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Industrial Waste Air Model (IWAIR) User's Guide

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Office of Solid Waste
U.S. Environmental Protection Agency
Washington, DC 20460

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Acronyms and Abbreviations

ATSDR	Agency for Toxic Substances and Disease Registry
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BOD	Biological oxygen demand
CAA	Clean Air Act
CalEPA	California Environmental Protection Agency
CAS	Chemical Abstract Service
COD	Chemical oxygen demand
CSF	Cancer slope factor
DCOM	Distributed component model
EPA	Environmental Protection Agency
HEAST	Health Effects Assessment Summary Tables
HQ	Hazard quotient
HSDB	Hazardous Substances Databank
IRIS	Integrated Risk Information System
ISCST3	Industrial Source Complex, Short-Term Model, Version 3
IWAIR	Industrial Waste Air Model
IWEM	Industrial Waste Management Evaluation Model
MLVSS	Mixed-liquor volatile suspended solids
MLSS	Mixed-liquor suspended solids
MRL	Minimum risk level
PAH	Polycyclic Aromatic Hydrocarbons
RfC	Reference concentration
REL	Reference exposure level
SCDM	Superfund Chemical Data Matrix
TOC	Total organic carbon
TSS	Total suspended solids
WMU	Waste management unit

1.0 Introduction

This document describes how to use the Industrial Waste Air Model (IWAIR). A companion document, the *Industrial Waste Air Model Technical Background Document*, provides technical background information. This section of the User's Guide provides an overview of IWAIR, its purpose, operation, and application; describes the three major components of the system—the emissions, dispersion, and results models; and provides an overview of the remainder of the User's Guide.

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 User's Guide to accompany the *Guide* to evaluate 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. The *IWAIR Technical Background Document* contains a more detailed explanation of each.

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. You can also add chemical properties to model additional chemical constituents. 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 you to provide the required waste- and unit-specific data. Once you have entered these data, the model calculates and displays chemical-specific emission rates. If you decide not to develop or use the CHEMDAT8 rates, you can enter your own site-specific emission rates (g/m^2-s).

Table 1-1. Constituents Included in IWAIR

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

*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 contaminants 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 µg/m^2- s) to obtain a dispersion factor, which is measured in µg/m^3 per µg/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 you 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 the unit you specify, IWAIR selects an appropriate dispersion factor from the default dispersion factors in the model.   If you specify a unit surface area or height that falls between two of the sizes already modeled, an interpolation method will estimate dispersion in relation to the modeled unit sizes.

Alternatively, you 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 allowable 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, 2001, 1997b); for a complete list of sources, see Appendix B, Section B.2.2.3. IWAIR uses these data to estimate risk or hazard quotients (HQs) or to estimate allowable waste concentrations. You may override the IWAIR health benchmarks with your own values.

1.3   Overview of Approach to Estimating Risk or Allowable Concentration

Figure 1-1 provides an overview of the stepwise approach you will follow to estimate risk or allowable waste concentrations with IWAIR. The seven steps of the estimation process are shown down the right side of the figure, and the user input requirements are specified to the left of each step. As you provide input data, the program proceeds to the next step. Each step of the estimation process is summarized below (later sections of this User's Guide provide more detailed instructions):

1.   **Select Calculation Method.** To begin, select one of two calculation methods—risk or allowable concentration. Use the risk calculation to arrive at chemical-specific and cumulative risk estimates; you must know the concentrations of constituents in the waste to use this option. Use the allowable concentration calculation method to estimate waste concentrations that may be managed protectively in new units.

2.   **Identify Waste Management Unit.** Four WMU types can be modeled: surface impoundments, land application units, active landfills, and waste piles. For each WMU, you will be asked to specify some design and operating parameters, such as waste quantity, surface area, and depth for surface impoundments and landfills; height for waste piles; and tilling depth for land application units. The amount of unit-specific data needed as input will vary depending on whether you elect to have IWAIR calculate CHEMDAT8 emission rates or enter your own. IWAIR provides default values for several of the operating parameters that you may use, if appropriate.

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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.
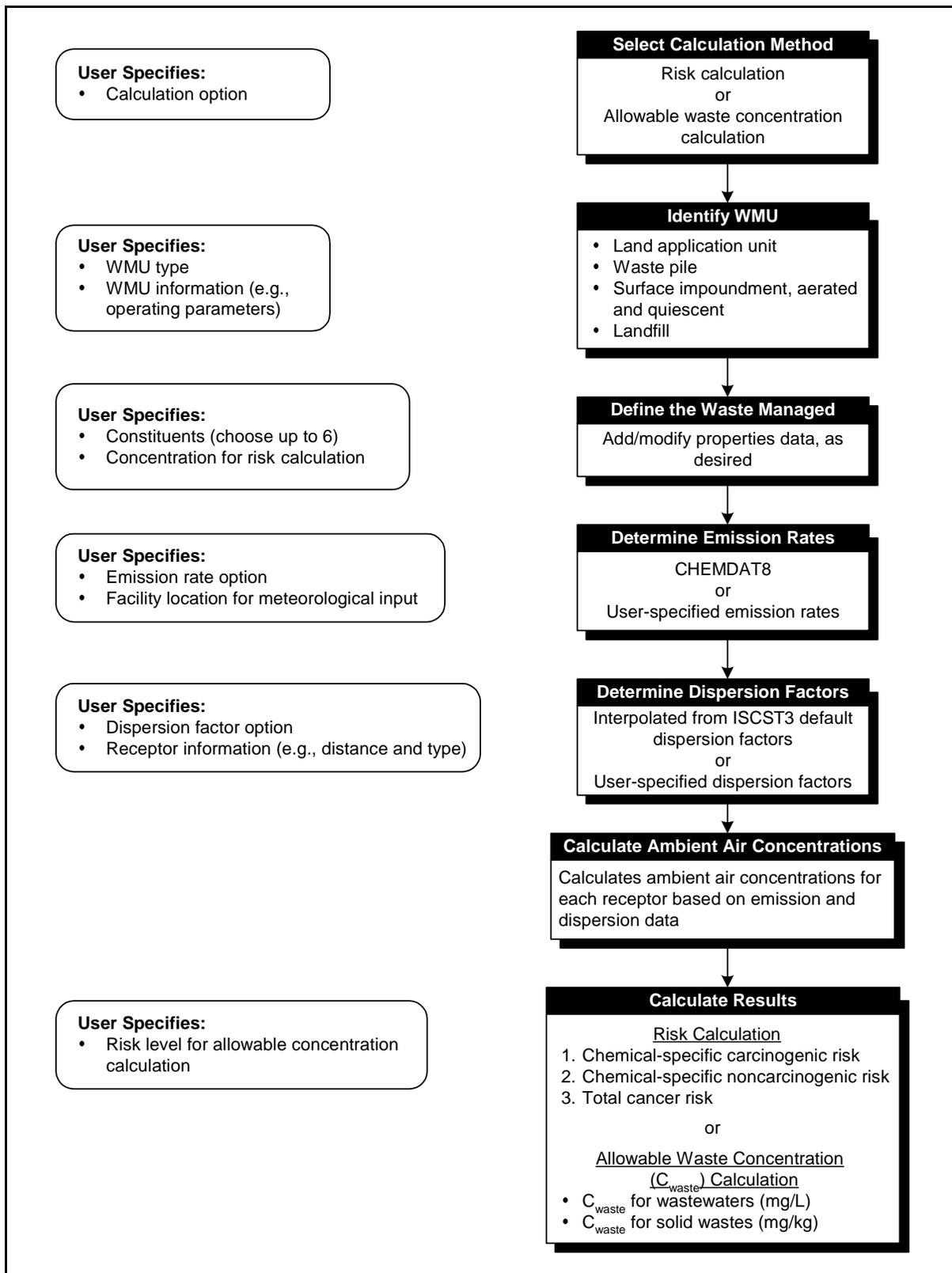
Figure 1-1. **IWAIR approach for estimating risk or allowable waste concentrations.**
This figure shows the steps in the tool to assist you in developing risk or allowable waste concentration estimates.

3.   **Define the Waste Managed.** If you choose to calculate chemical-specific risk estimates, specify constituents and concentrations in the waste. If you choose to calculate allowable waste concentrations, then specify only constituents of concern (no concentrations). You can also add chemicals or modify chemical property data in this step.

4.   **Determine Emission Rates.** You can elect to develop CHEMDAT8 emission rates or provide your own site-specific emission rates for use in calculations. IWAIR will also ask for facility location information to link the facility's location to one of the 60 IWAIR meteorological stations. Data from the meteorological stations provide wind speed and temperature information needed to develop emission estimates. In some circumstances, you may already have emissions information from monitoring or from a previous modeling exercise. As an alternative to using the CHEMDAT8 rates, you may provide your own site-specific emission rates developed with a different model or based on emission measurements.

5.   **Determine Dispersion Factors.** You can provide site-specific dispersion factors ($\mu g/m^3$ per $\mu g/m^2$-s) or have the model develop dispersion factors based on WMU information that you specify and the IWAIR default dispersion data. These dispersion factors are specific to the meteorological station selected. Because a number of assumptions were made in developing the IWAIR default dispersion data (for example, flat terrain was assumed), you may elect to provide site-specific dispersion factors that can be developed by conducting independent modeling with ISCST3 or with a different model. Whether you use IWAIR or provide dispersion factors from another source, specify distance to the receptor from the edge of the WMU, and the receptor type (i.e., resident or worker). These data are used to define points of exposure and exposure duration.

6.   **Calculate Ambient Air Concentration.** For each receptor, the model combines emission rates and dispersion data to estimate ambient air concentrations for up to six waste constituents you have specified.

7.   **Calculate Results.** The model calculates results by combining estimated ambient air concentrations at a specified exposure point with receptor exposure factors and toxicity benchmarks. Presentation of results depends on whether you chose to calculate risk or the allowable waste concentration.

        Risk Calculation: Results are estimates of cancer and noncancer risks from inhalation exposure to volatilized constituents in the waste. If risks are too high, your options are to (1) implement unit controls to reduce volatile air emissions; (2) implement pollution prevention programs or treatment measures to reduce volatile compound concentrations before the waste enters the unit; or (3) conduct a full, site-specific risk assessment to more precisely characterize risks from the unit.

Allowable Concentration Calculation: Results are estimates of constituent concentrations in waste that can be protectively managed in the unit so as not to exceed a defined risk level (e.g., 1E–6 or an HQ of 1) for specified receptors. This information should be used to determine preferred characteristics for wastes entering the unit. There are several options if it appears that planned waste concentrations may be too high: (1) implement pollution prevention programs or treatment measures to reduce volatile compound concentrations in the waste; (2) modify waste management practices to better control volatile compounds (for example, use closed tanks rather than surface impoundments); or (3) conduct a full site-specific risk assessment to more precisely characterize risks from the unit.

1.4   Capabilities and Appropriate Application of the Model

In many cases, IWAIR will provide a reasonable alternative to conducting a full-scale site-specific risk analysis to determine if a WMU poses unacceptable risk to human health. However, because the model can accommodate only a limited amount of site-specific information, it is important to understand its capabilities and recognize situations when it may be most appropriate to use in a specific way, when it may not be appropriate to use at all, or when another model would be a better choice.

Capabilities

■   The model provides a reasonable, protective representation of volatile compound inhalation risks associated with WMUs.

■   The model is easy to use and requires a minimal amount of data and expertise.

■   The model is flexible and provides features to meet a variety of user needs.

■   You can enter emission and/or dispersion factors derived from another model (perhaps to avoid some of the limitations below) and still use IWAIR to conduct a risk evaluation.

■   The model can calculate risk from specified waste concentrations or allowable concentrations based on a target risk or HQ.

■   You can modify health benchmarks and target risk level, when appropriate and in consultation with other stakeholders.

■   You can add additional volatile organic chemicals to the 95 chemicals included with IWAIR.

Appropriate Applications

■　*Release Mechanisms and Exposure Routes*. The model considers exposures from breathing ambient air. It does not address potential risks attributable to particulate releases, nor does it address risks associated with indirect routes of exposure (i.e, noninhalation routes of exposure). Appendix A discusses the potential for indirect risks. Additionally, in the absence of user-specified emission rates, volatile emission estimates are developed with CHEMDAT8 based on unit- and waste-specific data. The CHEMDAT8 model was developed to address only volatile emissions from WMUs. The model does not account for all competing removal mechanisms; specifically, runoff, erosion, and leaching are not modeled. In so much as these competing processes actually occur, the model would tend to slightly overestimate the volatile emissions.

■　*Waste Management Practices*. Although you specify a number of unit-specific parameters that have a significant impact on the inhalation pathway (e.g., size, type, and location of WMU, which is important in identifying meteorological conditions), the model cannot accommodate information concerning control technologies, such as covers, that might influence the degree of volatilization (e.g., whether a waste pile is covered immediately after application of new waste). In this case, it may be necessary to generate site-specific emission rates and enter those into IWAIR. In addition, IWAIR cannot be used to estimate emissions from land application units using spray techniques for waste application; the emissions model component for land application units is only applicable to tilled land application units; again, in this case, it will be necessary to generate site-specific emission rates and enter them into IWAIR. IWAIR also cannot be used to model tanks; the surface impoundment component should *not* be used to model tanks, as most tanks have some height above the ground, and the dispersion factors used in IWAIR for surface impoundments are all for a ground-level source.

■　*Terrain and Meteorological Conditions*. If a facility is located in an area of intermediate or complex terrain or with unusual meteorological conditions, it may be necessary to either generate site-specific air dispersion modeling results for the site and enter those results into the program, or use a site-specific risk modeling approach other than IWAIR. The model will inform you which of the 60 meteorological stations is used for a facility. If the local meteorological conditions are very different from the meteorological conditions at the site chosen by the model, it would be more accurate to choose a different model or enter a different location that results in the selection of a more appropriate meteorological station.

The terrain type surrounding a facility can influence air dispersion modeling results and, ultimately, risk estimates. In performing air dispersion modeling to develop the IWAIR default dispersion factors, it was assumed that the facility was located in an area of flat terrain. The *Guideline on Air Quality Models* (U.S. EPA,

1993) can assist you in determining whether a facility is in an area of simple, intermediate, or complex terrain.

■   *Receptor Type and Location*. IWAIR has predetermined worker and resident receptors and predetermined exposure factors. The program cannot be used to characterize risk for other possible exposure scenarios. The model contains dispersion factors for six receptor locations. IWAIR cannot evaluate other receptor locations unless you enter your own dispersion factors.

1.5   About This User's Guide

The focus of this User's Guide is to help you understand how to use IWAIR. The remainder of this document is organized into five sections and three appendices:

■   Section 2, *Getting Started*, identifies system requirements for running IWAIR, provides stepwise guidance for installing the program, and introduces you to program screens and navigational tools (e.g., tabs, menus, and buttons). This section covers saving and retrieving data and printing reports. It also includes a troubleshooting guide.

■   Section 3, *Selecting Calculation Method, WMU Type, and Modeling Pathway*, assists you in selecting the appropriate calculation method (i.e., calculation of risk estimates or calculation of allowable waste concentration), WMU type, and modeling pathway. This section describes the types of units IWAIR addresses.

With both risk and allowable concentration calculations, you can select from the following four modeling pathways:

—   Pathway 1: Using CHEMDAT8 emission rates and ISCST3 default dispersion factors

—   Pathway 2: Using CHEMDAT8 emission rates and user-specified dispersion factors

—   Pathway 3: Using user-specified emission rates and ISCST3 default dispersion factors

—   Pathway 4: Using user-specified emission rates and dispersion factors.

Depending on the calculation method, you will be directed to follow the detailed guidance provided in Section 4 for completing a risk calculation or in Section 5 for completing an allowable concentration calculation. Each of these sections provides pathway-specific guidance, as needed.

■ Section 4, *Completing Risk/Hazard Quotient Calculations*, provides detailed guidance to develop risk estimates for wastes of known chemical concentration(s). Follow the screen-by-screen guidance to arrive at risk estimates.

■ Section 5, *Completing Allowable Waste Concentration Calculations*, provides detailed guidance to predict allowable waste levels based on a user-specified risk level. Again, follow the screen-by-screen guidance to complete an allowable concentration calculation.

■ Section 6, *Example Calculations*, provides a detailed example of how the program calculates air concentration and inhalation risk or allowable waste concentrations. It does not cover emission or dispersion calculations.

■ Appendix A, *Considering Risks from Indirect Pathways*, describes the types of pathways by which an individual may be exposed to a contaminant, explains which pathways are accounted for in IWAIR, and discusses exposures unaccounted for in IWAIR.

■ Appendix B, *Parameter Guidance*, describes and provides additional information on all parameter values needed to run IWAIR.

■ Appendix C, *Physical-Chemical Property Values*, provides molecular weights and densities for IWAIR constituents.

A separate document, *Industrial Waste Air Model Technical Background Document*, provides detailed discussions on the CHEMDAT8 emission model, the ISCST3 model and modeling efforts conducted to develop the IWAIR default dispersion factors, and health benchmarks included in IWAIR.

2.0 Getting Started

2.1 Hardware and Software Requirements

The IWAIR tool consists of a 32-bit Visual Basic application and an Access 2000 database. It is designed to run on an IBM-compatible computer with Windows 95, 98, NT4, or 2000. The recommended hardware configuration to run IWAIR includes at least 32 MB of RAM (preferably 64 MB), a Pentium 120 MHz CPU processor (preferably Pentium II or above), and 30 MB of free hard-drive space (preferably 50 MB).

The most recent version of the appropriate Windows operating system must be installed on the computer. As of the publication of this document, the most recent versions are Windows 95B, Windows 98 SE, Windows NT4 with Service Pack 6a, and Windows 2000 with Service Pack 2. Service packs are available from the Microsoft Web site (www.microsoft.com). Microsoft recommends that these service packs be re-installed after any software is installed or uninstalled. If the computer is running Windows 95B or Windows 98SE, the distributed component model (DCOM) software also must be installed. This software is available from the Microsoft Web site (www.microsoft.com/com/dcom/dcom95/dcom1_3.asp for Windows 95, www.microsoft.com/com/dcom/dcom98/dcom1_3.asp for Windows 98). The program does not require any additional software when running under Windows NT or Windows 2000 (other than the latest service packs mentioned above).

2.2 Installing and Uninstalling the Program

You receive the IWAIR computer program on the Guidance CD-ROM. The installation consists of three files: setup.exe, setup.lst, and iwair.cab. Depending on the security settings of your operating system, this software may need to be installed and uninstalled by someone with administrator privileges. Instructions for installing and uninstalling the program are provided below. Any updated instructions are located on the Guidance CD-ROM in readme.txt.

Installing

1.   Close all applications, such as word processors and e-mail programs. Close or disable virus protection software.[1]

2.   Insert the CD-ROM into your CD-ROM drive.

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[1] Many virus protection programs interfere with or slow down the installation of software. You should scan any software files for viruses before installing.

3.   Open MY COMPUTER.

4.   Select the CD-ROM drive.

5.   Double-click on setup.exe.

6.   You will see some files being copied to your hard drive. The WELCOME TO THE IWAIR INSTALLATION PROGRAM screen then appears. If all your other applications were closed (Step 1), then click |OK|.

7.   The next screen is IWAIR SETUP. This screen displays the default location for the IWAIR files to be installed. If you want to change the location, click the |CHANGE DIRECTORY| button and specify a different directory. Otherwise, just click the large button (shows a computer with an open box in front of it).

8.   The next screen is IWAIR - CHOOSE PROGRAM GROUP. The default is to create a new program group named "IWAIR." You can change the program group if you prefer a different one. Press the |CONTINUE| button to install the program.

9.   The next screen is IWAIR SETUP. The progress bar shows the progress of the files that are being installed to your hard drive.

10.   The final screen displays the message, "IWAIR setup was completed successfully." Click on the |OK| button.

11.   If you are using Windows 2000 or Windows NT4, you should install the latest Service Pack.

12.   Restart your computer.

OR

1.   Close all applications, such as word processors and e-mail programs. Close or disable virus protection software.[2]

2.   Insert the CD-ROM into your CD-ROM drive.

3.   Click on the Windows |START| button and select RUN.

4.   Type "D:\SETUP" or, as appropriate, replace "D:" in this command with the correct drive designation for your CD-ROM drive.

5.   Proceed with Step 6 above.

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[2] Many virus protection programs interfere with or slow down the installation of software. You should scan any software files for viruses before installing.

Uninstalling

1. Click on the Windows |Start| button.

2. Select Settings, and then Control Panel.

3. Select Add/Remove Programs.

4. Select IWAIR and then Change/Remove. When asked "Are you sure you want to completely remove IWAIR and all of its components," select the |Yes| button.

5. If you are using Windows 2000 or Windows NT4, you should re-install your latest Service Pack and restart your computer.

2.3 Running IWAIR

To execute the program, press the Windows |Start| button. Select Programs, IWAIR, IWAIR. (If you selected a different name for the group during the installation process, you must select Programs, then the group name you selected, then IWAIR.)

Begin working in IWAIR by clicking on the |Start| button of the program title screen. IWAIR can model one unit (choice of four unit types: surface impoundment, land application unit, active landfill, and waste pile), up to six chemicals of concern, and up to five different receptors during a single simulation. Once IWAIR's |Start| button is selected, the program automatically opens the Method, Met. Station, WMU screen.

2.4 Navigating in IWAIR

The following tools facilitate interaction with the IWAIR program:

- Tabs
- Menus
- Command buttons
- Message prompts.

Each of these tools is explained in more detail in this section. Although this guide assumes the use of a mouse to navigate through the screens and features, you may also navigate using key strokes (see the "Navigation without the Mouse" explanation at the end of this section).

Tabs

Tabs facilitate navigation between the different screens in the program. Clicking a tab opens the screen associated with it. You can enter information and edit data on an open screen. There are six tabs, one for each of the following screens:

- Method, Met. Station, WMU

■   WASTES MANAGED
■   WMU DATA FOR CHEMDAT8
■   EMISSION RATES
■   DISPERSION FACTORS
■   RESULTS.

Table 2-1 describes each of these tabs and how each screen associated with a tab assists you in providing the program with the inputs needed to perform the calculations. The program automatically opens the next screen after the required information is entered into the data fields and the |DONE| command button is clicked.

At any time in the program, you can return to a screen that has already been visited by clicking the tab associated with the screen. You can view information entered on the screen and can also change any information entered on a previously visited screen. Changing data on a previously visited screen has no effect on screens before the changed screen, but does affect screens following the changed screen. Whenever you change data on a previously visited screen, you will have to proceed through the following screens in order (even if the data on them have been retained) to return to where you were before you went back and made the change; this is so that calculated values will be recalculated with the new data. For example, if you were on the EMISSION RATES screen and returned to the METHOD, MET STATION, WMU screen to change meteorological stations, you would still have to proceed through the WASTES MANAGED and WMU DATA FOR CHEMDAT8 screens, clicking on |DONE|, to return to the EMISSION RATES screen. If you enter data on a screen, return to a previous screen without clicking |DONE|, and make changes to the previous screen, the new data you entered will be lost, and you will need to re-enter them when you return to the screen you were working on. These data will not be lost if you do not change anything on the previous screen and if you return to the subsequent screen using |TAB| rather than |DONE|.

Menus

As shown in Figure 2-1, a menu is also provided with IWAIR that allows you to perform tasks such as starting a new run, loading data from a previous run, saving data from the current run, printing reports, and exiting the program. The menu options are covered in detail in Section 2.5.

Command Buttons

In addition to tabs and menus, one or more command buttons are provided on each screen that initiate an action by the program. For instance, click the |DONE| command button after you have entered all data on a screen to calculate and proceed to the next screen.

Message Prompts

The program uses message boxes to communicate important information and to confirm actions before executing a command. For instance, an error message is shown when incorrect, invalid, or incomplete information is entered.

Table 2-1. IWAIR Tabs and Associated Screens

Tab	Description of Screen Associated with Tab
Method, Met. Station, WMU	■ Select calculation method (i.e., risk calculation or allowable waste concentration calculation). ■ Select WMU type. The WMU choices include surface impoundment, land application unit, active landfill, and waste pile. ■ Enter zip code or latitude and longitude of site to allow the program to select the most representative meteorological station from the program's 60 stations. ■ Select whether estimations will be made based on program-generated CHEMDAT8 emission rates and default ISCST3 dispersion factors, user-specified emission rates and default dispersion factors, or a combination of both IWAIR-generated and user-specified estimates.
Wastes Managed	■ Identify up to six chemicals that are present in the waste managed in the WMU of concern. You can choose to view chemicals by CAS number or by chemical name (95 chemicals are included in the database that is installed with the IWAIR program). ■ Add or modify chemical data. ■ If you selected to perform a risk calculation and to use CHEMDAT8, you must provide the concentration of each chemical in the WMU.
WMU Data for CHEMDAT8	This tab is enabled and its associated screens are opened if you elected to have IWAIR develop chemical-specific emission rates using EPA's CHEMDAT8 model. You must provide a variety of site-specific data (e.g., unit dimensions and waste loading information). Default values are provided adjacent to the data box for several of the input parameters.
Emission Rates	View and confirm CHEMDAT8 emission rates or enter user-specified emission rates. Enter source and justification for user-specified emission rates on this screen.
Dispersion Factors	Calculate dispersion factors or provide user-specified dispersion factors. Identify up to five receptors (i.e., potentially exposed individuals). For each receptor, specify the distance to the receptor and the receptor type (i.e., resident or worker). The program calculates the dispersion factors based on distance to the receptor, as well as WMU area and meteorological station. Alternatively, you may enter your own dispersion factors. Enter source and justification for the user-supplied dispersion factors on this screen.
Results	Two different results screens are associated with this tab, one for risk calculation and one for allowable concentration calculation. You can ■ Select the receptor for which the calculation is to be performed. ■ View the chemicals of concern that were selected under the WASTES MANAGED screen. ■ View input data determined in the previous screen (distance from the unit to the receptor, receptor type, and dispersion factors). IWAIR uses these data in the risk or waste concentration calculations. ■ View and override program-supplied health benchmarks. If you choose to override these data, you should also provide the source and justification for the user-supplied benchmarks. ■ In the risk calculation mode, click the |CALCULATE| button to generate and display risk estimates for carcinogens, and HQs for noncarcinogens. ■ In the allowable concentration mode, select target risk level (e.g., 1E–5, 1E–6) and/or an HQ (e.g., 0.5, 1) to serve as the starting point for the allowable concentration calculation for each chemical. Then click the |CALCULATE| button to generate and display the allowable waste concentrations for each chemical of concern.
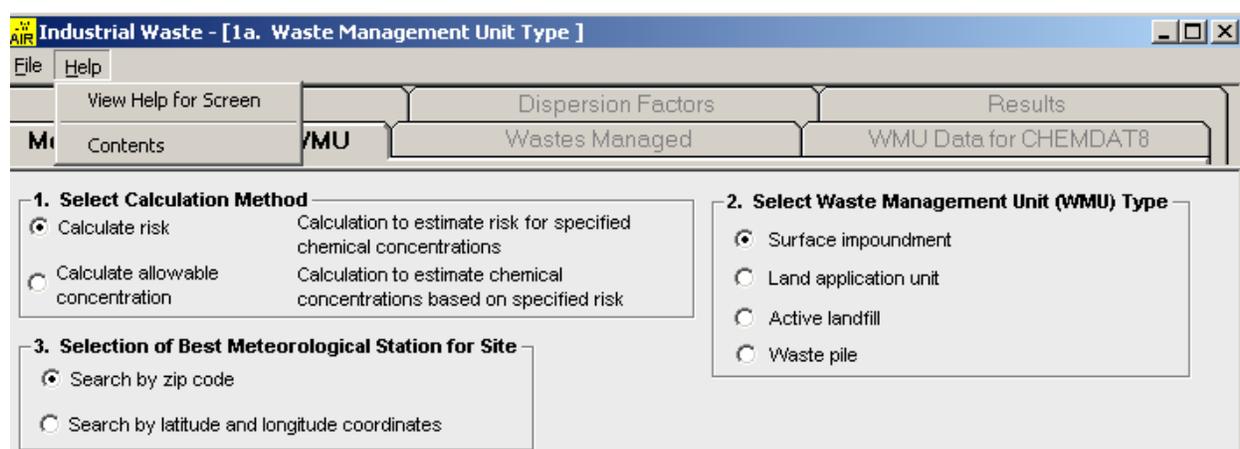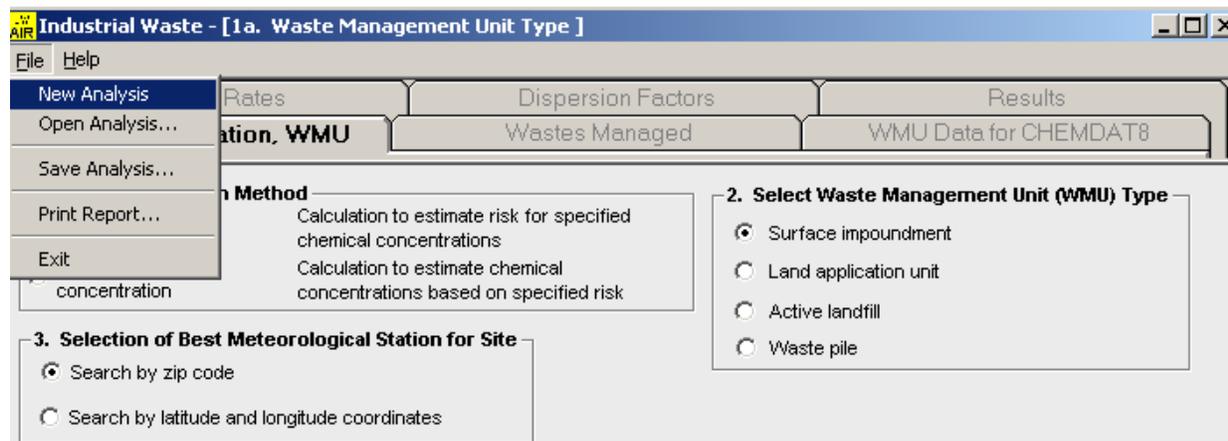
Figure 2-1. Menu bar in the IWAIR program.

