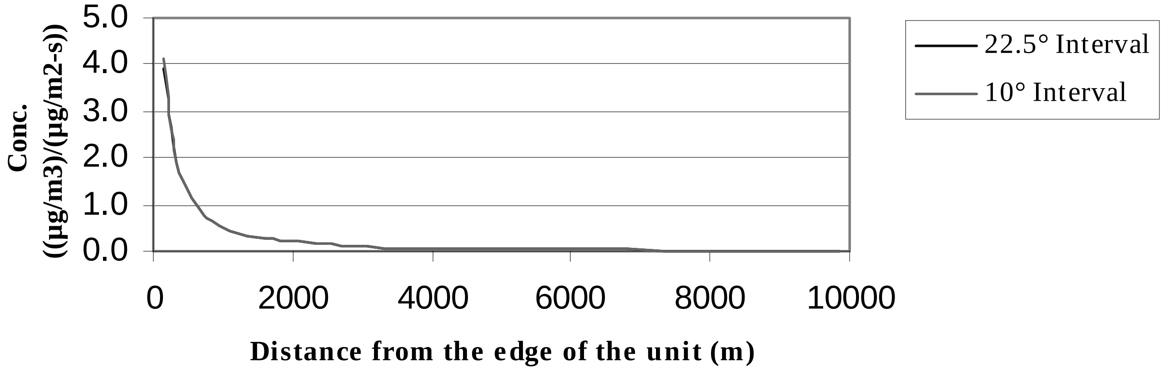


Figure C-7b. Maximum concentrations, polar grid (50th percentile area, land application unit, Los Angeles, CA).

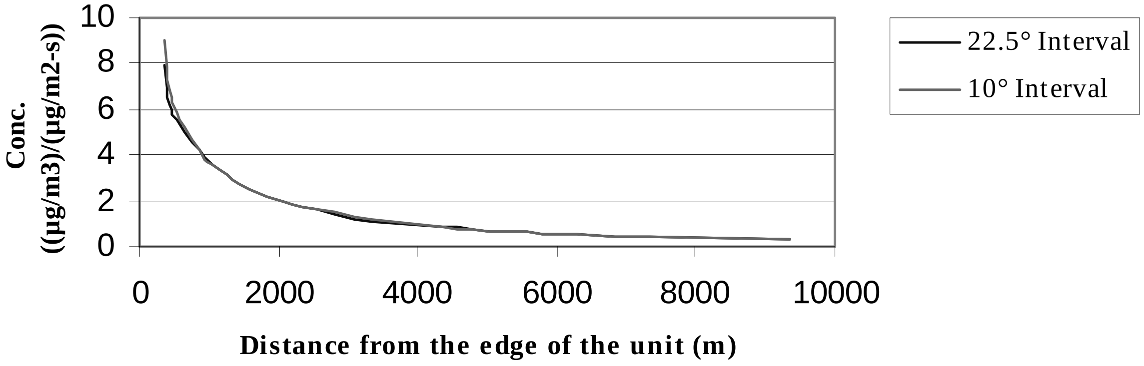


Figure C-7c. Maximum concentrations, polar grid (95th percentile area, land application unit, Los Angeles, CA).

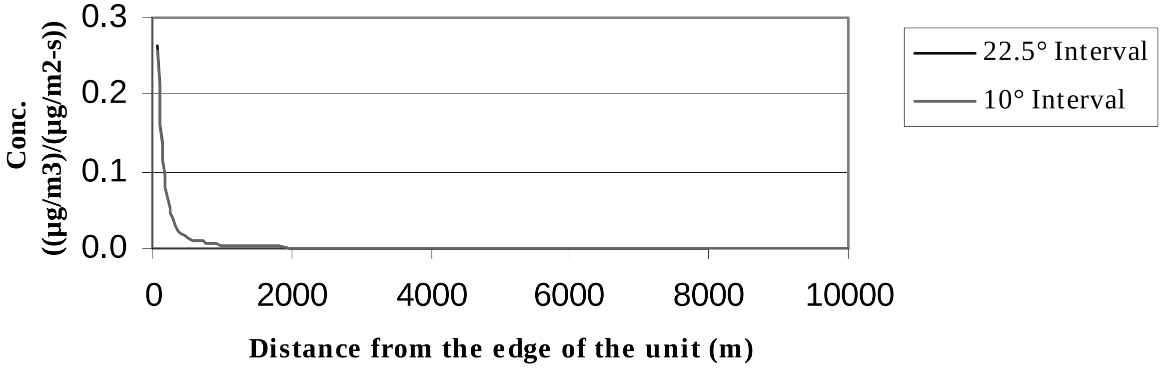


Figure C-7d. Maximum concentrations, polar grid (5th percentile area, land application unit, Little Rock, AR).

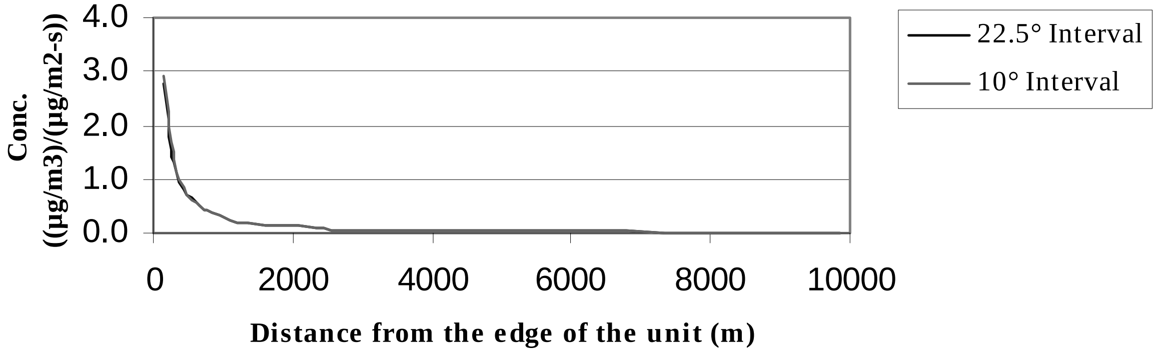


Figure C-7e. Maximum concentrations, polar grid (50th percentile area, land application unit, Little Rock, AR).

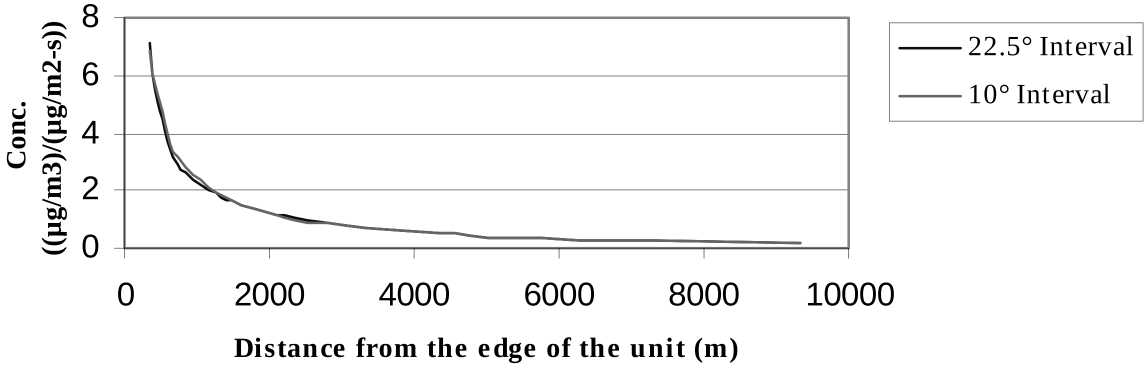


Figure C-7f. Maximum concentrations, polar grid (95th percentile area, land application unit, Little Rock, AR).

Appendix D

Selection of Meteorological Stations

Appendix D

Selection of Meteorological Stations

Meteorological data for more than 200 meteorological stations in the United States are available on the SCRAM Bulletin Board (http://www.epa.gov/scram001) and from a number of other sources. Because of the time required to develop dispersion factors, it was not feasible to include dispersion factors in IWAIR for all of these stations. Therefore, EPA developed an approach to select a subset of these stations for use in IWAIR. This approach considers the factors most important for the inhalation pathway risk modeling done by IWAIR.

The approach used involved two main steps:

1. Identify contiguous areas that are sufficiently similar with regard to the parameters that affect dispersion that they can be reasonably represented by one meteorological station. The parameters used were

   - Surface-level meteorological data (e.g., wind patterns and atmospheric stability)
   - Physiographic features (e.g., mountains, plains)
   - Bailey’s ecoregions and subregions
   - Land cover (e.g., forest, urban areas).

2. For each contiguous area, select one meteorological station to represent that area. The station selection step considered the following parameters:

   - Industrial activity
   - Population density
   - Location within the area
   - Years of meteorological data available
   - Average wind speed.

These steps are described in the following sections.

D.1 Identify Contiguous Areas

A hierarchical procedure based on features affecting wind flow was used to divide the country into regions. The primary delineation of areas was based on geographic features affecting synoptic (broad area) winds, including mountain ranges and plains. These features are also known as physiography. Data were obtained from Fenneman and Johnson (1946), Wahrhaftig (1965), and State of Hawaii (1997). The secondary delineation was based on features affecting mesoscale (10 to 1,000 km) winds, including coastal regions and basic land cover classifications of forest, agriculture, and barren lands. These land cover features were obtained from U.S. Geological Survey (1999).

The methodology for identifying contiguous areas used wind data and atmospheric stability data derived from surface-level meteorological data as the primary consideration, modified by physiography, Bailey's ecoregions and subregions, and land cover. The approach focused on how well the wind speed and direction and atmospheric stability patterns measured at a surface-level meteorological station represented the surrounding area. The limit of appropriate representation varied by area of the country and was substantially determined by terrain and topography. For example, a station in the Midwest, where topography and vegetation are uniform, may adequately represent a very large area, while a mountainous station, where ridges and valleys affect the winds, may represent a much smaller area.

D.1.1 Primary Grouping on Wind-Rose and Atmospheric Stability Data

The surface-level meteorological data were downloaded from EPA's SCRAM Web site (www.epa.gov/scram001). SCRAM has these data for 1984 to 1991. A 5-year period is commonly used to obtain an averaged depiction of the winds for each station; 5 years covers most of the usual variation in meteorological conditions. EPA selected a single 5-year period (1986 to 1990) from the middle of the available period for the purpose of comparing wind roses. A single period provided consistency across stations. Not all stations had 5 years of data in this time period. Three years of data was considered a desirable minimum; therefore, stations that had less than 3 years of data during this time period were not considered for selection. A total of 223 stations in the contiguous 48 states were considered, plus 17 in Alaska, 3 in Hawaii, and 1 in Puerto Rico.

Two types of wind data were considered: wind directionality and wind speed. Wind directionality describes the tendency of winds to blow from many different directions (weakly directional) or primarily from one direction (strongly directional). Strongly directional winds will tend to disperse air pollutants in a consistent direction, resulting in higher air concentrations in that direction and higher overall maximum air concentrations. Weakly directional winds will tend to disperse pollutants in multiple directions, resulting in lower air concentrations in any one direction and lower overall maximum air concentration.

Wind speed also affects dispersion. A greater average wind speed tends to disperse pollutants more quickly, resulting in lower air concentrations than lower average wind speeds would produce. Wind speed was used in the station selection process, but not to identify contiguous areas of the country.

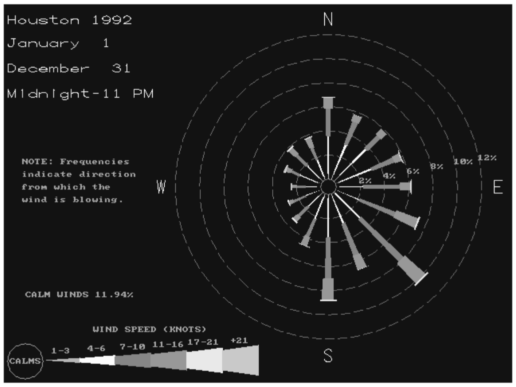
A wind rose is a graphical depiction of the frequency of wind speeds by wind direction (see Figure D-1). Wind roses were produced from the surface-level meteorological data for each station using WRPLOT (available from www.epa.gov/scram001/models/relat/wrplot.zip). Winds are plotted in 16 individual directions; thus, if every direction has the same frequency, the wind would blow from each direction 6.25 percent of the time. Based on the wind roses, each station was assigned to one of four bins based on the frequency of wind in the predominant direction (the direction from which the wind blows the greatest percentage of the time). These bins were as follows:

- W, weakly directional: blowing from the predominant direction less than 10 percent of the time
- A, mildly directional: blowing from the predominant direction 10 to 14 percent of the time
- B, moderately directional: blowing from the predominant direction 15 to 20 percent of the time
- C, strongly directional: blowing from the predominant direction more than 20 percent of the time.

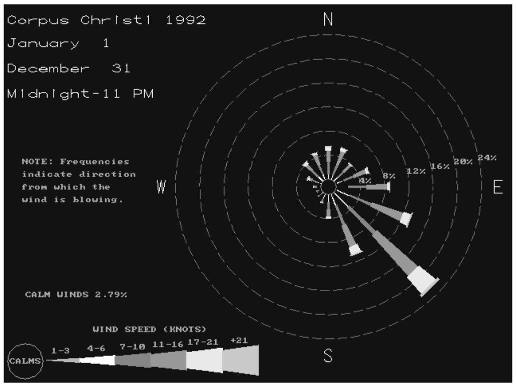
Atmospheric stability class frequency distributions were also used for some stations. Atmospheric stability is a measure of vertical movement of air and can be classified as stable, unstable, or neutral. For sources at ground level and slightly elevated (i.e., not tall stacks), such as are modeled in IWAIR, pollutants tend to stay close to the ground in a stable atmosphere, thereby increasing the air concentration of the pollutant. In an unstable atmosphere, the pollutants will tend to disperse more in the vertical direction, thereby decreasing the air concentration of the pollutant. Atmospheric stability varies throughout the day and year, as well as by location, because atmospheric stability is determined from variable factors such as wind speed, strength of solar radiation, and the vertical temperature profile above the ground. In addition, the presence of large bodies of water, hills, large urban areas, and types and height of vegetation all affect atmospheric stability. If all other factors are the same at two stations, the one with stable air a larger percentage of the time will have higher air concentrations than the station with stable air a smaller percentage of the time.

