United States
Environmental Protection
Agency

Solid Waste and
Emergency Response
(5305W)

EPA530-R-99-004
May 1999
www.epa.gov/osw

Industrial Waste Air Model Technical Background Document

Printed on paper that contains at least 30 percent postconsumer fiber

Industrial Waste Air Model Technical Background Document

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

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1.0 Introduction

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

1.1 Guide for Industrial Waste Management and IWAIR

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

- Adopt a multimedia approach to protect human health and the environment.
- Tailor management practices to risk in this 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 their programs.
- Foster partnerships among facility managers, the public, and regulatory agencies.

The *Guide* recommends best management practices and key factors to take into account to protect groundwater, surface water and ambient air quality in siting, operation, design, monitoring, corrective action, and closure and post closure care. In particular, the guidance recommends risk-based approaches to choose liner systems and waste application rates for groundwater protection and to evaluate the need for air controls. The CD ROM version of the *Guide* includes user-friendly air and groundwater models to conduct these risk evaluations.

The chapter of the *Guide* entitled "Protecting Air Quality" highlights several key recommendations:

- Adopt controls to minimize particulate emissions.
- Determine whether waste management units at a facility are addressed by Clean Air Act requirements and comply with those requirements.

- If waste management units are not specifically addressed by Clean Air Act requirements, use IWAIR to assess risks associated with volatile air emissions from units.

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

EPA developed the IWAIR model and this Technical Background Document to accompany the *Guide* for use in evaluating inhalation risks. Workers and residents in the vicinity of a waste management unit (WMU) may be exposed to volatile chemicals from the WMU 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 the fetus or neurological effects in an adult). With a limited amount of site-specific information, IWAIR can estimate whether specific wastes and management practices may pose an unacceptable risk to human health.

1.2 Model Design

IWAIR is an interactive computer program with three main components: an emissions model; a dispersion model to estimate fate and transport of constituents through the atmosphere and determine ambient air concentrations at specified receptor locations; and a risk model to calculate either the risk to exposed individuals or waste constituent concentrations that can be managed in the unit while being protective of human health. 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.*

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. The emission model selected for incorporation into IWAIR is EPA's CHEMDAT8 model. This model has undergone extensive review by both EPA and industry representatives and is publicly available from EPA's Web page (http://www.epa.gov/ttn/chief/software.html).

To facilitate emission modeling with CHEMDAT8, IWAIR prompts the user to provide the required waste- and unit-specific data. Once these data are entered, the model calculates and displays chemical-specific emission rates. If users decide not to develop or use the CHEMDAT8 rates, they can enter their own site-specific emission rates (g/m^2-s).

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).

Table 1-1. Constituents Included in IWAIR

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

ISCST3 was run to calculate dispersion for a standardized unit emission rate (1 $\mu g/m^2$ - s) to obtain a unitized air concentration (UAC), also called a dispersion factor, which is measured in micrograms/cubic meter per microgram/square meter-second. The total air concentration estimates are then developed by multiplying the constituent-specific emission rates derived from CHEMDAT8 (or from another source) with a site-specific dispersion factor. Running ISCST3 to develop a new dispersion factor for each location/WMU is very time consuming, and requires extensive meteorological data and technical expertise. Therefore, IWAIR incorporates default dispersion factors developed by ISCST3 for many separate scenarios designed to cover a broad range of unit characteristics, including:

- 29 meteorological stations chosen to represent the nine general climate regions of the continental United States
- 4 unit types
- 14 surface area sizes for landfills, land application units, and surface impoundments and 7 surface area sizes and 2 heights for wastepiles
- 6 receptor distances from the unit (25, 50, 75, 150, 500, 1,000 meters)
- 16 directions in relation to the edge of the unit.

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

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

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

1.2.3 Risk Model

The third component combines the constituent's air concentration with receptor exposure factors and toxicity benchmarks to calculate either the risk from concentrations managed in the unit or the waste concentration (C_w) 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 maintains standard health benchmarks (cancer slope factors for carcinogens and reference concentrations for noncarcinogens) for 95 constituents. These health benchmarks are from the Integrated Risk Information System (IRIS) and the Health Effects Assessment Summary Tables (HEAST) (U.S. EPA, 1997b, 1998a). The IWAIR uses these data to perform either a forward calculation to

obtain risk estimates or a backward calculation to obtain protective waste concentration estimates.

1.3 About This Document

The remainder of this background document is organized as follows:

- Section 2, *Source Emission Estimates Using CHEMDAT8*, describes the CHEMDAT8 model used to calculate emissions
- Section 3, *Development of Dispersion Factors Using ISCST3*, describes how dispersion factors were developed using ISCST3 and how these are used in the model
- Section 4, *Exposure Factors*, describes the exposure factors used in the model
- Section 5, *Development of Inhalation Health Benchmarks,* describes the health benchmarks used in the model, and how these were developed if health benchmarks were not available from standard sources
- Section 6, *Calculation of Risk/Hazard Quotient or Waste Concentration*, describes the forward risk calculation, and the iterative method used by the model for performing backward calculations
- Section 7, *References*.