Navigation without the Mouse

Although you typically navigate IWAIR's graphical user interface using a mouse or other pointing device, the keyboard may be used to make selections and proceed through the screens. The |TAB| key moves the cursor from one input box or control (e.g., command button, option button, drop-down list) to the next. The |BACK-TAB| key (|SHIFT| + |TAB|) moves the cursor in the reverse order on the current screen. When the cursor is on a command button, press the |ENTER| key to "click" the button. Option buttons always appear in a set of at least two options; when the cursor is on any option button, press a cursor arrow key to mark a different option button as being selected and then use the |TAB| key to move out of that option button group. A drop-down box displays one choice of several; when the cursor is on the box, use the up-arrow and down-arrow keys to display the desired choice. At any time, you can press the |ALT| key to access the FILE and HELP menus at the top of the window.

2.5 Menus

As shown in Figure 2-1, the IWAIR menu bar consists of two choices: FILE and HELP. HELP is described in Section 2.6. The FILE menu options are described in this section.

The FILE menu provides the following features: start a new analysis, save and re-open an analysis, print reports, and exit IWAIR. Each of these features is discussed below.

2.5.1 Start a New Analysis

During an IWAIR session, you may want to discard all data and start over with a new analysis, so as to model a different WMU, different chemicals, or a different scenario. The NEW ANALYSIS option lets you clear the current analysis without exiting and restarting IWAIR. It is not necessary to select NEW ANALYSIS when you start IWAIR.

NEW ANALYSIS clears all entered data and resets IWAIR to initial defaults, with one exception: the facility information for printed report headers is retained when you select NEW ANALYSIS. This information may be edited when you print a report.

To start a new analysis, select FILE, NEW ANALYSIS. You will be prompted with "Discard all changes and restart calculations?"

- ■ Click on |YES| to start a new analysis.
- ■ Click on |NO| to return to your existing analysis.

2.5.2 Save and Re-Open an Analysis

You can save an analysis and re-open it later using the FILE, SAVE ANALYSIS and FILE, OPEN ANALYSIS features. IWAIR saves all user-entered data, as well as calculated and user-override emission rates and dispersion factors, and current facility information for report headers (if any has been entered during the session). It does not save calculated values from the RESULTS screen (air concentrations, risks, HQs, and allowable concentrations); these must be recalculated from the RESULTS screen.

IWAIR does not save chemical properties data or user-defined health benchmarks with a saved analysis, but uses the current chemical properties and user-defined health benchmark values in the chemical database at the time an analysis is re-opened. Therefore, the results may change if you have changed the chemical properties or user-defined health benchmarks of any chemical in the saved analysis since you saved the analysis. Changes to user-defined health benchmarks will be reflected when you recalculate the results, as you are required to do. Changes to other chemical properties that affect emission rates will not be reflected unless you recalculate emission rates by clicking |DONE| on the WMU DATA FOR CHEMDAT8 screen. In addition, the chemical database must contain entries for all chemicals in the saved analysis, or the analysis will not reload. This would only occur if you had saved an analysis containing user-defined chemicals, then subsequently deleted any of those chemicals from the chemical database, or if you tried to open a file saved by another user containing user-defined chemicals specific to his or her

chemical database and not found in yours. See Appendix A, Sections A.4.2 and A.5.2, for more details on adding or modifying chemical data.

IWAIR can only reload analyses saved from the current version of IWAIR.

You can save an analysis only from the RESULTS screen. You can open a saved analysis from any screen, but once the analysis is reloaded, you will be returned to the METHOD, MET. STATION, WMU screen. You should then move through the tabs in sequence by clicking |DONE|, even if you have not changed anything. This will recalculate your analysis (though you will have to re-enter any user-override emission rates or dispersion factors) and ensure the accuracy of the results. If you wish to view saved user-override emission rates or dispersion factors before you do this, you can use the tabs to move directly to other screens without clicking |DONE| on each screen. IWAIR was not designed to do calculations other than as part of a complete sequence through the screens. Therefore, although you may be able to view results by recalculating only on the RESULTS screen (without clicking through the previous screens using the |DONE| buttons), doing so may result in model errors.

If an analysis fails to reload (either because it is missing a chemical or was saved from a previous version of IWAIR), you will be returned to the METHOD, MET. STATION, WMU tab with all values reset, as if you had selected NEW ANALYSIS.

To save the current analysis, navigate to the RESULTS screen, and select FILE, SAVE ANALYSIS. This opens a SAVE AS dialog box.

- ■ Enter the desired file name in the FILE NAME box and click on |SAVE| to save the analysis to a new file.

- ■ Click on an existing file name and click on |SAVE| to save the analysis over an existing file. You will be warned that the file already exists and asked if you want to replace it.

    – Click on |YES| to replace the existing file.
    – Click on |NO| to return to the SAVE AS box and change the file name.

- ■ Click on |CANCEL| to abort saving the analysis; you will be returned to the current analysis.

To reload a previously saved analysis, select FILE, OPEN ANALYSIS. You will be prompted with "You will lose unsaved data. Continue?"

- ■ Click on |YES| to open a FILE OPEN dialog box; from this box, select the desired file by clicking on it.

    – Click on |OPEN| or double-click on the file name to open it. You may see the IWAIR screens flashing on your screen as IWAIR reloads your data.

–   Click on |CANCEL| to abort opening a saved analysis and return to your existing analysis.

■   Click on |NO| to return to your existing analysis.

2.5.3   Print Reports

You can print a report containing the data and results from the current analysis using the PRINT REPORT function. Reports are divided into five sections:

■   Part 1a: General Parameters. This section includes facility information; information on the meteorological station, WMU type, and computation options used; and WMU characteristics. The facility information for the header includes facility name, facility type, address, date of sample analysis, name of user, and additional information; you will be prompted to enter or edit this, if you desire, before printing the report.

■   Part 1b: Chemical Properties. This section includes the CAS number and all chemical properties except health benchmarks for each chemical in the analysis.

■   Part 2: Health Benchmark Information. This section includes the IWAIR and user-defined health benchmarks and references for each chemical in the analysis.

■   Part 3: Receptors and Dispersion Factors. This section includes the receptor data, IWAIR and user-override dispersion factors, and exposure duration for each receptor.

■   Part 4: Final Results. This section includes the waste concentration, IWAIR and user-override emission rates, and the risk and HQ for each chemical and receptor.

The exact data in each report vary somewhat depending on the type of WMU and the type of analysis. The reports are 5 to 8 pages long, depending on how many chemicals and receptors you have selected. The report only prints in full and to the default printer. You cannot print selected pages or sections, nor can you print reports to a file.

The facility information you enter for the report header is retained until you exit IWAIR; each time you print a report, you have the option to edit it. This information is saved in a saved analysis; therefore, if you open a saved analysis, the saved information will overwrite the current information.

You can print a report only once you have completed an analysis (i.e., you have reached the RESULTS screen). Once you have done this, you can print a report from any screen (i.e., if you have gone back to look at a previous screen); however, printing a report always returns you to the RESULTS screen, regardless of where you printed from.

To print a report, select FILE, PRINT REPORT. You will be prompted with "Edit facility information for report header?"

- ■ Click on |YES| to enter or edit facility information to be printed in the report header.

- ■ Click on |NO| to retain the current facility information for the report header (or to leave it blank if you have not entered facility information during the current IWAIR session).

- ■ Click on |CANCEL| to abort printing.

Once you have edited (or chosen not to edit) the facility information for the report header, you will be prompted to "Click OK to route the reports to local printer." The report cannot be aborted at this point. Reports are printed to the default printer defined on your system.

2.5.4 Exit IWAIR

To exit IWAIR, select FILE, EXIT, or click on the X in the upper right corner of the screen. IWAIR will ask "Do you want to exit IWAIR?"

- ■ Click on |YES| to exit IWAIR. Any unsaved data will be lost.
- ■ Click on |NO| to return to your analysis.

2.6 Online Help

The program provides online help that can be accessed from any screen, either by pressing the |F1| key or by selecting the HELP menu. The |F1| key and the VIEW HELP FOR SCREEN selection on the HELP menu display the information corresponding to Sections 4 and 5 of this document that is pertinent to the currently displayed program screen. A hyperlink at the top of the HELP screen brings up the parameter guidance help corresponding to Appendix B of this document. In some cases, this may be preceded by hyperlinks for risk versus allowable concentration calculations. The CONTENTS selection on the HELP menu displays the table of contents for the online help.

2.7 Troubleshooting

Table 2-2 lists some common problems you may encounter and how to solve them.

Table 2-2. Troubleshooting Common Problems in IWAIR

Problem Category	Description of Problem	Solutions
Installation	Windows 95B and NT4 SP6a ask to restart computer to update Windows system files.	Click on |YES|. After restart is complete, double-click on setup.exe again to finish the install. Windows system files updated will be in the system folders in the Windows directory, and the old ones will be renamed "filename.dll.old".

(continued)

Table 2-2. (continued)

Problem Category	Description of Problem	Solutions
	Windows NT4 SP6a, error occurs installing CRVIEWER.DLL.	Choose |IGNORE|, and the program will install completely. This does not in any way affect the functionality of the software.
Display	The gray screens in the program appear "blotched" and are not uniformly gray.	Changing your monitor's display settings will fix this problem. Under the CONTROL PANEL, DISPLAY, SETTINGS tab, make sure that the Color Pallette is set for High Color (16 bit) or True Color (32 bit) or higher. Note that these options may not be available on all machines, depending on the type of monitor, graphics card, and video driver used.
	Screens are not displayed correctly, display is not optimized.	The IWAIR program display is optimized for screen resolutions of 800×600 pixels. At lower resolutions, not all of the IWAIR screens are displayed. The screens appear smaller at higher resolutions.
Printing	Text is cut off at the edges.	Due to the large quantity of data to be displayed on the reports, the margins selected for the reports are only 0.25 inches. Text may be cut off if the printer has a larger unprintable area. Printing functions were tested on an HP Laser Jet 4/4M and higher-grade printers.
	Override values print in reports even though no override values were entered.	If no override values are entered, IWAIR may repeat the calculated emission rates or dispersion factors in the override column of the printed report.
Miscellaneous	Low system resources message is displayed, program crashes, program runs slowly.	IWAIR may be unstable when other applications are also open because of the memory required for running IWAIR. Close all other applications before starting IWAIR to free up the maximum resources for the program. If your computer's resources are still low, reboot the computer and restart IWAIR.

3.0 Selecting Calculation Method, WMU Type, and Modeling Pathway

3.1   Selecting Calculation Method

Each time you begin the program, select the mode of calculation. You can choose from two calculation methods: risk and allowable concentration. Click on the option button associated with either the risk calculation or the allowable concentration calculation mode. Each of these options is discussed below.

Risk Calculation Method

The first calculation method, risk calculation, allows you to develop inhalation risk estimates based on waste concentration levels that you specify. Results from the risk calculation method include (1) chemical-specific cancer risk estimates, (2) total cancer risk estimates (i.e., the summation of the chemical-specific risk estimates), and (3) noncancer risk estimates (i.e., HQs for noncarcinogens in the waste). Use the risk calculation option to develop risk estimates when you know the concentrations of the constituents in the waste. If the program results indicate that the waste poses an unacceptable risk to exposed individuals, then you should consider conducting a more site-specific analysis or implementing corrective measures to reduce the fraction of constituents released to the atmosphere. Such measures could include pretreatment of waste to reduce volatile chemical concentrations before the waste enters the unit or applying unit control technologies or practices to reduce volatile air emissions. Chapter 5 of the *Guide for Industrial Waste Management*, "Protecting Air Quality," identifies and discusses some emission control options.

Allowable Concentration Calculation Method

The second calculation method is an allowable concentration calculation that results in the development of waste concentrations (C_{waste}) that are protective of human health when managed as described. The calculation method can be applied in calculating waste concentrations for both wastewaters (C_{waste} in mg/L) and solid waste (C_{waste} in mg/kg). Concentrations are estimated based on user-defined target cancer and noncancer risk levels (e.g., 1E‒5 for carcinogens, or an HQ of 1 for noncarcinogens), which you will set on a later screen, the RESULTS SCREEN. The program uses information gathered on the IWAIR screens to calculate for each chemical an allowable waste concentration that would not pose an inhalation risk to the receptor greater than the selected target level. You can use the allowable concentration calculation option to estimate waste concentrations for a WMU that has not yet received a waste,

to determine what concentration(s) would pose an unacceptable risk to potentially exposed individuals.

3.2   Selecting WMU Type

Identify the WMUs that are used to manage wastes of concern at your facility and run the model separately for each WMU. Each of the four IWAIR unit types (described below) reflects waste management practices that are likely to occur at Industrial Subtitle D facilities.

Surface Impoundment. In the IWAIR tool, surface impoundments are considered to be ground-level, flowthrough units. The major source of volatile emissions associated with surface impoundments is the uncovered liquid surface exposed to the air (U.S. EPA, 1991). Impoundments can be quiescent (nonaerated) or aerated. Aeration or agitation is applied to aid in the treatment of the waste. Emissions tend to increase with an increase in surface turbulence because of enhanced mass transfer between the liquid and air (U.S. EPA, 1991). IWAIR can conduct emission modeling for both aerated and nonaerated surface impoundments. Parameters to which emissions are most sensitive include surface area, unit depth, waste concentration, retention time, wind speed for quiescent systems, and biodegradation.

The surface impoundment component of the IWAIR tool should not be used to model tanks. Although tanks have many common characteristics with surface impoundments with respect to volatile emissions, tanks are usually aboveground units, and height of the unit above the ground has a significant effect on dispersion factors. Therefore, the dispersion factors included in IWAIR for surface impoundments (which are presumed to be ground-level) are inappropriate for tanks and would produce erroneous results if so used.

Tilled Land Application Units. Wastes managed in land application units can be tilled or sprayed directly onto the soil and subsequently mixed with the soil by discing or tilling. Waste in a land application unit is a mixture of waste and soil.   IWAIR allows the modeling of tilled land application units only. Spray application was not included because the degree of volatilization associated with this type of application practice is very site-specific and is influenced by a number of variables, including meteorological conditions and application equipment. Therefore, IWAIR is unsuitable for modeling spray land application units. Important characteristics for the tilled land application unit include surface area (the exposed area from which volatile emissions can be released) and the application rate (which affects the depth of the contamination, which, along with area, defines the extent of the source for volatile emissions).

Landfills. IWAIR allows modeling of emissions released from the surface of an active (i.e., receiving wastes) landfill. Volatilization can occur from the surface of the landfill. Important unit characteristics for the landfill include surface area and unit depth. IWAIR assumes that the landfill being modeled is a ground-level emission source.

Waste Piles. Waste piles are typically elevated sources used as temporary storage units for solid wastes. Important characteristics for the waste pile include surface area and height. These parameters define the exposed area from which volatile emissions can be released.

3.3   Determining Appropriate Modeling Pathway

Regardless of the calculation method selected (risk or allowable concentration), determine which modeling pathway to follow in using the tool. After deciding on the appropriate calculation method and modeling pathway, proceed to either Section 4 for detailed guidance on completing risk calculations or Section 5 for guidance on allowable waste calculations.

You can choose from four pathways that provide you with the flexibility of conducting modeling using IWAIR-generated emissions rates and dispersion factors, user-specified emission and dispersion estimates, or a combination of both IWAIR-generated and user-specified estimates:

- ■   Pathway 1: Using CHEMDAT8 emission rates and ISCST3 default dispersion factors

- ■   Pathway 2: Using CHEMDAT8 emission rates and user-specified dispersion factors

- ■   Pathway 3: Using user-specified emission rates and ISCST3 default dispersion factors

- ■   Pathway 4: Using user-specified emission rates and dispersion factors.

In selecting a pathway, consider the availability of site-specific information. For example, if you have access to a limited amount of site-specific data and do not have access to emissions measurement data, then you will likely want to follow either Pathway 1 or 2 to allow IWAIR to develop CHEMDAT8 emissions rates. Similarly, if you do not have the ability (i.e., resources or access to technical capabilities) to conduct site-specific air dispersion modeling, then you will want to follow either Pathway 1 or 3 to allow IWAIR to develop dispersion factors. If site-specific emission and dispersion rates are accessible or if resources are available to develop these data, Pathway 4 will provide the most refined site-specific results.

Additionally, consider model assumptions and capabilities. Because a number of assumptions are made by IWAIR in modeling emissions and dispersion, use of these features may not be appropriate in all cases. Review the following overviews of CHEMDAT8 emission modeling and ISCST3 default dispersion factors, as well as Section 1.4 on IWAIR's capabilities and limitations, prior to choosing a pathway.

Using CHEMDAT8 Emission Rates

EPA's CHEMDAT8 model has been incorporated into the IWAIR program to assist you in the development of chemical-specific emission rates. 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).

CHEMDAT8 considers many of the competing removal pathways that might limit air emissions, including adsorption and hydrolysis in surface impoundments and biodegradation in all types of units. Adsorption is the tendency of a chemical to attach or bind to the surface of particles in the waste and therefore to not volatilize into the air. Biodegradation is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by organisms in the waste or soil; because this is a highly site-specific process, IWAIR allows you to choose whether to model biodegradation for all WMU types. Similarly, hydrolysis is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by reaction with water. IWAIR does not model these breakdown products produced as a result of biodegradation or hydrolysis. Chemicals that decompose by either biodegradation or hydrolysis have lower potential for volatile emission to the air.

Loss of contaminant by leaching or runoff is not included in the CHEMDAT8 model. Both leaching and runoff are a function of a chemical's tendency to become soluble in water and follow the flow of water (e.g., due to rainfall) down through the soil to groundwater (leaching) or downhill to surface water (runoff). These two mechanisms would also result in less chemical being available for volatile emission to the air. CHEMDAT8 is considered to provide reasonable to slightly high (environmentally conservative) estimates of air emissions from the various emission sources. See the *IWAIR Technical Background Document* for a more detailed discussion of the emissions modeling.

IWAIR Assumptions Made for Modeling Volatile Emissions with CHEMDAT8

- Annual average temperature is determined by assigned meteorological station; user may override.
- Waste is homogeneous.

Quiescent and Aerated Surface Impoundment Assumptions:

- Flowthrough unit is operating at steady state.
- For aqueous-phase wastes, waste in the surface impoundment is well mixed.
- Organic-phase wastes are modeled under plug flow conditions.
- For aqueous-phase wastes, biodegradation rate is first order with respect to biomass concentrations.
- For aqueous-phase wastes, biodegradation rate follows Monod kinetics with respect to contaminant concentrations.
- For aqueous-phase wastes, hydrolysis rate is first order with respect to contaminant concentrations.
- For aqueous-phase wastes, biodegradation is modeled by default; user may turn off.

Tilled Land Application Unit Assumptions:

- The volume of the land application unit remains constant. As new waste is applied, an equal volume of waste/soil mixture becomes buried or otherwise removed from the active tilling depth.
- Biodegradation is modeled by default; user may turn off.
- For organic-phase wastes, biodegradation and hydrolysis are not modeled.

Landfill Assumptions:

- Only one cell is active at a time.
- The active cell is modeled as instantaneously filled at time t = 0 and open for the life of the landfill divided by the number of cells. Cells are either depleted of the constituent or capped at the end of this period.
- Biodegradation is not modeled by default; user may turn on.

Waste Pile Assumptions:

- Waste pile operates with fixed volume.
- Waste pile is modeled as a square box with essentially vertical sides.
- Biodegradation is not modeled by default; user may turn on.

Using ISCST3 Default Dispersion Factors

The IWAIR default dispersion factors were developed by conducting air dispersion modeling with EPA's ISCST3 (U.S. EPA, 1995). This model is capable of modeling ground-level and elevated area sources. For IWAIR, landfills, land application units, and surface impoundments were modeled as ground-level area sources and waste piles were modeled as elevated area sources.

Because the ISCST3 model has considerable run times for area sources, modeling was conducted for a limited number of WMUs of representative sizes (i.e., surface areas, and heights for waste piles) using meteorological data obtained from 60 meteorological stations. The representative WMU sizes were selected from the range of sizes seen in the 1985 Screening Survey of Industrial Subtitle D Establishments (Shroeder et al., 1987). This database was the

Assumptions Made for Dispersion Modeling
■ 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.
■ Modeling was conducted using a unit emission rate of 1 µg/m^2-s.
■ 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.
■ 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.

most comprehensive database that EPA had on waste unit characteristics. It contains data on 6,254 surface impoundments, 1,281 waste piles, 702 land application units, and 790 landfills. The IWAIR program is designed to cover the range of unit characteristics contained in the database. Specific areas to be modeled were selected from the skewed distribution of areas found in the Industrial D Survey database so that all WMUs in the database would be adequately represented and interpolation errors would be minimized. As a result, 17 surface areas were selected for modeling for the landfills, land application units, and surface impoundments. Eleven surface areas were selected for waste piles. In addition, 7 heights were selected to be modeled for waste piles, and waste piles were modeled at all possible combinations of the 11 areas and 7 heights.

The ISCST3 modeling was conducted with data obtained from 60 meteorological stations chosen to represent the various climatic and geographical regions of the contiguous 48 states, Hawaii, Puerto Rico, and parts of Alaska. The dispersion modeling was conducted using 5 years of data from each of the 60 meteorological stations. The meteorological data required as input to the ISCST3 model included hourly readings for

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.

the following parameters: wind direction, wind speed (m/s), ambient temperature (K), mixing height, and stability class.

Dispersion factors were obtained as output by running the model with a unit emission rate (i.e., 1 µg/m^2-s). The selected areas for each type of WMU were modeled using meteorological inputs obtained from the 60 representative meteorological locations. Receptors were placed in 16 directions at distances of 25, 50, 75, 150, 500, and 1,000 meters from the edge of the WMU. Figure 3-1 illustrates the pattern of receptor placement around the unit for a 10,000 m^2 unit; only receptors at 150 m or less are shown for clarity reasons. Receptor placement was made based on a sensitivity analysis that was conducted to determine the locations and spacings that would provide adequate resolution without modeling an excessive number of receptors. The resulting maximum annual average air concentrations at each distance serve as the IWAIR default dispersion factors.

Figure 3-1. Receptor Locations.

Based on the WMU surface area (and height, for waste piles) that you provide, the IWAIR tool selects an appropriate dispersion factor. If the entered WMU surface area or height lies between two modeled areas or heights, dispersion factors for the WMU are estimated by an interpolation between dispersion factors for WMUs in the database with areas and heights above and below that of the WMU area you entered. For example, if you specify a landfill with a surface area of 8,000 m^2, the program will determine that this surface area falls between two modeled units with surface areas of 4,047 m^2 and 12,546 m^2. A linear interpolation method is then applied to estimate a dispersion factor for the 8,000 m^2 landfill, based on the default dispersion factors stored in the IWAIR database for two similarly sized units. For waste piles, a two-dimensional nonlinear interpolation method (called a spline) is used. See the *IWAIR Technical Background Document* for more information on the spline approach.

3.0 Selecting Calculation Method, WMU Type, and Modeling Pathway

3.1 Selecting Calculation Method

Each time you begin the program, select the mode of calculation. You can choose from two calculation methods: risk and allowable concentration. Click on the option button associated with either the risk calculation or the allowable concentration calculation mode. Each of these options is discussed below.

Risk Calculation Method

The first calculation method, risk calculation, allows you to develop inhalation risk estimates based on waste concentration levels that you specify. Results from the risk calculation method include (1) chemical-specific cancer risk estimates, (2) total cancer risk estimates (i.e., the summation of the chemical-specific risk estimates), and (3) noncancer risk estimates (i.e., HQs for noncarcinogens in the waste). Use the risk calculation option to develop risk estimates when you know the concentrations of the constituents in the waste. If the program results indicate that the waste poses an unacceptable risk to exposed individuals, then you should consider conducting a more site-specific analysis or implementing corrective measures to reduce the fraction of constituents released to the atmosphere. Such measures could include pretreatment of waste to reduce volatile chemical concentrations before the waste enters the unit or applying unit control technologies or practices to reduce volatile air emissions. Chapter 5 of the *Guide for Industrial Waste Management*, "Protecting Air Quality," identifies and discusses some emission control options.

Allowable Concentration Calculation Method

The second calculation method is an allowable concentration calculation that results in the development of waste concentrations (C_{waste}) that are protective of human health when managed as described. The calculation method can be applied in calculating waste concentrations for both wastewaters (C_{waste} in mg/L) and solid waste (C_{waste} in mg/kg). Concentrations are estimated based on user-defined target cancer and noncancer risk levels (e.g., 1E−5 for carcinogens, or an HQ of 1 for noncarcinogens), which you will set on a later screen, the RESULTS SCREEN. The program uses information gathered on the IWAIR screens to calculate for each chemical an allowable waste concentration that would not pose an inhalation risk to the receptor greater than the selected target level. You can use the allowable concentration calculation option to estimate waste concentrations for a WMU that has not yet received a waste,

to determine what concentration(s) would pose an unacceptable risk to potentially exposed individuals.

3.2   Selecting WMU Type

Identify the WMUs that are used to manage wastes of concern at your facility and run the model separately for each WMU. Each of the four IWAIR unit types (described below) reflects waste management practices that are likely to occur at Industrial Subtitle D facilities.

Surface Impoundment. In the IWAIR tool, surface impoundments are considered to be ground-level, flowthrough units. The major source of volatile emissions associated with surface impoundments is the uncovered liquid surface exposed to the air (U.S. EPA, 1991). Impoundments can be quiescent (nonaerated) or aerated. Aeration or agitation is applied to aid in the treatment of the waste. Emissions tend to increase with an increase in surface turbulence because of enhanced mass transfer between the liquid and air (U.S. EPA, 1991). IWAIR can conduct emission modeling for both aerated and nonaerated surface impoundments. Parameters to which emissions are most sensitive include surface area, unit depth, waste concentration, retention time, wind speed for quiescent systems, and biodegradation.

The surface impoundment component of the IWAIR tool should not be used to model tanks. Although tanks have many common characteristics with surface impoundments with respect to volatile emissions, tanks are usually aboveground units, and height of the unit above the ground has a significant effect on dispersion factors. Therefore, the dispersion factors included in IWAIR for surface impoundments (which are presumed to be ground-level) are inappropriate for tanks and would produce erroneous results if so used.

Tilled Land Application Units. Wastes managed in land application units can be tilled or sprayed directly onto the soil and subsequently mixed with the soil by discing or tilling. Waste in a land application unit is a mixture of waste and soil.   IWAIR allows the modeling of tilled land application units only. Spray application was not included because the degree of volatilization associated with this type of application practice is very site-specific and is influenced by a number of variables, including meteorological conditions and application equipment. Therefore, IWAIR is unsuitable for modeling spray land application units. Important characteristics for the tilled land application unit include surface area (the exposed area from which volatile emissions can be released) and the application rate (which affects the depth of the contamination, which, along with area, defines the extent of the source for volatile emissions).

Landfills. IWAIR allows modeling of emissions released from the surface of an active (i.e., receiving wastes) landfill. Volatilization can occur from the surface of the landfill. Important unit characteristics for the landfill include surface area and unit depth. IWAIR assumes that the landfill being modeled is a ground-level emission source.

Waste Piles. Waste piles are typically elevated sources used as temporary storage units for solid wastes. Important characteristics for the waste pile include surface area and height. These parameters define the exposed area from which volatile emissions can be released.

3.3   Determining Appropriate Modeling Pathway

Regardless of the calculation method selected (risk or allowable concentration), determine which modeling pathway to follow in using the tool. After deciding on the appropriate calculation method and modeling pathway, proceed to either Section 4 for detailed guidance on completing risk calculations or Section 5 for guidance on allowable waste calculations.

You can choose from four pathways that provide you with the flexibility of conducting modeling using IWAIR-generated emissions rates and dispersion factors, user-specified emission and dispersion estimates, or a combination of both IWAIR-generated and user-specified estimates:

- ■   Pathway 1: Using CHEMDAT8 emission rates and ISCST3 default dispersion factors

- ■   Pathway 2: Using CHEMDAT8 emission rates and user-specified dispersion factors

- ■   Pathway 3: Using user-specified emission rates and ISCST3 default dispersion factors

- ■   Pathway 4: Using user-specified emission rates and dispersion factors.

In selecting a pathway, consider the availability of site-specific information. For example, if you have access to a limited amount of site-specific data and do not have access to emissions measurement data, then you will likely want to follow either Pathway 1 or 2 to allow IWAIR to develop CHEMDAT8 emissions rates. Similarly, if you do not have the ability (i.e., resources or access to technical capabilities) to conduct site-specific air dispersion modeling, then you will want to follow either Pathway 1 or 3 to allow IWAIR to develop dispersion factors. If site-specific emission and dispersion rates are accessible or if resources are available to develop these data, Pathway 4 will provide the most refined site-specific results.

Additionally, consider model assumptions and capabilities. Because a number of assumptions are made by IWAIR in modeling emissions and dispersion, use of these features may not be appropriate in all cases. Review the following overviews of CHEMDAT8 emission modeling and ISCST3 default dispersion factors, as well as Section 1.4 on IWAIR's capabilities and limitations, prior to choosing a pathway.

Using CHEMDAT8 Emission Rates

EPA's CHEMDAT8 model has been incorporated into the IWAIR program to assist you in the development of chemical-specific emission rates. 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).

CHEMDAT8 considers many of the competing removal pathways that might limit air emissions, including adsorption and hydrolysis in surface impoundments and biodegradation in all types of units. Adsorption is the tendency of a chemical to attach or bind to the surface of particles in the waste and therefore to not volatilize into the air. Biodegradation is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by organisms in the waste or soil; because this is a highly site-specific process, IWAIR allows you to choose whether to model biodegradation for all WMU types. Similarly, hydrolysis is the tendency of a chemical to be broken down or decomposed into less-complex chemicals by reaction with water. IWAIR does not model these breakdown products produced as a result of biodegradation or hydrolysis. Chemicals that decompose by either biodegradation or hydrolysis have lower potential for volatile emission to the air.