Stability class distributions were readily available for only 108 of the 223 stations considered for the United States. To apply the stability class data, the distributions were summarized as percent unstable, percent neutral, and percent stable.

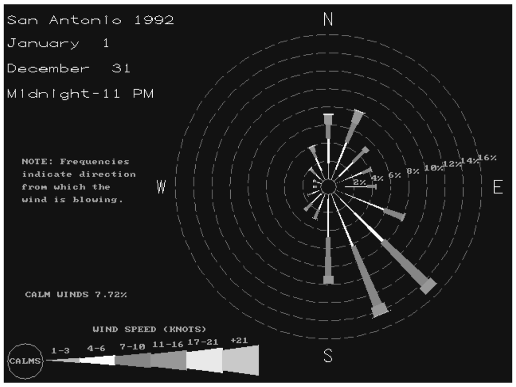
All stations with their assigned wind-rose bins and stability class distributions were marked on a map and then grouped geographically with others nearby with the same or an adjacent assigned bin and a similar stability class distribution. Figure D-1 illustrates the usefulness of this approach with respect to wind-rose data. It shows the 1992 wind roses for eight cities in Texas and Louisiana. A visual inspection of these graphics reveals that the wind patterns for these stations differ significantly.



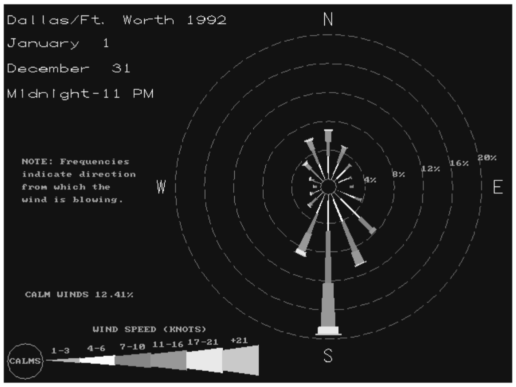
Houston, Texas, 1992.



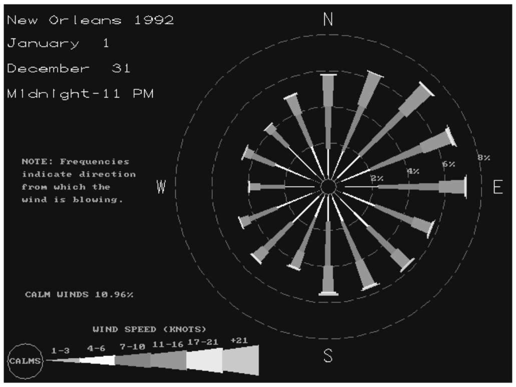
Corpus Christi, Texas, 1992.



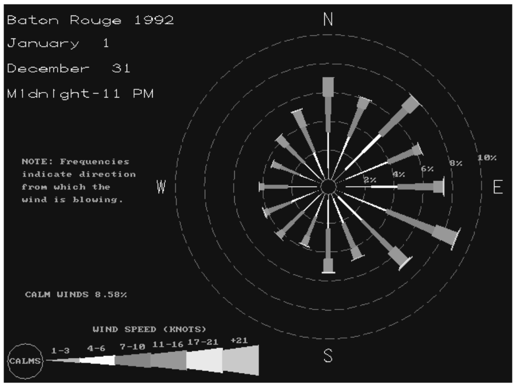
San Antonio, Texas, 1992.



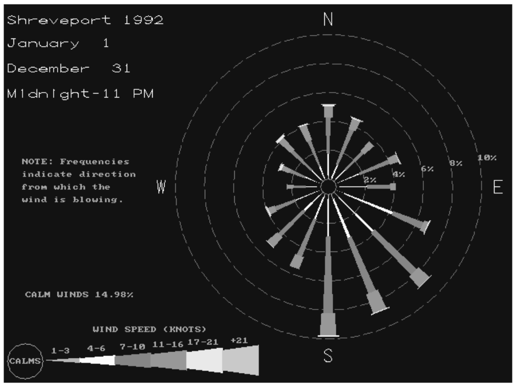
Dallas/Ft. Worth, Texas, 1992.



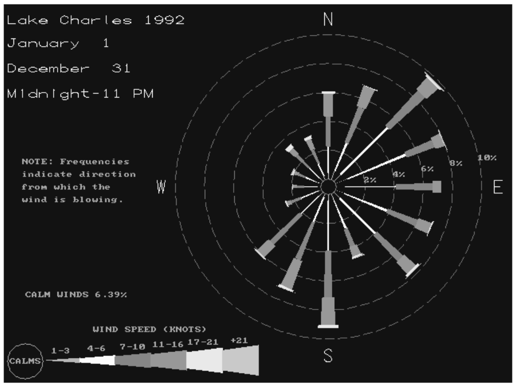
New Orleans, Louisiana, 1992.



Baton Rouge, Louisiana, 1992.



Shreveport, Louisiana, 1992.



Lake Charles, Louisiana, 1992.

Figure D-1. Wind-rose data for Texas and Louisiana.

D.1.2 Secondary Grouping Considerations

After spatially grouping the wind roses in similar bins, the next step was to delineate geographic areas around these groups of meteorological stations using maps of physiography, Bailey's ecoregions, and land cover. Physiography includes major topographic features, such as mountains or plains. Land cover classifications include urban, crop land, grassland, forest, large waterbody, wetland, barren, and snow or ice. Regional boundaries were chosen to coincide with physiographic, Bailey's ecoregion, and land cover boundaries to the extent possible.

D.2 Station Selection

The above approach used to delineate contiguous areas ensures that the stations grouped together are fairly similar in most cases. Therefore, the selection of an appropriate station to represent each area was based on other considerations, including

- **Previous EPA work on meteorological station selection.** Earlier efforts already identified stations that were representative of broad regions.
- **Number of years of surface-level meteorological data available.** More years of data provide a more realistic long-term estimate of air concentration.
- **Industrial activity**, based on TRI facility locations. More industrial activity suggests these locations are representative of more potential IWAIR users.
- **Population density**, based on land cover data. High population density in urban areas indicates more potential receptors; therefore, these are areas EPA would like to represent very well, so as to minimize potential error and uncertainty.
- **Central location within the area.** All other factors being equal, central locations are more likely to be representative of the entire contiguous geographic area because they have the smallest average distance from all points in the region.
- **Wind speed.** Lower wind speeds lead to less dispersion and higher air concentrations.

EPA considered two previous studies covering meteorological station selection. An assessment for EPA's Superfund program Soil Screening Levels (SSLs) (EQM and Pechan, 1993) selected a set of 29 meteorological stations as being representative of the nine general climate regions of the contiguous 48 states. In EPA's SSL study, it was determined that 29 meteorological stations would be a sufficient sample to represent the population of 200 meteorological stations and predict mean dispersion values with a high (95 percent) degree of confidence. The 29 meteorological stations were distributed among nine climate regions based on meteorological representativeness and variability across each region. These 29 stations have been used in a variety of EPA studies. The 2001 Surface Impoundment Study (SIS) (U.S. EPA, 2001) added 12 stations to the list of 29 for assessment of inhalation risks.

Industrial activity was based on a map of the locations of the WMUs in the 1985 Industrial D database (Schroeder et al., 1987) and facilities listing on-site land disposal-based emissions in the 1998 TRI (U.S. EPA, 2000). Population density was considered by identifying urban areas on the land cover map. Wind speed was summarized as average speed in the prevailing wind direction. This value is not readily extractable from the wind roses; therefore, it was obtained from the *International Station Meteorological Climate Summary* CD (NOAA, 1992) of meteorological data. For a few stations, this value was unrealistically low; in those cases, an average wind speed in the prevailing wind direction was estimated from the wind rose data.

EPA used a hierarchical procedure to select a representative station, as follows:

- If the area contained one of the 29 SSL stations, it was selected.
- If the area contained one of the stations added to the SSL list for the SIS, it was selected.
- Stations with less than 5 years of data in SCRAM were eliminated, unless no station had 5 years of data.
- Stations in locations with greater industrial activity (as indicated by TRI facilities reporting on-site land-based disposal) or greater population (based on urban areas from land cover maps) were preferred.
- Stations centrally located in the area were preferred if the above factors did not identify a clear choice.
- If all other factors were equal, stations with lower average wind speeds were selected to ensure that air concentration was not underestimated. Variations in wind speed within regions were minor.

D.3 New Meteorological Station Boundaries by Region

As a result of this work, the list of 60 stations shown in Table D-1, sorted by state and station name, was chosen for use in IWAIR. Appendix D-1 provides additional data on all of the meteorological stations considered. Selection of the stations is discussed in the following sections; for purposes of that discussion, the United States was divided into the following sections: West Coast, Desert Southwest, Western Mountains, Texas (excluding the Gulf Coast), Gulf Coast, Southeast, Middle Atlantic, Northeast, Great Lakes, Central States, Alaska, Hawaii, and Puerto Rico. The process of selecting stations and delineating the region assigned to each station is discussed by these sections.

Figure D-2 shows the selected stations and their assigned regions for the contiguous 48 states. Figures D-3, D-4, and D-5 show these boundaries on a larger scale for the western, southeastern, and northeastern United States overlaid on the location of facilities from the 1998 TRI data. The Bailey's ecoregions, physiographic features, and land cover were instrumental in

Table D-1. Surface-Level Meteorology Stations in IWAIR

Station Number	Station Name	State
26451	Anchorage/WSMO Airport	AK
25309	Juneau/International Airport	AK
13963	Little Rock/Adams Field	AR
23183	Phoenix/Sky Harbor International Airport	AZ
93193	Fresno/Air Terminal	CA
23174	Los Angeles/International Airport	CA
24257	Redding/AAF	CA
23234	San Francisco/International Airport	CA
23062	Denver/Stapleton International Airport	CO
14740	Hartford/Bradley International Airport	CT
12839	Miami/International Airport	FL
12842	Tampa/International Airport	FL
13874	Atlanta/Atlanta-Hartsfield International	GA
03813	Macon/Lewis B Wilson Airport	GA
22521	Honolulu/International Airport	HI
94910	Waterloo/Municipal Airport	IA
24131	Boise/Air Terminal	ID
94846	Chicago/O'Hare International Airport	IL
03937	Lake Charles/Municipal Airport	LA
12916	New Orleans/International Airport	LA
13957	Shreveport/Regional Airport	LA
14764	Portland/International Jetport	ME
94847	Detroit/Metropolitan Airport	MI
14840	Muskegon/County Airport	MI
14922	Minneapolis-St Paul/International Airport	MN
13994	St. Louis/Lambert International Airport	MO
13865	Meridian/Key Field	MS
24033	Billings/Logan International Airport	MT
03812	Asheville/Regional Airport	NC
13722	Raleigh/Raleigh-Durham Airport	NC

(continued)

Table D-1. (continued)

Station Number	Station Name	State
24011	Bismarck/Municipal Airport	ND
14935	Grand Island/Airport	NE
23050	Albuquerque/International Airport	NM
23169	Las Vegas/McCarran International Airport	NV
24128	Winnemucca/WSO Airport	NV
14820	Cleveland/Hopkins International Airport	OH
93815	Dayton/International Airport	OH
13968	Tulsa/International Airport	OK
94224	Astoria/Clatsop County Airport	OR
24232	Salem/McNary Field	OR
14751	Harrisburg/Capital City Airport	PA
13739	Philadelphia/International Airport	PA
14778	Williamsport-Lycoming/County	PA
11641	San Juan/Isla Verde International Airport	PR
13880	Charleston/International Airport	SC
13877	Bristol/Tri City Airport	TN
13897	Nashville/Metro Airport	TN
23047	Amarillo/International Airport	TX
13958	Austin/Municipal Airport	TX
12924	Corpus Christi/International Airport	TX
03927	Dallas/Fort Worth/Regional Airport	TX
12960	Houston/Intercontinental Airport	TX
23023	Midland/Regional Air Terminal	TX
24127	Salt Lake City/International Airport	UT
13737	Norfolk/International Airport	VA
14742	Burlington/International Airport	VT
24233	Seattle/Seattle-Tacoma International	WA
24157	Spokane/International Airport	WA
03860	Huntington/Tri-State Airport	WV
24089	Casper/Natrona Co International Airport	WY

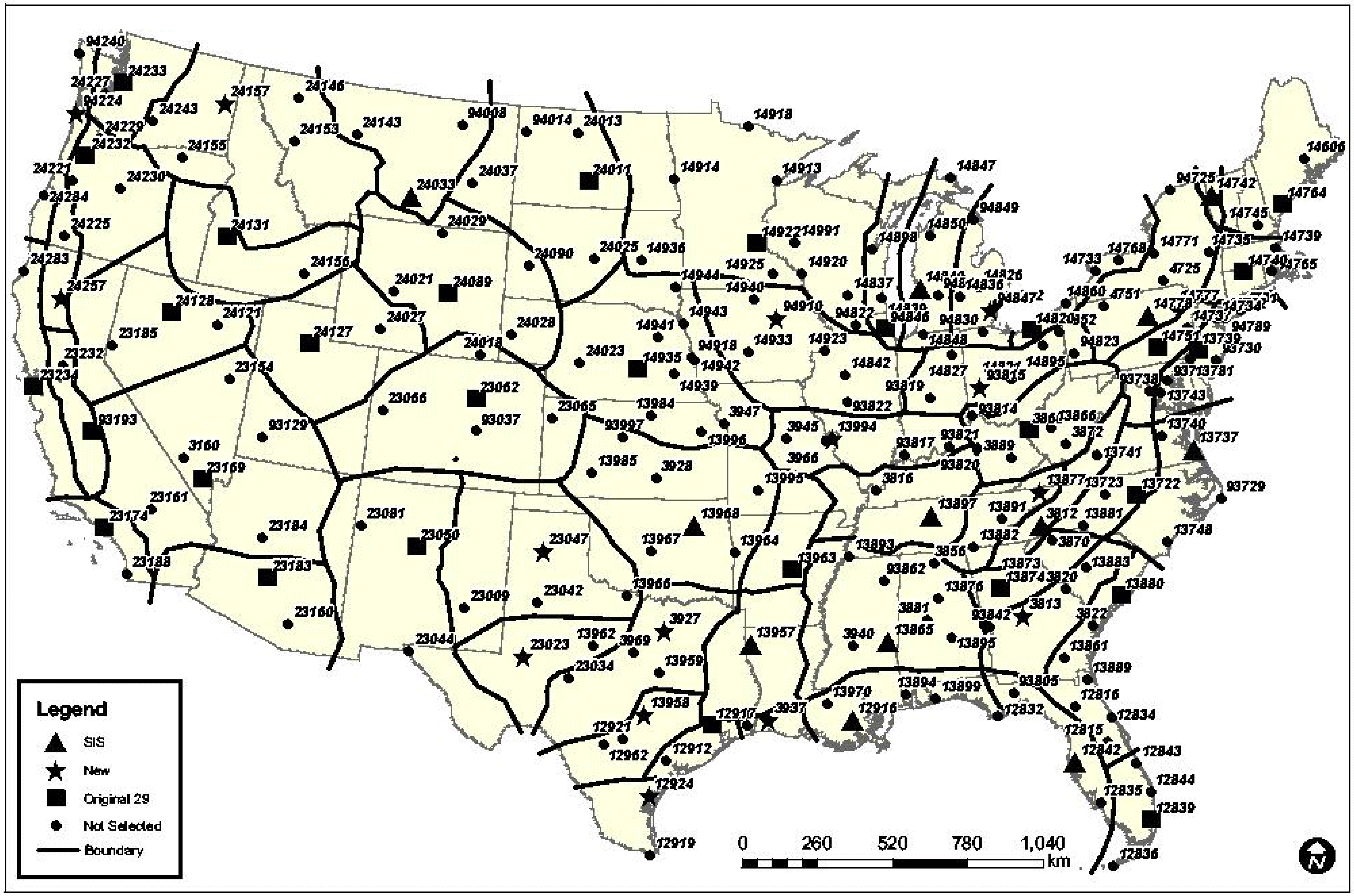


Figure D-2. Meteorological stations and region boundaries for the contiguous 48 states.

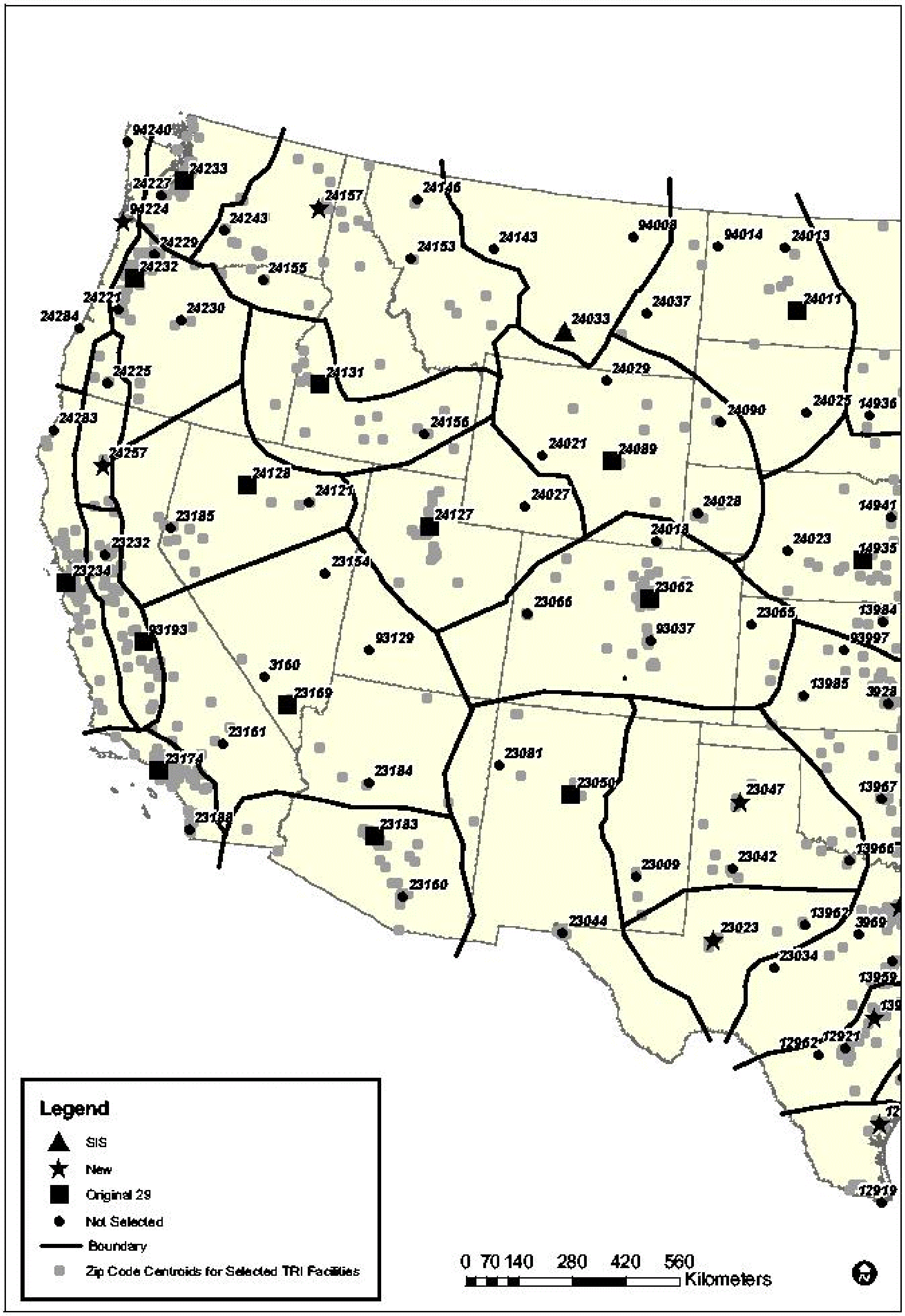


Figure D-3. Meteorological stations and region boundaries for the western United States with TRI facilities.

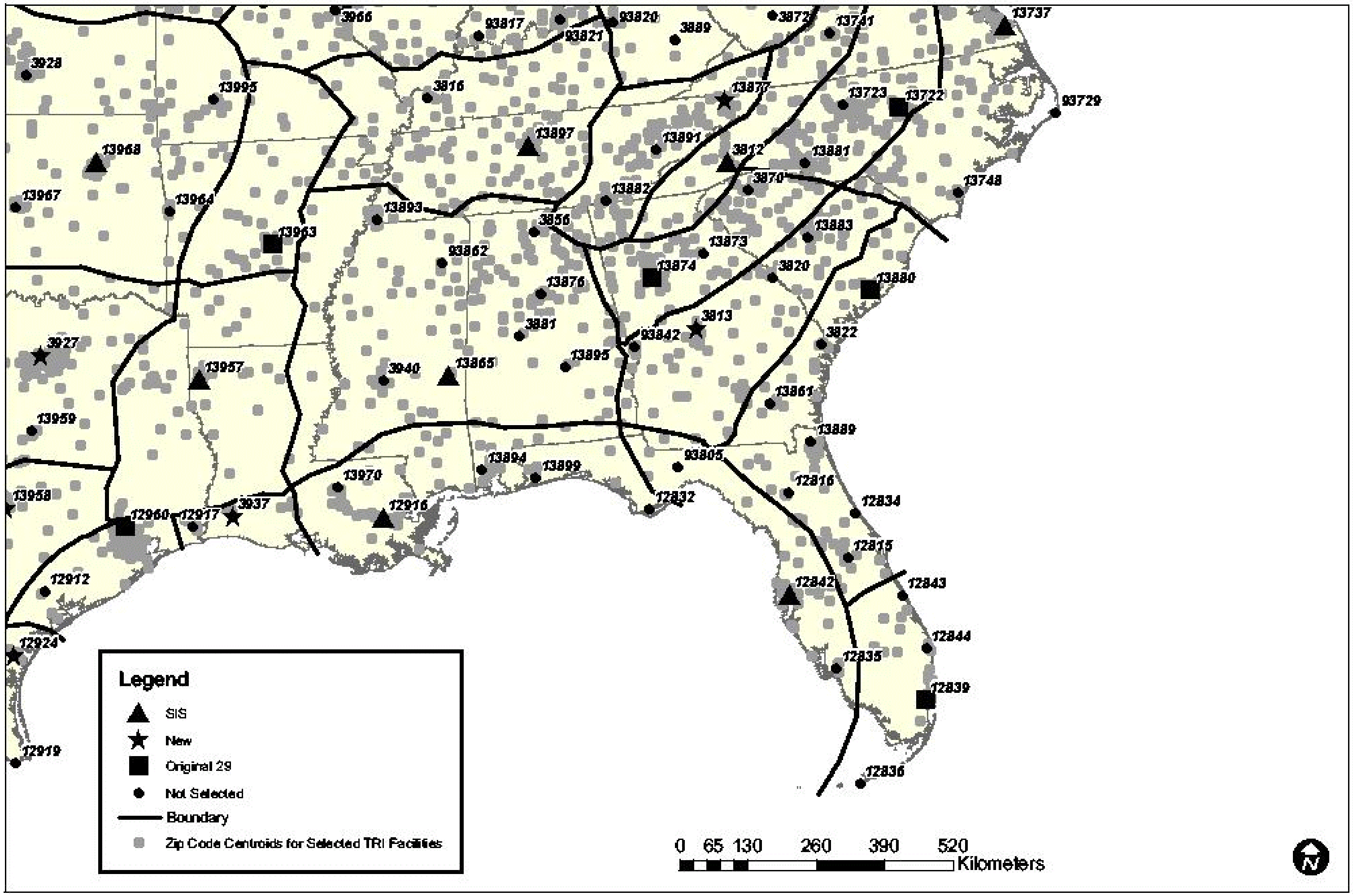


Figure D-4. Meteorological stations and region boundaries for the southeastern United States with TRI facilities.

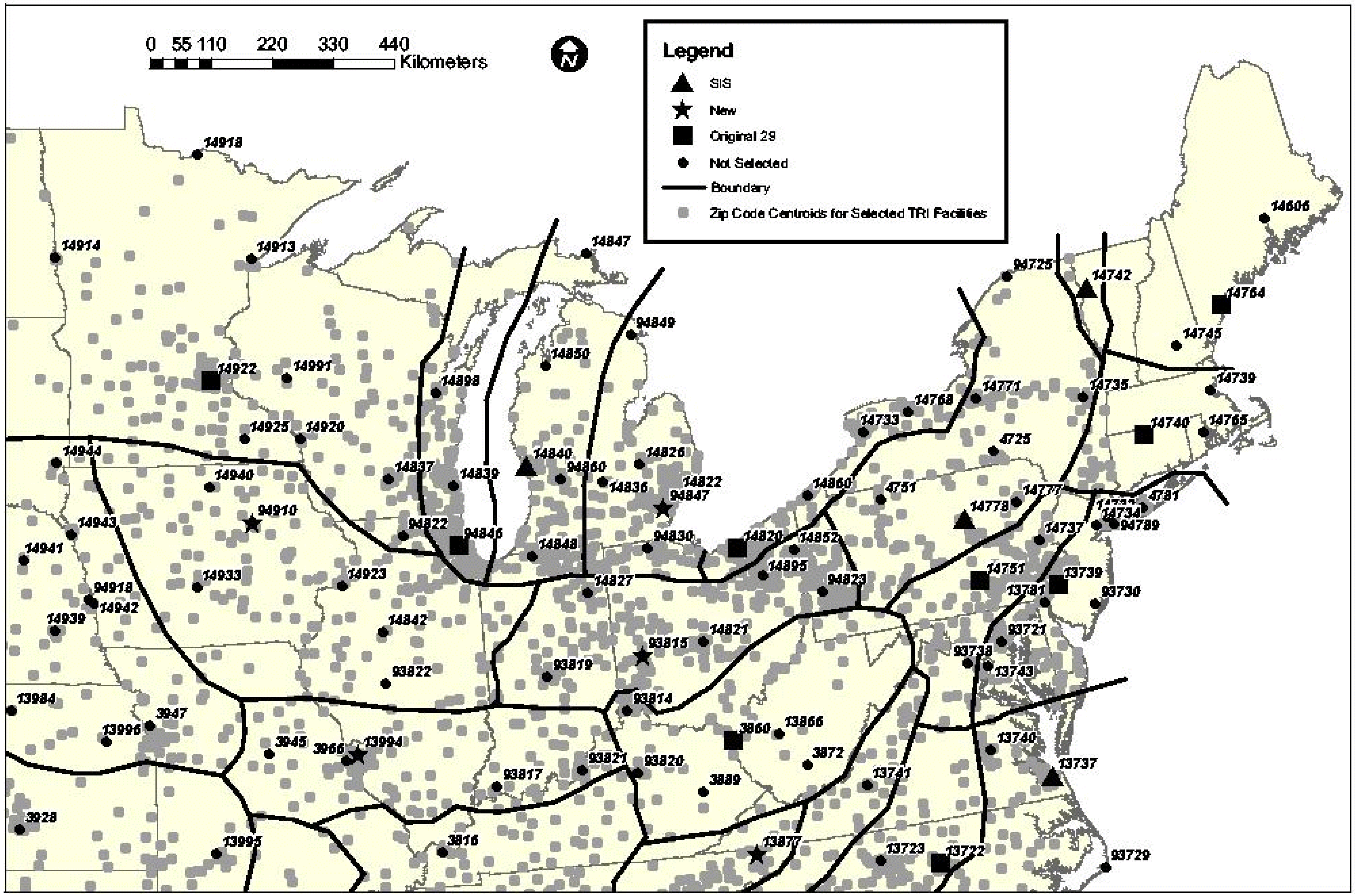


Figure D-5. Meteorological stations and region boundaries for the northeastern United States with TRI facilities.

assigning final boundaries for each selected station. Figures D-6, D-7, and D-8 also show the contiguous 48 states and the selected stations overlaid on Bailey's ecoregions, physiographic features, and land cover, respectively. Figures D-9 and D-10 show physiographic features for Alaska and Hawaii, respectively.

D.3.1 West Coast

The West Coast is defined by a narrow coastal plain and mountain chains running parallel to the coast of the Pacific Ocean. In many areas, the mountainous region is broken by a large central valley, such as in California. Due to the potential number of facilities in California that may use IWAIR, the California central valley was regionally delineated; the central valleys in Washington and Oregon were combined with some rural mountainous areas to their east.

The northwestern Pacific coast contains a narrow plain between the Pacific Ocean and the Coast Ranges. The **Astoria/Clatsop** County Airport station (94224) in Oregon represents the region from the Strait of Juan de Fuca south to the Oregon/California border. The wind rose shows generally weak directionality (bin W), and the average wind speed is 8 knots.