Loss of contaminant by leaching or runoff is not included in the CHEMDAT8 model. Both leaching and runoff are a function of a chemical's tendency to become soluble in water and follow the flow of water (e.g., due to rainfall) down through the soil to groundwater (leaching) or downhill to surface water (runoff). These two mechanisms would also result in less chemical being available for volatile emission to the air. CHEMDAT8 is considered to provide reasonable to slightly high (environmentally conservative) estimates of air emissions from the various emission sources. See the *IWAIR Technical Background Document* for a more detailed discussion of the emissions modeling.

IWAIR Assumptions Made for Modeling Volatile Emissions with CHEMDAT8

- Annual average temperature is determined by assigned meteorological station; user may override.
- Waste is homogeneous.

Quiescent and Aerated Surface Impoundment Assumptions:

- Flowthrough unit is operating at steady state.
- For aqueous-phase wastes, waste in the surface impoundment is well mixed.
- Organic-phase wastes are modeled under plug flow conditions.
- For aqueous-phase wastes, biodegradation rate is first order with respect to biomass concentrations.
- For aqueous-phase wastes, biodegradation rate follows Monod kinetics with respect to contaminant concentrations.
- For aqueous-phase wastes, hydrolysis rate is first order with respect to contaminant concentrations.
- For aqueous-phase wastes, biodegradation is modeled by default; user may turn off.

Tilled Land Application Unit Assumptions:

- The volume of the land application unit remains constant. As new waste is applied, an equal volume of waste/soil mixture becomes buried or otherwise removed from the active tilling depth.
- Biodegradation is modeled by default; user may turn off.
- For organic-phase wastes, biodegradation and hydrolysis are not modeled.

Landfill Assumptions:

- Only one cell is active at a time.
- The active cell is modeled as instantaneously filled at time t = 0 and open for the life of the landfill divided by the number of cells. Cells are either depleted of the constituent or capped at the end of this period.
- Biodegradation is not modeled by default; user may turn on.

Waste Pile Assumptions:

- Waste pile operates with fixed volume.
- Waste pile is modeled as a square box with essentially vertical sides.
- Biodegradation is not modeled by default; user may turn on.

Using ISCST3 Default Dispersion Factors

The IWAIR default dispersion factors were developed by conducting air dispersion modeling with EPA's ISCST3 (U.S. EPA, 1995). This model is capable of modeling ground-level and elevated area sources. For IWAIR, landfills, land application units, and surface impoundments were modeled as ground-level area sources and waste piles were modeled as elevated area sources.

Because the ISCST3 model has considerable run times for area sources, modeling was conducted for a limited number of WMUs of representative sizes (i.e., surface areas, and heights for waste piles) using meteorological data obtained from 60 meteorological stations. The representative WMU sizes were selected from the range of sizes seen in the 1985 Screening Survey of Industrial Subtitle D Establishments (Shroeder et al., 1987). This database was the most comprehensive database that EPA had on waste unit characteristics. It contains data on 6,254 surface impoundments, 1,281 waste piles, 702 land application units, and 790 landfills. The IWAIR program is designed to cover the range of unit characteristics contained in the database. Specific areas to be modeled were selected from the skewed distribution of areas found in the Industrial D Survey database so that all WMUs in the database would be adequately represented and interpolation errors would be minimized. As a result, 17 surface areas were selected for modeling for the landfills, land application units, and surface impoundments. Eleven surface areas were selected for waste piles. In addition, 7 heights were selected to be modeled for waste piles, and waste piles were modeled at all possible combinations of the 11 areas and 7 heights.

The ISCST3 modeling was conducted with data obtained from 60 meteorological stations chosen to represent the various climatic and geographical regions of the contiguous 48 states, Hawaii, Puerto Rico, and parts of Alaska. The dispersion modeling was conducted using 5 years of data from each of the 60 meteorological stations. The meteorological data required as input to the ISCST3 model included hourly readings for

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Assumptions Made for Dispersion Modeling

- 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.

- Modeling was conducted using a unit emission rate of 1 $\mu g/m^2$-s.

- 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.

- 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.

**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.

the following parameters: wind direction, wind speed (m/s), ambient temperature (K), mixing height, and stability class.

Dispersion factors were obtained as output by running the model with a unit emission rate (i.e., 1 µg/m^2-s). The selected areas for each type of WMU were modeled using meteorological inputs obtained from the 60 representative meteorological locations. Receptors were placed in 16 directions at distances of 25, 50, 75, 150, 500, and 1,000 meters from the edge of the WMU. Figure 3-1 illustrates the pattern of receptor placement around the unit for a 10,000 m^2 unit; only receptors at 150 m or less are shown for clarity reasons. Receptor placement was made based on a sensitivity analysis that was conducted to determine the locations and spacings that would provide adequate resolution without modeling an excessive number of receptors. The resulting maximum annual average air concentrations at each distance serve as the IWAIR default dispersion factors.

Figure 3-1. Receptor Locations.

Based on the WMU surface area (and height, for waste piles) that you provide, the IWAIR tool selects an appropriate dispersion factor. If the entered WMU surface area or height lies between two modeled areas or heights, dispersion factors for the WMU are estimated by an interpolation between dispersion factors for WMUs in the database with areas and heights above and below that of the WMU area you entered. For example, if you specify a landfill with a surface area of 8,000 m^2, the program will determine that this surface area falls between two modeled units with surface areas of 4,047 m^2 and 12,546 m^2. A linear interpolation method is then applied to estimate a dispersion factor for the 8,000 m^2 landfill, based on the default dispersion factors stored in the IWAIR database for two similarly sized units. For waste piles, a two-dimensional nonlinear interpolation method (called a spline) is used. See the *IWAIR Technical Background Document* for more information on the spline approach.

5.0 Completing Allowable Waste Concentration Calculations

IWAIR allows you to develop allowable waste concentrations (C_{waste}) that may be protectively managed in a WMU. The calculation method can be applied in calculating waste concentrations for both wastewaters (C_{waste} in mg/L) and solid waste (C_{waste} in mg/kg). These concentrations are estimated based on user-defined target cancer and noncancer risk levels (e.g., 1E‑5 or 1E‑6 for carcinogens, or an HQ of 0.5 or 1 for noncarcinogens), which you define on the RESULTS screen.

The release of a chemical into the atmosphere is influenced by whether a waste is an aqueous- or organic-phase waste. IWAIR can apply either an aqueous or organic waste equilibrium partitioning algorithm. These partitioning algorithms are discussed in detail in the *IWAIR Technical Background Document*.

> **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.

EPA anticipates that most Industrial D wastes managed by the users of IWAIR will be aqueous-phase wastes with no chemicals above the typical solubility or saturation limits; therefore, the allowable concentration calculation is initially based on an aqueous-phase waste. For some chemicals in some units, it may not be possible to reach the target risk without the concentration exceeding the solubility limit (in wastewaters) or the soil saturation limit (in solid wastes) of the chemical. Once these limits are exceeded, the waste is better modeled as organic. In this case, IWAIR will switch to organic-phase emission rates and continue.[1] If the target risk is still not reached when the concentration reaches the maximum 1,000,000 mg/kg or mg/L, then the program will output a concentration of 1,000,000 and will note the maximum risk (or HQ) achievable.

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[1] For formaldehyde, the organic-phase emissions are higher than aqueous-phase emissions, and in order to be protective, the allowable concentration calculation is always based on an organic-phase waste.

IWAIR is structured in a stepwise framework. Through the use of a series of screens, IWAIR assists in selecting calculation options, identifying and entering required inputs, and generating desired outputs. There are four different pathways you can follow in performing a calculation:

■   Pathway 1: Using CHEMDAT8 emission rates and ISCST3 default dispersion factors

■   Pathway 2: Using CHEMDAT8 emission rates and user-specified dispersion factors

■   Pathway 3: Using user-specified emission rates and ISCST3 default dispersion factors

■   Pathway 4: Using user-specified emission rates and dispersion factors.

Guidance for determining which modeling pathway to follow is provided in Section 3.3. The stepwise approach employed by IWAIR to assist in calculating waste concentration, whether you are following Pathway 1, 2, 3, or 4, is shown in Figures 5-1, 5-2, 5-3, and 5-4, respectively. The seven steps of the estimation process are shown down the right side of each figure, and the user input requirements are specified to the left of each step. The types of input data required will vary depending on the modeling pathway chosen. Screen-by-screen, IWAIR walks you through the steps of an allowable concentration calculation to arrive at protective waste concentration estimates.

This section provides screen-by-screen guidance that describes the data that are required as input to each screen and the assumptions that are interwoven in the calculation being performed. The guidance provided in this section will assist you in completing an allowable concentration calculation. You will not need to reference all of the information provided in this section because the guidance addresses all four of the modeling pathways. Follow only those subsections that are applicable to your chosen pathway.

Select Calculation Method

Allowable concentration calculation

Identify WMU

- Land application unit
- Waste pile
- Surface impoundment
- Landfill

Define the Waste Managed

Add/modify chemical properties data, as desired

Determine Emission Rates

CHEMDAT8

Determine Dispersion Factors

Interpolated from ISCST3 default dispersion factors

Calculate Ambient Air Concentrations

Calculates ambient air concentrations for each receptor based on emission and dispersion data

Calculate Results

Allowable Waste Concentration Calculation

C_{waste} for wastewaters (mg/L)
C_{waste} for solid wastes (mg/kg)

User Specifies:
- Calculation option

User Specifies:
- WMU type

User Specifies:
- Constituents (choose up to 6)

User Specifies:
- CHEMDAT8 option
- Facility location for meteorological input
- WMU information (i.e., design and operating parameters)

User Specifies:
- Receptor information (i.e., distance and type)
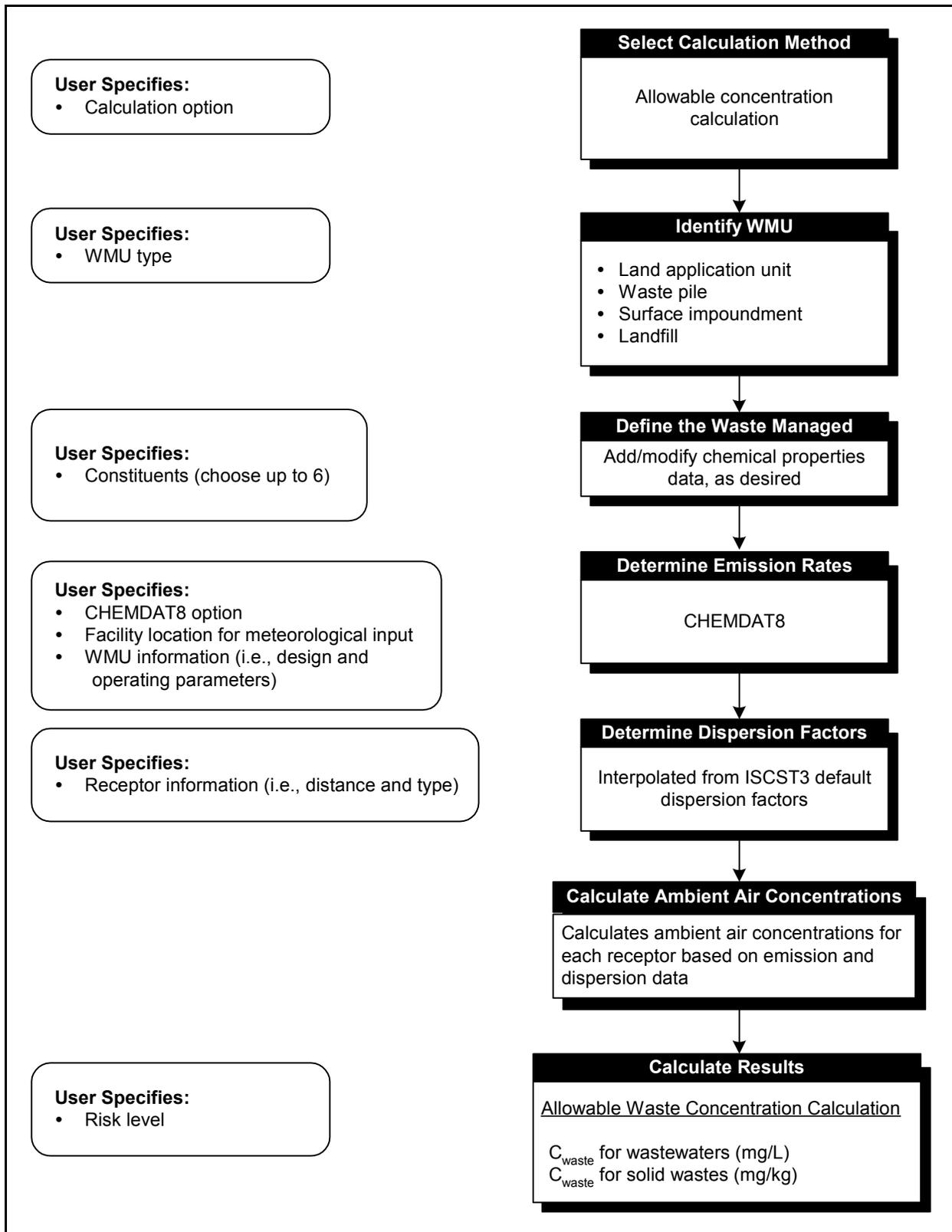
User Specifies:
- Risk level

Figure 5-1.   IWAIR approach for completing allowable waste concentration calculations, Pathway 1: Using CHEMDAT8 emission rates and ISCST3 default dispersion factors.

User Specifies:
• Calculation option

User Specifies:
• WMU type

User Specifies:
• Constituents (choose up to 6)

User Specifies:
• CHEMDAT8 option
• Facility location for meteorological input
• WMU information (i.e., design and operating parameters)

User Specifies:
• Dispersion factors
• Receptor information (i.e., distance and type)

User Specifies:
• Risk level

Select Calculation Method

Allowable concentration calculation

Identify WMU

• Land application unit
• Waste pile
• Surface impoundment
• Landfill

Define the Waste Managed

Add/modify chemical properties data, as desired

Determine Emission Rates

CHEMDAT8

Determine Dispersion Factors

User-specified dispersion factors

Calculate Ambient Air Concentrations

Calculates ambient air concentrations for each receptor based on emission and dispersion data

Calculate Results

Allowable Waste Concentration Calculation

C_{waste} for wastewaters (mg/L)
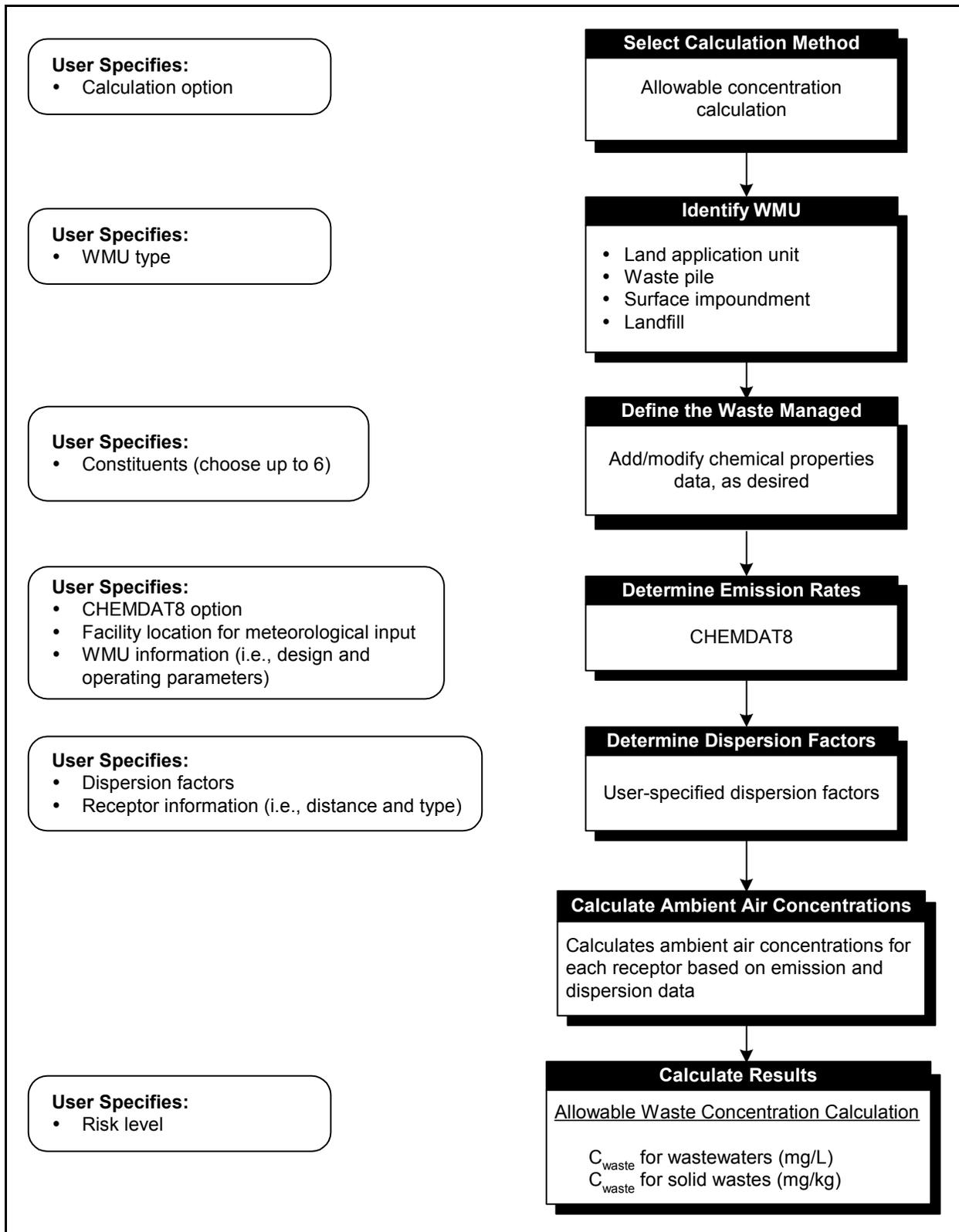C_{waste} for solid wastes (mg/kg)

Figure 5-2.   IWAIR approach for completing allowable waste concentration calculations, Pathway 2: Using CHEMDAT8 emission rates and user-specified dispersion factors.

Select Calculation Method

Allowable concentration
calculation

Identify WMU

- Land application unit
- Waste pile
- Surface impoundment
- Landfill

Define the Waste Managed

Add/modify chemical properties,
as desired

Determine Emission Rates

User-specified emission rates

Determine Dispersion Factors

Interpolated from ISCST3 default
dispersion factors

Calculate Ambient Air Concentrations

Calculates ambient air concentrations for
each receptor based on emission and
dispersion data

Calculate Results

Allowable Waste Concentration Calculation
3
   C_{waste} for wastewaters (mg/L)
   C_{waste} for solid wastes (mg/kg)

User Specifies:
- Calculation option

User Specifies:
- WMU type

User Specifies:
- Constituents (choose up to 6)

User Specifies:
- Emission rates

User Specifies:
- WMU area (and height for waste pile)
- Facility location for meteorological input
- Receptor information (i.e., distance and type)

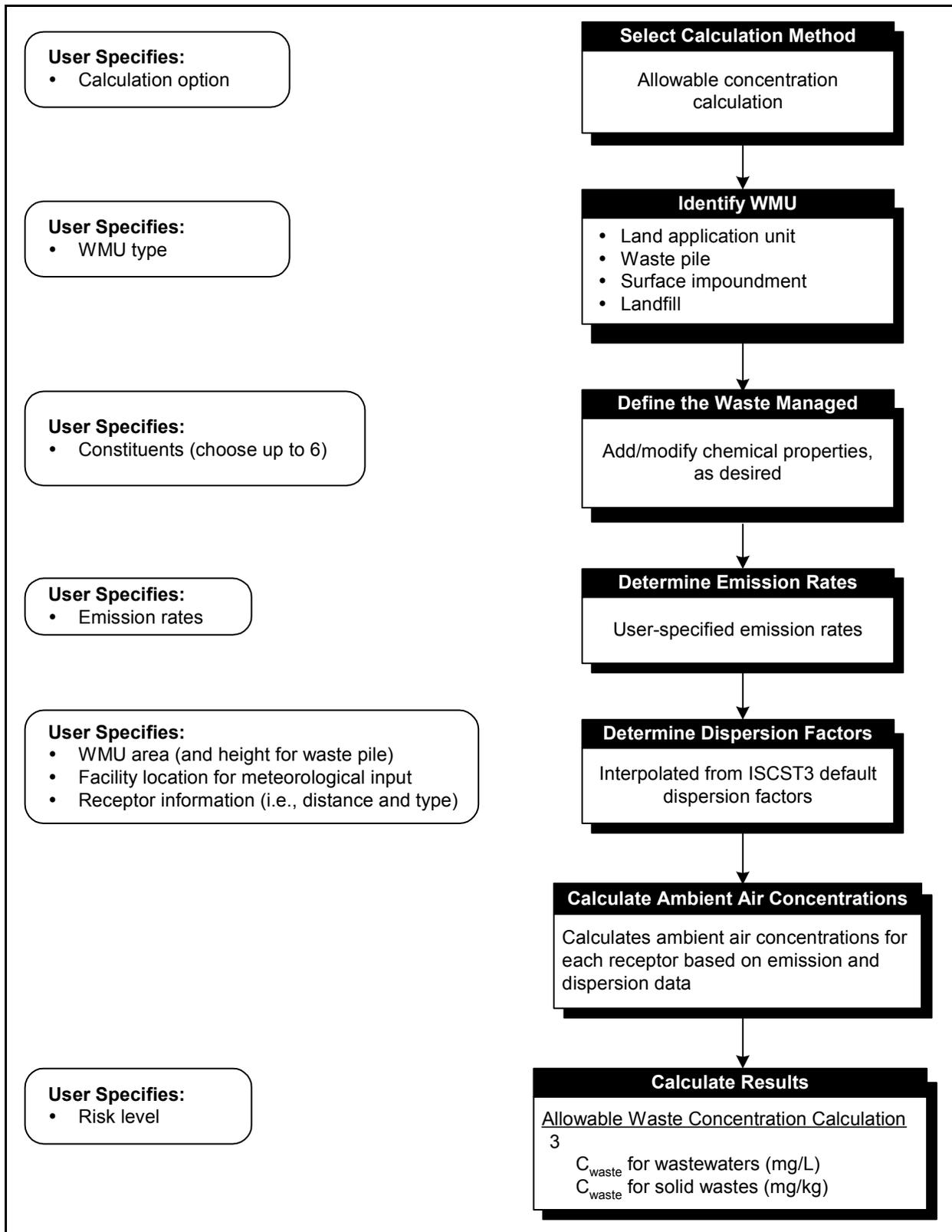**User Specifies:**
- Risk level

**Figure 5-3.   IWAIR approach for completing allowable waste concentration calculations,
Pathway 3: Using user-specified emission rates and ISCST3 default
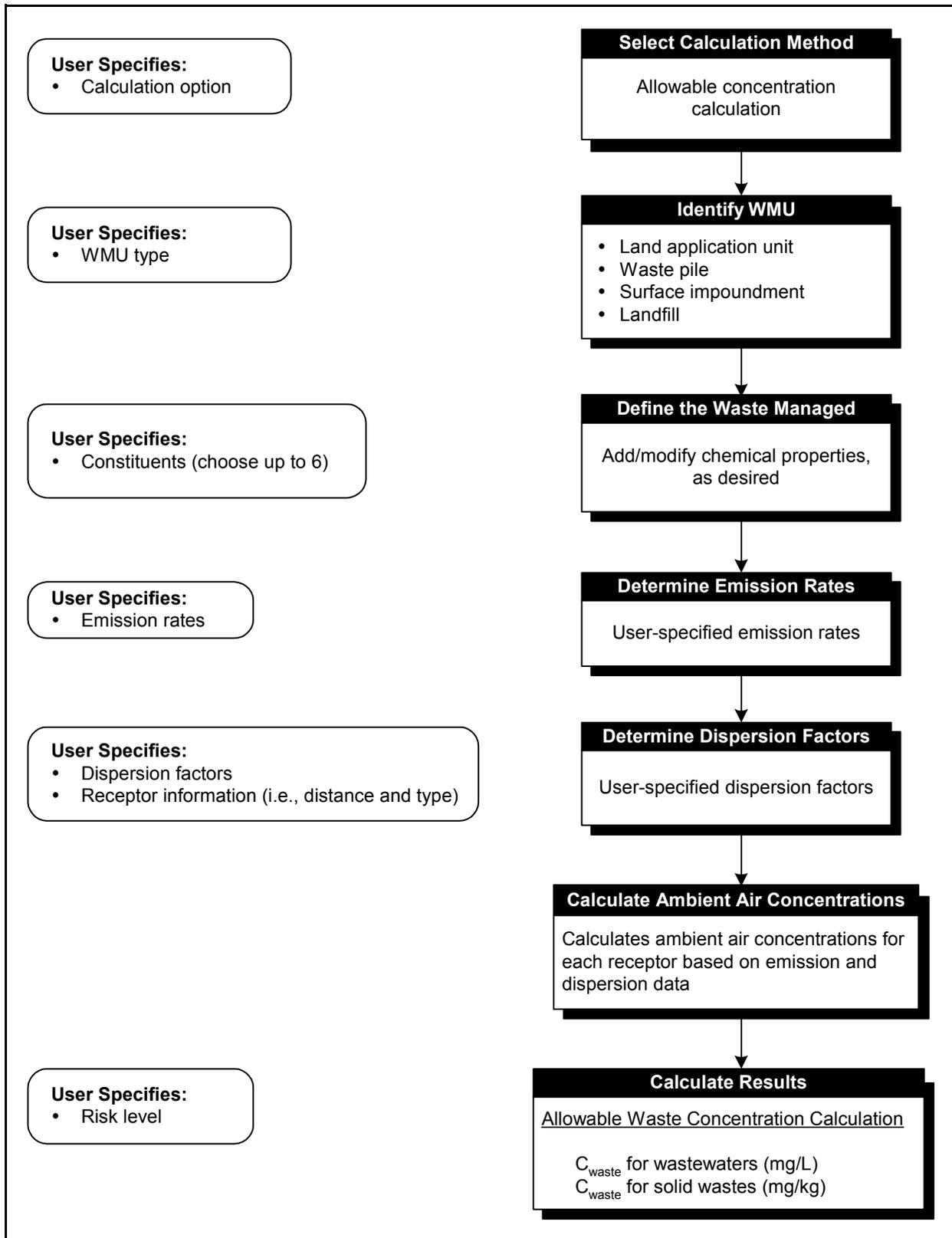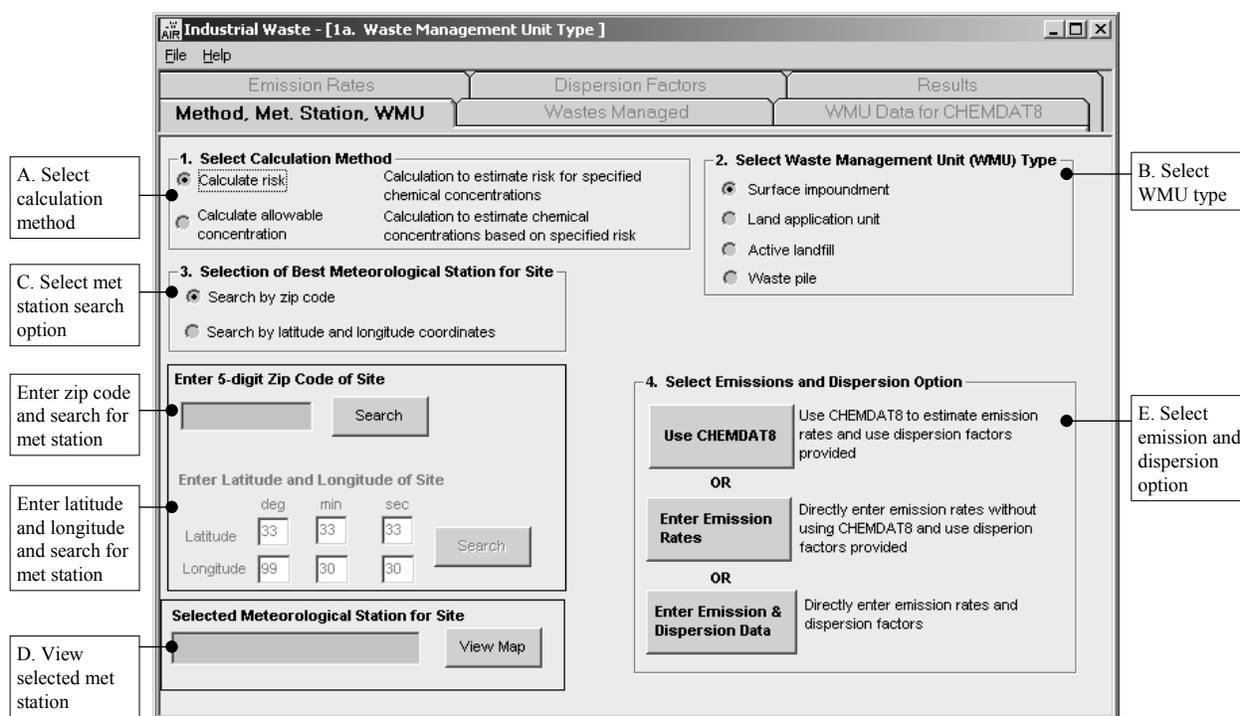dispersion factors.**

User Specifies:
- Calculation option

User Specifies:
- WMU type

User Specifies:
- Constituents (choose up to 6)

User Specifies:
- Emission rates

User Specifies:
- Dispersion factors
- Receptor information (i.e., distance and type)

User Specifies:
- Risk level

Select Calculation Method

Allowable concentration calculation

Identify WMU
- Land application unit
- Waste pile
- Surface impoundment
- Landfill

Define the Waste Managed

Add/modify chemical properties, as desired

Determine Emission Rates

User-specified emission rates

Determine Dispersion Factors

User-specified dispersion factors

Calculate Ambient Air Concentrations

Calculates ambient air concentrations for each receptor based on emission and dispersion data

Calculate Results

Allowable Waste Concentration Calculation

C_{waste} for wastewaters (mg/L)
C_{waste} for solid wastes (mg/kg)

Figure 5-4. **IWAIR approach for completing allowable waste concentration calculations, Pathway 4: Using user-specified emission rates and dispersion factors.**

Screen 1A. Method, Meteorological Station, WMU

5.1   Method, Meteorological Station, WMU (Screen 1A)

A.   *Select Calculation Method (Screen 1A)*

Select the calculation method by clicking on the |CALCULATE ALLOWABLE CONCENTRATION| option button. Detailed guidance for selecting the appropriate mode of calculation is provided in Section 3.1.