The California coast is divided just north of Point Conception above Los Angeles. The northern section is represented by the **San Francisco** International Airport (23234). The wind rose shows strong directionality (bin C), and the average wind speed is 12 knots.

The southern California coast contains the Los Angeles basin south to the California/ Mexico border. This region is represented by the **Los Angeles** International Airport (23174). The wind rose shows strong directionality (bin C), and the average wind speed is 8 knots.

The California central valley region, which encompasses the Sacramento Valley to the north and the San Joaquin Valley to the south, is defined by the Coast Range and Diablo Range on the west and the Sierra Nevada mountains on the east. The valley extends south to the northern rim of the Los Angeles basin. This valley was divided into two sections between Sacramento and Redding because of the variation in wind regimes. The southern section is represented by **Fresno** Air Terminal (93193). The wind rose shows strong directionality (bin C). The northern division, whose northern border is represented by an ecoregion change to the Willamette Valley and Puget Trough Section, is represented by the **Redding** AAF (24257). The wind rose shows moderate directionality (bin B).

The inland portion of Washington is bounded by the Coast Ranges on the west, the edge of the Humid Temperate Domain to the east, the Washington/Canada border to the north, and the Columbia River to the south. This region is represented by the **Seattle**-Tacoma International Airport (24233). The wind rose shows moderate directionality (bin B), and the average wind speed is 10 knots.

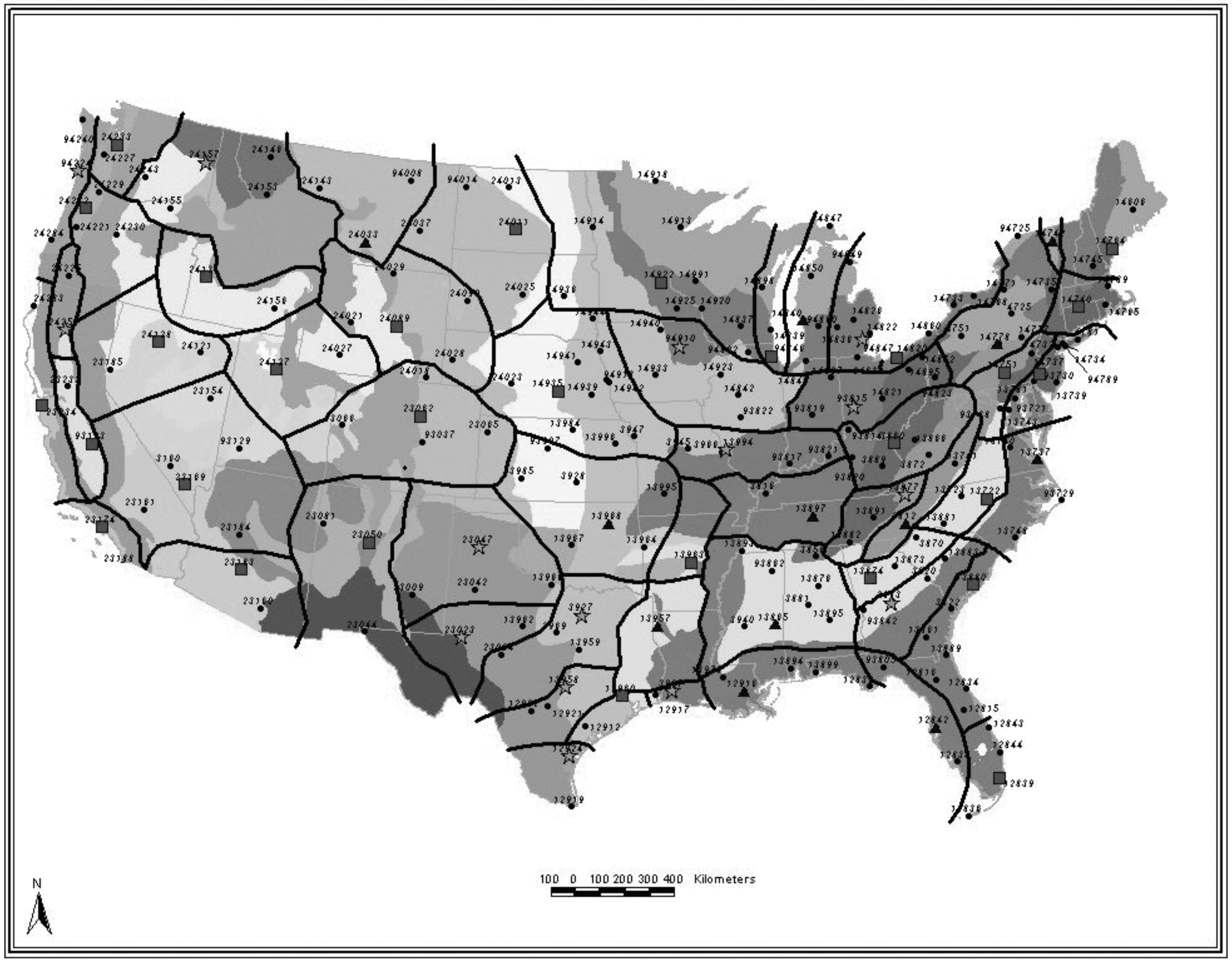


Figure D-6. **Meteorological stations and region boundaries for the continental United States with Bailey's ecoregions (Bailey et al., 1994).**

(continued)

🟥 Original 29
☆ NEW
▲ SIS
• Not Selected
∧∨ Boundary

Baileys Provinces
🟫 Adirondack-New England Mixed Forest-Coniferous Forest-Alpine Meadow Province
🟨 American Semi-Desert and Desert Province
🟩 Arizona-New Mexico Mountains Semi-Desert-Open Woodland-Coniferous Forest-Alpine Meadow Province
🟧 Black Hills Coniferous Forest Province
⬜ California Coastal Chapparral Forest and Shrub Province
🟧 California Coastal Range Open Woodland-Shrub-Coniferous Forest-Meadow Province
🟨 California Dry Steppe Province
🟩 Cascade Mixed Forest-Coniferous Forest-Alpine Meadow Province
🟫 Central Appalachian Broadleaf Forest-Coniferous Forest-Meadow Province
🟫 Chihuahuan Semi-Desert Province
🟨 Colorado Plateau Semi-Desert Province
🟩 Eastern Broadleaf Forest (Continental) Province
🟫 Eastern Broadleaf Forest (Oceanic) Province
🟩 Everglades Province
⬜ Great Plains Steppe Province
🟨 Great Plains Steppe and Shrub Province
🟨 Great Plains-Palouse Dry Steppe Province
⬜ Intermountain Semi-Desert Province
🟧 Intermountain Semi-Desert and Desert Province
🟩 Laurentian Mixed Forest Province
🟧 Lower Mississippi Riverine Forest Province
🟧 Middle Rocky Mountain Steppe-Coniferous Forest-Alpine Meadow Province
🟧 Nevada-Utah Mountains-Semi-Desert-Coniferous Forest-Alpine Meadow Province
🟩 Northern Rocky Mountain Forest-Steppe-Coniferous Forest-Alpine Meadow Province
🟩 Ouachita Mixed Forest - Meadow Province
🟫 Outer Coastal Plain Mixed Forest Province
🟨 Ozark Broadleaf Forest - Meadow Province
🟨 Pacific Lowland Mixed Forest Province
🟧 Prairie Parkland (Subtropical) Province
⬜ Prairie Parkland (Temperate) Province
🟧 Sierran Steppe-Mixed Forest-Coniferous Forest-Alpine Meadow Province
🟨 Southeastern Mixed Forest Province
🟩 Southern Rocky Mountain Steppe-Open Woodland-Coniferous Forest-Alpine Meadow Province
🟫 Southwest Plateau and Plains Dry Steppe and Shrub Province

Figure D-6. (continued)

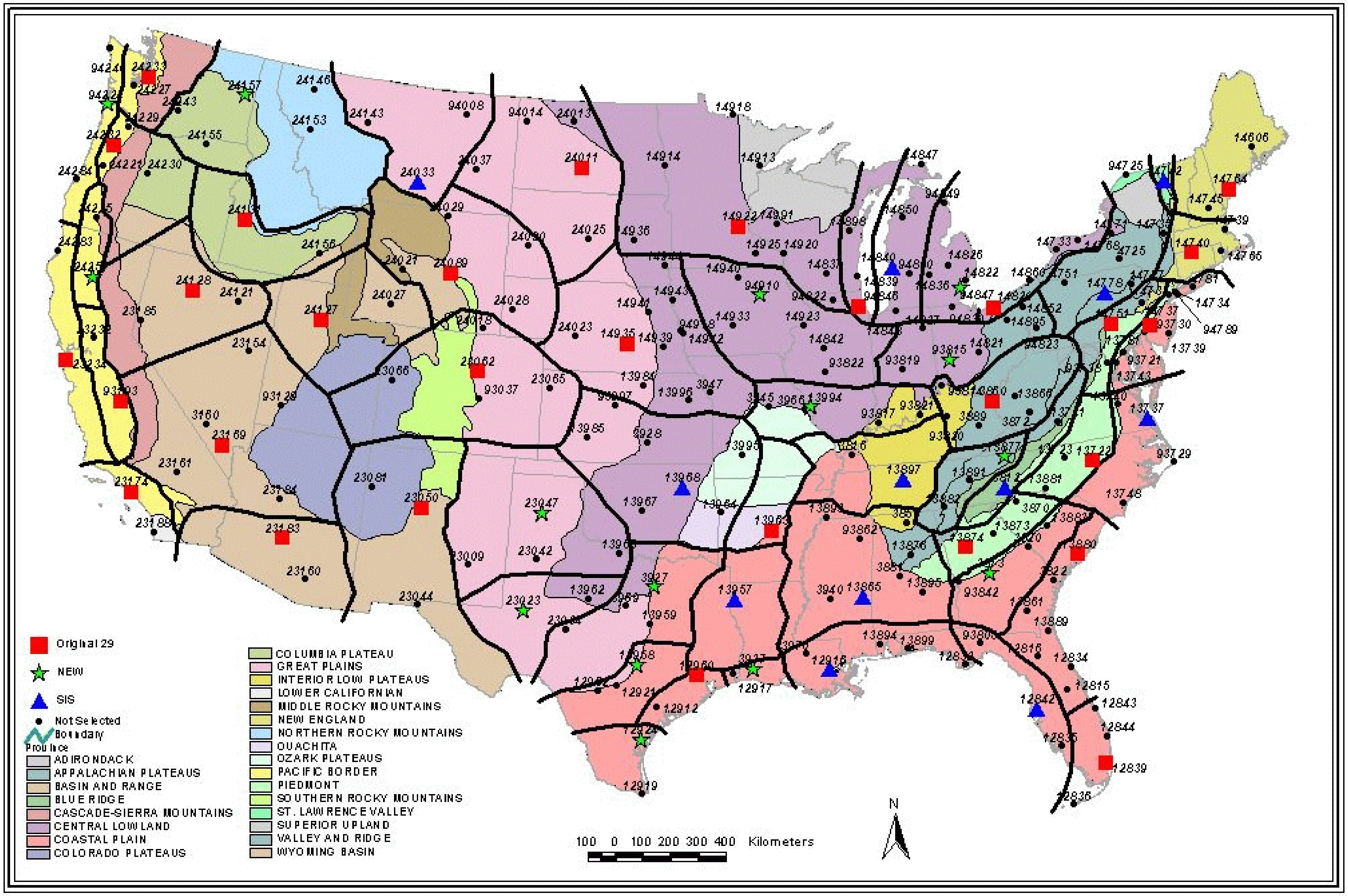


Figure D-7. Meteorological stations and region boundaries for the continental United States with physiography (Fenneman and Johnson, 1946).

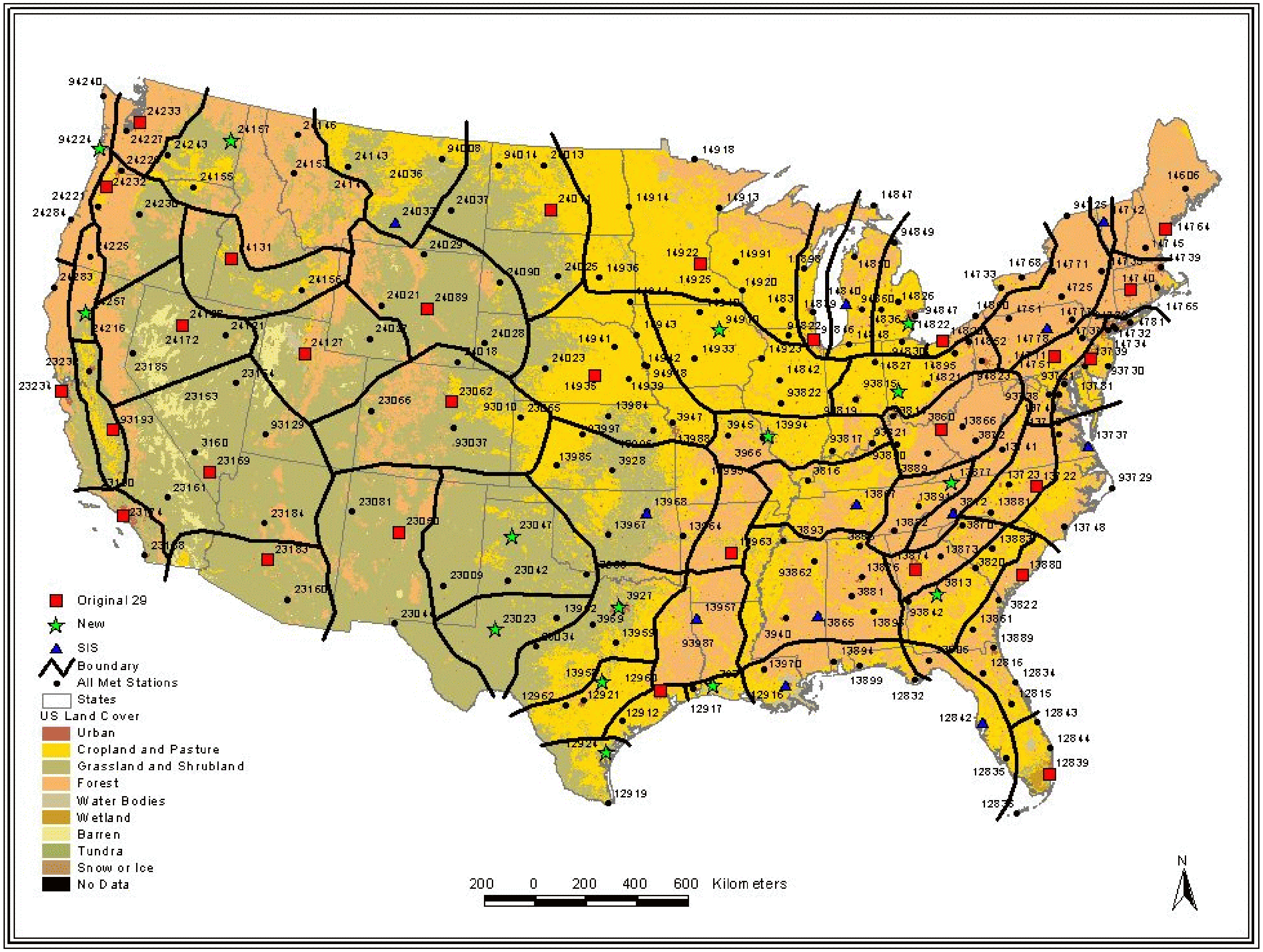


Figure D-8. Meteorological stations and region boundaries for the continental United States with land cover (USGS, 1999).

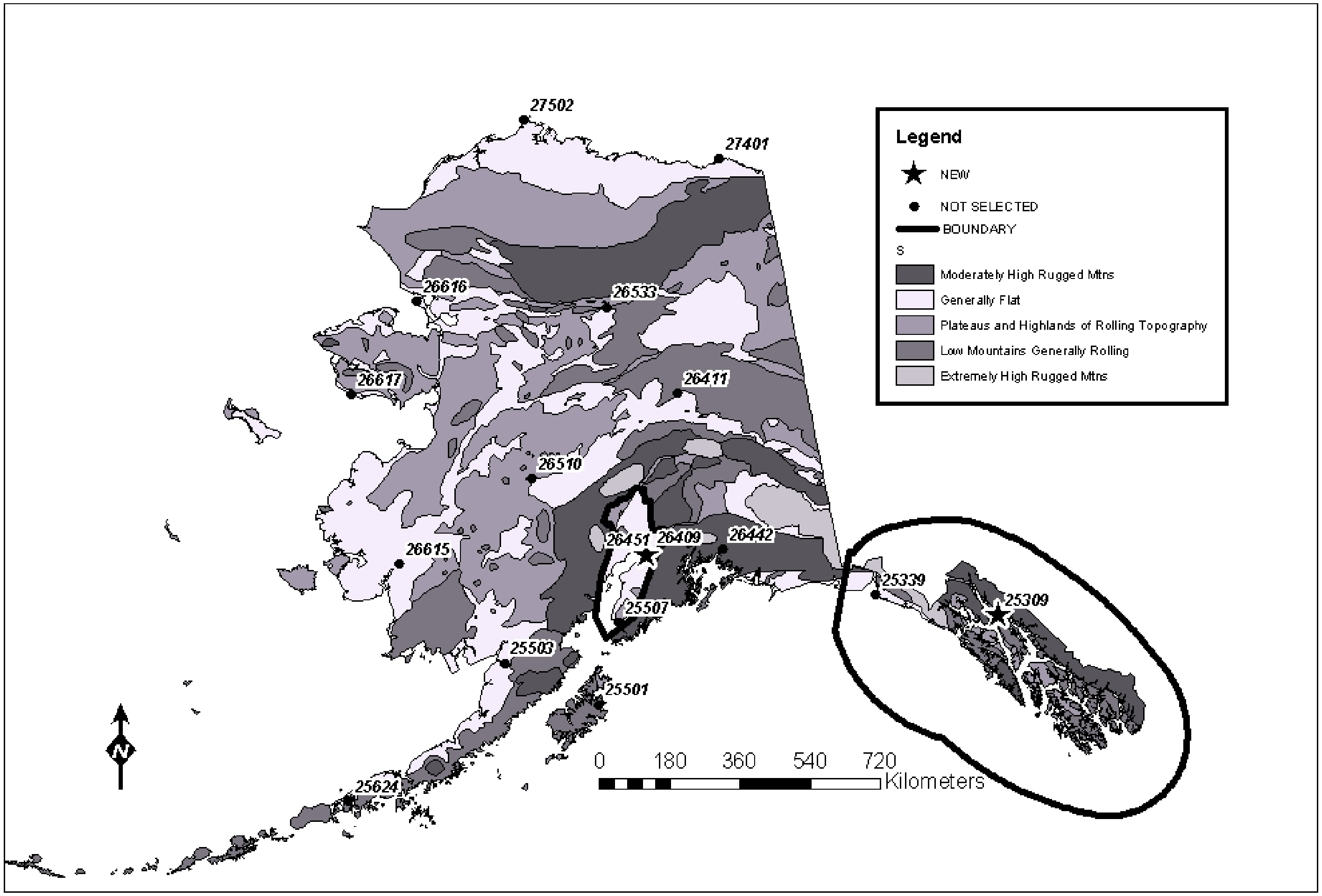


Figure D-9. Meteorological stations and region boundaries for Alaska with physiography (Wahrhaftig, 1965).

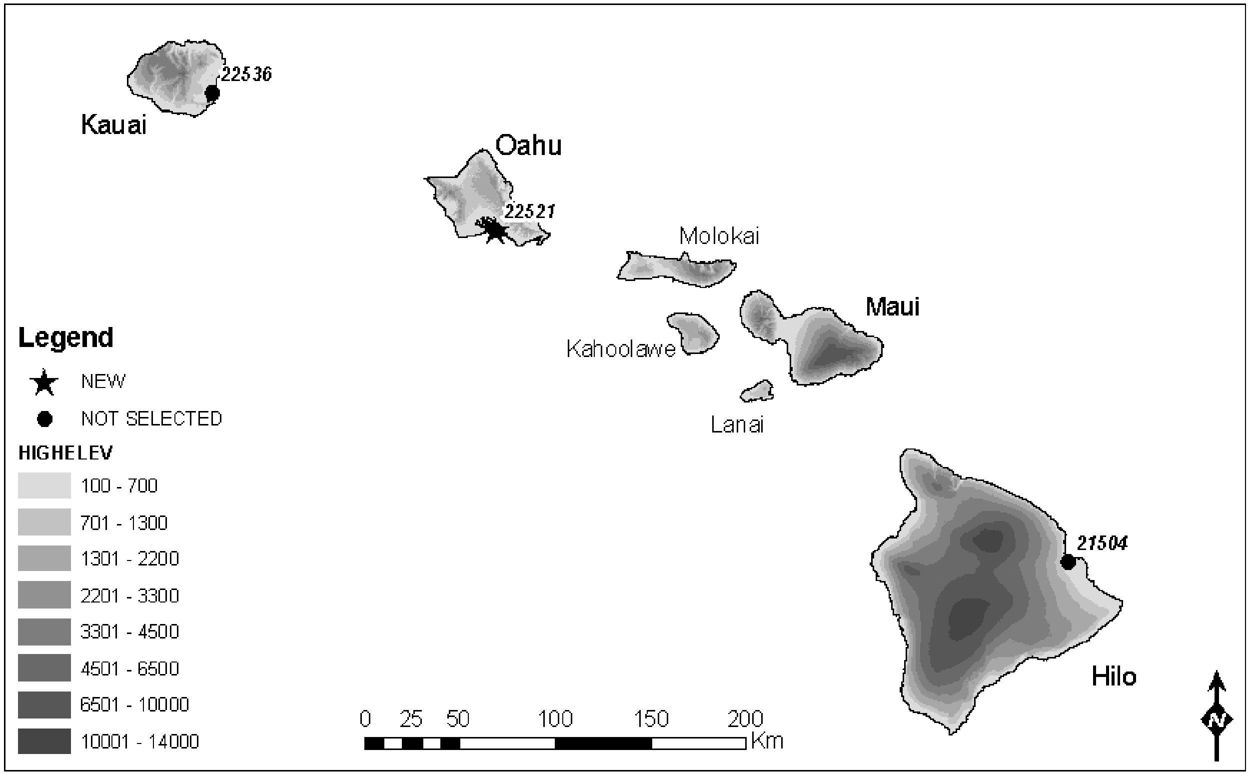


Figure D-10. Meteorological stations for Hawaii with physiography (State of Hawaii, 1997).

D.3.2 Desert Southwest

The Desert Southwest is defined by various deserts and mountain ranges. One distinguishing feature is the transition between low desert in southern Arizona and high desert in northern Arizona. The southern boundary of this section is the United States/Mexico border.

Southern Arizona contains the Sonoran Desert. This region of low desert is represented by the station at **Phoenix**/Sky Harbor International Airport (23183). The region is bounded to the north between Phoenix and Prescott, Arizona, along the southern edge of the Columbia Plateau, which represents the transition from low to high desert. The wind rose shows moderate directionality (bin B), and the average wind speed is 6 knots.

Northern Arizona, southeastern California, southern Nevada, and southern Utah are represented by the station at **Las Vegas**/McCarran International Airport (23169). This region is characterized by high desert, including the Columbia Plateau. Relatively few facilities and people are located here. The wind rose shows mild directionality (bin A), and the average wind speed is 10 knots.

The mountainous region of western New Mexico and far west Texas is represented by the station at **Albuquerque** International Airport (23050). This region is bounded on the east by the Sacramento Mountains east of El Paso, Texas, and by the Sangre de Cristo Mountains east of Albuquerque, New Mexico. The wind rose shows weak directionality (bin W), and the average wind speed is 8 knots.

D.3.3 Western Mountains

The Western Mountains include numerous mountain ranges, plateaus, and valleys that affect wind flows. The northern portion of the Western Mountains is bounded on the west by the eastern edge of the Humid Temperate Domain and on the east by the Great Plains in western Montana. The southern boundary is approximately at the southern edge of the Temperate Steppe Regime Mountains. This region is represented by the station at **Spokane** International Airport. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

The inland region of Oregon includes both the central valley area and the Great Sandy Desert, east to the Columbia Plateau. The western boundary is the Coast Ranges. The Black Rock Desert forms the southern boundary. This region is represented by the station at McNary Field in **Salem, Oregon** (24232). The wind rose shows moderate directionality (bin B), and the average wind speed is 9 knots. Facilities in the eastern portion of this region should consider obtaining local meteorological data and running the ISCST3 model to obtain local dispersion factors for IWAIR; this area is not well-represented by any of the surrounding stations but did not have enough population or TRI facilities to warrant adding another station to IWAIR.

The Snake River Plain of southern Idaho forms the region represented by **Boise** Air Terminal (24131) in Idaho. This region is bounded by the Salmon River Mountains on the north and the Columbia Plateau to the west and south. The wind rose shows moderate directionality (bin B), and average wind speed is 9 knots.

Northern Nevada and northeastern California are represented by the station at **Winnemucca** WSO Airport (24128) in Nevada. This is the Great Basin area. The wind rose shows mild directionality (bin A), and the average wind speed is 8 knots.

The Salt Lake Basin and the Great Divide Desert in Utah and Colorado are represented by the station at **Salt Lake City** International Airport (24127) in Utah. The eastern boundary of this region is formed by the Wind River Range and the Front Range. The wind rose shows moderate directionality (bin B), and the average wind speed is 9 knots.

D.3.4 Texas (Excluding the Gulf Coast)

The state of Texas is a very large section encompassing many wind regimes. These are bounded by mountains, deserts, forests, the Gulf of Mexico, and plains. The Gulf Coast region is covered in Section D.3.5.

The Texas Panhandle region is represented by the station at **Amarillo** International Airport (23047). The western boundary is formed by the Sangre de Cristo Mountains in New Mexico. The northern boundary is the southern edge of the Great Plains. The southern boundary divides this region from the West Texas region to its south. The wind rose shows mild directionality (bin A), and the average wind speed is 13 knots.

The West Texas region includes high plateaus and is represented by the station at **Midland** Regional Airport (23023). The western boundary of this region is formed by the Sacramento Mountains. The wind rose for this region shows moderate directionality (bin B), and the average wind speed is 10 knots.

Central Texas is represented by the station at **Dallas/Ft. Worth** airport (03927). The majority of the population in this region is located in the vicinity of Dallas and Ft. Worth. Also, most of the industrial facilities in this region are located in that vicinity. The southwestern portion of this region encompasses the Edwards Plateau. The eastern boundary is formed by the transition to forest in eastern Texas. The wind rose shows strong directionality (bin C), and the average wind speed is 11 knots.

South Central Texas includes the area north of the southern coastal region and south Texas. The eastern boundary is formed by the eastern edge of the Prairie Parkland (Subtropical) Province. The southern boundary is formed by the transition from grassland and crop land to the shrub land in Southern Texas. This region is represented by the station at **Austin** Municipal Airport (13958). The wind rose shows moderate directionality (bin B), and the average wind speed is 8 knots.

Southern Texas includes the southern coast of the Gulf of Mexico, including Corpus Christi and Brownsville, Texas. This region is represented by the station at **Corpus Christi** International Airport (12924). The southern and western borders are formed by the Rio Grande River. The eastern border is the Gulf of Mexico. The northern boundary is formed by the transition from shrub land in Southern Texas to grassland and crop land in South Central Texas. The wind rose shows strong directionality (bin C), and the average wind speed is 12 knots.

D.3.5 Gulf Coast

The wind regime along the Gulf of Mexico is strongly influenced by that body of water. However, its effects do not reach very far inland. A series of regions have been designated to represent the coastal section.

The middle Texas Gulf Coast is represented by the station at **Houston** Intercontinental Airport (12960). Although Houston itself is somewhat inland, it is expected to have a more coastal environment due to Galveston Bay. This region extends south past Victoria to the vegetative boundary marking Southern Texas. The wind rose in this region shows mild directionality (bin A), and the average wind speed is 8 knots.

The western portion of the Louisiana Gulf Coast and the far eastern portion of the Texas Gulf Coast has the vegetative land cover change to forest as its northern border. This relatively small area includes a high concentration of industrial facilities along the coast. The station at **Lake Charles** Municipal Airport (03937) represents this region. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

The Central Gulf Coast extends from eastern Louisiana through the Florida panhandle. This entire region is part of the Outer Coastal Plain Mixed Forest Province and is characterized by weakly directional winds. The station at **New Orleans** International Airport (12916) in Louisiana represents this region. The wind rose shows weak directionality (bin W), and the average wind speed is 8 knots.