B.   *Select Waste Management Unit (WMU) Type (Screen 1A)*

Identify the WMUs that are used to manage wastes of concern at your facility and run the model separately for each unit type. The four unit types that are addressed as part of this guidance include surface impoundments (aerated and quiescent), active landfills, waste piles, and tilled land application units. A detailed description of these unit types is provided in Section 3.2. Select one of the four WMU types shown in Screen 1A by clicking on the appropriate option button.

C.   *Select Meteorological Station Search Option (Screen 1A)*

The two search options available include searching by the site's 5-digit zip code or by its latitude and longitude. Select the appropriate search option and enter the appropriate information. This information is used to link the facility's location to one of the 60 IWAIR meteorological stations. The 60 stations cover the 48 contiguous states, Hawaii, Puerto Rico, and

parts of Alaska. Data from the 60 stations (shown on maps in Screen 1B, viewed by clicking on the |Vɪᴇᴡ Mᴀᴘ| button shown on Screen 1A) were used as inputs to the air dispersion modeling effort conducted to develop the default dispersion factors contained in the IWAIR tool. They are also used as inputs to CHEMDAT8 emission modeling (e.g., annual average temperature and wind speed). Additional information on this air dispersion modeling effort and the 60 representative meteorological stations is provided in Section 3.3.

Enter 5-Digit Zip Code and Search for Meteorological Station

Enter a 5-digit zip code and click on the |Sᴇᴀʀᴄʜ| button to identify the default meteorological station. If the zip code was entered incorrectly or if no data were provided at all, message boxes will appear to indicate the specific problem that the tool encountered so that you can supply the needed data. The zip code database includes zip codes established through 1999. If your facility has a new zip code that was established more recently, you will get an error message indicating that it is not a valid zip code because it is not in IWAIR's database. If this occurs, you can use your old zip code, use a nearby zip code, or select a meteorological station using latitude and longitude.

Enter Latitude and Longitude Information and Search for Meteorological Station

As shown in Screen 1A, enter the latitude and longitude of the site in degrees, minutes, and seconds. At a minimum, the program requires degrees for latitude and longitude to be entered. If available, the minutes and seconds should be supplied to ensure that the most appropriate station is selected for a site. After these data are entered, click on the |Sᴇᴀʀᴄʜ| button to identify the default meteorological station. If the latitude and longitude information was entered incorrectly or if no data were provided at all, message boxes will be displayed that indicate the specific problem that the tool encountered so that you can supply the needed data.

D.   *View Selected Meteorological Station (Screen 1A)*

The meteorological station selected by the tool will be displayed in the text box. Once the meteorological station is selected, you are encouraged to click on the |Vɪᴇᴡ Mᴀᴘ| button to view the maps showing the 60 meteorological stations to ensure that the selection was made correctly. For example, if the latitude of a site was entered incorrectly, then the selected meteorological station would likely not be the most representative station. In this case, the map will help you identify this error before proceeding with the calculations. Clicking on the |Vɪᴇᴡ Mᴀᴘ| button will bring up a map of the 48 contiguous states (Screen 1B, shown here). You may view six additional maps (regional maps for the northeastern, southeastern, and western areas of the 48 contiguous states, as well as maps of Hawaii, Alaska, and Puerto Rico) by clicking on the appropriate button at the bottom of Screen 1B. The |Cʟᴏsᴇ| button returns you to the Mᴇᴛʜᴏᴅ, Mᴇᴛ. Sᴛᴀᴛɪᴏɴ, WMU Sᴄʀᴇᴇɴ (Screen 1A).
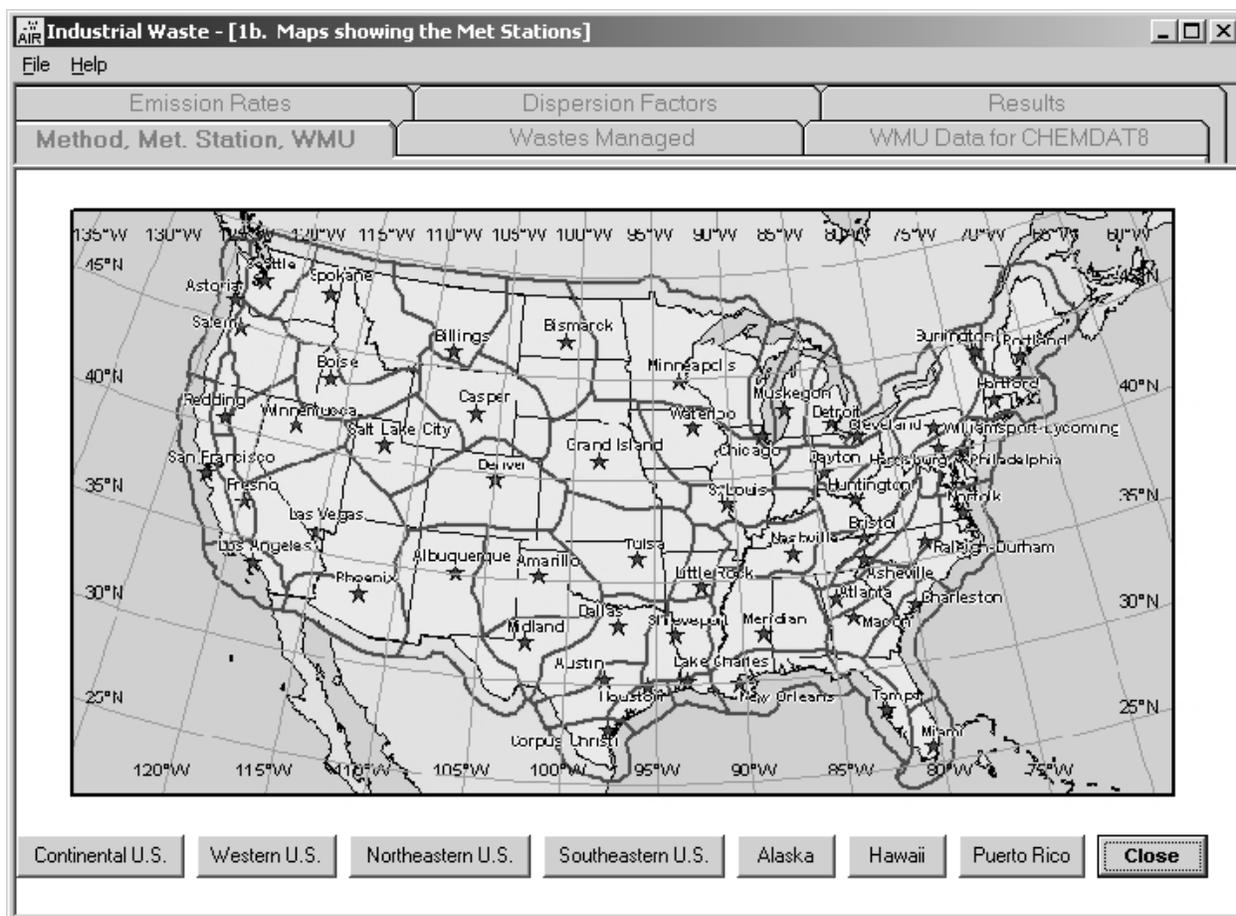
Screen 1B. Map of 48 Contiguous States Showing 60 Meteorological Station

E.   Select Emission and Dispersion Option (IWAIR-Generated or User-Specified) (Screen 1A)

You must select from the IWAIR emission and dispersion data options. Under these options, you have the flexibility of conducting modeling using IWAIR-generated emission rate and dispersion factor estimates, user-specified emission and dispersion estimates, or a combination of IWAIR-generated and user-specified estimates.

The tool uses emission rate and dispersion factor estimates in both the risk and allowable concentration modes. As seen in Screen 1A, you must select one of the three options provided for obtaining emission and dispersion data:

■ *Use CHEMDAT8*

Select |USE CHEMDAT8| to use CHEMDAT8 for calculating the emissions from your unit regardless of whether you want to calculate or enter dispersion factors. This allows you to enter a variety of unit-specific information that IWAIR will use to develop chemical-specific emission rate estimates through the use of EPA's CHEMDAT8 model. These inputs also provide the information needed to use the ISCST3 dispersion factors provided with IWAIR; however, you may also enter your own dispersion factors. You will not be allowed to override the IWAIR emission estimates on subsequent screens in allowable concentration mode. This option corresponds to Pathways 1 and 2 (see Section 3.3 and Figures 5-1 and 5-2).

■ *Enter Emission Rates*

Select |ENTER EMISSION RATES| to enter your own site-specific emission rates (g/m^2-s per mg/kg of mg/L) on a subsequent screen. Rates may be developed based on monitoring data or measurements or by conducting modeling with a different emission model. If your emission rates are in g/s, they will also have to be normalized by dividing by the area of the unit in m^2. In addition, these emission rates must be unitized (i.e., normalized to a unit waste concentration). This can be done by dividing the emission rate in g/m^2-s by the waste concentration in mg/L or mg/kg. Under this option, IWAIR can be used to estimate dispersion based on ISCST3 default dispersion factors. If this option is selected, you will still be allowed to override the IWAIR dispersion factors on subsequent screens with site-specific unitized dispersion factors ($\mu g/m^3$ per $\mu g/m^2$-s). Once the |ENTER EMISSION RATES| command button is selected, a message box will appear that directs you to enter WMU area (m^2). If a waste pile is being modeled, a subsequent box will appear for the height of the unit to be entered. These WMU data are used by the model to calculate dispersion estimates. This option corresponds to Pathway 3 (see Section 3.3 and Figure 5-3).

■ *Enter Emission, Dispersion Data*

Select |ENTER EMISSION & DISPERSION DATA| to enter your own emission estimates (g/m^2-s per mg/kg or mg/L) and unitized dispersion factors ($\mu g/m^3$ per $\mu g/m^2$-s). Emission rates may be developed based on monitoring data or measurements or by conducting modeling with a different emission model. If your emission rates are in g/s, they will also have to be normalized by dividing by the area of the unit in m^2. In addition, these emission rates must be unitized (i.e., normalized to a unit waste concentration). This can be done by dividing the emission rate in g/m^2-s by the waste concentration in mg/L or mg/kg. Dispersion factors may also need to be unitized by dividing by the emission rate (in g/m^2-s) used in dispersion modeling. This option corresponds to Pathway 4 (see Section 3.3 and Figure 5-4).
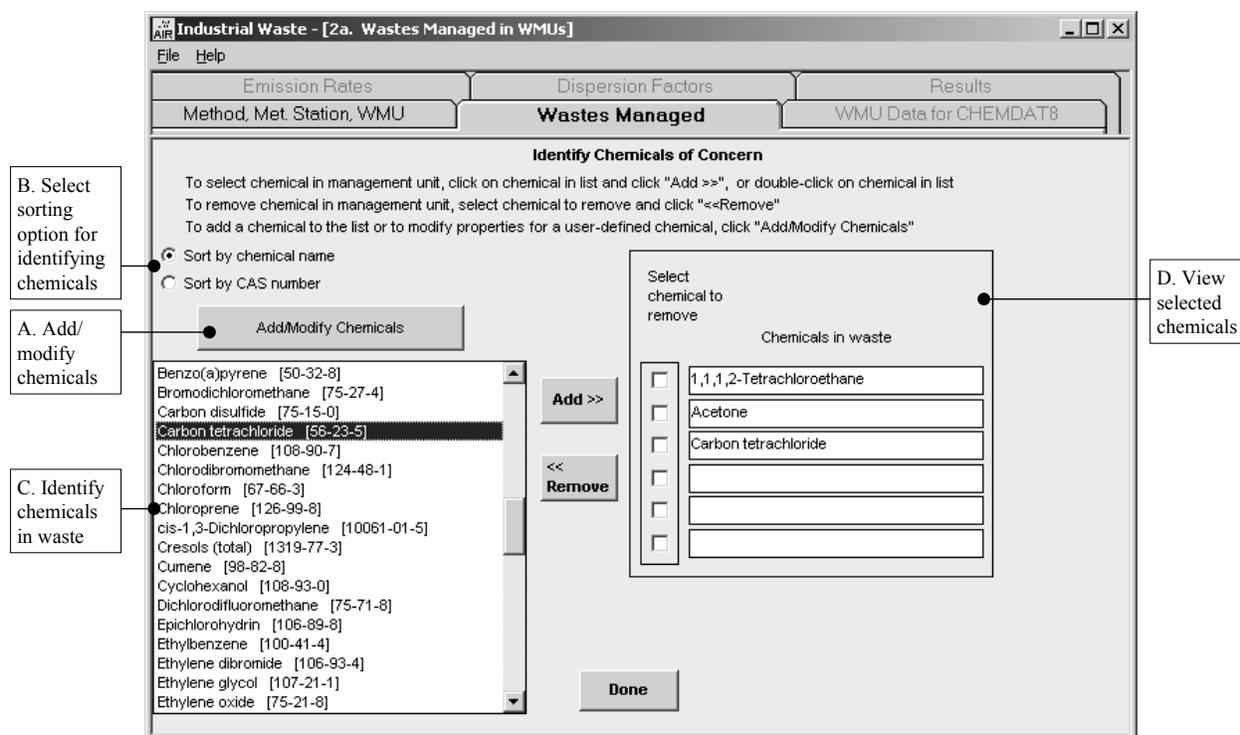
Screen 2A. Wastes Managed

5.2   Wastes Managed (Screen 2A)

To perform an allowable concentration calculation, identify the chemical(s) of concern in the waste.

A.   Add/Modify Chemicals (Screen 2A)

IWAIR includes a list of chemicals from which you can identify waste constituents. As a convenience to the user, IWAIR includes data on 95 constituents (shown with their CAS number in Section 1, Table 1-1). However, this list of chemicals may not include all the organic chemicals in your waste, and the data for these 95 chemicals may not match your site-specific conditions for some properties. Therefore, IWAIR has the capability to add or modify chemicals. To add or modify chemical data, click on the |ADD/MODIFY CHEMICALS| button. This will bring up Screen 2B, ADD/MODIFY CHEMICALS.

Screen 2B. Add/Modify Chemicals

The ADD/MODIFY CHEMICALS screen will initially appear with no data in any of the fields. You have four options:

- **Add a new chemical.** To do this, enter all data, including chemical name and CAS number, manually.

- **Add a new entry for a chemical already in the database.** To do this, select an existing entry for the chemical for which you wish to add an entry; if you select a user-defined entry, IWAIR will ask if you want to create a new entry. Click on |YES|. If you select an original IWAIR entry, IWAIR will automatically create a new entry.

- **Modify the data in an existing user-defined entry**. To do this, select the chemical to modify; when IWAIR asks if you want to create a new entry, click on |NO|. Original IWAIR entries may not be modified; if you select one, IWAIR will automatically create a new entry.

- **Delete an existing user-defined entry**. Select the entry to delete. Original IWAIR entries may not be deleted.

To ensure the integrity of the original IWAIR data and distinguish user-defined entries, IWAIR will automatically generate a unique identifier for each chemical entry added to the data set in the format "User X," where "X" is an entry number and "User" indicates it is a user-defined entry. This identifier will be appended to the chemical name to uniquely identify each entry. This identifier will be shown on screens and reports whenever the chemical is identified to clearly indicate which chemical entry has been used.

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), you may not create additional or modified entries for mercury.

A1. *Select Sorting Order for Identifying Chemicals (Screen 2B)*

The list of chemicals that is currently available in the database is shown here so that you can select constituents to modify. This list includes the 95 constituents included with IWAIR, as well as any you have already added to the IWAIR database. To facilitate the chemical selection process, IWAIR allows you to sort this list of chemicals alphabetically by chemical name, or by CAS number. As shown in Screen 2B, select a sort order by clicking on the button to the left of the sorting option of choice.

A2. *Select a Chemical to Modify (Screen 2B)*

If you wish to add a new entry for an existing chemical or modify an existing user-defined entry, double-click on the chemical name in the list of chemicals. This will display the data for that chemical on the ADD/MODIFY CHEMICALS screen. If you select one of the 95 original IWAIR chemicals, a new entry will be generated automatically with a new, unique user-defined identifier. If you select a user-defined entry, IWAIR will ask if you want to create a new entry. Click on |YES| to create a new entry (you will be able to modify the data) or |NO| to edit the existing entry.

A3. *Enter or View Chemical Name and CAS Number (Screen 2B)*

If you selected a chemical to modify or to update with a new entry, the chemical name and CAS number will be displayed. These may not be edited, to preserve the integrity of the unique chemical identifiers. If you are adding a new chemical and therefore entering all data manually, you will need to enter an appropriate chemical name and CAS number in these text boxes. Do not include a "User X" designation in your chemical name—IWAIR will append that automatically. Chemical names may not contain apostrophes (') or quotations marks ("). CAS numbers that are shorter than the maximum length should be prefaced with leading spaces, not zeros.

A4. *Enter Chemical Properties Data (Screen 2B)*

Enter values for all chemical properties shown on the screen. Use the mouse to click in each text box, or use the |TAB| key to move between the boxes. Except for health benchmarks, you may only enter numeric values (although you may enter numeric values

in scientific notation). For health benchmarks, you may also enter "NA." Be sure to enter values in the units shown. Additional guidance on obtaining values for these parameters is available in Appendix B, Section B.2.2.3.

You may enter user-defined health benchmarks may be entered both here, in a user-defined chemical record, and on the RESULTS screen. On the RESULTS screen, you can enter them directly into an IWAIR chemical record without overwriting the original IWAIR value. If you are entering a new or modified chemical entry, you should enter any user-defined health benchmarks here. However, you need not create a new chemical entry here just to change the benchmark of an IWAIR chemical; you can enter the user-defined health benchmark on the RESULTS screen.

A5.   *Clear Entry (Screen 2B)*

To clear an unwanted entry from the ADD/MODIFY CHEMICALS screen without saving, click on the |CLEAR| button. You will be asked to confirm that you want to clear the data.

A6.   *Save Entry (Screen 2B)*

Once all data have been entered, you can save by clicking on the |SAVE| button. IWAIR does some limited range checking to ensure values are within physically possible ranges; if an entry is not in the acceptable range, IWAIR will display an error message with the accepted range. These ranges are intended to eliminate only impossible entries (e.g., negative values for many properties) or values that will cause the model to fail. The actual typical range for most of the chemical properties is likely smaller than the accepted range. Once all data values have been validated and the entry added to the database, the form will be cleared.

A7.   *Delete a Chemical (Screen 2B)*

You may delete a user-defined chemical entry on the ADD/MODIFY CHEMICALS screen by selecting the chemical from the list of chemical entries and clicking on the |DELETE USER-DEFINED CHEMICAL| button. It is not necessary to double-click on the chemical to bring up its data before deleting; a single click to select the entry in the list is sufficient. If you have selected an original IWAIR chemical entry, an error message will appear indicating that the entry cannot be deleted. If you have selected a user-defined entry, a message will appear to confirm that you want to delete the entry. If you select |YES|, the entry will be deleted from the database and you will be returned to the ADD/MODIFY CHEMICALS screen. The list of chemicals on this screen will be updated to reflect the removal of the entry. If you select |NO|, you will be returned to the screen, and the chemical will not be deleted.

Note that the deletion of a chemical entry used in a saved analysis will lead to the failure of the saved analysis to reload.

A8. ***Return to Wastes Managed Screen (Screen 2B)***

Once you have completed all desired data additions, modifications, and deletions, click the |Rᴇᴛᴜʀɴ| button to return to the Wᴀsᴛᴇs Mᴀɴᴀɢᴇᴅ screen. If you have unsaved data, IWAIR will warn you and ask if you want to proceed. If you select |Yᴇs|, the unsaved data will be lost. If you select |Nᴏ|, you will be returned to the Aᴅᴅ/Mᴏᴅɪғʏ Cʜᴇᴍɪᴄᴀʟs screen, where you can save your data by selecting |Sᴀᴠᴇ|. The list of available chemicals in the Wᴀsᴛᴇs Mᴀɴᴀɢᴇᴅ screen will be updated to include any new entries and to omit any deleted entries.

B. ***Select Sorting Option for Identifying Chemicals (Screen 2A)***

Once you have returned to the Wᴀsᴛᴇs Mᴀɴᴀɢᴇᴅ screen, you can identify waste constituents from the list of chemicals included in IWAIR. This list includes the 95 constituents included with IWAIR, as well as any you add to the IWAIR database using the Aᴅᴅ/Mᴏᴅɪғʏ Cʜᴇᴍɪᴄᴀʟs feature. The 95 constituents included with IWAIR are shown with their CAS number in Section 1, Table 1-1. To facilitate the chemical identification process, IWAIR allows you to sort this list of chemicals alphabetically by chemical name, or by CAS number. As shown in Screen 2A, select a sort order by clicking on the button to the left of the sorting option of choice.

C. ***Identify Chemicals in Waste (Screen 2A)***

Identify up to six chemicals in a waste for modeling with IWAIR. Identify a chemical by clicking on the chemical name or CAS number and clicking on the |Aᴅᴅ>>| command button. To remove a waste constituent from consideration, select the check box located to the left of the chemical name and click the |<<Rᴇᴍᴏᴠᴇ| command button. User-defined entries are identified in this list by the modifier "User X" appended to the chemical name, where "X" is a unique number.

You may choose to simultaneously model the same chemical using multiple entries from the chemical database. You may want to do this to compare results based on changes you have made in chemical properties.

D. ***View Selected Chemicals (Screen 2A)***

The chemicals you identified for consideration are displayed in text boxes shown on Screen 2A. You can remove waste constituents from consideration by selecting the check box to the left of the chemical and clicking the |<<Rᴇᴍᴏᴠᴇ| command button.

5.3 Enter WMU Data for Using CHEMDAT8 Emission Rates

If you elected to use CHEMDAT8 emission rates in the calculations (i.e., selected the |Usᴇ CHEMDAT8| command button shown previously on Screen 1A), you will need to enter WMU data as specified in this section. If you did not elect to use CHEMDAT8 emission rates, then you should skip this section and proceed to Section 5.4, *Emission Rates*. If you elected to enter

emission rates and use ISCST3 dispersion factors, you will be asked to enter the WMU area (and height, if a waste pile) for ISCST3 before proceeding to the emissions screen.

This section provides guidance on providing input data needed to develop CHEMDAT8 emission estimates for the four unit types addressed by IWAIR.

Surface Impoundments. The major source of volatile emissions associated with surface impoundments is the uncovered liquid surface exposed to the air (U.S. EPA, 1991). Aeration and/or agitation are applied to aid in treatment of the waste, and emissions tend to increase with an increase in surface turbulence because of enhanced transfer of liquid-phase contaminants to the air (U.S. EPA, 1991). Parameters to which emissions are most sensitive include surface area, unit depth, waste concentration, retention time, wind speed for quiescent systems, and biodegradation. Retention time is not an explicit input, but a function of impoundment volume and flow.

Land Application Units. Waste can be tilled or sprayed directly onto the soil and subsequently mixed with the soil by discing or tilling. Waste in a land application unit is a mixture of sludge and soil. IWAIR allows the modeling of tilled land application units. If your unit uses spray application, another model may be more appropriate. Air emissions from land treatment units are dependent on the chemical/physical properties of the organic constituents, such as vapor pressure, diffusivity, and biodegradation rate. Operating and field parameters affect the emission rate, although their impact is not as great as that of the constituent properties.

Active Landfills. IWAIR allows the modeling of emissions released from the surface of an active (i.e., receiving wastes) landfill. The landfill model is sensitive to the air porosity of the solid waste, the liquid loading in the solid waste, the waste depth (assumed to be the same as the unit depth), the constituent concentration in the waste, and the volatility of the constituent (U.S. EPA, 1991).

Waste Piles. The waste pile emission model is sensitive to the air porosity of the solid waste, the liquid loading in the solid waste, the waste pile height, the constituent concentration in the waste, and the volatility of the constituent (U.S. EPA, 1991).

Screens 3A, 3B, 3C, and 3D, respectively, identify the CHEMDAT8 input requirements for surface impoundments, land application units, landfills, and waste piles. Guidance for completing each screen is provided below. For some of the required inputs, default values are provided in the screen text boxes, as well as to the right of the text boxes. These default values were selected to represent average or typical operating conditions. If appropriate, the defaults can be applied in the absence of site-specific data; however, you always have the option of overriding any defaults. The basis for these default values is provided in the *IWAIR Technical Background Document*.

Screen 3A. WMU Data for CHEMDAT8: Surface Impoundment

Screen 3B. WMU Data for CHEMDAT8: Land Application Unit

Screen 3C. WMU Data for CHEMDAT8: Landfill
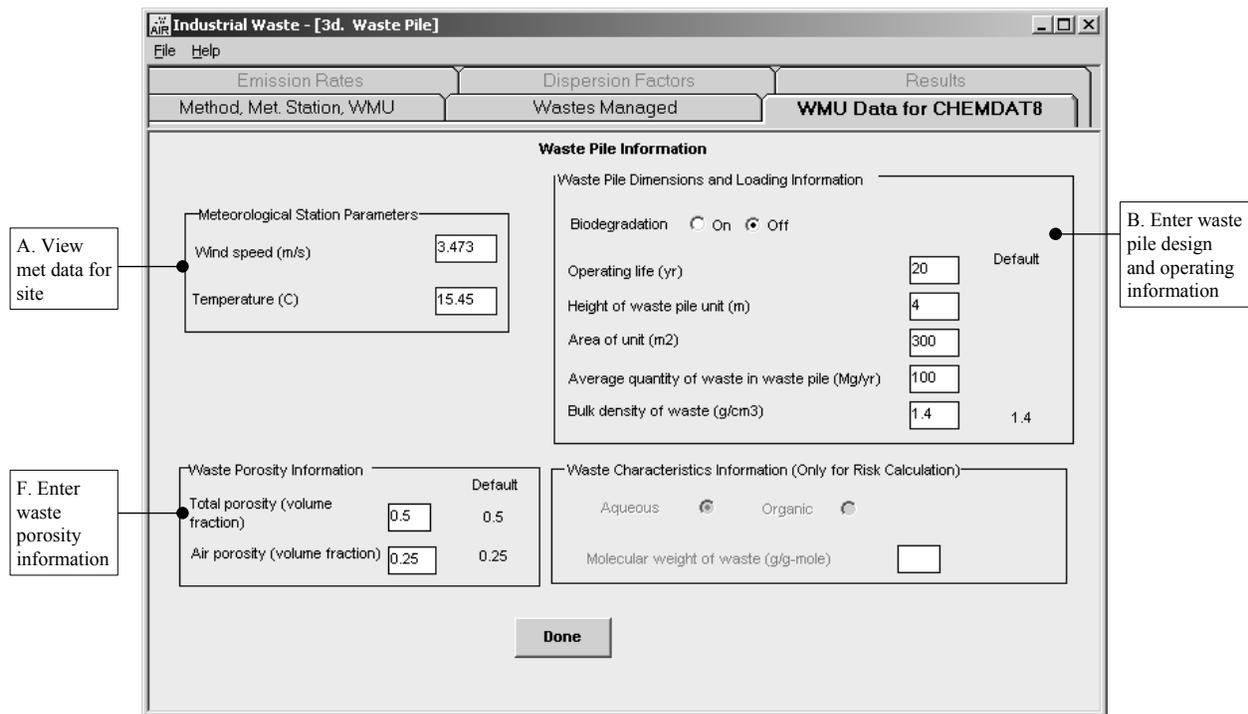
Screen 3D. WMU Data for CHEMDAT8: Waste Pile

A.   View Meteorological Data for Site (Screens 3A, 3B, 3C, and 3D)

Both wind speed and temperature can affect the volatilization rate of a chemical. Average wind speed and temperature are used as input to the CHEMDAT8 model. Average annual 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. Average annual temperature is used to adjust Henry's law constant and vapor pressure values (temperature-dependent chemical properties) from a standard temperature to the ambient temperature at the unit. Drawing from the meteorological data stored in IWAIR, the program will display the average annual temperature and wind speed available for the representative meteorological station that was determined for the site in Screen 1A. You can enter average wind speed and temperature for your site if the default values are significantly different.[2]

B.   Enter Unit Design and Operating Data

For all unit types, you may select whether or not biodegradation occurs in your unit. Select the |On| option to turn biodegradation on and the |Off| option to turn it off. The default setting varies by unit type. See Appendix B, Sections B.3.1.2, B.3.2.3, B.3.3.3, and B.3.4.3, for further details about the implications of turning biodegradation on or off and the appropriateness of difference choices for different unit types.

Enter Surface Impoundment Design Data (Screen 3A)

Enter the unit dimensions and loading information in the text boxes shown in Screen 3A. The data include the operating life of the unit (yrs), the depth of the unit (m), the area of the unit (m^2), and the annual flow of the waste (m^3/yr).