The West Coast of the Florida Peninsula is heavily influenced by the Gulf of Mexico, which has warmer water than the Atlantic Ocean off the East Coast of the Florida Peninsula. This region extends from the Florida Panhandle to the north to Cape Romano, just north of the Everglades in South Florida. The station at **Tampa** International Airport (12842) represents this region. The wind rose shows mild directionality (bin A), and the average wind speed is 7 knots.

D.3.6 Southeast

The Southeast section extends from the Atlantic coastal region of Florida and the Florida Keys northward through Georgia and South Carolina. This region has an extremely broad coastal plain, requiring it to be divided between coastal region and more inland regions for Georgia and South Carolina. This section also includes the inland areas of Louisiana, Mississippi, and Alabama.

The southern tip of Florida includes the Everglades, which have been drained along the Atlantic coast to provide land for Miami, Ft. Lauderdale, West Palm Beach, and other coastal cities. This region, which includes the Florida Keys, is represented by the station at **Miami** International Airport (12839). Its wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

A long stretch of the Southeastern Atlantic Coast extends from north of Vero Beach, Florida (i.e., just south of Cape Canaveral), through Georgia and South Carolina. The Atlantic

Ocean forms the eastern boundary, and the land cover boundary between the more forested coast and more agricultural inland area forms the western boundary. The station at **Charleston** International Airport (13880) represents this region. The wind rose shows weak directionality (bin W), and the average wind speed is 8 knots.

The inland coastal plain of Georgia and South Carolina extends inland from the coastal forest/agriculture land cover boundary to the physiographic boundary between the Coastal Plain and the Blue Ridge. This region is represented by the station at **Macon**'s Lewis B. Wilson Airport (03813) in Georgia. The wind rose shows weak directionality (bin W), and the average wind speed is 8 knots.

Further inland in Georgia and South Carolina lies the Blue Ridge region. This region is delineated by physiographic boundaries—the transition to the Coastal Plain on the coastal side and to the Appalachian Plateaus on the inland side. The station at **Atlanta** Hartsfield International Airport (13874) represents this region. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

The inland areas of Alabama and Mississippi are represented by the station at **Meridian** Key Field (13865), which is located in Mississippi close to the Alabama border. This region extends from the Central Gulf Coast region northward into southern Tennessee (including Memphis) and westward into the Coastal Plain region of eastern Arkansas. The wind rose shows mild directional (bin A), and the average wind speed is 7 knots.

The inland portion of Louisiana and eastern Texas is part of the Coastal Plain. This region extends northward to the Ouachita Mountains, which are just south of the Ozark Plateau in Arkansas. The western boundary is the vegetative transition from the forests in this region to the prairies in Texas. This region is represented by the station at **Shreveport** Regional Airport (13957) in Louisiana. The wind rose is mildly directional (bin A), and the average wind speed is 9 knots.

D.3.7 Middle Atlantic

The Middle Atlantic section includes coastal areas with bays, sounds, inlets, and barrier islands; a broad coastal plain; and the southern Appalachian Mountains. The physiographic features generally extend from northeast to southwest, parallel to the coast of the Atlantic Ocean.

The coastal region of North Carolina and Virginia is represented by the station at **Norfolk** International Airport (13737) in Virginia. This region is bounded by the Atlantic Ocean on the east, the physiographic boundary to the Piedmont section to the west, the political border between North Carolina and South Carolina to the south, and a line bisecting the Chesapeake Bay to the north. The wind rose shows mild directionality (bin A), and the average wind speed is 10 knots.

The Piedmont region of North Carolina and Virginia is just inland from the coastal region. This region is delineated on the east by the physiographic boundary with the coastal plain, and on the west with the physiographic boundary with the Appalachian Mountains. This region is also part of the Southeastern Mixed Forest Province of Bailey's ecoregions. The station at **Raleigh-Durham** Airport (13722) in North Carolina represents this region. The wind rose shows weak directionality (bin W), and the average wind speed is 8 knots.

The eastern portion of the southern Appalachian Mountains lies to the west of the Piedmont region of North Carolina and Virginia. This region extends to the southwest to include a portion of western South Carolina and northeastern Georgia. The station at **Asheville** Regional Airport (03812) in North Carolina represents this region. The wind rose shows moderate directionality (bin B), and the average wind speed is 10 knots.

The western portion of the southern Appalachian Mountains, including the Cumberland Plateau, lies in western Virginia, eastern Tennessee, northwestern Georgia, and northeastern Alabama. The western edge of this region follows the physiographic boundary between the Appalachian Plateaus and the Interior Low Plateaus. The station at **Bristol** Tri City Airport (13877) in Tennessee represents this region. The wind shows weak directionality (bin W), and the average wind speed is 8 knots.

The Appalachian Mountains of West Virginia and eastern Kentucky are characterized by mountainous ridges and valleys extending from northeast to southwest. This region is represented by the station at **Huntington** Tri-State Airport (03860) in West Virginia. The wind rose shows mild directionality (bin A), and the average wind speed is 7 knots.

The inland region encompassing northern Virginia, part of Maryland, and eastern Pennsylvania is composed of another section of the Appalachian Mountains. Boundaries are approximated by the Bailey's Central Appalachian Forest province. The station at **Harrisburg**/Capital City Airport (14751) in Pennsylvania represents this region. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

The northern portion of the Chesapeake Bay northward through New Jersey, eastern Pennsylvania, and New York City is characterized by the Eastern Broadleaf Forest (Oceanic) Province in the coastal plain. The station at **Philadelphia** International Airport (13739) in Pennsylvania represents this region. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

D.3.8 Northeast

The Northeast section includes New England. This region is characterized by forests to the north, large urban areas along the southern coastal plain, and the mountain ridges and valleys of the northern Appalachian Mountains. This section is bounded by the Atlantic Ocean on the east, the U.S./Canada border on the north, and the coastal plain of the eastern Great Lakes to the west.

The station at Bradley International Airport (14740) in **Hartford**, Connecticut, represents the New England region, which encompasses Connecticut, Massachusetts, Rhode Island and a small portion of Vermont, New Hampshire, and eastern New York. The wind rose shows mild directionality (bin A), and the average wind speed is 8 knots.

Northern New England is represented by the station located at the International Jetport (14764) in **Portland**, Maine. This region includes Maine and most of New Hampshire and Vermont. The northwest portion of Vermont is not included in this region. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

The station at the International Airport (14742) in **Burlington**, Vermont, represents a very small region. Burlington is located in a valley between mountainous areas of the northern Appalachian Mountains. The wind rose shows moderate directionality (bin B), and the average wind speed is 10 knots.

The remainder of the northern Appalachian Mountains in New York and Pennsylvania is represented by the station at **Williamsport**-Lycoming (14778) in Pennsylvania. This region is bounded on the west by the Adirondack Mountains, just to the east of the coastal plain of Lake Ontario. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

D.3.9 Great Lakes

The Great Lakes are bodies of water large enough to affect weather patterns in that portion of the country. Land and sea breezes affect wind patterns along the coasts, especially along Lake Michigan in the summer. The moisture of the lakes also affects winter precipitation patterns (i.e., lake effect snow storms).

The Eastern Great Lakes divide the United States and Canada. On the U.S. side, the western portion of New York, a small portion of Pennsylvania, and northeastern Ohio border the eastern shores of Lake Ontario and Lake Erie. Mountains form the eastern boundary. The southwestern border is drawn southward from the southern shore of Lake Erie. The station at Hopkins International Airport (14820) in **Cleveland**, Ohio, represents this region. The wind rose shows moderate directionality (bin B), and the average wind speed is 10 knots.

The Lower Peninsula of Michigan is bordered by the Great Lakes on three sides. Although this region has relatively few topographic features, the presence of the lakes may result in different dispersion analyses for the eastern and western portions of the state. Therefore, the Lower Peninsula has been divided into two regions—East and West.

The eastern region of the Lower Peninsula of Michigan is bordered by Lake Erie, Lake St. Clair, and Lake Huron and includes Saginaw Bay and a small abutment with Canada. This region is represented by the station at **Detroit** Metropolitan Airport (94847). The wind rose shows mild directionality (bin A), and the average wind speed is 10 knots.

The western region of the Lower Peninsula of Michigan is bordered by Lake Michigan on the west and the Straits of Mackinac on the north. The eastern portion of the Upper Peninsula of Michigan is also included in this region. The station at **Muskegon** County Airport (14840) represents this region. The wind rose shows weak directionality (bin W), and the average wind speed is 11 knots.

The western shore of Lake Michigan, which includes Green Bay, is formed by the northeastern portion of Illinois, eastern Wisconsin, and part of the Upper Peninsula of Michigan. Lake Superior forms the northern boundary of this region, and the western boundary is formed by the hills to the east of the Wisconsin River and the Upper Mississippi River. This region is represented by the station at O'Hare International Airport (94846) in **Chicago**, Illinois. The wind rose shows mild directionality (bin A), and the average wind speed is 9 knots.

D.3.10 Central States

This section includes the Central Lowlands (south of the Great Lakes), the Midwest, and the Great Plains. The elevation for this section is generally lowest in the Mississippi Valley, which extends through the Midwest and drains a large portion of the center of the continental United States. This section also includes other major river valleys, including the Ohio, Tennessee, and Missouri. This section is bordered on the east by the Appalachian Mountains, on the west by the Rocky Mountains, on the north by the border with Canada, and on the south by the Southeast, Texas, and the Desert Southwest.

The Central Lowland is the area south of the Great Lakes and west of the Appalachian Mountains. This area is divided into several regions based on wind rose data. The region that includes central Indiana, Ohio, and western Pennsylvania is represented by the new station at **Dayton** International Airport (93815) in Ohio. The western boundary is formed by a transition from hills in this region to flat land to its west. The northern boundary is formed by the Great Lakes section, and the eastern and southeastern boundaries are formed by the Appalachian Mountains. The wind rose shows mild directionality (bin A), and the average wind speed is 10 knots.

The region encompassing parts of Illinois, northeastern Missouri, and most of Iowa is relatively flat farmland. The station at **Waterloo** Municipal Airport (94910) in Iowa represents this region. The wind rose shows mild directionality (bin A), and the average wind speed is 11 knots.

The region of southern Indiana, south-central Illinois, and east-central Missouri includes the industrial area surrounding St. Louis, Missouri. The station at Lambert International Airport (13994) in **St. Louis**, Missouri, represents this region. The wind rose shows mild directionality (bin A), and the average wind speed is 10 knots.

The region to the south of the one represented by St. Louis includes western Kentucky, central and western Tennessee north of Memphis, and southeastern Missouri east of the Ozark Plateau. This region is represented by the station at **Nashville** Metropolitan Airport (13897) in Tennessee. The wind rose shows moderately directionality (bin B), and the average wind speed is 8 knots.

Adams Field (13963) in **Little Rock**, Arkansas, represents a small region that includes the higher portions of the Ozark Plateau in southern Missouri and northern Arkansas and the Ouachita Mountains in central Arkansas. The wind rose shows weak directionality (bin W), and the average wind speed is 7 knots.

The northern portion of the Midwest includes the portion of Wisconsin west of the Lake Michigan coastal plain, Minnesota, and the eastern portion of North and South Dakota. The western boundary through the Dakotas is the physiographic boundary between the Central Lowland and the Great Plains. This region is represented by the station at **Minneapolis-St. Paul** International Airport (14922) in Minnesota. The wind rose shows mild directionality (bin A), and the average wind speed is 11 knots.

The Great Plains lie between the Central Lowlands to the east and the Rocky Mountains to the west. The headwaters of the Mississippi and the Missouri rivers are located in the Great Plains. Lands at higher elevations are more grassland and shrub land used for cattle ranges, while the lower elevations are used more frequently for crops. The region that includes the western portion of North and South Dakota and eastern Montana is represented by the station at **Bismarck** Municipal Airport (24011) in North Dakota. The wind rose shows weak directionality (bin W), and the average wind speed is 12 knots.

The central portion of Montana is more rugged, but still part of the Great Plains. The Rocky Mountains form the western and southwestern boundaries of this region, which is represented by the station at **Billings** Logan International Airport (24033) in Montana. The wind rose shows strong directionality (bin C), and the average wind speed is 10 knots.

The original station at **Casper**/Natrona County International Airport (24089) in Wyoming represents Wyoming east of the Front Range of the Rocky Mountains, southwestern South Dakota, and western Nebraska. The wind rose shows strong directionality (bin C), and the average wind speed is 14 knots. In this region, most cities are located in valleys or near the base of a mountain ridge. The wind regime at Casper, therefore, may not adequately represent facilities at other locations in this region.

The region represented by the station at Stapleton International Airport (23062) in **Denver**, Colorado, has facilities clustered in the Denver vicinity. The southern boundary is formed by the southern edge of the Great Plains. The wind rose shows mild directionality (bin A), and the average wind speed is 8 knots. Grand Junction, Colorado, which is located in the western portion of the state, is included in this region although it exhibits a different wind regime. Facilities located in the western portion of Colorado should consider entering dispersion factors based on their local meteorological data; this area is not well-represented by any of the surrounding stations, and did not have enough population or TRI facilities to warrant adding another station to IWAIR.

The north-central portion of the Great Plains includes most of Nebraska, northern Kansas, western Iowa, southwestern South Dakota, and northwestern Missouri. This region is represented by the station at **Grand Island** Airport (14935) in Nebraska. The wind rose shows moderate directionality (bin B), and the average wind speed is 12 knots.

The southern portion of the Great Plains includes eastern Oklahoma, most of Kansas, and the lower area of the western Ozark Plateau in southwestern Missouri and northwestern Arkansas. This region is represented by the station at **Tulsa** International Airport (13968). The wind rose shows moderate directionality (bin B), and the average wind speed is 11 knots.

D.3.11 Alaska

Alaska contains a wide variety of topography and land cover (see Figure D-9). The northern portion of the state, which includes the North Shore oil fields, is primarily tundra on flat topography. The southwestern portion is grassland and shrub land on flat to rolling topography. The remainder of the state includes large, forested valleys and rugged mountains with glaciers. The coastal areas include numerous islands. IWAIR includes two stations in Alaska, but cannot represent the entire state. The 1998 TRI data were used to select the locations of the included stations.