Enter Land Application Unit Design and Operating Information (Screen 3B)

Enter the unit dimensions and loading information in the text boxes shown in Screen 3B. The data include the operating life of the unit (yrs), tilling depth of the unit (m), area of the unit (m^2), annual waste quantity (Mg/yr), number of applications per year, and waste bulk density (g/cm^3).

Enter Landfill Design and Operating Information (Screen 3C)

Enter the unit dimensions and loading information in the text boxes in Screen 3C. The model assumes that the landfill is divided into cells, with only one cell active at a time. Emissions are modeled from the active cell. The data to be entered include the operating life of the unit (yrs), total area of the unit (m^2), depth of the unit (m), number of cells in your unit, annual quantity of wastes disposed in the unit (Mg/yr), and bulk density of waste (g/cm^3).

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[2] These inputs are not used in the dispersion modeling, which uses hourly data, not annual averages. Therefore, changes to these inputs will not affect the dispersion factors.

Enter Waste Pile Design and Operating Information (Screen 3D)

Enter the unit dimensions and loading information in the text boxes in Screen 3D. The data include the operating life of the unit (yrs), the height of the pile (m), area of the unit (m^2), annual quantity of waste in the pile (Mg/yr), and bulk density of the waste (g/cm^3).

C.   *For Aerated Surface Impoundments Only – Enter Aeration Data (Screen 3A)*

IWAIR models both quiescent (nonaerated) and aerated impoundments. Aeration or agitation of a liquid waste in an impoundment enhances transfer air (oxygen) to the liquid to improve mixing or to increase biodegradation (U.S. EPA, 1991). Aeration is achieved through the use of mechanical mixers, such as impellers (i.e., mechanically aerated), or by sparging air, which bubbles up from the bottom of the unit (i.e., diffused air aerated). First, select the aeration option that best describes your unit by clicking the appropriate option button. If you selected one of the aerated options, provide information to characterize the aeration in your unit. For all aeration options, you will need to enter the fraction of the surface area agitated (unitless). If you selected an option including diffused air aeration (diffused air only or both diffused air and mechanical aeration), you will also need to enter the total submerged air flow (m^3/s) of all diffusers in the impoundment.

If you choose to model an aerated impoundment, you will not have the option of modeling an organic-phase waste; IWAIR cannot model an organic-phase waste in an aerated impoundment because of limitations in CHEMDAT8.

D.   *For Mechanically Aerated Surface Impoundments Only – Enter Mechanical Aeration Information (Screen 3A)*

If a surface impoundment is mechanically aerated, you will need to provide additional operating parameter information. These data include oxygen transfer rate (lb O$_2$/hr-hp), number of aerators, total power (hp), power efficiency (fraction), impeller diameter (cm), and impeller speed (rad/s).

E.   *For Surface Impoundments Only – Enter Waste Characteristics Data (Screens 3A)*

The waste characteristic information to be entered for surface impoundments includes active biomass (g/L), total suspended solids into WMU (mg/L), total organics into WMU (mg/L), and total biorate (mg/g biomass-hr). These parameters are discussed in more detail in Appendix B.

F.   *For Land Application Units, Landfills, and Waste Piles Only – Enter Waste Porosity Information (Screens 3B, 3C, and 3D)*

Waste (or soil/waste mixture for land application units) porosity information required as input includes total porosity (unitless) and air porosity (unitless). Total porosity includes air porosity and the space occupied by oil and water within waste. Total porosity (ϵ_t), also sometimes called saturated water content, can be calculated from the bulk density (BD) of the waste and particle density (ρ_s) as follows:

$$\epsilon_t \;=\; 1 \;-\; \frac{BD}{\rho_s}$$

where BD and ρ_s are expressed in the same units.

In the absence of site-specific data, IWAIR identifies default values of 0.5 and 0.25, respectively, for total porosity and air porosity. Air porosity cannot exceed total porosity.

Done. Once you provide the required WMU inputs, click the |DONE| button to enable the EMISSION RATES tab and open the EMISSION RATES screen. Proceed to Section 5.4, *Emission Rates*. IWAIR must calculate emission rates before displaying the EMISSION RATES screen. This is usually very quick, but if your computer is slow, or if you are modeling a land application unit and with a large number of total applications (i.e., number of applications per year times operating life), there can be a noticeable delay before the EMISSION RATES screen is displayed. This is normal, but should typically not exceed 1 minute on a fast machine or 5 minutes on a slow machine.

5.4   Emission Rates

Guidance for using CHEMDAT8 emission rates or entering your own emission rates is provided in this section. View and confirm the CHEMDAT8 emission rates as directed in Section 5.4.1. If you did not elect to use CHEMDAT8 (i.e., if you selected the |ENTER EMISSION RATES| or |ENTER EMISSION & DISPERSION DATA| command buttons shown previously on Screen 1A), proceed to Section 5.4.2, *User-Specified Emission Rates*.

Please note that all calculated and entered values on the EMISSION RATES screen will be lost if you return to a previous screen and make changes. This includes both calculated and entered override emission rate values.
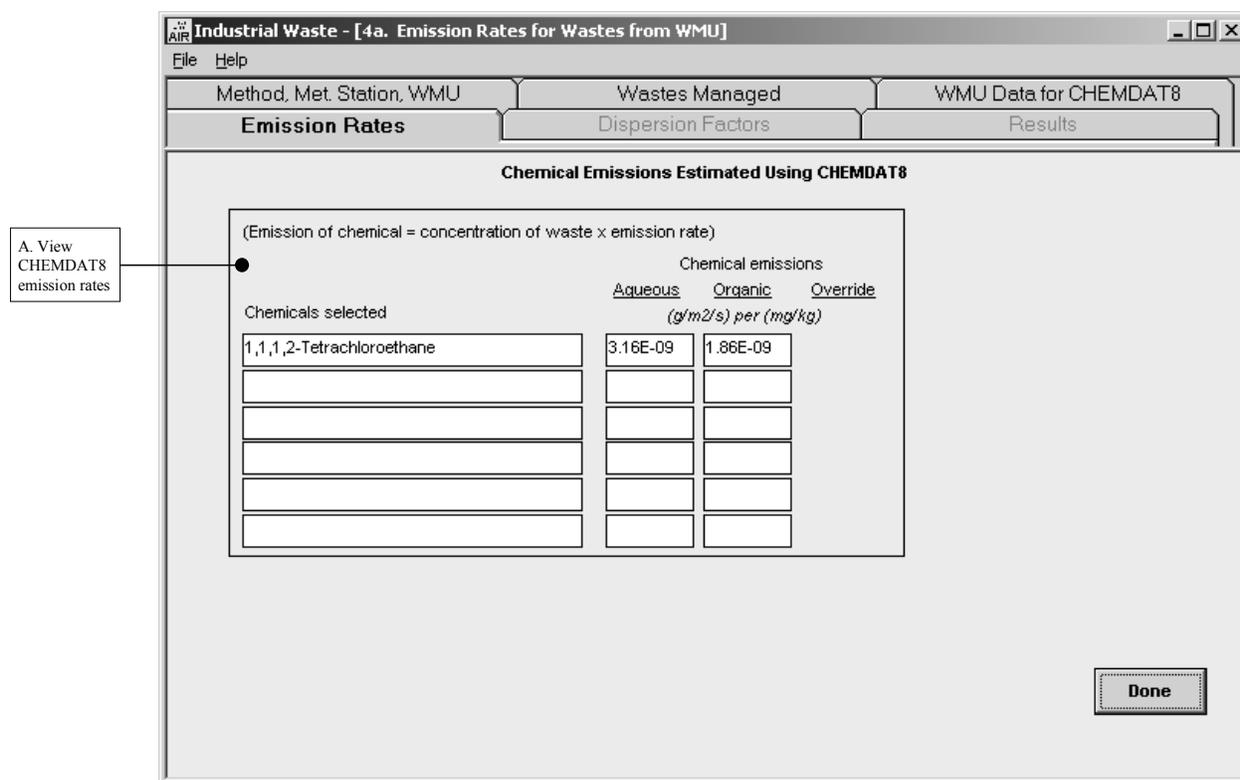
Screen 4A. CHEMDAT8 Emission Rates

5.4.1   Using CHEMDAT8 Emission Rates (Screen 4A)

A.   View CHEMDAT8 Emission Rates (Screen 4A)

Screen 4A shows the calculated CHEMDAT8 emission rates. Emission rates for the allowable concentration mode are unitized to a unit waste concentration (i.e., a waste concentration of 1 mg/kg). For land application units, landfills, and waste piles, emission rates are linear with concentration; therefore, this unitized emission rate can be adjusted to any specific concentration by multiplying by the concentration. For surface impoundments, however, emissions are not linear in the aqueous phase because of biodegradation, which is first order at low concentrations and shifts to zero order at higher concentrations. The concentration at which this occurs is chemical-specific. Therefore, for surface impoundments, this screen does not display emission rates. The actual emission rate used in risk calculations is calculated later, during the risk calculations.

For landfills and waste piles, emissions are modeled at equilibrium and are assumed to reflect a long-term average emission rate, normalized to a waste concentration of 1 mg/kg, which is shown on this screen. In contrast, land application units are not assumed to be at equilibrium; rather, emissions are calculated for each year of the specified operating life, plus 30 years postclosure. The emission rates shown on this screen are the maximum single-year emission

rates for each chemical (which may not reflect the same year for all chemicals), normalized to a waste concentration of 1 mg/kg. This emission rate is used directly to calculate air concentration for calculating noncarcinogenic risk. However, for carcinogenic risk, the maximum 7- or 30-year average emission rate (7-year for a worker and 30-year for a resident, corresponding to the default exposure durations for each receptor type) is used to calculate air concentration and then risk.

For all unit types other than surface impoundments, emission rates will be displayed under both the AQUEOUS and ORGANIC column headings; IWAIR will determine which of these to use during calculation of the allowable concentration depending on the target risk or HQ and the chemical's solubility or saturation limit.

These emission rates may not be overridden. Confirm the emission rates to be used in the calculations by clicking the |DONE| button. The program will automatically enable the DISPERSION FACTORS tab and open the DISPERSION FACTORS screen. Proceed to Section 5.5, *Dispersion Factors*.

Screen 4B. User-Specified Emission Rates

5.4.2   User-Specified Emission Rates (Screen 4B)

A.   *Enter User-Specified Emissions (Screen 4B)*

Enter site-specific normalized emission rates (g/m^2-s per mg/kg or g/m^2-s per mg/L) in the text box located under User Override. Your emission rates *must* be normalized to a unit concentration. If you have measured or calculated emission rates in g/s for your entire unit, you will need to divide that emission rate by the total area of your unit (in m^2) to obtain area-normalized emission rates in g/m^2-s. You can normalize this emission rate to a unit concentration by dividing by the waste concentration in mg/L or mg/kg at the time when the emission rate was measured or calculated. These emission rates should reflect long-term average emissions, not a short-term peak.

B.   *Enter Source and Justification for User-Specified Emission Rates (Screen 4B)*

The program will prompt you to provide justification for using user-specified emission rates and documentation of the estimation method applied. It is important to provide this documentation as a reference that will allow you or another user to view and understand saved files at a later date.

Done. Once you have entered emission data and source/justification, click the |Done| button to enable the Dispersion Factors menu tab and open the Dispersion Factors screen. Proceed to Section 5.5, *Dispersion Factors*.

5.5   Dispersion Factors

Dispersion modeling outputs are used to estimate air concentrations to which the various human receptors are exposed. Guidance for using the ISCST3 default dispersion factors or entering your own site-specific dispersion factors is provided in Sections 5.5.1 and 5.5.2, respectively. If you elected to use ISCST3 dispersion factors provided in IWAIR (i.e., selected the |Use CHEMDAT8| or |Enter Emission Rates| command buttons shown previously on Screen 1A), you will need to follow the guidance provided in Section 5.5.1. If you did not elect to use the default dispersion factors, you should proceed to Section 5.5.2, *User-Specified Dispersion Factors*.

Please note that all calculated and entered dispersion factors on the Dispersion Factors screen will be lost if you return to a previous screen and make changes. This does not include receptor locations and types but does include calculated and entered override dispersion factor values.

Screen 5A. Using ISCST3 Default Dispersion Factors

5.5.1 Using ISCST3 Default Dispersion Factors (Screen 5A)

In Screen 5A, you will provide receptor information (i.e., receptor type and distance to the receptor) and click on the |CALCULATE| button; IWAIR will develop site-specific dispersion factors based on default dispersion data. If you wish to override the IWAIR-developed dispersion factors, enter alternate site-specific unitized dispersion factors. If you enter alternative dispersion factors, you should document the source and the justification for these data in the text box on the screen.

A.   Select Receptor Type and Distance (Screen 5A)

Enter information concerning the receptors of concern (i.e., potentially exposed individuals). You can specify up to five receptors, including the distance to receptor and the receptor type. You can specify two receptor types at six distances (25, 50, 75, 150, 500, and 1,000 meters) from the edge of the WMU. You can delete the last receptor entered by deleting both the distance to receptor and receptor type entries.

Distance to Receptor – For each receptor of concern, determine the distance from the edge of the unit to the receptor. Based on this distance, select from the six default distances (25, 50, 75, 150, 500, and 1,000 meters) the one that best approximates the location of your receptor, using the drop-down box positioned under the DISTANCE TO RECEPTOR column heading. Note that selecting a distance smaller than the actual distance to receptors near your unit will overestimate

risk, and selecting a distance larger than the actual distance will underestimate risk. These distances correspond to the distances for which air dispersion modeling was conducted to develop the IWAIR default dispersion factors. The *IWAIR Technical Background Document* discusses the analysis that was conducted in determining the appropriateness of these default distances.

Receptor Type – Two different types of exposed individuals, worker and resident, can be modeled with IWAIR. The dispersion factors do not vary with receptor type; however, receptor type is chosen here for convenience. The difference between these two receptors is in the exposure factors, such as body weight and inhalation rate, used to calculate risk for carcinogens. There is no difference between them for noncarcinogens because calculation of noncarcinogenic risk does not depend on exposure factors. The *IWAIR Technical Background Document* describes the exposure factors used for residents and workers. The assumptions for workers reflect a full-time, outdoor worker. The exposure duration for workers is the smaller of 7.2 years or the operating life of the unit. The assumptions for residents reflect males and females from birth through age 30; it is important to consider childhood exposures because children typically have higher intake rates per kilogram of body weight than adults. The actual exposure duration used for residents is the smaller of 30 years or the operating life that you entered for the unit. For exposure durations less than 30 years, exposure starts at birth and continues for the length of the exposure duration, using the appropriate age-specific exposure factors. Use the drop-down box positioned under the RECEPTOR TYPE column heading to select either WORKER or RESIDENT.

B.   *Direct IWAIR to Estimate Dispersion Factors (Screen 5A)*

After the requested receptor information is provided, click on the |CALCULATE| button to direct the program to determine an appropriate dispersion factor based on the IWAIR default dispersion data. The resulting dispersion factor will be displayed for each receptor of concern. A discussion of the development of IWAIR default dispersion data and the methodology used by the program in selecting an appropriate dispersion factor for each WMU/receptor combination is provided in Section 3.3. A more detailed discussion of the air dispersion modeling effort is provided in the *IWAIR Technical Background Document*.

For waste piles, IWAIR uses a two-dimensional nonlinear spline to interpolate dispersion factors for areas and heights different from those included in the dispersion factor database. This technique is more accurate than a two-dimensional linear interpolation and is less likely to underestimate the actual dispersion factor. However, on rare occasions, the spline may produce results inconsistent with the data points nearest the actual area and height. If this occurs, IWAIR shifts to the linear interpolation technique, which generally produces somewhat lower dispersion factors. If this occurs, you will see a message to that effect. The interpolation techniques used for dispersion factors are discussed in greater detail in the *IWAIR Technical Background Document*.

C.   *View IWAIR Dispersion Factors or Enter User-Specified Dispersion Factors (Screen 5A)*

        You may override the program-calculated dispersion factors by entering alternative dispersion data in the text box located under the USER OVERRIDE column (see Screen 5A).

D.   *Enter Source and Justification for User-Specified Dispersion Factors (Section 5A)*

        If you choose to provide alternative dispersion factors, document the source and the justification for these data in the text box that will appear. It is important to provide this documentation as a reference that will allow you or another user to view and understand saved files at a later date.

        Done. Once the program has developed dispersion factors, click the |DONE| button to open the RESULTS tab. Proceed to Section 5.6, *Results*.

Screen 5B. User-Specified Dispersion Factors

5.5.2   User-Specified Dispersion Factors (Screen 5B)

A.   *Select Receptor Type and Distance (Screen 5B)*

        Enter information concerning the receptors of concern (i.e., potentially exposed individuals). You can specify up to five receptors. The receptor information includes the

distance to receptor and the receptor type. You can specify two receptor types in sixteen directions at six distances (25, 50, 75, 150, 500, and 1,000 meters) from the edge of the WMU. You can delete the last receptor entered by deleting both the distance to receptor and receptor type entries.

Distance to Receptor – For each receptor of concern, determine the distance from the edge of the unit to the receptor. Based on this distance, select from the six default distances (25, 50, 75, 150, 500, and 1,000 meters) the one that best approximates the location of your receptor, using the drop-down box positioned under the DISTANCE TO RECEPTOR column heading. These values are only for your reference and are not used in calculations, since you are entering your own dispersion factors.

Receptor Type – Two different types of exposed individuals, worker and resident, can be modeled with IWAIR. The dispersion factors do not vary with receptor type; however, receptor type is chosen here for convenience. The difference between these two receptor types lies in the exposure factors, such as body weight and inhalation rate, used to calculate risk for carcinogens. There is no difference between them for noncarcinogens because calculation of noncarcinogenic risk does not depend on exposure factors. The *IWAIR Technical Background Document* describes the exposure factors used for residents and workers. The assumptions for workers reflect a full-time, outdoor worker. The exposure duration for workers is the smaller of 7.2 years or the operating life of the unit. The assumptions for residents reflect males and females from birth through age 30; it is important to consider childhood exposures because children typically have higher intake rates per kilogram of body weight than adults. The actual exposure duration used for residents is the smaller of 30 years or the operating life of the unit that you entered. For exposure durations less than 30 years, exposure starts at birth and continues for the length of the exposure duration, using the appropriate age-specific exposure factors. Use the drop-down box positioned under the RECEPTOR TYPE column heading to select either WORKER or RESIDENT.

B.   Enter User-Specified Dispersion Factors (Screen 5B)

For each receptor specified, enter site-specific unitized dispersion factors (μg/m^3 per μg/m^2-s) in the text box located under USER OVERRIDE. You may need to normalize modeled dispersion factors to a unit concentration by dividing the modeled dispersion factor by the emission rate used in dispersion modeling (in μg/m^2-s) if it was not 1 μg/m^2-s. For example, if you ran your dispersion model using an emission rate of 1E–6 μg/m^2-s, then you would need to divide all your dispersion factors by 1E–6 to normalize them to a concentration of 1 μg/m^2-s.

C.   Enter Source and Justification for User-Specified Dispersion Factors (Screen 5B)

The program will prompt you to provide justification for using user-specified dispersion data and documentation of the estimation method applied. It is important to provide this documentation as a reference that will allow you or another user to view and understand saved files at a later date.

Done. Once you have entered dispersion data, click the |DONE| button to open the RESULTS tab. Proceed to Section 5.6, *Results*.

5.6   Allowable Concentration Results (Screen 6)

Allowable waste concentrations can be calculated from user-specified risk levels. The program combines the constituent's air concentration with receptor exposure factors and toxicity benchmarks to calculate the waste concentrations that are protective of human health. For each receptor, IWAIR calculates air concentrations using emission and dispersion data specified or calculated in previous screens. To reflect exposure that would occur in a lifetime (i.e., from childhood through adulthood), the model applies a time-weighted-average approach. This approach considers exposure that would occur during five different phases of life (i.e., Child < 1 yr, Child 1–5 yrs, Child 6–11 yrs, Child 12–18 yrs, and Adult). The exposure factors addressed as part of this approach include inhalation rate, body weight, exposure duration, and exposure frequency. The default values that are applied in developing these time-weighted-average exposures were identified based on data presented in EPA's *Exposure Factors Handbook* (U.S. EPA, 1997a) and represent average exposure conditions. IWAIR incorporates standard toxicity benchmarks (CSFs for carcinogens and RfCs for noncarcinogens) for 95 constituents. These health benchmarks were obtained primarily from the EPA's IRIS and the HEAST (U.S. EPA, 2001, 1997b). IWAIR uses these data to perform an allowable concentration calculation. See the *IWAIR Technical Background Document* for documentation of the equations.

The approach applied by IWAIR to calculate allowable concentration employs an iterative calculation algorithm. The program sets an initial waste concentration, calculates risk, compares that to the target risk, then adjusts the waste concentration and recalculates until the target risk is achieved.

If you are modeling a land application unit, landfill, waste pile, or quiescent surface impoundment and have elected to use CHEMDAT8 to calculate emissions, IWAIR will perform allowable concentration calculations for both an aqueous-phase waste and an organic-phase waste and will output the lower (or more protective) of the two resulting concentrations. For most chemicals, that will be the aqueous-phase concentration, but for a few chemicals (most notably formaldehyde), it will be the organic-phase concentration.[3] If you elected to enter your own emission rates, or if you are modeling an aerated surface impoundment, IWAIR will only calculate and output concentrations for an aqueous-phase waste.

In performing allowable concentration calculations, IWAIR ensures that calculated aqueous-phase concentrations do not exceed the soil saturation limit (for land-based units) or the solubility limit (for surface impoundments) for that chemical. This prevents impossible results from occurring. Similarly, the program also ensures that calculated organic-phase concentrations do not exceed 1,000,000 mg/kg. If the target risk or HQ cannot be achieved by any possible concentration (i.e., in an aqueous-phase waste up to the soil saturation or solubility limit, or in an organic-phase waste up to 1,000,000 mg/kg), then the program will note the maximum risk or HQ that can be reached, and the calculated concentration will be set to the concentration that

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[3] Any concentration at or below the soil saturation limit or solubility limit may occur in either an aqueous-phase waste or an organic-phase waste. The phase of the waste is not solely determined by the concentration of any one chemical. For most chemicals, the same concentration in an aqueous-phase waste will produce higher emissions than in an organic-phase waste; however, formaldehyde is a notable exception.

results in the maximum possible risk or HQ. This will be either the soil saturation limit or 1,000,000 if you are modeling a land-based unit using CHEMDAT8; the soil saturation limit if you are modeling a land-based unit with your own emission factors; or the solubility if you are modeling a surface impoundment.

For chemicals with both a CSF and an RfC, allowable concentrations are calculated based on both of these health benchmarks, and the final allowable concentration is based on the one that leads to the lowest, most protective concentration. This is almost always the one based on the CSF.

Please note that all calculated values on the RESULTS screen will be lost if you return to a previous screen and make changes.

Screen 6. Allowable Concentration Results

A. *Select Receptor (Screen 6)*

Select a single receptor to serve as the focal exposure point for the calculations by clicking on the option button associated with the receptor of choice. As discussed above in Section 5.5, you can specify up to five receptors of concern; however, results can only be seen on the screen for one receptor at a time. Once results are calculated and displayed for one receptor, you can select another receptor by clicking on one of the other receptor option buttons. You do not need to enter exposure duration because it is set by IWAIR and will be displayed when you click on the |CALCULATE| button.

B. *Specify Risk Level (Screen 6)*

Specify target cancer and noncancer risk levels. As shown in Screen 6, a drop-down box is used to allow you to select an appropriate risk level (e.g., an HQ of 1 for noncarcinogens or 1E‒6 for carcinogens).

C. *View or Override Health Benchmarks (Screen 6)*

Screen 6 allows you to view the health benchmarks that IWAIR will use in calculating risk estimates. For each benchmark, the table on the RESULTS screen shows the value and a brief reference. To see more-complete citations, click on the |FULL CITATIONS| button in the SOURCE AND JUSTIFICATION box in the upper right corner of the screen.

IWAIR gives you the option of entering your own health benchmarks. If you choose not to use the IWAIR data, you can enter alternative health benchmarks by opening the drop-down box in the RFC REF. column of the desired health benchmark and selecting USER-DEFINED, and then entering a value in the text box for the benchmark. Enter CSFs (per mg/kg-d) in text boxes located under the CSF heading and RfCs (mg/m^3) under the RFC heading. Do not use a reference *dose* in the place of a reference *concentration*. Once you have entered alternative benchmarks, they are available in future runs, and you may toggle between them and the IWAIR values using the drop-down reference box.

You must enter a user-defined health benchmark for two chemicals in IWAIR's chemical database: divalent mercury and 3,4-dimethylphenol. At the time IWAIR was released, no accepted health benchmarks were available for these chemicals from the hierarchy of sources used to populate the IWAIR health benchmark database, nor were there data available from these sources to allow the development of a health benchmark with any confidence. Thus, if you want to model one of these chemicals, you will have to enter at least one user-defined health benchmark. See Section 5 of the *IWAIR Technical Background Document* for further discussion of how health benchmarks were developed for IWAIR.

D. *Enter Source and Justification for User-Specified Values (Screen 6)*

If you choose to override the IWAIR-provided benchmarks, you should specify the source and the justification of the alternative data in the text box. It is important to provide this documentation as a reference that will allow you or another user to view and understand saved files at a later date.

E. *Direct IWAIR to Calculate Allowable Waste Concentrations (Screen 6)*

Click on the |CALCULATE| button to calculate exposure duration, air concentration, and waste concentration estimates.

F.   *View Air Concentration (Screen 6)*

Air concentration at the selected receptor point is displayed for each chemical identified as managed. For land application units, IWAIR calculates three different air concentrations, based on three different underlying emission rates: a 30-year average for residents for carcinogens, a 7-year average for workers for carcinogens, and a 1-year maximum for residents or workers exposed to noncarcinogens. Depending on the receptor selected and the chemical, IWAIR displays the appropriate air concentration. However, for chemicals that are both carcinogens and noncarcinogens, only the 30- or 7-year average used for the carcinogenic risk calculation is displayed. To calculate the 1-year maximum used in the noncarcinogenic HQ calculation, multiply the emission rate shown on the EMISSION RATES screen by the dispersion factor and then multiply by 1,000,000 (to convert units).

G.   *View Allowable Waste Concentration (Screen 6)*

Waste concentration estimates will be displayed for each chemical of concern. If CHEMDAT8 emission rates were used in the calculations, the waste phase (aqueous or organic) that served as the basis for these rates will be displayed to the right of the waste concentration text boxes.

For chemicals with both a CSF and an RfC, allowable concentrations are calculated based on both of these health benchmarks, and the final allowable concentration is based on the one that leads to the lowest, most protective concentration. This is almost always the one based on the CSF.

When using the IWAIR tool in allowable concentration calculation mode, you need to remember that the specified target levels are chemical-specific and do not represent total or cumulative cancer risk levels (i.e., the summation of the chemical-specific risk estimates). If multiple chemicals of concern are present in the waste, the cumulative cancer risk will likely be greater than the specific target risk level unless the target risk could not be reached for some or all of the chemicals. If the target risk is reached for all chemicals, you can estimate the cumulative risk posed to the receptor of concern by multiplying the number of carcinogens in the waste by the specified target risk level. For example, if a waste being managed contains five carcinogens and the single target risk level specified is 1E–6, then the cumulative risk posed to the receptor of concern would be equal to the product of the number of carcinogens in the waste (5) times the target risk level (1E–6) or 5E–6.

Done. Click the |DONE| button to initiate a new run or save the run that you have just completed. A dialog box will appear to guide you through starting a new run or saving the current run.

6.0 Example Calculations

With IWAIR, you can calculate estimates of cancer and noncancer inhalation risk or estimates of allowable waste concentration from a specified target risk level. The following example calculations demonstrate how IWAIR calculates risk or allowable concentration from emission rates and dispersion factors, using the equations presented in Section 6 of the *IWAIR Technical Background Document,* "Calculation of Risk/Hazard Quotient or Allowable Waste Concentration." You may either use IWAIR-calculated emission rates and dispersion factors or enter your own values; these example calculations do not cover how IWAIR calculates emission rates and dispersion factors.

The example calculations are based on a hypothetical exposure situation with the following conditions:

■   The WMU modeled is a landfill.

■   The waste managed in the landfill contains the carcinogen hexachlorobenzene and the noncarcinogen acrolein.

■   The emission rates and dispersion factors are IWAIR-calculated values, not user-override values.

■   The exposed individual is a resident living 25 meters from the edge of the unit.

Additional inputs used for the emission and dispersion modeling are summarized in Table 6-1.

6.1   Calculation of Risk and Hazard Quotient

To calculate risk from a specified chemical to a specified receptor, IWAIR uses the following steps:

1.   Calculate emission rates from your inputs or use the emission rates that you entered; the emission rates are chemical-specific and, if calculated by IWAIR, depend on the waste concentrations that you entered.

2.   Calculate dispersion factors from your inputs or use your entered 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.

Table 6-1. Inputs Used for Example Calculation: Landfill

Parameter	Example Calculation Value
Method, Met. Station, WMU Parameters	
Meteorological Station	Huntington, WV
WMU Type	Landfill
Wastes Managed Parameters	
Chemicals	Hexachlorobenzene, Acrolein
Concentration (mg/kg)	Hexachlorobenzene: 10 Acrolein: 3
Waste Management Unit Parameters	
Temperature (°C)	13.12 (met station default)
Wind speed (m/s)	3.179 (met station default)
Total porosity (volume fraction)	0.5 (default)
Air porosity (volume fraction)	0.25 (default)
Biodegradation	Off (default)
WMU operating life (yr)	30
WMU area (m^2)	10,000
WMU depth (m)	2
Number of cells	25
Annual waste quantity (Mg/y)	500
Waste bulk density (g/cm^3)	1.2 (default)
Receptor Parameters	
Receptor type	Resident
Receptor distance (m)	25

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

This example calculation does not cover the calculation of emission rates and dispersion factors in Steps 1 and 2. Using the inputs shown in Table 6-1, IWAIR calculates an emission rate of $1.56\text{E}{-}8$ g/m^2-s for hexachlorobenzene, an emission rate of $5.36\text{E}{-}9$ g/m^2-s for acrolein, and a dispersion factor of 3.37 [µg/m^3]/[µg/m^2-s], which is not chemical-specific (but corresponds to a receptor at 25 m).