The station at **Juneau** International Airport (25309) represents the southeastern portion of Alaska. This region extends from just west of Yakutat Bay southward to Dixon Entrance. Canada forms the northeastern border, and the Gulf of Alaska is on the west. The wind rose shows strong directionality (bin C).

The station at **Anchorage** WSMO Airport is in a unique wind regime in a coastal valley surrounded by mountains. However, several TRI facilities report land-based air emissions for this region. Anchorage is located at the northern end of Cook Inlet. Industrial facilities are located just to its south on the western portion of the Kenai Peninsula. This region, therefore, is bounded by the Alaska Range to the west and north, the Chugach Mountains to the east, and the Gulf of Alaska to the south. The wind rose shows mild directionality (bin A), and the average wind speed is 8 knots.

All Alaska zip codes and coordinates that are not located within the regions assigned to the stations at Juneau and Anchorage are assigned to a “no data” region. Users entering coordinates in the “no data” region will be required to enter user-defined dispersion factors, based on local meteorological data.

D.3.12 Hawaii

The station at **Honolulu** International Airport (22521) on Oahu represents Hawaii. The wind rose shows strong directionality (bin C).

D.3.13 Puerto Rico

The station at **San Juan** represents Puerto Rico; this is the only station in Puerto Rico. The wind rose shows strong directionality (bin C), and the averge wind speed is 11 knots.

D.4 References

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Appendix D-1

Data for Meteorological Stations Considered for Inclusion in IWAIR

Table D1-1. Data for All Meteorological Stations Considered; Grouped by Region and Final Assignment

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
West Coast								
23174	**LOS ANGELES/INT'L ARPT**	**CA**	**original**	**8**	**C**	**30/52**	**20/43/37**	
23188	SAN DIEGO/LINDBERGH FIELD	CA		8	B	17/41	NA	
23234	**SAN FRANCISCO/INT'L ARPT**	**CA**	**original**	**12**	**C**	**24/52**	**17/54/29**	
24283	ARCATA/ARPT	CA		NA	A	11/24	NA	3 yrs data
24233	**SEATTLE/SEATTLE-TACOMA INT'L**	**WA**	**original**	**10**	**B**	**18/45**	**15/60/25**	
24227	OLYMPIA/ARPT	WA		8	B	17/41	NA	
24257	**REDDING/AAF**	**CA**	**new**	**NA**	**B**	**17/39**	**NA**	**4 yrs data**
24225	MEDFORD/JACKSON COUNTY ARPT	OR		6	A	11/28	24/38/38	
93193	**FRESNO/AIR TERMINAL**	**CA**	**original**	**7**	**C**	**24/45**	**29/29/42**	
23232	SACRAMENTO/EXECUTIVE ARPT	CA		9	A	12/34	24/35/40	4 yrs data
94224	**ASTORIA/CLATSOP COUNTY ARPT**	**OR**	**new**	**8**	**W**	**9/26**	**NA**	
94240	QUILLAYUTE/WSO AIRPORT	WA		7	W	8/22	NA	
24284	NORTH BEND/FAA AIRPORT	OR		NA	B	15/30	NA	3 yrs data
Desert Southwest								
23050	**ALBUQUERQUE/INT'L ARPT**	**NM**	**original**	**8**	**W**	**9/23**	**26/36/37**	
23081	GALLUP/FAA AIRPORT	NM		NA	A	11/26	NA	
23044	EL PASO/INT'L ARPT	TX		8	W	8/18	28/30/42	local mountain effects
23169	**LAS VEGAS/MCCARRAN INT'L ARPT**	**NV**	**original**	**10**	**A**	**13/33**	**27/38/35**	
23184	PRESCOTT/MUNICIPAL	AZ		NA	C	25/52	NA	
23161	DAGGETT/FAA AIRPORT	CA		NA	C	24/60	NA	3 yrs data
03160	DESERT ROCK	NV		NA	A	13/29	NA	4 yrs data
23154	ELY/YELLAND FIELD	NV		10	C	22/49	NA	
93129	CEDAR CITY/FAA AIRPORT	UT		NA	A	13/31	NA	
23183	**PHOENIX/SKY HARBOR INT'L ARPT**	**AZ**	**original**	**6**	**B**	**16/35**	**33/18/49**	
23160	TUCSON/INT'L ARPT	AZ		7	B	18/41	28/31/41	
Western Mountains								
24127	**SALT LAKE CITY/INT'L ARPT**	**UT**	**original**	**9**	**B**	**18/46**	**22/44/34**	
24027	ROCK SPRINGS/FAA AIRPORT	WY		NA	B	20/42	NA	4 yrs data

(continued)

Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
24128	**WINNEMUCCA/WSO AIRPORT**	**NV**	**original**	**8**	**A**	**10/23**	**23/39/38**	**2 yrs data only**
24121	ELKO/MUNICIPAL ARPT	NV		8	W	9/24	NA	4 yrs data
23185	RENO/CANNON INT'L ARPT	NV		10	W	9/22	NA	
24131	**BOISE/AIR TERMINAL**	**ID**	**original**	**9**	**B**	**16/37**	**21/45/34**	
24156	POCATELLO/MUNICIPAL ARPT	ID		10	B	16/44	18/51/31	
24157	**SPOKANE/INT'L ARPT**	**WA**	**new**	**9**	**A**	**13/35**	**17/55/28**	
24243	YAKIMA/AIR TERMINAL	WA		7	B	18/40	26/39/35	4 yrs data
24146	KALISPELL/GLACIER PK INT'L AP	MT		8	A	11/25	NA	
24153	MISSOULA/JOHNSON-BELL FLD	MT		7	W	9/24	NA	4 yrs data
24155	PENDLETON/MUNICIPAL ARPT	OR		NA	A	11/28	22/47/31	
24232	**SALEM/MCNARY FIELD**	**OR**	**original**	**9**	**B**	**16/31**	**16/53/31**	
24221	EUGENE/MAHLON SWEET ARPT	OR		9	A	14/30	NA	
24229	PORTLAND/INT'L ARPT	OR		7	A	11/29	15/58/26	
24230	REDMOND/FAA AIRPORT	OR		NA	A	13/29	NA	4 yrs data
Texas (excluding Gulf Coast)								
03927	**DALLAS/FORT WORTH/REGIONAL AR**	**TX**	**new**	**11**	**C**	**22/43**	**17/53/30**	
23034	SAN ANGELO/WSO AIRPORT	TX		10	C	21/42	NA	
03969	STEPHENVILLE	TX		NA	C	22/44	NA	3 yrs data
13959	WACO/MADISON-COOPER ARPT	TX		12	C	22/43	NA	
12924	**CORPUS CHRISTI/INT'L ARPT**	**TX**	**new**	**12**	**C**	**21/48**	**NA**	
12919	BROWNSVILLE/INT'L ARPT	TX		12	C	21/48	NA	
13958	**AUSTIN/MUNICIPAL ARPT**	**TX**	**new**	**8**	**B**	**17/40**	**19/48/32**	
12962	HONDO/WSMO AIRPORT	TX		NA	B	15/36	NA	3 yrs data
12921	SAN ANTONIO/WSFO	TX		9	B	16/41	NA	
23023	**MIDLAND/REGIONAL AIR TERMINAL**	**TX**	**new**	**10**	**B**	**16/37**	**NA**	
13962	ABILENE/MUNICIPAL ARPT	TX		11	B	17/45	NA	

(continued)

Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
23047	**AMARILLO/INT'L ARPT**	**TX**	**new**	**13**	**A**	**14/39**	**14/64/23**	
23009	ROSWELL/INDUSTRIAL AIR PARK	NM		9	A	12/32	NA	4 yrs data
23042	LUBBOCK/REGIONAL ARPT	TX		11	A	12/31	14/60/26	
13966	WICHITA FALLS/MUNICIPAL ARPT	TX		12	A	14/39	NA	
Gulf Coast								
03937	**LAKE CHARLES/MUNICIPAL ARPT**	**LA**	**new**	**9**	**A**	**10/25**	**19/46/36**	
12917	PORT ARTHUR/JEFFERSON COUNTY	TX		9	A	12/29	18/48/34	
12842	**TAMPA/INT'L ARPT**	**FL**	**SIS**	**7**	**A**	**10/28**	**23/36/41**	
12835	FORT MYERS/PAGE FIELD	FL		7	A	10/29	NA	
93805	TALLAHASSEE/MUNICIPAL ARPT	FL		7	A	13/29	24/32/44	
12916	**NEW ORLEANS/INT'L ARPT**	**LA**	**SIS**	**8**	**W**	**8/22**	**22/41/38**	
13894	MOBILE/WSO AIRPORT	AL		9	W	9/26	NA	
12832	APALACHICOLA/MUNICIPAL ARPT	FL		NA	W	9/21	NA	3 yrs data
13899	PENSACOLA/REGIONAL ARPT	FL		9	A	11/26	NA	
13970	BATON ROUGE/RYAN ARPT	LA		8	W	8/21	21/40/38	
12960	**HOUSTON/INTERCONTINENTAL ARPT**	**TX**	**original**	**8**	**A**	**12/29**	**18/46/36**	
12912	VICTORIA/WSO AIRPORT	TX		10	A	13/37	NA	
Southeast								
03813	**MACON/LEWIS B WILSON ARPT**	**GA**	**new**	**8**	**W**	**9/26**	**22/39/40**	
03820	AUGUSTA/BUSH FIELD	GA		7	W	6/17	NA	3 yrs data
93842	COLUMBUS/METROPOLITAN ARPT	GA		8	A	11/25	NA	
13883	COLUMBIA/METRO ARPT	SC		6[a]	A	11/27	21/40/39	
12839	**MIAMI/INT'L ARPT**	**FL**	**original**	**9**	**A**	**13/34**	**18/43/39**	
12836	KEY WEST/INT'L ARPT	FL		11	B	16/39	NA	not representative of rest of region
12843	VERO BEACH/MUNICIPAL AIRPORT	FL		NA	A	10/27	NA	3 yrs data
12844	WEST PALM BEACH/INT'L ARPT	FL		10	A	12/34	NA	

(continued)

Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
13865	**MERIDIAN/KEY FIELD**	**MS**	**SIS**	**7**	**A**	**12/28**	**22/38/40**	
03881	CENTREVILLE/WSMO	AL		NA	W	9/24	NA	
13895	MONTGOMERY/WSO ARPT	AL		7	W	7/19	NA	
13876	BIRMINGHAM/MUNICIPAL ARPT	AL		7	A	11/24	NA	
03856	HUNTSVILLE/MADISON COUNTY JET	AL		8	A	11/27	20/45/36	4 yrs data
03940	JACKSON/THOMPSON FIELD	MS		8	A	10/30	21/41/38	
93862	TUPELO	MS		NA	A	12/28	NA	
13893	MEMPHIS/INT'L ARPT	TN		7	A	11/27	20/44/36	
13874	**ATLANTA/ATLNC-HARTSFIELD INT'**	**GA**	**original**	**9**	**A**	**14/32**	**20/46/34**	
13873	ATHENS/MUNICIPAL ARPT	GA		8	A	11/25	22/41/37	
03870	GREER/GREENV'L-SPARTANBRG AP	SC		8[a]	A	13/32	21/43/36	
13880	**CHARLESTON/INT'L ARPT**	**SC**	**original**	**8**	**W**	**9/24**	**18/43/38**	
12834	DAYTONA BEACH/REGIONAL ARPT	FL		9	W	8/19	NA	4 yrs data
12816	GAINESVILLE/MUNICIPAL AIRPORT	FL		NA	W	7/18	NA	
13889	JACKSONVILLE/INT'L ARPT	FL		8	W	6/16	NA	
12815	ORLANDO/INT'L ARPT	FL		7	W	9/25	NA	
03822	SAVANNAH/MUNICIPAL ARPT	GA		8	W	7/19	20/40/40	4 yrs data
13861	WAYCROSS/WSMO	GA		NA	W	8/21	NA	4 yrs data
13957	**SHREVEPORT/REGIONAL ARPT**	**LA**	**SIS**	**9**	**A**	**12/29**	**20/43/37**	
Middle Atlantic								
03812	**ASHEVILLE/REGIONAL ARPT**	**NC**	**SIS**	**10**	**B**	**19/41**	**18/49/32**	**4 yrs data**
13741	ROANOKE/WOODRUM ARPT	VA		10	A	11/28	18/48/34	
03860	**HUNTINGTON/TRI-STATE ARPT**	**WV**	**original**	**7**	**A**	**13/31**	**20/47/34**	
93814	COVINGTON/GREATER CINCINNATI	KY		9	A	13/31	NA	
03889	JACKSON/JULIAN CARROLL ARPT	KY		NA	A	13/35	NA	
93820	LEXINGTON/BLUEGRASS FIELD	KY		9	A	13/32	18/51/32	
03872	BECKLEY/RALEIGH CO MEMORIAL A	WV		10	A	11/25	NA	
13866	CHARLESTON/KANAWHA ARPT	WV		8	A	10/26	NA	
13722	**RALEIGH/RALEIGH-DURHAM ARPT**	**NC**	**original**	**8**	**W**	**9/26**	**20/44/37**	
13881	CHARLOTTE/DOUGLAS INT'L ARPT	NC		8	W	9/25	21/42/37	
13723	GREENSBORO,HIGH POINT / WINSTO	NC		7	A	13/31	20/43/37	

(continued)

Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
13737	**NORFOLK/INT'L ARPT**	**VA**	**SIS**	**10**	**A**	**11/28**	**14/60/26**	
93729	CAPE HATTERAS/WSO	NC		11[a]	A	12/31	NA	
13748	WILMINGTON/NEW HANOVER COUNTY	NC		9[a]	A	11/26	NA	
13740	RICHMOND/R E BYRD INT'L ARPT	VA		7	A	11/28	NA	
13739	**PHILADELPHIA/INT'L ARPT**	**PA**	**original**	**9**	**A**	**11/31**	**16/54/30**	
13781	WILMINGTON/GREATER WILMINGTON	DE		9	A	12/29	15/53/31	
93721	BALTIMORE/BLT-WASHNGTN INT'L	MD		9	A	13/33	16/51/33	4 yrs data
93730	ATLANTIC CITY/AIRPORT NAFEC	NJ		10	A	10/25	14/53/32	
14734	NEWARK/INT'L ARPT	NJ		NA	A	11/26	13/61/26	
04781	ISLIP	NY		NA	A	10/25	NA	
94789	NEW YORK/J F KENNEDY INT'L AR	NY		12	A	10/25	NA	
14732	NEW YORK/LAGUARDIA ARPT	NY		12	A	11/27	NA	
13743	WASHINGTON DC/NATIONAL ARPT	VA		9	B	17/33	NA	
13877	**BRISTOL/TRI CITY AIRPORT**	**TN**	**new**	**8**	**W**	**9/21**	**22/40/38**	
13882	CHATTANOOGA/LOVELL FIELD	TN		7	W	9/23	NA	
13891	KNOXVILLE/MC GHEE TYSON ARPT	TN		7	A	12/27	21/44/35	4 yrs data
14751	**HARRISBURG/CAPITAL CITY ARPT**	**PA**	**original**	**9**	**A**	**11/29**	**17/51/33**	
14737	ALLENTOWN/BETLEHEM-EASTON ARP	PA		10	A	10/27	14/57/29	
93738	WASHINGTON DC/DULLES INT'L AR	VA		9	A	11/27	NA	4 yrs data
Northeast								
14740	**HARTFORD/BRADLEY INT'L ARPT**	**CT**	**original**	**8**	**A**	**14/27**	**15/54/31**	
14739	BOSTON/LOGAN INT'L ARPT	MA		NA	A	12/29	10/72/17	
14765	PROVIDENCE/T F GREEN STATE AR	RI		10	A	10/26	NA	
14742	**BURLINGTON/INT'L ARPT**	**VT**	**SIS**	**10**	**B**	**20/37**	**13/61/26**	**position in valley funnels winds**
14764	**PORTLAND/INT'L JETPORT**	**ME**	**original**	**9**	**A**	**11/25**	**14/55/31**	
14606	BANGOR/FAA AIRPORT	ME		NA	A	11/24	NA	
14745	CONCORD/MUNICIPAL ARPT	NH		9	A	13/28	NA	

(continued)

Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
14778	**WILLIAMSPORT-LYCOMING /COUNTY**	**PA**	**SIS**	**9**	**A**	**12/32**	**16/56/28**	
14735	ALBANY/COUNTY ARPT	NY		10	A	13/30	14/60/27	
04725	BINGHAMTON/EDWIN A LINK FIELD	NY		10	A	10/28	12/64/23	
94725	MASSENA/FAA AIRPORT	NY		NA	A	11/28	NA	
14771	SYRACUSE/HANCOCK INTʼL ARPT	NY		10	A	11/31	NA	
04751	BRADFORD/FAA AIRPORT	PA		NA	A	11/31	NA	
14777	WILKES-BARRE/WB-SCRANTON WSO	PA		8	A	12/29	15/56/29	3 yrs only
Great Lakes								
14820	**CLEVELAND/HOPKINS INT'L ARPT**	**OH**	**original**	**10**	**B**	**19/42**	**13/63/24**	
14733	BUFFALO/GREATER BUFFALO INTʼL	NY		12	A	14/37	11/67/21	
14768	ROCHESTER/ROCHESTER-MONROE CO	NY		11	B	15/37	13/64/24	
14860	ERIE/INTʼL ARPT	PA		10	B	17/38	NA	
14840	**MUSKEGON/COUNTY ARPT**	**MI**	**SIS**	**11**	**W**	**9/23**	**12/66/22**	**2 yrs data**
14848	SOUTH BEND/MICHIANA REGIONAL	IN		10	A	12/31	13/62/25	
94860	GRAND RAPIDS/KENT CO INTʼL AR	MI		10	A	11/27	13/61/26	
14847	SAULT STE MARIE/NWSO	MI		9	A	13/28	NA	4 yrs data
14850	TRAVERSE CITY/FAA AIRPORT	MI		NA	A	11/31	NA	
94846	**CHICAGO/O'HARE INT'L ARPT**	**IL**	**original**	**9**	**A**	**11/29**	**14/59/27**	
14898	GREEN BAY/AUSTIN STRAUBEL FIE	WI		10	A	10/27	14/57/29	
14839	MILWAUKEE/GENERAL MITCHELL FI	WI		11	A	11/29	NA	
94847	**DETROIT/METROPOLITAN ARPT**	**MI**	**new**	**10**	**A**	**11/27**	**12/62/26**	
94849	ALPENA/PHELPS COLLINS AP	MI		8	W	9/25	NA	4 yrs data
14822	DETROIT/CITY AIRPORT	MI		NA	W	9/25	NA	3 yrs data
14826	FLINT/BISHOP ARPT	MI		10	A	10/30	13/61/26	
14836	LANSING/CAPITAL CITY ARPT	MI		11	A	10/28	NA	
94830	TOLEDO/EXPRESS ARPT	OH		10	A	14/33	NA	3 yrs data
Central States								
13897	**NASHVILLE/METRO ARPT**	**TN**	**SIS**	**8**	**B**	**16/32**	**20/44/36**	
03816	PADUCAH/WSO AIRPORT	KY		NA	B	18/33	NA	

(continued)

Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
13963	**LITTLE ROCK/ADAMS FIELD**	**AR**	**original**	**7**	**W**	**8/23**	**NA**	**in valley between mountain groups**
13968	**TULSA/INT'L ARPT**	**OK**	**SIS**	**11**	**B**	**19/42**	**15/53/31**	
13964	FORT SMITH/MUNICIPAL ARPT	AR		6	B	16/38	NA	
13985	DODGE CITY/MUNICIPAL ARPT	KS		14	B	18/37	13/65/22	
93997	RUSSELL/FAA AIRPORT	KS		NA	B	15/35	NA	
03928	WICHITA/MID-CONTINENT ARPT	KS		12	C	21/39	13/59/27	
13995	SPRINGFIELD/REGIONAL ARPT	MO		10	B	19/42	17/51/31	
13967	OKLAHOMA CITY/WILL ROGERS WOR	OK		12	C	21/45	14/59/27	
13994	**ST LOUIS/LAMBERT INT'L ARPT**	**MO**	**new**	**10**	**A**	**10/25**	**16/54/29**	
93817	EVANSVILLE/DRESS REGIONAL ARP	IN		9	W	8/22	18/48/34	
93821	LOUISVILLE/STANDIFORD FIELD	KY		8	A	11/28	NA	
03945	COLUMBIA/REGIONAL ARPT	MO		9	B	16/34	17/52/31	4 yrs data
03966	ST LOUIS/SPIRIT OF ST LOUIS	MO		NA	A	10/23	NA	3 yrs data
14922	**MINNEAPOLIS-ST PAUL/INT'L ARP**	**MN**	**original**	**11**	**A**	**10/23**	**14/59/28**	
94822	ROCKFORD/GREATER ROCKFORD ARP	IL		9	B	17/29	13/60/28	
14913	DULUTH/INT'L ARPT	MN		11	A	11/27	12/64/25	
14918	INTERNATIONAL FALLS/INT'L ARP	MN		9	W	9/25	NA	
14925	ROCHESTER/MUNICIPAL ARPT	MN		12	A	12/28	NA	4 yrs data
14914	FARGO/HECTOR FIELD	ND		13	A	14/32	NA	
14936	HURON/REGIONAL ARPT	SD		12	A	13/31	NA	
14991	EAU CLAIRE/FAA AIRPORT	WI		NA	W	7/20	NA	
14920	LA CROSSE/MUNICIPAL ARPT	WI		NA	A	14/31	NA	4 yrs data
14837	MADISON/DANE CO REGIONAL ARPT	WI		9	B	15/28	NA	
14935	**GRAND ISLAND/ARPT**	**NE**	**original**	**12**	**B**	**15/31**	**14/57/29**	**a.k.a. Lincoln**
14943	SIOUX CITY/MUNICIPAL ARPT	IA		11	A	14/27	NA	
13984	CONCORDIA/BLOSSER MUNICIPAL A	KS		13	A	12/29	NA	
13996	TOPEKA/MUNICIPAL ARPT	KS		11	A	10/28	NA	

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Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
03947	KANSAS CITY/INT'L ARPT	MO		11	B	15/34	15/56/29	
14939	LINCOLN/MUNICIPAL ARPT	NE		10	A	13/30	NA	
14941	NORFOLK/KARL STEFAN MEM ARPT	NE		NA	A	11/27	NA	
94918	NORTH OMAHA/NWSFO ARPT	NE		NA	A	11/31	NA	
24023	NORTH PLATTE/LEE BIRD FLD	NE		11	A	11/26	NA	
14942	OMAHA/EPPLEY AIRFIELD	NE		10	B	18/38	NA	
14944	SIOUX FALLS/FOSS FIELD	SD		NA	W	9/24	NA	
23062	**DENVER/STAPLETON INT'L ARPT**	**CO**	**original**	**8**	**A**	**14/34**	**25/38/37**	**a.k.a. Boulder 94018**
93037	COLORADO SPRINGS/MUNICIPAL AR	CO		10	A	12/33	NA	
23066	GRAND JUNCTION/WALKER FIELD	CO		8	B	16/38	NA	
23065	GOODLAND/RENNER FIELD	KS		12	A	13/30	NA	
24018	CHEYENNE/MUNICIPAL ARPT	WY		13	B	16/40	13/63/24	
24011	**BISMARCK/MUNICIPAL ARPT**	**ND**	**original**	**12**	**W**	**9/24**	**14/53/33**	
24037	MILES CITY/MUNICIPAL ARPT	MT		9	A	12/27	18/50/32	3 yrs data
24013	MINOT/FAA AIRPORT	ND		NA	A	13/31	NA	3 yrs data
94014	WILLISTON/SLOULIN INT'L ARPT	ND		9	W	8/22	NA	
24025	PIERRE/FAA AIRPORT	SD		NA	A	11/27	NA	
24033	**BILLINGS/LOGAN INT'L ARPT**	**MT**	**SIS**	**10**	**C**	**24/41**	**17/60/23**	
94008	GLASGOW/INT'L ARPT	MT		11	B	16/32	NA	
24143	GREAT FALLS/INT'L ARPT	MT		13	C	26/52	NA	
24089	**CASPER/NATRONA CO INT'L ARPT**	**WY**	**original**	**14**	**C**	**26/49**	**13/61/26**	
24028	SCOTTSBLUFF/COUNTY AIRPORT	NE		11	C	22/40	NA	
24090	RAPID CITY/REGIONAL ARPT	SD		15	B	16/40	NA	
24021	LANDER/HUNT FIELD	WY		8	A	11/27	NA	4 yrs only
24029	SHERIDAN/COUNTY ARPT	WY		11	A	13/32	NA	
93815	**DAYTON/INT'L ARPT**	**OH**	**new**	**10**	**A**	**11/28**	**15/57/28**	
14827	FORT WAYNE/BAER FIELD	IN		11	A	13/27	NA	
93819	INDIANAPOLIS/INT'L ARPT	IN		9	A	11/28	16/54/30	
14895	AKRON/AKRON-CANTON REGIONAL	OH		9	A	12/31	13/60/26	
14821	COLUMBUS/PORT COLUMBUS INT'L	OH		8	W	7/21	15/53/31	

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Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
14852	YOUNGSTOWN/MUNICIPAL ARPT	OH		10	A	11/28	13/62/25	
94823	PITTSBURGH/WSCOM 2 AIRPORT	PA		10	A	10/29	13/57/29	
94910	**WATERLOO/MUNICIPAL ARPT**	**IA**	**new**	**11**	**A**	**12/27**	**NA**	
14933	DES MOINES/INT'L ARPT	IA		11	A	12/28	NA	
14940	MASON CITY/FAA AIRPORT	IA		NA	A	11/26	NA	4 yrs data
14923	MOLINE/QUAD-CITY ARPT	IL		11	A	10/25	13/58/29	
14842	PEORIA/GREATER PEORIA ARPT	IL		9	A	14/29	15/56/29	
93822	SPRINGFIELD/CAPITAL ARPT	IL		11	A	13/30	14/59/27	
Alaska								
25309	**JUNEAU/INT'L ARPT**	**AK**	**new**	**NA**	**C**	**21/43**	**NA**	**3 yrs data, large facility in the Toxics Release Inventory (TRI), unique location due to coastal mountains**
26451	**ANCHORAGE/WSMO AIRPORT**	**AK**	**new**	**8**	**A**	**12/29**	**NA**	**multiple facilities in TRI, unique wind regime due to location surrounded by mountains and water**
26409	ANCHORAGE	AK						
27502	BARROW/W POST-W ROGERS ARPT	AK						
27401	BARTER ISLAND/WSO AIRPORT	AK						
26615	BETHEL/WSO AIRPORT	AK						
26533	BETTLES/BETTLES FIELD	AK						
25624	COLD BAY/ARPT	AK						
26411	FAIRBANKS/INT'L ARPT	AK		6				
25507	HOMER/ARPT	AK						
25503	KING SALMON/ARPT	AK						
25501	KODIAK/U S C G BASE	AK		11				

(continued)

Table D1-1. (continued)

Station No.	Station Name	State	Status	Wind Speed (knots)	Wind-Rose Bin[b]	Wind Directionality[c]	Stability Class[d]	Notes
26616	KOTZEBUE/RALPH WEIN MEMORIAL	AK						
26510	MC GRATH/ARPT	AK		6				
26617	NOME/MUNICIPAL ARPT	AK						
26442	VALDEZ/WSO	AK		8				
25339	YAKUTAT/STATE ARPT	AK		8				
Hawaii								
22521	**HONOLULU/INT'L ARPT**	**HI**	**new**	**NA**	**C**	**39/66**	**NA**	
21504	HILO/GENERAL LYMAN FIELD	HI		NA	B	16/37	NA	winds affected by mountains, so not representative of entire island
22536	LIHUE/ARPT	HI		NA	C	34/69	NA	3 yrs data, adequately represented by Honolulu
Puerto Rico								
11641	**SAN JUAN/ISLA VERDE INT'L ARP**	**PR**	**new**	**11**	**C**	**22/56**	**NA**	

[a] International Station Meteorological Climate Summary (ISMCS) value unrealistically low; estimated from wind-rose data.

[b] Key to wind-rose bins:

W: Weakly directional, one-directional wind < 10%
A: Mildly directional, one-directional wind 10–14%
B: Moderately directional, one-directional wind 15–20%
C: Strongly directional, one-directional wind > 20%

[c] % in 1 direction/% in 3 directions

[d] % Unstable/% Neutral/% Stable