Starting with Step 3, IWAIR calculates air concentration, as follows:

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

where

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

Plugging the values for emission rates and dispersion factor shown above into Equation 6-1 gives the following air concentration values:

$$\begin{aligned} C_{air,hcb} &= 1.56\text{E}{-}8 \times 10^6 \times 3.37 \\ &= 5.26\text{E}{-}2 \end{aligned}$$

$$\begin{aligned} C_{air,acrolein} &= 5.36\text{E}{-}9 \times 10^6 \times 3.37 \\ &= 1.806\text{E}{-}2 \end{aligned}$$

In Step 4, for carcinogens, IWAIR uses the calculated air concentration, the exposure factors, and the CSF to calculate carcinogenic risk, as follows:

$$Risk_j = \frac{C_{air,j} \times 10^{-3} \times CSF_j \times EF}{AT \times 365} \times \sum_{i=1}^{5} \frac{IR_i \times ED_i}{BW_i} \tag{6-2}$$

where

$Risk_j$ =   individual risk for chemical j (unitless)

$C_{air,j}$ = air concentration for chemical j ($\mu g/m^3$) = 5.26E-2 for hexachlorobenzene, calculated above

10^{-3} = unit conversion (mg/μg)

CSF_j = cancer slope factor for chemical j (per mg/kg-d) = 1.6 for hexachlorobezene

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) – varies by age group, see Table 6-2

ED_i = exposure duration for age group i (yr) – varies by age group, see Table 6-2

EF = exposure frequency (d/yr) = 350

365 = unit conversion (d/yr)

AT = averaging time (yr) = 70

BW_i = body weight for age group i (kg) – varies by age group, see Table 6-2.

Table 6-2. Parameter Values Used in Estimating Time-Weighted-Average Exposure

Age Range	Body Weight (kg)	Inhalation Rate (m³/day)	Exposure Duration (yrs)	Exposure Frequency (d/yr)
Child < 1 year	9.1	4.5	1	350
Child 1–5 years	15.4	7.55	5	350
Child 6–11 years	30.8	11.75	6	350
Child 12–18 years	57.2	14.0	7	350
Adult	69.1	13.3	11	350

Plugging the air concentration value for hexachlorobenzene and the exposure factors shown above into Equation 6-2 gives the following carcinogenic risk value:

$$Risk_{hcb} = \frac{5.26E\text{-}2 \times 10^{-3} \times 1.6 \times 350}{70 \times 365} \times \left(\frac{4.5 \times 1}{9.1} + \frac{7.55 \times 5}{15.4} + \frac{11.75 \times 6}{30.8} + \frac{14.0 \times 7}{57.2} + \frac{13.3 \times 11}{69.1} \right)$$

$$= 1.04E\text{-}5$$

In Step 4, for noncarcinogens, IWAIR uses the calculated air concentration and the RfC to calculate noncarcinogenic risk (HQ), as follows:

$$HQ_j = \frac{C_{air,j} \times 10^{-3}}{RfC_j} \qquad (6\text{-}3)$$

where

$\qquad$ HQ$_j$ $\quad$ = $\quad$ hazard quotient for chemical *j* (unitless)

$\qquad$ C$_{air,j}$ $\quad$ = $\quad$ air concentration for chemical *j* (μg/m^3) = 1.806E-2 for acrolein, calculated above

$\qquad$ 10^{-3} $\quad$ = $\quad$ unit conversion (mg/μg)

$\qquad$ RfC$_j$ $\quad$ = $\quad$ reference concentration for chemical *j* (mg/m^3) = 2E-5 for acrolein.

Plugging the air concentration value for acrolein into Equation 6-3 above gives the following HQ, or noncarcinogenic risk value:

$$HQ_{acrolein} = \frac{1.806E-2 \times 10^{-3}}{2E-5}$$

$$= 9.03E-1$$

6.2 Calculation of Allowable Concentration

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

1. Calculate unitized emission rates from your inputs or use your entered 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 your inputs or use your entered 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.

This example calculation does not cover the calculation of unitized emission rates and dispersion factors in Steps 1 and 2. Using the inputs shown in Table 6-1, IWAIR calculates the unitized emission rates for aqueous and organic phases for hexachlorobenzene and acrolein, shown in Table 6-3, and a dispersion factor of 3.37 [μg/m^3]/[μg/m^2-s], which is not chemical-specific. These will be used in Step 4.

**Table 6-3. Unitized Emission Rates for Allowable Concentration
Mode Example Calculation ([g/m²-s]/[mg/kg])**

Chemical	Aqueous-phase	Organic-phase
Hexachlorobenzene	1.56E$-$9	1.12E$-$13
Acrolein	1.79E$-$9	7.28E$-$10

Starting with Step 3, IWAIR calculates target air concentrations by solving Equations 6-2 and 6-3 above for air concentration. For carcinogens,

$$C_{air,j} = \frac{Risk_j \times AT \times 365}{10^{-3} \times CSF_j \times EF \times \sum\limits_{i=1}^{5} \dfrac{IR_i \times ED_i}{BW_i}} \tag{6-4}$$

Plugging a target risk value of 1E$-$5 into Equation 6-4 gives the following air concentration:

$$C_{air,hcb} = \frac{1E-5 \times 70 \times 365}{10^{-3} \times 1.6 \times 350 \times \left(\dfrac{4.5 \times 1}{9.1} + \dfrac{7.55 \times 5}{15.4} + \dfrac{11.75 \times 6}{30.8} + \dfrac{14.0 \times 7}{57.2} + \dfrac{13.3 \times 11}{69.1} \right)}$$

$$= 5.03E-2$$

For noncarcinogens,

$$C_{air,j} = HQ_j \times RfC_j \times 10^3 \tag{6-5}$$

Plugging a target HQ of 1 into Equation 6-5 gives the following air concentration:

$$C_{air,j} = 1 \times 2E-5 \times 10^3$$

$$= 2E-2$$

In Step 4, IWAIR uses an equation comparable to Equation 6-1 to relate target 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. The emission rate, E_j, is replaced by $C_{waste} \times E_{j,unitized}$, where C_{waste} is waste concentration in mg/kg and $E_{j,unitized}$ is the unitized emission rate for chemical j in [g/m²-s]/[mg/kg]. This new equation, which assumes that emissions are linear with waste concentration, is as follows:

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

where

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

Equation 6-6 may be solved for waste concentration, as follows:

$$C_{waste} = \frac{C_{air}}{E_{unit} \times 10^6 \times DF} \qquad (6\text{-}7)$$

IWAIR uses this equation with both an aqueous-phase emission rate and an organic-phase emission rate, to estimate an aqueous-phase waste concentration and an organic-phase waste concentration.

For hexachlorobenzene in an aqueous-phase waste, plugging the air concentration calculated above, the unitized emission rate for aqueous-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{5.03E\text{-}2}{1.56E\text{-}9 \times 10^6 \times 3.37}$$

$$= 9.57$$

For hexachlorobenzene in an organic-phase waste, plugging the air concentration calculated above, the unitized emission rate for organic-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{5.03E\text{-}2}{1.12E\text{-}13 \times 10^6 \times 3.37}$$

$$= 1.33E\text{+}5$$

In Step 5, IWAIR then examines these waste concentrations to ensure that they do not exceed physical limits (i.e., soil saturation concentration for aqueous-phase wastes and 1E+6 mg/kg for organic-phase wastes). If either waste concentration exceeds the applicable limit, it is

discarded.[1] If both values are possible, IWAIR selects the lower of the two as the allowable concentration.

The soil saturation concentration for hexachlorobenzene, given the inputs in Table 6-1, is 26 mg/kg. Because the aqueous-phase concentration for hexachlorobenzene calculated above (C_{waste} = 9.57) does not exceed 26 mg/kg, it is possible and is not discarded. Similarly, the organic-phase concentration does not exceed 1E+6 mg/kg, and is therefore possible and not discarded. Since both aqueous-phase and organic-phase concentrations are possible, IWAIR selects the lower of the two as the allowable concentration. In this case, the aqueous-phase waste value is lower for the target risk of 1E−5; consequently, the allowable concentration for hexachlorobenzene is 9.57 mg/kg, based on an aqueous-phase waste.

The calculations for Steps 4 and 5 are similar for acrolein. In an aqueous-phase waste, plugging the air concentration calculated above, the unitized emission rate for aqueous-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{2E-2}{1.79E-9 \times 10^6 \times 3.37}$$

$$= 3.32$$

For acrolein in an organic-phase waste, plugging the air concentration calculated above, the unitized emission rate for organic-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{2E-2}{7.28E-10 \times 10^6 \times 3.37}$$

$$= 8.15$$

The soil saturation concentration for acrolein, given the inputs in Table 6-1, is about 45,700 mg/kg. Because the calculated aqueous-phase concentration for acrolein is below this level, the value is possible and is not discarded.

Similarly, the organic-phase concentration does not exceed 1E+6 mg/kg and is therefore possible and not discarded. Since both aqueous-phase and organic-phase concentrations are possible, IWAIR selects the lower of the two as the allowable concentration. In this case, the aqueous-phase waste value is lower. Thus, for a target HQ of 1, the allowable concentration of acrolein is 3.32 mg/kg, based on an aqueous-phase waste.

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[1] If they are both discarded, the soil saturation limit or 1E+6 is used, whichever results in the greatest risk.

6.0 Example Calculations

With IWAIR, you can calculate estimates of cancer and noncancer inhalation risk or estimates of allowable waste concentration from a specified target risk level. The following example calculations demonstrate how IWAIR calculates risk or allowable concentration from emission rates and dispersion factors, using the equations presented in Section 6 of the *IWAIR Technical Background Document,* "Calculation of Risk/Hazard Quotient or Allowable Waste Concentration." You may either use IWAIR-calculated emission rates and dispersion factors or enter your own values; these example calculations do not cover how IWAIR calculates emission rates and dispersion factors.

The example calculations are based on a hypothetical exposure situation with the following conditions:

- ■   The WMU modeled is a landfill.

- ■   The waste managed in the landfill contains the carcinogen hexachlorobenzene and the noncarcinogen acrolein.

- ■   The emission rates and dispersion factors are IWAIR-calculated values, not user-override values.

- ■   The exposed individual is a resident living 25 meters from the edge of the unit.

Additional inputs used for the emission and dispersion modeling are summarized in Table 6-1.

6.1   Calculation of Risk and Hazard Quotient

To calculate risk from a specified chemical to a specified receptor, IWAIR uses the following steps:

1.   Calculate emission rates from your inputs or use the emission rates that you entered; the emission rates are chemical-specific and, if calculated by IWAIR, depend on the waste concentrations that you entered.

2.   Calculate dispersion factors from your inputs or use your entered 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.

Table 6-1. Inputs Used for Example Calculation: Landfill

Parameter	Example Calculation Value
Method, Met. Station, WMU Parameters	
Meteorological Station	Huntington, WV
WMU Type	Landfill
Wastes Managed Parameters	
Chemicals	Hexachlorobenzene, Acrolein
Concentration (mg/kg)	Hexachlorobenzene: 10 Acrolein: 3
Waste Management Unit Parameters	
Temperature (°C)	13.12 (met station default)
Wind speed (m/s)	3.179 (met station default)
Total porosity (volume fraction)	0.5 (default)
Air porosity (volume fraction)	0.25 (default)
Biodegradation	Off (default)
WMU operating life (yr)	30
WMU area (m^2)	10,000
WMU depth (m)	2
Number of cells	25
Annual waste quantity (Mg/y)	500
Waste bulk density (g/cm^3)	1.2 (default)
Receptor Parameters	
Receptor type	Resident
Receptor distance (m)	25

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

This example calculation does not cover the calculation of emission rates and dispersion factors in Steps 1 and 2. Using the inputs shown in Table 6-1, IWAIR calculates an emission rate of $1.56E{-}8$ g/m^2-s for hexachlorobenzene, an emission rate of $5.36E{-}9$ g/m^2-s for acrolein, and a dispersion factor of 3.37 [μg/m^3]/[μg/m^2-s], which is not chemical-specific (but corresponds to a receptor at 25 m).

Starting with Step 3, IWAIR calculates air concentration, as follows:

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

where

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

 Plugging the values for emission rates and dispersion factor shown above into Equation 6-1 gives the following air concentration values:

$$C_{air,hcb} = 1.56E{-}8 \times 10^6 \times 3.37$$
$$= 5.26E{-}2$$

$$C_{air,acrolein} = 5.36E{-}9 \times 10^6 \times 3.37$$
$$= 1.806E{-}2$$

In Step 4, for carcinogens, IWAIR uses the calculated air concentration, the exposure factors, and the CSF to calculate carcinogenic risk, as follows:

$$Risk_j = \frac{C_{air,j} \times 10^{-3} \times CSF_j \times EF}{AT \times 365} \times \sum_{i=1}^{5} \frac{IR_i \times ED_i}{BW_i} \qquad\qquad (6\text{-}2)$$

where

$Risk_j$ =   individual risk for chemical j (unitless)

$$C_{air,j} \quad = \quad \text{air concentration for chemical } j \text{ (}\mu\text{g/m}^3\text{)} = 5.26\text{E}{-}2 \text{ for hexachlorobenzene,}$$
calculated above

10^{-3} = unit conversion (mg/µg)

CSF_j = cancer slope factor for chemical j (per mg/kg-d) = 1.6 for hexachlorobezene

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 (m³/d) – varies by age group, see Table 6-2

ED_i = exposure duration for age group i (yr) – varies by age group, see Table 6-2

EF = exposure frequency (d/yr) = 350

365 = unit conversion (d/yr)

AT = averaging time (yr) = 70

BW_i = body weight for age group i (kg) – varies by age group, see Table 6-2.

Table 6-2. Parameter Values Used in Estimating Time-Weighted-Average Exposure

Age Range	Body Weight (kg)	Inhalation Rate (m³/day)	Exposure Duration (yrs)	Exposure Frequency (d/yr)
Child < 1 year	9.1	4.5	1	350
Child 1–5 years	15.4	7.55	5	350
Child 6–11 years	30.8	11.75	6	350
Child 12–18 years	57.2	14.0	7	350
Adult	69.1	13.3	11	350

Plugging the air concentration value for hexachlorobenzene and the exposure factors shown above into Equation 6-2 gives the following carcinogenic risk value:

$$Risk_{hcb} = \frac{5.26\text{E}{-}2 \times 10^{-3} \times 1.6 \times 350}{70 \times 365} \times \left(\frac{4.5 \times 1}{9.1} + \frac{7.55 \times 5}{15.4} + \frac{11.75 \times 6}{30.8} + \frac{14.0 \times 7}{57.2} + \frac{13.3 \times 11}{69.1} \right)$$

$$= 1.04\text{E}{-}5$$

In Step 4, for noncarcinogens, IWAIR uses the calculated air concentration and the RfC to calculate noncarcinogenic risk (HQ), as follows:

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

where

HQ_j = hazard quotient for chemical *j* (unitless)

$\text{C}_{air,j}$ = air concentration for chemical *j* ($\mu g/m^3$) = 1.806E–2 for acrolein, calculated above

10^{-3} = unit conversion (mg/μg)

RfC_j = reference concentration for chemical *j* (mg/m^3) = 2E–5 for acrolein.

Plugging the air concentration value for acrolein into Equation 6-3 above gives the following HQ, or noncarcinogenic risk value:

$$\text{HQ}_{acrolein} = \frac{1.806\text{E}-2 \times 10^{-3}}{2\text{E}-5}$$

$$= 9.03\text{E}-1$$

6.2   Calculation of Allowable Concentration

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

1. Calculate unitized emission rates from your inputs or use your entered 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 your inputs or use your entered 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.

This example calculation does not cover the calculation of unitized emission rates and dispersion factors in Steps 1 and 2. Using the inputs shown in Table 6-1, IWAIR calculates the unitized emission rates for aqueous and organic phases for hexachlorobenzene and acrolein, shown in Table 6-3, and a dispersion factor of 3.37 [$\mu g/m^3$]/[$\mu g/m^2$-s], which is not chemical-specific. These will be used in Step 4.

Table 6-3. Unitized Emission Rates for Allowable Concentration Mode Example Calculation ([g/m²-s]/[mg/kg])

Chemical	Aqueous-phase	Organic-phase
Hexachlorobenzene	1.56E−9	1.12E−13
Acrolein	1.79E−9	7.28E−10

Starting with Step 3, IWAIR calculates target air concentrations by solving Equations 6-2 and 6-3 above for air concentration. For carcinogens,

$$C_{air,j} = \frac{Risk_j \times AT \times 365}{10^{-3} \times CSF_j \times EF \times \sum_{i=1}^{5} \frac{IR_i \times ED_i}{BW_i}} \tag{6-4}$$

Plugging a target risk value of 1E−5 into Equation 6-4 gives the following air concentration:

$$C_{air,hcb} = \frac{1E-5 \times 70 \times 365}{10^{-3} \times 1.6 \times 350 \times \left(\frac{4.5 \times 1}{9.1} + \frac{7.55 \times 5}{15.4} + \frac{11.75 \times 6}{30.8} + \frac{14.0 \times 7}{57.2} + \frac{13.3 \times 11}{69.1} \right)}$$

$$= 5.03E-2$$

For noncarcinogens,

$$C_{air,j} = HQ_j \times RfC_j \times 10^3 \tag{6-5}$$

Plugging a target HQ of 1 into Equation 6-5 gives the following air concentration:

$$C_{air,j} = 1 \times 2E-5 \times 10^3$$

$$= 2E-2$$

In Step 4, IWAIR uses an equation comparable to Equation 6-1 to relate target 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. The emission rate, E_j, is replaced by $C_{waste} \times E_{j,unitized}$, where C_{waste} is waste concentration in mg/kg and $E_{j,unitized}$ is the unitized emission rate for chemical j in [g/m²-s]/[mg/kg]. This new equation, which assumes that emissions are linear with waste concentration, is as follows:

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

where

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

Equation 6-6 may be solved for waste concentration, as follows:

$$C_{waste} = \frac{C_{air}}{E_{unit} \times 10^6 \times DF} \tag{6-7}$$

IWAIR uses this equation with both an aqueous-phase emission rate and an organic-phase emission rate, to estimate an aqueous-phase waste concentration and an organic-phase waste concentration.

For hexachlorobenzene in an aqueous-phase waste, plugging the air concentration calculated above, the unitized emission rate for aqueous-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{5.03E{-}2}{1.56E{-}9 \times 10^6 \times 3.37}$$

$$= 9.57$$

For hexachlorobenzene in an organic-phase waste, plugging the air concentration calculated above, the unitized emission rate for organic-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{5.03E{-}2}{1.12E{-}13 \times 10^6 \times 3.37}$$

$$= 1.33E{+}5$$

In Step 5, IWAIR then examines these waste concentrations to ensure that they do not exceed physical limits (i.e., soil saturation concentration for aqueous-phase wastes and 1E+6 mg/kg for organic-phase wastes). If either waste concentration exceeds the applicable limit, it is

discarded.[1] If both values are possible, IWAIR selects the lower of the two as the allowable concentration.

The soil saturation concentration for hexachlorobenzene, given the inputs in Table 6-1, is 26 mg/kg. Because the aqueous-phase concentration for hexachlorobenzene calculated above (C_{waste} = 9.57) does not exceed 26 mg/kg, it is possible and is not discarded. Similarly, the organic-phase concentration does not exceed 1E+6 mg/kg, and is therefore possible and not discarded. Since both aqueous-phase and organic-phase concentrations are possible, IWAIR selects the lower of the two as the allowable concentration. In this case, the aqueous-phase waste value is lower for the target risk of 1E–5; consequently, the allowable concentration for hexachlorobenzene is 9.57 mg/kg, based on an aqueous-phase waste.

The calculations for Steps 4 and 5 are similar for acrolein. In an aqueous-phase waste, plugging the air concentration calculated above, the unitized emission rate for aqueous-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{2E{-}2}{1.79E{-}9 \times 10^6 \times 3.37}$$

$$= 3.32$$

For acrolein in an organic-phase waste, plugging the air concentration calculated above, the unitized emission rate for organic-phase waste shown in Table 6-3, and the dispersion factor shown earlier into Equation 6-7 gives the following waste concentration:

$$C_{waste} = \frac{2E{-}2}{7.28E{-}10 \times 10^6 \times 3.37}$$

$$= 8.15$$

The soil saturation concentration for acrolein, given the inputs in Table 6-1, is about 45,700 mg/kg. Because the calculated aqueous-phase concentration for acrolein is below this level, the value is possible and is not discarded.

Similarly, the organic-phase concentration does not exceed 1E+6 mg/kg and is therefore possible and not discarded. Since both aqueous-phase and organic-phase concentrations are possible, IWAIR selects the lower of the two as the allowable concentration. In this case, the aqueous-phase waste value is lower. Thus, for a target HQ of 1, the allowable concentration of acrolein is 3.32 mg/kg, based on an aqueous-phase waste.

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[1] If they are both discarded, the soil saturation limit or 1E+6 is used, whichever results in the greatest risk.

Appendix A

Considering Risks from Indirect Pathways

Appendix A

Considering Risks from Indirect Pathways

A.1   What are "Indirect Risks"?

IWAIR assesses exposures by direct inhalation of a contaminant. 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 contaminant 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.

> Direct Pathways: An individual is directly exposed to the contaminated medium, such as air or groundwater, into which the chemical was released.
>
> Indirect Pathways: An individual is indirectly exposed when a contaminant 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.

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.
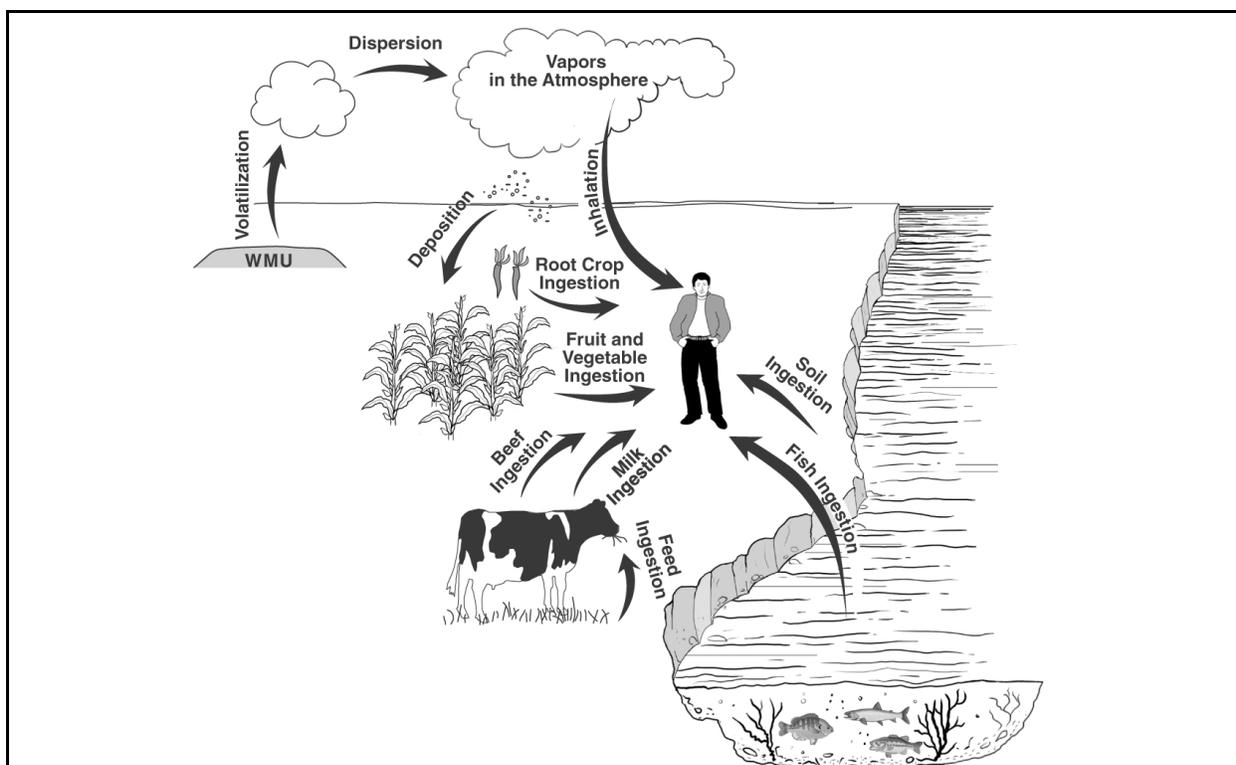
Figure A-1. Indirect exposure pathways.

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 of the *IWAIR Technical Background Document*; 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. Chemical contaminants 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 contaminant 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 of the *IWAIR Technical Background Document*; 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 contaminant 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 the *IWAIR Technical Background Document* 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

Parameter Guidance

Appendix B

Parameter Guidance

This appendix provides you with guidance on all parameter values needed to run IWAIR. This guidance covers all parameters that you may enter in text boxes and most selections from drop-down boxes. It does not include most option buttons, as those are covered in the operational guidance in Sections 4 and 5. However, a few options are covered here, as well as in Sections 4 and 5.

This appendix is organized by screen. Some parameters are applicable only to risk mode or allowable concentration mode; those are so noted.

B.1   Method, Met. Station, WMU (Screen 1A)

Most of the options on Screen 1A are covered in the operational guidance in Sections 4 and 5. There are only two parameters for this screen: zip code and latitude/longitude. You will only need to enter data for one or the other.

Zip Code. This is the 5-digit zip code for the physical location of your facility. IWAIR uses this zip code to assign the most appropriate meteorological station to your site; therefore, you should not use the zip code from a mailing address, such as a post office box or a company headquarters. The zip code database includes zip codes established through 1999. If your facility has a new zip code that was established more recently, you will get an error message indicating that it is not a valid zip code, because it is not in IWAIR's database. If this occurs, you can use your old zip code, use a nearby zip code, or select a meteorological station using latitude and longitude.

Latitude and Longitude. These are the latitude and longitude coordinates for the physical location of your facility. At a minimum, the program requires that degrees for latitude and longitude be entered. If available, the minutes and seconds should be supplied to ensure that the most appropriate station is selected for a site. Latitude and longitude can be obtained from most maps of the area where your facility is located.

B.2   Wastes Managed and Add/Modify Chemicals (Screens 2A and 2B)

B.2.1   Wastes Managed

Sections 4 and 5 cover the selection of chemicals for your waste. There is only one parameter to be entered on Screen 2A: waste concentration. This is only needed for risk calculations.

Waste Concentration (mg/L or mg/kg). This is the concentration of each chemical in your waste. It should reflect the waste or influent going into your unit, not the concentration within the unit. For surface impoundments, it should be in mg/L or ppm. For land application units, landfills, and waste piles, it should be in mg/kg or ppm. This value must be greater than zero; the sum of all concentrations entered must be less than or equal to one million.

B.2.2   Add/Modify Chemicals (Screen 2B)

The ADD/MODIFY CHEMICALS screen requires you to enter numerous chemical-specific parameters. These are organized below into chemical identifiers, physical-chemical properties, and health benchmarks.

B.2.2.1 Chemical Identifiers

Chemical Name. If you are entering a new chemical, you can enter the chemical name here. If you are modifying or making a new entry for an existing chemical, you will not need to enter a chemical name; IWAIR will fill it in automatically. Do not add any user designation to the end of the chemical name you enter—IWAIR will do that automatically. Enter the chemical name exactly as you would like it to sort and display. For example, if you want 1,2,4-trichlorobenzene to sort under T instead of 1, enter it as "trichlorobenzene, 1,2,4-".

CAS Number. If you are entering a new chemical, you can enter the Chemical Abstracts Service (CAS) number here. If you are modifying or making a new entry for an existing chemical, you will not need to enter a CAS number; IWAIR will fill it in automatically. IWAIR does not use leading zeros on CAS numbers; therefore, for consistency with the data provided with IWAIR, it is recommended that you use leading spaces instead of leading zeros for CAS numbers shorter than the maximum length.

B.2.2.2 Physical-Chemical Properties. Data on many physical-chemical properties can be obtained from the following sources:

- ■   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), and

■ Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles (ATSDR, 2001).

In addition, a useful source of data on chemical properties for dioxins is EPA's *Dioxin Reassessment* (U.S. EPA, 2000a).

Molecular Weight (g/mol). Molecular weight is used to estimate emissions. Values can be obtained from the literature, including from the SCDM; HSDB; and CHEMFATE. This value must be greater than or equal to 1 g/mol (the molecular weight of a single hydrogen ion). No maximum limit is enforced. IWAIR has been tested for molecular weights between 1 and 400 g/mol.

Density (g/cm³). 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 that water). Unless the value is very near 1 g/cm³ (the density of water), the model is not sensitive to variations in the value. Values can be obtained from the literature, including from the SCDM; Merck Index; and HSDB. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for densities between 0.01 and 14 g/cm³.

Vapor Pressure (mmHg). Vapor pressure and the mole fraction 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. Values can be obtained from the literature, including from the SCDM and HSDB. Vapor pressure may be reported in other units, such as atmospheres or torr; torr is equivalent to mmHg, but data in atmospheres will need to be converted. Different vapor pressures may be reported for the same chemical at different temperatures. For best results, choose a vapor pressure reported at a temperature around 20–25°C. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for vapor pressures between 0 and 5,300 mmHg.

Henry's Law Constant (atm-m³/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, including from the SCDM; 2000 *Dioxin Reassessment* (for dioxins); HSDB; CHEMFATE; and ChemFinder. If Henry's law constant is not available, it can be calculated from the chemical's vapor pressure, molecular weight, and solubility using the following equation (Lyman et al., 1990):

$$H = \frac{\left(\dfrac{VP}{760}\right)}{\left(\left(\dfrac{S}{MW}\right) \times \left(\dfrac{1000}{1000}\right)\right)}$$

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).

The value for Henry's law constant must be greater than zero. No maximum limit is enforced. IWAIR has been tested for Henry's law constants between 4E‒11 and 1.2 atm-m^3/mol-K.

   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). Values can be obtained from the literature, including from the SCDM; Merck Index; *Dioxin Reassessment* (for dioxins); HSDB; and CHEMFATE. This value must be greater than zero and less than or equal to one million. IWAIR has been tested for solubilities from 1.93E‒5 to 1,000,000 mg/L.

   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; this is not comparable to biodegradation rate and should not be used in IWAIR. However, you can calculate the soil biodegradation rate from the half-life as follows:

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

where

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

An excellent reference for soil biodegradation data (and the one used for all soil biodegradation rates included with IWAIR) is Howard et al. (1991). This reference provides both high-end and low-end half-life data for soil biodegradation. The high-end values were used in IWAIR. In general, half-lives are reported in hours. Values for very short half-lives are given in minutes or seconds. All values, except the ones already given in seconds, must be converted to seconds before using the above equation to convert to biodegradation rate. The soil biodegradation rate may be zero if the chemical does not biodegrade; however, because a zero value would cause IWAIR to try to divide by zero, IWAIR converts values entered as zero to 1E‒20, which results

in negligible biodegradation. No maximum limit is enforced. IWAIR has been tested for soil biodegradation rates from 1E–20 to 0.0004 s^{-1}.

Antoine's Constants: A, B, or C. Antoine's constants are used to adjust vapor pressure and Henry's law constant to ambient temperature. While not explicitly reported with units, they are intended to adjust vapor pressure in mmHg based on temperature in degrees Celsius. Values for Antoine's constants are available in Reid et al. (1977). A and B must be greater than or equal to zero. C may be negative. No maximum limits are enforced. IWAIR has been tested for A values from 0 to 14; B values from 0 to 5,400; and C values from 0 to 292.

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, 2001c):

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

where

$$
\begin{aligned}
D_W &= \text{diffusivity in water (cm}^2\text{/s)} \\
T &= \text{temperature (°C)} \\
273.16 &= \text{unit conversion (°C to °K)} \\
MW &= \text{molecular weight (g/mol)} \\
\rho &= \text{density (g/cm}^3\text{).}
\end{aligned}
$$

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

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

The value for diffusivity in water must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of diffusivity in water from 5E–6 to 3E–5 cm²/s.

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, 2001c):

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

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:

$$MW_{cor} = (1 - 0.000015 \times MW^2)$$

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

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

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

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

$$D_a = \left(\frac{154}{MW} \right)^{0.5} \times 0.068$$

Diffusivity in air values must be greater than or equal to zero. No maximum limit is enforced. IWAIR has been tested for values of diffusivity in air from 0 to 0.25 cm^2/s.

      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} and should be entered as the log in IWAIR. Values can be obtained from the literature, including the SCDM. Log K_{ow} is unitless. Log K_{ow} may have negative values, reflecting K_{ow} values less than 1. Due to model limitations, log K_{ow} may not be less than -10 or greater than 10; IWAIR has been tested for this entire range.

      Hydrolysis Constant (s^{-1}). This value, which is used to estimate losses by hydrolysis, is the hydrolysis rate constant at neutral pH. An excellent source of data on hydrolysis rate constants (and the one used for all hydrolysis rate constants included with IWAIR) is Kollig (1993). The hydrolysis constant may be zero if the chemical does not hydrolyze; it cannot be less than zero. No maximum limit is enforced. IWAIR has been tested for values of hydrolysis constants from 0 to 22 s^{-1}.

K_1 (L/g-h). K_1 is used to estimate biodegradation losses in surface impoundments. There are very few literature sources for K_1. The primary source of data is Coburn et al. (1988). Values for K_1 in CHEMDAT8 and IWAIR were taken from this source. If you have rate study data at very low concentrations, that rate can be used for K_1. K_1 may be zero if the chemical does not biodegrade; it cannot be less than zero. No maximum limit is enforced. IWAIR has been tested for values of K_1 from 0 to 25 L/g-h.

K_{max} (mg volatile organics/g-h). K_{max} is used to estimate biodegradation losses in surface impoundments. There are very few literature sources for K_{max}. The primary source of data is Coburn et al. (1988). Values for K_{max} in CHEMDAT8 and IWAIR were taken from this source. If you have rate study data at very high concentrations, that rate can be used for K_{max}. K_{max} may be zero if the chemical does not biodegrade; it cannot be less than zero. No maximum limit is enforced. IWAIR has been tested for values of K_{max} from 0 to 100 mg VO/g-h.

B.2.2.3 <u>Health Benchmarks</u>

Cancer Slope Factor (CSF) $(mg/kg/d)^{-1}$. The inhalation CSF is used to evaluate risk for carcinogens. 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. Inhalation CSFs are used in the model for carcinogenic constituents, regardless of the availability of an RfC. If a value for the inhalation CSF is not available, you should enter "NA" in the CSF field, rather than zero. IWAIR must have a numeric value for either the inhalation CSF or RfC to calculate risk or allowable concentration. If a numeric value is entered, it must be greater than zero. No maximum limit is enforced. IWAIR has been tested for CSF values from 0.00001 to 150,000 $(mg/kg/d)^{-1}$.

Reference Concentration (RfC) (mg/m^3). The RfC is used to evaluate noncancer hazards posed by inhalation exposures to chemicals. 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. If a value for the RfC is not available, you should enter "NA" in the RfC field, rather than zero. IWAIR must have a numeric value for either the inhalation CSF or RfC to calculate risk or allowable concentration. If a numeric value is entered, it must be greater than zero. No maximum limit is enforced. IWAIR has been tested for RfC values from 0.00001 to 40 mg/m^3.

Human health benchmarks contained in databases developed by EPA were used whenever available. Benchmarks were obtained in the following order of preference:

- ■   Integrated Risk Information System (IRIS) (U.S. EPA, 2001b)

- ■   Superfund Technical Support Center Provisional Benchmarks (U.S. EPA, 1998b, 1999a, 1999b, 2000b)

- ■   Health Effects Assessment Summary Tables (HEAST) (U.S. EPA, 1997a)

■   Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels
          (MRLs) (ATSDR, 2001)

■   California Environmental Protection Agency (CalEPA) chronic inhalation
          reference exposure levels (RELs) and cancer potency factors (CalEPA, 1999a,
          1999b, 2000)

■   EPA health assessment documents (U.S. EPA, 1986, 1987a, 1998a)

■   Various other EPA health benchmark sources.

B.3   WMU Data for CHEMDAT8 (Screens 3A through 3D)

B.3.1   WMU Data for CHEMDAT8 – Surface Impoundment (Screen 3A)

B.3.1.1 <u>Meteorological Station Parameters</u>. These inputs are used only for the
emissions modeling, not the dispersion modeling, which uses hourly meteorological data, not
annual averages. Therefore, changes to these inputs will not affect the dispersion factors.

Wind Speed (m/s). IWAIR uses wind speed 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. By default, IWAIR uses the
average annual wind speed from the meteorological station that was assigned to your location.
However, you may wish to override the default if you have site-specific data on wind speed. If
you do override, you should use an overall annual average in all directions, not any measure of
peak wind speed or average only in the prevailing wind direction. Also, wind speed is often
reported in knots or mph. However, for use in IWAIR, wind speed must be converted to m/s.
This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested
for values of wind speed from 0.01 to 100 m/s; however, a realistic range for average annual
wind speed is about 2 to 10 m/s.

Temperature (°C). IWAIR uses temperature to correct various temperature-dependent
chemical properties used in emissions modeling (Henry's law constant and vapor pressure) from
a standard temperature to the ambient temperature. By default, IWAIR uses the average annual
temperature from the meteorological station that was assigned to your location. However, you
may wish to override the default if you have site-specific data on temperature. If you do
override, you should use an annual average temperature. Temperature may be reported in
degrees Fahrenheit (°F); however, for use in IWAIR, temperature must be converted to degrees
Celsius (°C). This value must be greater than or equal to -100°C. No maximum limit is
enforced.   IWAIR has been tested for values of temperature from 0 to 50°C.

B.3.1.2 <u>SI Dimensions, Loading Information</u>

Biodegradation (on/off). This option, in conjunction with the ACTIVE BIOMASS input, allows
you to determine what type of biodegradation is modeled for your unit. 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 compose 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 acclimate and adapt to the chemicals present.

Setting biodegradation to |OFF| turns off direct biodegradation. It 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. Setting active biomass to zero also turns off direct biodegradation (in fact, if you have set biodegradation |ON| and then set active biomass to zero, IWAIR will automatically reset the biodegradation option to |OFF|). If you set biodegradation to |OFF|, IWAIR will remove the default value for active biomass, and you will have to enter a value (typically zero, but this is not required, and it may be greater than zero if you wish to model the transitional period before direct biodegradation occurs).

If your impoundment is biologically active, it recommended that you leave biodegradation set to |ON| (the default). If your impoundment is not biologically active, it is recommended that you set biodegradation to |OFF| and active biomass to zero.

Operating Life (yr). This parameter is the expected remaining operating life of your unit, from the time you are modeling until you expect it to be closed. Operating life does not affect emissions estimates for surface impoundments, which are modeled at steady state. However, operating life may affect exposure duration. IWAIR uses default exposure durations of 30 years for residents and 7.2 years for workers. However, proper closure of a surface impoundment typically ends all exposures. Therefore, if the operating life you specify is less than 30 or 7.2 years, IWAIR caps the exposure duration at the operating life. Values in excess of 30 years will not affect the results for residents, and values in excess of 7.2 years will not affect the results for workers. Operating life should be entered in years. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of operating life from 0.01 to 100 years.

Depth of Unit (m). This is the average depth of your unit in meters (m). If your unit is not a constant depth, use the average or most typical depth. If you have depth reported in units such as feet, you will need to convert them to meters. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of depth from 0.01 to 30 m.

Area of Unit (m²). This is the total surface area of your unit in m². Areas may be reported in acres or hectares; these values will need to be converted to m² for use in IWAIR. This value must be greater than or equal to 81 m² and less than or equal to 8,090,000 m²; these are the smallest and largest areas for which IWAIR can interpolate dispersion factors for ground-level sources. IWAIR has been tested for this full range.

Annual Flow of Waste (m³/yr). This is the total amount of waste that flows through your impoundment in a year, in m³/yr. Flow is often reported in millions of gallons per day (MGD) or

other units; you will need to convert to m^3/yr for use in IWAIR. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of annual flow of waste from 0.01 to 10,000,000 m^3/yr.

B.3.1.3 Aeration Option Information

Type of Aeration. This option allows you to identify whether your impoundment is aerated and, if so, the specific type of aeration. IWAIR can model no aeration (quiescent), diffused air aeration, mechanical aeration, and both (diffused air and mechanical).

If your impoundment is not aerated, choose NO AERATION.

If your impoundment is aerated only by mechanical aerators (these are rotating impellers), choose MECHANICAL AERATION.

If your impoundment is aerated only by diffused air flow from submerged aerators, choose DIFFUSED AIR AERATION.

If your impoundment is aerated by both mechanical aerators and diffused air aerators, choose BOTH (DIFFUSED AIR & MECHANICAL).

Fraction of Surface Area Agitated. Unless you chose NO AERATION, you will need to enter the fraction of surface area agitated. If you have data on agitated area, you can divide the agitated area by the total area (in the same units) to obtain this fraction. Alternatively, you can estimate this visually. This input is a unitless fraction and must be greater than zero and less than or equal to one. IWAIR has been tested with values of fraction agitated from 0.01 to 1.

Submerged Air Flow (m^3/s). Submerged air flow is used for diffused air systems; you will need to enter a value if you chose either DIFFUSED AIR AERATION or BOTH (DIFFUSED AIR & MECHANICAL). This is the total air flow of all diffusers in the impoundment. For example, if you had two diffusers, each with an air flow of 0.1 m^3/s, you would enter 0.2 m^3/s here. If you enter a value here, it must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of submerged air flow from 0.01 to 100 m^3/s.

B.3.1.4 Waste Characteristics Information

Type of Waste. In order to generate an accurate estimate of a constituent's volatile emissions, you must define the physical and chemical characteristics of the waste you are modeling. In particular, you must identify whether or not the waste is best described as a

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 limits. However, it is possible for the specific components of the waste to raise the effective solubility level for a chemical, allowing it to remain in solution at concentrations above the typical solubility limit.

Organic-phase waste: a waste that is predominantly organic chemicals, with a high concentration of organics. Concentrations of some chemicals may exceed solubility, 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.

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 contaminant has for one phase (for example, air) relative to another phase (for example, water) that drives the volatilization of organic chemicals. Your choice of waste matrix will significantly affect the rate of emissions from the waste. The following discussion is intended to provide background on emissions modeling as it relates to waste type, guidance on making this selection, and clarification of the modeling consequences of choosing AQUEOUS versus ORGANIC in IWAIR. Note that you will only be asked to choose a waste type for risk calculations; for allowable concentration calculations, IWAIR calculates emission rates for both aqueous and organic waste types and selects the one that achieves the target risk or HQ at the lowest concentration applicable to the waste type.

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 absorbed to solids, dissolved in liquids, or assume a 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 more heavily to air, while others tend to partition more heavily 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 moles of the chemical per total moles) 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

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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.

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 may be 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 has exceeded the bounds of "dilute aqueous" and is more appropriately modeled using Raoult's law. Chemicals exceeding solubility limits will typically come out of solution and behave more like pure, organic-phase component. However, solubility 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 limit. This scenario (an aqueous-phase waste with concentrations above typical solubility 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.

For surface impoundments, where the waste is a liquid, the model uses an 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 resistance to transfer in the liquid phase), and the gas-phase mass transfer factor (which accounts for resistance 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.

In the two-film model for surface impoundments, the gas-phase and liquid-phase mass transfer coefficients are strongly affected by the turbulence of the surface impoundment 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.

When in allowable concentration calculation mode, IWAIR calculates both aqueous-phase and organic-phase emission rates. However, aqueous-phase emission rates, as discussed above, are only applicable up to the solubility limit. If the use of the aqueous-phase emission

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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.

rate results in an allowable concentration in excess of the solubility limit, IWAIR will use the organic-phase rate instead.

   Molecular Weight of Waste (g/mol) (Only for Risk Calculation). If you choose to model an organic-phase waste, you will need to enter the average molecular weight of the waste. This may be calculated from the molecular weights of the component constituents as follows:

$$MW_{waste} = \frac{\Sigma\ (C_i) \times (1\ m^3)}{\Sigma\ (C_i/MW_i) \times (1\ m^3)}$$

where

   MW_{waste} =   molecular weight of waste (g/mol)
   C_i =   waste concentration of contaminant i (mg/L = g/m^3)
   MW_i =   molecular weight of contaminant i (g/mol).

This assumes that the average molecular weight of the unspecified fraction of the organic waste matrix has the same average molecular weight as the specified fraction (i.e., the input contaminant concentrations). Appendix C provides values for molecular weight for all IWAIR chemicals.

   This value must be greater than or equal to 1 (the molecular weight of a hydrogen ion). No maximum limit is enforced. IWAIR has been tested for values from 1 to 400 g/mol.

   Density of Waste (g/cm³) (Only for Risk Calculation). If you choose to model an organic-phase waste, you will need to enter the density of the waste. It is best to use a measured value for this, but you can estimate it as follows:

$$\rho_{waste} = \frac{\Sigma\ (C_i)}{\Sigma\ (C_i/\rho_i)}$$

where

   ρ_{waste} =   density of waste (g/cm^3)
   C_i =   waste concentration of contaminant i (mg/L = g/m^3)
   ρ_i =   density of contaminant i (g/cm^3).

Appendix C provides values for density for all IWAIR chemicals.

   This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values from 0.01 to 3 g/cm^3.

   Active Biomass (g/L). This input, in conjunction with the BIODEGRADATION option, allows you to determine what type of biodegradation is modeled for your unit. 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 compose 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 acclimate and adapt to the chemicals present. See also the discussion in Section B.3.1.2 on biodegradation and how active biomass interacts with the biodegradation setting.

This input refers to the biomass concentration within the surface impoundment. Most of the biodegradation rate constants use mixed-liquor volatile suspended solids (MLVSS) as the measure of bioconcentration. Therefore, MLVSS in the impoundment is the preferred source for this input if you have those data available. If not, you can approximate this (in order of preference) using biomass concentration in the impoundment, mixed-liquor suspended solids (MLSS) in the impoundment, MLVSS in the effluent, biomass concentration in the effluent, or MLSS in the effluent. Alternatively, you may choose to use the IWAIR default of 0.05 g/L; however, this default is only appropriate for biologically active impoundments. If you are modeling a biologically inactive impoundment, this value should be set to zero, which turns off direct biodegradation and biomass growth, so that adsorption losses are limited to adsorption to inlet solids. This value must be greater than or equal to zero and less than or equal to 1,000 g/L. IWAIR has been tested for this full range.

Total Suspended Solids in Influent (g/L). Total suspended solids (TSS) is used, in conjunction with total organics, to estimate growth of solids in the impoundment. This input is the TSS in the impoundment influent, not within the impoundment. If those data are not available, you can approximate this (in order of preference) using total solids in the influent, MLSS in the influent, MLVSS in the influent, biomass concentration in the influent, TSS within the impoundment, total solids within the impoundment, or MLSS within the impoundment. Alternatively, you may choose to use the IWAIR default of 0.2 g/L. This value must be greater than or equal to zero and less than or equal to 1,000 g/L. IWAIR has been tested for this full range.

Total Organics into WMU (mg/L). Total organics is used, in conjunction with TSS, to estimate new biomass growth, so it most accurately refers to biodegradable organics. For this reason, the most preferred data source is biological oxygen demand (BOD) in the influent. If BOD is not available, you can estimate this using chemical oxygen demand (COD) or total organic carbon (TOC) in the influent. Values of BOD, COD, or TOC in the effluent may be used if influent values are not available, but these need to be adjusted up to account for removal in the impoundment by dividing by (1 – removal efficiency). Alternatively, you can use the IWAIR default value of 200 mg/L. This value must be greater than or equal to the sum of the concentrations you entered for organic chemicals in the WASTES MANAGED screen and must be less than or equal to 1,000,000 mg/L. IWAIR has been tested for this full range.

Total Biorate (mg/g biomass-h). This is the degradation rate of total organics in the impoundment. Total biorate can be measured from the maximum oxygen uptake rate from respirometry studies, converting the oxygen uptake rate to grams carbon assuming mineralization (formation of CO_2). Alternatively, you can use the IWAIR default value of 19 mg/g biomass-h). This value must be greater than or equal to zero. No maximum limit is enforced. IWAIR has been tested for values from 0 to 100 mg/g biomass-h.

B.3.1.5 <u>Mechanical Aeration Information</u>

These inputs are needed for only if you selected Mechanical aeration or Both (diffused air & mechanical).

Oxygen Transfer Rate (lb O_2/h-hp). This is the oxygen transfer rating of your aerator, measured using water, and should be available from the design specifications of your aerator. If no data are available, you can use the IWAIR default of 3.0 lb O_2/h-hp. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values from 0.01 to 3 lb O_2/h-hp.

Number of Aerators. This is the number of impellers in your impoundment. You should be able to count them visually if you do not have these data readily available. This value must be greater than or equal to 1 and should be an integer. No maximum limit is enforced. IWAIR has been tested for values from 1 to 150.

Total Power (hp). This is the power from all impellers in the impoundment combined. You can calculate it by summing the power of each impeller (make sure they are all in the same units first). Impeller power should be part of the design specifications for your aerators. In a survey of surface impoundments managing nonhazardous wastes (U.S. EPA, 2001a), the reported average power per aerator ranged from 4 to 100 hp. If you cannot determine the power of your aerators, you can estimate aerator power. Aeration and mixing power requirements often depend on the volume of liquid needing aeration or mixing, although the range of appropriate values can be wide. Additionally, many impoundments are aerated near the unit's influent, but a large portion of the impoundment may remain unaerated. Consequently, the lower limit for aeration may be more difficult to assess than the upper limit. A reasonable upper limit for aeration power based on high aeration requirements is approximately 150 hp per million gallons of impoundment volume (Metcalf and Eddy, 1979). This factor can be applied to the total volume of the unit to assess a maximum power limit. A lower limit based on mixing is approximately 10 hp/million gallons; this factor can be applied to the unit volume times the fraction aerated to yield a lower limit. The minimum value for total power must be greater the 0.25 hp. No maximum limit is enforced. IWAIR has been tested for values from 0.26 to 3,000 hp.

Power Efficiency (fraction). 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. 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. 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.

This correction factor is used to adjust the oxygen transfer rate input (which applies to pure water) for application to wastewaters. A value for your aerator should be available from your aerator supplier. If no data are available, you can use the IWAIR default of 0.83; this value is consistent with its use as the oxygen correction factor. This value must be greater than zero and less than or equal to 1. IWAIR has been tested for values from 0.01 to 1.

Impeller Diameter (cm). This is the diameter of each impeller, from one end of the impeller to the other. If you have different impellers of different diameters, use either an average or the most typical. If this value is in meters, feet, or inches, it must be converted to centimeters for use in IWAIR. If you cannot determine the diameter of your impellers, you can use the IWAIR default value of 61 cm. This value must be greater than zero and less than 100 times the square root of the area of the unit in m^2 (i.e., the impeller cannot be longer than the side length of the unit, assuming the unit is square, which maximizes the smallest side length). IWAIR has been tested for this full range.

Impeller Speed (rad/s). This is a measure of rotational speed (in radians per second). It should be part of the specifications of your aerators, although it may be reported in rotations per minute (rpm). If so, you will need to convert it to radians per second. One rotation is equal to 360 degrees, or 6.28 radians. If your aerators have different speeds, use an average or the most typical value. If you cannot determine the speed of your impellers, you can use the IWAIR default value of 130 rad/s. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for a range from 0.01 to 1,000 rad/s.

B.3.2   WMU Data for CHEMDAT8 – Land Application Unit (Screen 3B)

B.3.2.1 <u>Meteorological Station Parameters</u>. These inputs are used only for the emissions modeling, not the dispersion modeling, which uses hourly meteorological data, not annual averages. Therefore, changes to these inputs will not affect the dispersion factors.

Wind Speed (m/s). IWAIR uses wind speed 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. By default, IWAIR uses the average annual wind speed from the meteorological station that was assigned to your location. However, you may wish to override the default if you have site-specific data on wind speed. If you do override, you should use an overall annual average in all directions, not any measure of peak wind speed or average only in the prevailing wind direction. Also, wind speed is often reported in knots or mph. However, for use in IWAIR, wind speed must be converted to m/s. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of wind speed from 0.01 to 100 m/s; however, a realistic range for average annual wind speed is about 2 to 10 m/s.

Temperature (°C). IWAIR uses temperature to correct various temperature-dependent chemical properties used in emissions modeling (Henry's law constant and vapor pressure) from

a standard temperature to the ambient temperature. By default, IWAIR uses the average annual temperature from the meteorological station that was assigned to your location. However, you may wish to override the default if you have site-specific data on temperature. If you do override, you should use an annual average temperature. Temperature may be reported in degrees Fahrenheit (°F); however, for use in IWAIR, temperature must be converted to degrees Celsius (°C). This value must be greater than or equal to -100°C. No maximum limit is enforced. IWAIR has been tested for values of temperature from 0 to 50°C.

B.3.2.2 Waste/Soil Mixture Porosity Information

Total Porosity (volume fraction). Porosity refers to the spaces in a soil or waste matrix that are not soil particles. These spaces may be filled with air or water. Total porosity is the sum of both air- and water-filled porosity. Sometimes porosity is referred to as saturated water content. Porosity values are used in the emissions model, and they can be used to estimate soil saturation concentration limits. If measured data on porosity are not available, porosity can be estimated from the bulk density and particle density of the waste as follows:

$$\epsilon_t \ = \ 1 - BD/\rho_s$$

where

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

If particle density is not available, a typical value for mineral material is 2.65 g/cm^3 (Mason and Berry, 1968).

Porosity must be greater than zero and less than 1. IWAIR has been tested for values from 0.01 to 0.99.

Air Porosity (volume fraction). Air-filled porosity is the porosity that is filled with air instead of water. This can be calculated from volumetric moisture content (which is equivalent to water-filled porosity) and total porosity as follows:

$$\epsilon_a \ = \ \epsilon_t - \epsilon_w$$

where

ϵ_a = air-filled porosity (unitless)
ϵ_t = total porosity (unitless)
ϵ_w = water-filled porosity = volumetric water content (unitless).

Air-filled porosity must be greater than zero and less than or equal to the total porosity. IWAIR has been tested for this full range.

B.3.2.3 LAU Dimensions and Loading Information

Biodegradation (on/off). This option lets you choose whether to model biodegradation losses in the unit. Land application units are designed to biodegrade wastes; therefore, the biodegradation option is turned on by default. Biodegradation rates can be very site-specific. If you believe that the actual rates in your unit are different than those included in the IWAIR chemical properties database, the best choice would be to enter user-defined chemical entries using your own soil biodegradation rates and select biodegradation |ON|. However, if you wish to model a land application unit without biodegradation, you can select biodegradation |OFF|.

Operating Life (yr). This parameter is the expected remaining operating life of your unit, from the time you are modeling until you expect it to be closed. Operating life does not affect exposure duration for land application units the way it does for other unit types, because exposures can continue postclosure for land application units. Operating life does affect average emission rates for land application units. Emissions are estimated for each year of operation plus 30 years postclosure, and then the maximum 7- and 30-year averages are calculated. For land application units, IWAIR uses default exposure durations used by IWAIR of 30 years for residents and 7.2 years for workers, regardless of operating life. Operating life should be entered in years. This value must be greater than zero. No maximum limit is enforced; however, see the discussion below under number of applications per year on how operating life affects the maximum number of applications per year. IWAIR has been tested for values of operating life from 0.01 to 100 years.

Tilling Depth of Unit (m). This is the depth to which your land application unit is tilled and the depth to which wastes are mixed with soil; once constituents get below this depth, they are no longer mixed with newly applied waste. Tilling depth should be entered in m; if it is in other units, it must be converted to m. Tilling depth must be greater than zero. No maximum limit is enforced. IWAIR has been tested for tilling depths from 0.01 to 1 m.

Area of Unit (m^2). This is the total surface area of your unit in m^2. Areas may be reported in acres or hectares; these values will need to be converted to m^2 for use in IWAIR. This value must be greater than or equal to 81 and less than or equal to 8,090,000 m^2; these are the smallest and largest areas for which IWAIR can interpolate dispersion factors for ground-level sources. IWAIR has been tested for this full range of values.

Annual Waste Quantity (Mg/yr). This is the total amount of waste that you manage in your land application unit in a year, in Mg/yr. You may need to estimate this by multiplying the waste quantity applied per application by the number of applications per year. This value must be greater than zero. The maximum limit depends on the other inputs. The waste quantity, number of applications per year, bulk density, and area imply a depth of application as follows:

$$d_{app} = Q/(N_{appl} \times BD \times A)$$

where

d_{app} = depth of application (m)
Q = annual waste quantity (Mg/yr)
N_{appl} = number of applications per year (yr^{-1})
BD = bulk density of waste (g/cm^3 = Mg/m^3)
A = area of unit (m^2).

This depth of application may not exceed the tilling depth and, realistically, should be considerably less than the tilling depth. IWAIR has been tested for values of annual waste quantity from 0.01 to 10,000,000 Mg/yr.

   Number of Applications per Year. This is the number of times you apply waste to the land application unit per year. You may need to convert a frequency of application to the corresponding number of applications per year. For example, if you apply waste weekly, you would enter 52 applications per year in IWAIR. This value must be an integer greater than or equal to 1. The maximum number of applications per year depends on the operating life you specified. IWAIR models land application unit emissions in time steps equal to the time between applications (so, if you entered 52 applications per year, IWAIR would model in 1-week time steps), for a period equal to the operating life of the unit plus 30 years. The total number of time steps modeled is thus:

$$N_{steps} = (t_{life} + 30) \times N_{appl}$$

where

N_{steps} = total number of time steps modeled (unitless)
t_{life} = operating life of unit (yr)
N_{appl} = number of applications per year (yr^{-1}).

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, you could have daily applications (365 applications/year) for 59 years and still be just within this limitation. IWAIR has been tested for values from 1 to 52.

   Waste Bulk Density (g/cm^3). This is the overall, or bulk, density of your waste. This should be available from measurements. Bulk density must be in g/cm^3. This value must be greater than zero. IWAIR has been tested for values from 0.01 to 14 g/cm^3.

B.3.2.4 <u>Waste Characteristics Information (Only for Risk Calculation)</u>

Type of Waste. In order to generate an accurate estimate of a constituent's volatile emissions, you must define the physical and chemical characteristics of the waste you are modeling. In particular, you 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 contaminant has for one phase (for example, air) relative to another phase (for example,

> **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 saturation limits. However, it is possible for the specific components of the waste to raise the effective saturation level for a chemical, allowing it to remain in solution at concentrations above the typical saturation limit.
>
> **Organic-phase waste:** a waste that is predominantly organic chemicals, with a high concentration of organics. Concentrations of some chemicals may exceed saturation limits, causing those chemicals to come out of solution and form areas of free product in the WMU.

water) that drives the volatilization of organic chemicals. Your choice of waste matrix will significantly affect the rate of emissions from the waste. The following discussion is intended to provide background on emissions modeling as it relates to waste type, guidance on making this selection, and clarification of the modeling consequences of choosing AQUEOUS versus ORGANIC in IWAIR. Note that you will only be asked to choose a waste type for risk calculations; for allowable concentration calculations, IWAIR calculates emission rates for both aqueous and organic waste types and selects the one that achieves the target risk or HQ at the lowest concentration applicable to the waste type.

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 absorbed to solids, dissolved in liquids, or assume a 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 more heavily to air, while others tend to partition more heavily 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 moles of the chemical per total moles) 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.[3] 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 may be 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 soil saturation concentration has exceeded the bounds of "dilute aqueous" and is more appropriately modeled using Raoult's law. Chemicals exceeding saturation limits will typically come out of solution and behave more like pure, organic-phase component. However, saturation limits can vary depending on site-specific parameters, such as temperature and pH of the waste. In addition, waste matrix effects[4] can cause chemicals to remain in solution at concentrations above their typical saturation limit. This scenario (an aqueous-phase waste with concentrations above typical 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.

For land application units, 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 contaminant through the porous waste/soil media.

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[3] 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.

[4] "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.

When in allowable concentration calculation mode, IWAIR calculates both aqueous-phase and organic-phase emission rates. However, aqueous-phase emission rates, as discussed above, are only applicable up to the saturation limit. If the use of the aqueous-phase emission rate results in an allowable concentration in excess of the saturation limit, IWAIR will use the organic-phase rate instead.

Molecular Weight of Waste (g/mol). If you choose to model an organic-phase waste, you will need to enter the average molecular weight of the waste. This may be calculated from the molecular weights of the component constituents as follows:

$$MW_{waste} = \frac{\Sigma \ (C_i) \times (1 \ Mg)}{\Sigma \ (C_i/MW_i) \times (1 \ Mg)}$$

where

MW_{waste} = molecular weight of waste (g/mol)
C_i = waste concentration of contaminant i (mg/kg = g/Mg)
MW_i = molecular weight of contaminant i (g/mol).

This assumes that the average molecular weight of the unspecified fraction of the organic waste matrix has the same average molecular weight as the specified fraction (i.e., the input contaminant concentrations). This value must be greater than or equal to 1 (the molecular weight of a single hydrogen ion). No maximum limit is enforced.

B.3.3   WMU Data for CHEMDAT8 – Landfill (Screen 3C)

B.3.3.1 Meteorological Station Parameters. These inputs are used only for the emissions modeling, not the dispersion modeling, which uses hourly meteorological data, not annual averages. Therefore, changes to these inputs will not affect the dispersion factors.

Wind Speed (m/s). IWAIR uses wind speed 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. By default, IWAIR uses the average annual wind speed from the meteorological station that was assigned to your location. However, you may wish to override the default if you have site-specific data on wind speed. If you do override, you should use an overall annual average in all directions, not any measure of peak wind speed or average only in the prevailing wind direction. Also, wind speed is often reported in knots or mph. However, for use in IWAIR, wind speed must be converted to m/s. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of wind speed from 0.01 to 100 m/s; however, a realistic range for average annual wind speed is about 2 to 10 m/s.

Temperature (°C). IWAIR uses temperature to correct various temperature-dependent chemical properties used in emissions modeling (Henry's law constant and vapor pressure) from a standard temperature to the ambient temperature. By default, IWAIR uses the average annual

temperature from the meteorological station that was assigned to your location. However, you may wish to override the default if you have site-specific data on temperature. If you do override, you should use an annual average temperature. Temperature may be reported in degrees Fahrenheit (°F); however, for use in IWAIR, temperature must be converted to degrees Celsius (°C). This value must be greater than or equal to -100°C. No maximum limit is enforced. IWAIR has been tested for values of temperature from 0 to 50°C.

B.3.3.2 Waste Porosity Information

Total Porosity (volume fraction). Porosity refers to the spaces in a soil or waste matrix that are not soil particles. These spaces may be filled with air or water. Total porosity is the sum of both air- and water-filled porosity. Sometimes porosity is referred to as saturated water content. Porosity values are used in the emissions model, and they can be used to estimate soil saturation concentration limits. If measured data on porosity are not available, porosity can be estimated from the bulk density and particle density of the waste as follows:

$$\epsilon_t \; = \; 1 - BD/\rho_s$$

where

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

If particle density is not available, a typical value for mineral material is 2.65 g/cm^3 (Mason and Berry, 1968).

Porosity must be greater than zero and less than 1. IWAIR has been tested for values from 0.01 to 0.99.

Air Porosity (volume fraction). Air-filled porosity is the porosity that is filled with air instead of water. This can be calculated from volumetric moisture content (which is equivalent to water-filled porosity) and total porosity as follows:

$$\epsilon_a \; = \; \epsilon_t - \epsilon_w$$

where

ϵ_a = air-filled porosity (unitless)
ϵ_t = total porosity (unitless)
ϵ_w = water-filled porosity = volumetric water content (unitless).

Air-filled porosity must be greater than zero and less than or equal to the total porosity. IWAIR has been tested for this full range.

B.3.3.3 Landfill Dimensions and Loading Information

Biodegradation (on/off). This option lets you choose whether to model biodegradation losses in the unit. Landfills are generally not designed to biodegrade wastes; therefore, the biodegradation option is turned off for landfills by default. However, biodegradation may occur in your landfill. If you believe it does and want to model it, you can select biodegradation |ON|. Soil biodegradation rates can be very site-specific. If you believe that the actual rates in your unit are different than those included in the IWAIR chemical properties database, you can enter user-defined chemical entries using your own soil biodegradation rates.

Operating Life (yr). This parameter is the expected remaining operating life of your unit, from the time you are modeling until you expect it to be closed. For landfills, this value is used in emissions calculations. In addition, it affects exposure duration. IWAIR uses default exposure durations of 30 years for residents and 7.2 years for workers. However, proper closure of a landfill typically ends all exposures. Therefore, if the operating life you specify is less than 30 or 7.2 years, IWAIR caps the exposure duration at the operating life. Values in excess of 30 years will not affect the results for residents, and values in excess of 7.2 years will not affect the results for workers. Operating life should be entered in years. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of operating life from 0.01 to 100 years.

Total Area of Landfill (m².) This is the total surface area of your unit in m². Be sure to enter total area and not just the area of the active cell. Areas may be reported in acres or hectares; these values will need to be converted to m² for use in IWAIR. This value must be greater than or equal to 81 and less than or equal to 8,090,000 m², which are the smallest and largest areas for which IWAIR can interpolate dispersion factors for ground-level sources. IWAIR has been tested for this full range of values.

Total Depth of Landfill (m). This is the average depth of your unit in meters (m). If your unit is not a constant depth, use the average or most typical depth. If you have depth reported in units such as feet, you will need to convert them to m. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of depth from 0.01 to 30 m.

Total Number of Cells in Landfill. Landfills are typically filled one cell at a time. This input is the total number of cells in your landfill. IWAIR models one open cell at a time, with each cell open for a period equal to the operating life divided by the total number of cells. This value must be greater than or equal to 1. No maximum limit is enforced. IWAIR has been tested for values from 1 to 10,000.

Annual Quantity of Waste Disposed in Landfill (Mg/yr). This is the total amount of waste that you manage in your landfill in a year, in Mg/yr. This value must be greater than zero. The maximum limit depends on other inputs. The waste quantity, operating life, area, and depth imply a loading rate as follows:

$$L = (Q \times t_{life})/(A \times D)$$

where

L   =   loading rate ($Mg/m^3 = g/cm^3$)
Q   =   annual waste quantity (Mg/yr)
t_{life} =   operating life (yr)
A   =   area of landfill (m^2)
D   =   depth (m).

This loading rate may not exceed the bulk density of the waste. IWAIR has been tested for values of annual waste quantity from 0.01 to 10,000,000 Mg/yr.

   Bulk Density of Waste (g/cm^3). This is the overall, or bulk, density of your waste. This should be available from measurements. Bulk density must be in g/cm^3. This value must be greater than zero. IWAIR has been tested for values from 0.01 to 14 g/cm^3.

B.3.3.4 Waste Characteristics Information (Only for Risk Calculation)

   Type of Waste. In order to generate an accurate estimate of a constituent's volatile emissions, you must define the physical and chemical characteristics of the waste you are modeling. In particular, you 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 contaminant has for one phase (for example, air) relative to another phase (for example, water) that drives the volatilization of organic chemicals. Your choice of waste matrix will significantly affect the rate of emissions from the waste. The following discussion is intended to provide background on emissions modeling as it relates to waste type, guidance on making this selection, and clarification of the modeling consequences of choosing AQUEOUS versus ORGANIC in IWAIR. Note that you will only be asked to choose a waste type for risk calculations; for allowable concentration calculations, IWAIR calculates emission rates for both aqueous and organic waste types and selects the one that achieves the target risk or HQ at the lowest concentration applicable to the waste type.

> **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 saturation limits. However, it is possible for the specific components of the waste to raise the effective saturation level for a chemical, allowing it to remain in solution at concentrations above the typical saturation limit.
>
> **Organic-phase waste:** a waste that is predominantly organic chemicals, with a high concentration of organics. Concentrations of some chemicals may exceed saturation limits, causing those chemicals to come out of solution and form areas of free product in the WMU.

   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 absorbed to solids, dissolved in liquids, or assume a 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 more heavily to air, while others tend to partition more heavily 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 moles of the chemical total moles) 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.[5] 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 may be 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 soil saturation concentration has exceeded the bounds of "dilute aqueous" and is more appropriately modeled using Raoult's law. Chemicals exceeding saturation limits will typically come out of solution and behave more like pure, organic-phase component. However, saturation limits can vary depending on site-specific parameters, such as temperature and pH of the waste. In addition, waste matrix effects[6] can cause chemicals to

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[5] 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.

[6] "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

remain in solution at concentrations above their typical saturation limit. This scenario (an aqueous-phase waste with concentrations above typical 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.

For landfills, 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 contaminant through the porous waste/soil media.

When in allowable concentration calculation mode, IWAIR calculates both aqueous-phase and organic-phase emission rates. However, aqueous-phase emission rates, as discussed above, are only applicable up to the saturation limit. If the use of the aqueous-phase emission rate results in an allowable concentration in excess of the saturation limit, IWAIR will use the organic-phase rate instead.

Molecular Weight of Waste (g/mol). If you choose to model an organic-phase waste, you will need to enter the average molecular weight of the waste. This may be calculated from the molecular weights of the component constituents as follows:

$$MW_{Waste} = \frac{\Sigma \ (C_i) \times (1 \ Mg)}{\Sigma \ (C_i/MW_i) \times (1 \ Mg)}$$

where

MW_{waste} = molecular weight of waste (g/mol)
C_i = waste concentration of contaminant i (mg/kg = g/Mg)
MW_i = molecular weight of contaminant i (g/mol).

This assumes that the average molecular weight of the unspecified fraction of the organic waste matrix has the same average molecular weight as the specified fraction (i.e., the input contaminant concentrations). This value must be greater than or equal to 1 (the molecular weight of a single hydrogen ion). No maximum limit is enforced.

B.3.4   WMU Data for CHEMDAT8 – Waste Pile (Screen 3D)

B.3.4.1 <u>Meteorological Station Parameters</u>. These inputs are used only for the emissions modeling, not the dispersion modeling, which uses hourly meteorological data, not annual averages. Therefore, changes to these inputs will not affect the dispersion factors.

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.

Wind Speed (m/s). IWAIR uses wind speed 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. By default, IWAIR uses the average annual wind speed from the meteorological station that was assigned to your location. However, you may wish to override the default if you have site-specific data on wind speed. If you do override, you should use an overall annual average in all directions, not any measure of peak wind speed or average only in the prevailing wind direction. Also, wind speed is often reported in knots or mph. However, for use in IWAIR, wind speed must be converted to m/s. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of wind speed from 0.01 to 100 m/s; however, a realistic range for average annual wind speed is about 2 to 10 m/s.

Temperature (°C). IWAIR uses temperature to correct various temperature-dependent chemical properties used in emissions modeling (Henry's law constant and vapor pressure) from a standard temperature to the ambient temperature. By default, IWAIR uses the average annual temperature from the meteorological station that was assigned to your location. However, you may wish to override the default if you have site-specific data on temperature. If you do override, you should use an annual average temperature. Temperature may be reported in degrees Fahrenheit (°F); however, for use in IWAIR, temperature must be converted to degrees Celsius (°C). This value must be greater than or equal to -100°C. No maximum limit is enforced. IWAIR has been tested for values of temperature from 0 to 50°C.

B.3.4.2 Waste Porosity Information

Total Porosity (volume fraction). Porosity refers to the spaces in a soil or waste matrix that are not soil particles. These spaces may be filled with air or water. Total porosity is the sum of both air- and water-filled porosity. Sometimes porosity is referred to as saturated water content. Porosity values are used in the emissions model, and they can be used to estimate soil saturation concentration limits. If measured data on porosity are not available, porosity can be estimated from the bulk density and particle density of the waste as follows:

$$\epsilon_t \; = \; 1 - BD/\rho_s$$

where

$$\epsilon_t \quad = \quad \text{total porosity (unitless)}$$
$$BD \quad = \quad \text{bulk density of waste (g/cm}^3\text{)}$$
$$\rho_s \quad = \quad \text{particle density of waste (g/cm}^3\text{).}$$

If particle density is not available, a typical value for mineral material is 2.65 g/cm^3 (Mason and Berry, 1968).

Porosity must be greater than zero and less than 1. IWAIR has been tested from 0.01 to 0.99.

Air Porosity (volume fraction). Air-filled porosity is the porosity that is filled with air instead of water. This can be calculated from volumetric moisture content (which is equivalent to water-filled porosity) and total porosity as follows:

$$\epsilon_a \; = \; \epsilon_t - \epsilon_w$$

where

ϵ_a =   air-filled porosity (unitless)
ϵ_t =   total porosity (unitless)
ϵ_w =   water-filled porosity = volumetric water content (unitless).

Air-filled porosity must be greater than zero and less than or equal to the total porosity. IWAIR has been tested for this full range.

B.3.4.3 Waste Pile Dimensions and Loading Information

Biodegradation (on/off). This option lets you choose whether to model biodegradation losses in the unit. Waste piles are generally not designed to biodegrade wastes; therefore, the biodegradation option is turned off for waste piles by default. However, biodegradation may occur in your waste pile, particularly if residence times of waste in the waste pile are long (on the order of 60 days to one year). With such residence times, naturally occurring microorganisms could potentially acclimate and degrade contaminants within the waste pile. If you believe that biodegradation does occur in your waste pile and you want to model it, you can select biodegradation |ON|. Soil biodegradation rates can be very site-specific. If you believe that the actual rates in your unit are different than those included in the IWAIR chemical properties database, you can enter user-defined chemical entries using your own soil biodegradation rates.

Operating Life (yr). This parameter is the expected remaining operating life of your unit, from the time you are modeling until you expect it to be closed. Operating life does not affect emissions estimates for waste piles, which are modeled at steady state. However, operating life may affect exposure duration. IWAIR uses default exposure durations of 30 years for residents and 7.2 years for workers. However, proper closure of a waste pile typically ends all exposures. Therefore, if the operating life you specify is less than 30 or 7.2 years, IWAIR caps the exposure duration at the operating life. Values in excess of 30 years will not affect the results for residents, and values in excess of 7.2 years will not affect the results for workers. Operating life should be entered in years. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of operating life from 0.01 to 100 years.

Height of Waste Pile Unit (m). This is the average height of your waste pile in meters (m). If your waste pile is not a constant height, use the average or most typical height. If you have height reported in units such as feet, you will need to convert them to m. This value must be greater than or equal to 1 m and less than or equal to 10 m; these are the smallest and largest heights for which IWAIR can interpolate dispersion factors for waste piles. IWAIR has been tested for this full range.

Area of Unit (m²). This is the total surface area of your unit in m². Areas may be reported in acres or hectares; these values will need to be converted to m² for use in IWAIR. This value must be greater than or equal to 20 and less than or equal to 1,300,000 m²; these are the smallest and largest areas for which IWAIR can interpolate dispersion factors for waste piles. IWAIR has been tested for this full range of values.

Average Quantity of Waste in Waste Pile (Mg/yr). This is the average amount of waste in your waste pile over a year, in Mg/yr. This value must be greater than zero. No maximum limit is enforced. IWAIR has been tested for values of annual waste quantity from 0.01 to 10,000,000 Mg/yr.

Bulk Density of Waste (g/cm³). This is the overall, or bulk, density of your waste. This should be available from measurements. Bulk density must be in g/cm³. This value must be greater than zero. IWAIR has been tested for values from 0.01 to 14 g/cm³.

B.3.4.4 <u>Waste Characteristics Information (Only for Risk Calculation)</u>

Type of Waste. In order to generate an accurate estimate of a constituent's volatile emissions, you must define the physical and chemical characteristics of the waste you are modeling. In particular, you 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 contaminant has for one phase (for example, air) relative to another phase (for example, water) that drives the volatilization of organic

> **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 saturation limits. However, it is possible for the specific components of the waste to raise the effective saturation level for a chemical, allowing it to remain in solution at concentrations above the typical saturation limit.
>
> **Organic-phase waste:** a waste that is predominantly organic chemicals, with a high concentration of organics. Concentrations of some chemicals may exceed saturation limits, causing those chemicals to come out of solution and form areas of free product in the WMU.

chemicals. Your choice of waste matrix will significantly affect the rate of emissions from the waste. The following discussion is intended to provide background on emissions modeling as it relates to waste type, guidance on making this selection, and clarification of the modeling consequences of choosing Aqueous versus Organic in IWAIR. Note that you will only be asked to choose a waste type for risk calculations; for allowable concentration calculations, IWAIR calculates emission rates for both aqueous and organic waste types and selects the one that achieves the target risk or HQ at the lowest concentration applicable to the waste type.

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 absorbed to solids, dissolved in liquids, or assume a 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 more heavily to air, while others tend to partition more heavily 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 moles of the chemical per total moles) 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.[7] 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 may be 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 soil saturation concentration has exceeded the bounds of "dilute aqueous" and is more appropriately modeled using Raoult's law. Chemicals exceeding saturation limits will typically come out of solution and behave more like pure, organic-phase component. However, saturation limits can vary depending on site-specific parameters, such as

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[7] 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.

temperature and pH of the waste. In addition, waste matrix effects[8] can cause chemicals to remain in solution at concentrations above their typical saturation limit. This scenario (an aqueous-phase waste with concentrations above typical 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.

For 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 contaminant through the porous waste/soil media.

When in allowable concentration calculation mode, IWAIR calculates both aqueous-phase and organic-phase emission rates. However, aqueous-phase emission rates, as discussed above, are only applicable up to the saturation limit. If the use of the aqueous-phase emission rate results in an allowable concentration in excess of the saturation limit, IWAIR will use the organic-phase rate instead.

Molecular Weight of Waste (g/mol). If you choose to model an organic-phase waste, you will need to enter the average molecular weight of the waste. This may be calculated from the molecular weights of the component constituents as follows:

$$MW_{waste} = \frac{\Sigma\ (C_i) \times (1\ Mg)}{\Sigma\ (C_i/MW_i) \times (1\ Mg)}$$

where

MW_{waste} = molecular weight of waste (g/mol)
C_i = waste concentration of contaminant i (mg/kg = g/Mg)
MW_i = molecular weight of contaminant i (g/mol).

This assumes that the average molecular weight of the unspecified fraction of the organic waste matrix has the same average molecular weight as the specified fraction (i.e., the input contaminant concentrations). This value must be greater than or equal to 1 (the molecular weight of a single hydrogen ion). No maximum limit is enforced.

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[8] "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.

B.4   User-Override Emission Rates (Screens 4A and 4B)

Override Emission Rates. You may choose either to enter your own emission rates for all chemicals modeled or to override IWAIR's calculated emission rates for some or all of the chemicals modeled. Override emission rates may be based on measured data or modeled results from an emissions model outside of IWAIR, but regardless of source, should reflect a long-term average, not a short-term peak.

This input has different units in risk calculation mode versus allowable concentration mode:

■ In risk mode, this input should be the actual measured or modeled emissions from your unit, normalized on area (in $g/m^2/s$). If emission rates are based on modeled rates, they should correspond to the actual waste concentrations in your unit. Emissions in g/s should be normalized to area by dividing by the area of the unit.

■ In allowable concentration mode, the emission rate should either be based on modeled emissions corresponding to a waste concentration of 1 mg/kg or 1 mg/L, or they should be normalized to concentration by dividing by the actual waste concentration present when the emissions were measured or modeled. The units for allowable concentration mode emission rates (g/m^2-s per mg/kg or mg/L) reflect this. Emissions measured or modeled in g/s should also be normalized to area by dividing by the area of the unit.

You may input one override emission rate per chemical. In risk mode, IWAIR assumes this emission rate corresponds to the waste type (aqueous or organic) you chose on Screen 3, WMU DATA FOR CHEMDAT8. In allowable concentration mode, IWAIR assumes this emission rate corresponds to an aqueous waste. As a result, IWAIR will not output concentrations in concentration mode in excess of each chemical's solubility or saturation limit if you have entered user-override emission factors.

Source and Justification for User-Override Values. If you enter override emission factors, you must document their source in this field. The justification field may not be left blank.

B.5   ISCST3 or User-Override Dispersion Factors (Screen 5A)

Distance to Receptor (m). This is the distance from the edge of your unit to the receptor for whom you want to estimate risk or allowable concentration. You must choose from one of the six values available in IWAIR: 25, 50, 75, 150, 500, or 1,000 m. Choose the distance that best approximates the location of your receptors. If you are using IWAIR's dispersion factors, they will correspond to the distance you select; selecting a distance smaller than the actual distance to receptors near your unit will overestimate risk, and selecting a distance larger than the actual distance will underestimate risk. If you enter your own dispersion factors, this input is only for your reference and is not used in calculations. Therefore, you should select the distance that most closely approximates the distance your dispersion factor applies to.

      Receptor Type. Two different types of exposed individuals, worker and resident, can be modeled with IWAIR. The dispersion factors do not vary with receptor type; however, receptor type is chosen here for convenience. The difference between these two receptor types lies in the exposure factors, such as body weight and inhalation rate, used to calculate risk for carcinogens. There is no difference between them for noncarcinogens because calculation of noncarcinogenic risk does not depend on exposure factors. The assumptions for residents reflect males and females from birth through age 30; it is important to consider childhood exposures because children typically have higher intake rates per kilogram of body weight than adults. The actual exposure duration used for residents is the smaller of 30 years or the operating life of the unit that you entered (except for land application units, for which the exposure duration for residents is always 30 years regardless of operating life). Exposure for residents starts at birth and continues for the length of the exposure duration, using the appropriate age-specific exposure factors. The assumptions for workers reflect a full-time, outdoor worker; all exposure is assumed to occur as an adult. The exposure duration for workers is the smaller of 7.2 years or the operating life of the unit (except for land application units, for which the exposure duration for workers is always 7.2 years regardless of operating life).   For more information on the specific exposure factors used for residents and workers, see the *IWAIR Technical Background Document.*

      User-Override Dispersion Factors. You may choose either to enter your own dispersion factors for all receptors modeled or to override IWAIR's calculated dispersion factors for some or all of the receptors modeled. Note that dispersion factors are not chemical-specific, nor are they specified to receptor type (resident or worker). Dispersion factors may be based on measured air concentrations or air concentrations modeled outside of IWAIR. If based on modeled air concentrations, they should correspond to an emission rate of 1 $\mu g/m^2$-s. If based on measured air concentration data, they should be normalized to emission rate by dividing by the actual emission rate measured or modeled. The units for dispersion factors ($\mu g/m^3$ per $\mu g/m^2$-s) reflect this. Note that when you enter your own dispersion factors, you are not limited to the six receptor distances included in IWAIR. In this circumstance, those distances are for your reference only.

      Source and Justification for User-Override Values. If you enter override dispersion factors, you must document their source in this field. If your receptor distances differ from the distances available in IWAIR, it may be useful to document here the actual receptor distances for each numbered receptor. The justification field may not be left blank.

B.6   Results Screen (Screen 6)

B.6.1   Target Risk and Hazard Quotient Value

      These inputs are needed for allowable concentration mode only. In risk mode, risk and HQ are calculated by IWAIR.

      Risk Value for Carcinogens. Choose one of the five values available. A higher risk value represents greater risk and will result in lower allowable concentrations. This value is not required if no carcinogens are being modeled (i.e., CSF is NA for all chemicals modeled).

Hazard Quotient Value for Noncarcinogens. Choose one of the five values available. A higher HQ value represents greater likelihood of health effects and will result in lower allowable concentrations. This value is not required if no noncarcinogens are being modeled (i.e., RfC is NA for all chemicals modeled).

B.6.2 Health Benchmarks

Parameter guidance for health benchmarks is provided in Section B.2.2.3.

B.7   References

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Appendix C

Physical-Chemical Property Values

Table C-1. Molecular Weights and Densities for IWAIR Constituents

CAS	Chemical Name	Molecular Weight (g/mole)	Density (g/cm3)
50000	Formaldehyde	30	0.82
50328	Benzo(a)pyrene	252	1.35
55185	N-Nitrosodiethylamine	102	0.94
56235	Carbon tetrachloride	154	1.59
56495	3-Methylcholanthrene	268	1.28
57976	7,12-Dimethylbenz[a]anthracene	256	1.02
62533	Aniline	93	1.02
67561	Methanol	32	0.79
67641	Acetone	58	0.79
67663	Chloroform	119	1.48
67721	Hexachloroethane	237	2.09
68122	N,N-Dimethyl formamide	73	0.94
71432	Benzene	78	0.88
71556	1,1,1-Trichloroethane	133	1.34
74839	Methyl bromide	95	1.68
74873	Methyl chloride	50	0.91
75014	Vinyl chloride	63	0.91
75058	Acetonitrile	41	0.79
75070	Acetaldehyde	44	0.78
75092	Methylene chloride	85	1.33
75150	Carbon disulfide	76	1.26
75218	Ethylene oxide	44	0.89
75252	Tribromomethane	253	2.90
75274	Bromodichloromethane	164	1.98
75354	1,1-Dichloroethylene	97	1.21
75569	Propylene oxide	58	0.86
75694	Trichlorofluoromethane	137	1.49
75718	Dichlorodifluoromethane	121	1.49
76131	1,1,2-Trichloro-1,2,2-trifluoroethane	187	1.56
77474	Hexachlorocyclopentadiene	273	1.70
78591	Isophorone	138	0.93
78875	1,2-Dichloropropane	113	1.16
78933	Methyl ethyl ketone	72	0.81
79005	1,1,2-Trichloroethane	133	1.44
79016	Trichloroethylene	131	1.46
79061	Acrylamide	71	1.12
79107	Acrylic acid	72	1.05
79345	1,1,2,2-Tetrachloroethane	168	1.60
79469	2-Nitropropane	89	0.98
80626	Methyl methacrylate	100	0.94

Table C-1. Molecular Weights and Densities for IWAIR Constituents

CAS	Chemical Name	Molecular Weight (g/mole)	Density (g/cm3)
85449	Phthalic anhydride	148	1.53
87683	Hexachloro-1,3-butadiene	261	1.56
91203	Naphthalene	128	1.03
92875	Benzidine	184	1.25
95501	o-Dichlorobenzene	147	1.31
95534	o-Toluidine	107	1.00
95578	2-Chlorophenol	129	1.26
95658	3,4-Dimethylphenol	122	0.98
96128	1,2-Dibromo-3-chloropropane	236	2.09
98011	Furfural	96	1.16
98828	Cumene	120	0.86
98953	Nitrobenzene	123	1.20
100414	Ethylbenzene	106	0.87
100425	Styrene	104	0.91
106467	p-Dichlorobenzene	147	1.25
106887	1,2-Epoxybutane	72	0.84
106898	Epichlorohydrin	93	1.18
106934	Ethylene dibromide	188	2.18
106990	1,3-Butadiene	54	0.61
107028	Acrolein	56	0.84
107051	Allyl chloride	77	0.94
107062	1,2-Dichloroethane	99	1.24
107131	Acrylonitrile	53	0.81
107211	Ethylene glycol	62	1.11
108054	Vinyl acetate	86	0.93
108101	Methyl isobutyl ketone	100	0.80
108883	Toluene	92	0.87
108907	Chlorobenzene	113	1.11
108930	Cyclohexanol	100	0.96
108952	Phenol	94	1.05
109864	2-Methoxyethanol	76	0.96
110496	2-Methoxyethanol acetate	118	1.01
110543	n-Hexane	86	0.65
110805	2-Ethoxyethanol	90	0.93
110861	Pyridine	79	0.98
111159	2-Ethoxyethanol acetate	132	0.98
118741	Hexachlorobenzene	285	2.04
120821	1,2,4-Trichlorobenzene	181	1.46
121142	2,4-Dinitrotoluene	182	1.32
121448	Triethylamine	101	0.73

Table C-1. Molecular Weights and Densities for IWAIR Constituents

CAS	Chemical Name	Molecular Weight (g/mole)	Density (g/cm3)
122667	1,2-Diphenylhydrazine	184	1.16
123911	1,4-Dioxane	88	1.03
124481	Chlorodibromomethane	208	2.45
126998	Chloroprene	89	0.96
127184	Tetrachloroethylene	166	1.62
630206	1,1,1,2-Tetrachloroethane	168	1.54
924163	N-Nitrosodi-n-butylamine	158	0.90
930552	N-Nitrosopyrrolidine	100	1.09
1319773	Cresols (total)	108	1.06
1330207	Xylenes	106	0.87
1634044	Methyl tert-butyl ether	88	0.74
1746016	2,3,7,8-TCDD	322	1.83
7439976	Mercury	201	13.53
7439977	Divalent Mercury	201	5.60
10061015	cis-1,3-Dichloropropylene	111	1.22
10061026	trans-1,3-Dichloropropylene	111	1.22