2.0 Source Emission Estimates Using CHEMDAT8

This section describes the CHEMDAT8 emission model used to develop the emission estimates for each WMU. Section 2.1 describes why CHEMDAT8 was chosen and provides an overview of CHEMDAT8. Section 2.2 describes the input parameters. Section 2.3 describes the important modeling assumptions and equations used to convert IWAIR inputs to those needed for CHEMDAT8 and to calculate actual emission rates from the fraction emitted estimated by CHEMDAT8.

2.1 Model Selection and Overview of CHEMDAT8

EPA's CHEMDAT8 model was selected as the model to estimate volatile emissions rates from the waste management units in IWAIR. CHEMDAT8 meets the goals that were considered during the model selection process. These goals were to:

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

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

The CHEMDAT8 model considers most of the competing removal pathways that might limit air emissions, including adsorption and hydrolysis for surface impoundments and

biodegradation for all units. While the land-based units do not consider adsorption per se, volatilization is limited by the relative air porosity of the soil or waste matrix. Hydrolysis is not considered in the land-based units, even for soil moisture or percolating rainwater. Adsorption is the tendency of a chemical or liquid media to attach or bind to the surface of particles in the waste and therefore 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. Similarly, hydrolysis is the tendency of a chemical to be broken down or decomposed into less complex chemicals by reaction with water. Chemicals that decompose due to either biodegradation or hydrolysis have lower potential for emission to the air as gases because the mass of chemical is reduced by these processes. Biodegradation and hydrolysis may generate daughter products; however, for the chemicals covered by IWAIR, the daughter products were found to be less toxic than the parents. CHEMDAT8 models only the parent. 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 emission to the air as gases or particles. As such, CHEMDAT8 is considered to provide reasonable to slightly high (environmentally conservative) estimates of air emissions from the various emission sources.

EPA's CHEMDAT8 model is provided as a modular component of IWAIR. **For complete documentation on the CHEMDAT8 model, refer to documents available on EPA's web page.** The CHEMDAT8 spreadsheet model and model documentation may be downloaded at no charge from EPA's web page (http://www.epa.gov/ttn/chief/software.html). This document provides information about CHEMDAT8 that is pertinent to the IWAIR program; however, it does not document the CHEMDAT8 equations. CHEMDAT8 is a Lotus 1-2-3 spreadsheet that includes analytical models for estimating volatile organic compound emissions from treatment, storage, and disposal facility processes under user-specified input parameters. The original CHEMDAT8 spreadsheet was converted to Visual Basic code for use in IWAIR. In addition, the chemical-specific data in the original code were evaluated for accuracy. Some of these values have been changed to reflect newer or better information. A list of the physical-chemical properties is provided in Appendix A of this document. Extensive testing was performed to ensure that the coded version produces results identical to the spreadsheet version.

CHEMDAT8 calculates the fraction of a waste constituent that is released to air and, for surface impoundments, the amount adsorbed and the amount remaining in the effluent. The fraction emitted is converted to annual emissions in the appropriate units required for the IWAIR program calculations.

2.2 Emission Model Input Parameters

Emission modeling using CHEMDAT8 is conducted using unit-specific data entered by the user. Most of the inputs are used directly by CHEMDAT8; a few are used to calculate inputs for CHEMDAT8. The IWAIR program provides default input data for some parameters. For example, the temperature and windspeed for a WMU site are automatically used as a default for a site once the site is assigned to one of the 29 meteorological stations in the IWAIR program. Users may choose to override the default data and enter their own estimates for these parameters.

Thus, modeling emissions using CHEMDAT8 can be performed with a very limited amount of site-specific information using the default data that are provided. The unit-specific input parameters required to run IWAIR and the default values for those parameters are listed in Tables 2-1 through 2-4.

This section discusses the various parameters that significantly impact the estimated emission rates. Inputs that influence these rates include input parameters specific to the physical and chemical properties of the constituent being modeled, the physical and chemical characteristics of the waste material being managed, input parameters specific to the process and operating conditions of the WMU being modeled, and meteorological parameters.

A general discussion of the physical and chemical properties of the constituents is provided in the Section 2.2.1. Critical input parameters for the remaining sets of inputs are discussed for land-based WMUs in Section 2.2.2 and for surface impoundments in Section 2.2.3. The input parameters used in IWAIR differ in some respects from those needed by CHEMDAT8. When the CHEMDAT8 inputs are not readily available but can be calculated from more readily available data, IWAIR uses the more readily available input parameters. The equations used to convert these to the CHEMDAT8 inputs are documented in Section 2.3.

Table 2-1. Input Parameters for Landfills

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design and Operating Parameters				
Operating Life of Landfill	years	None	0-100	Required input
Total Area of Landfill - All Cells	m^2	None	$0\text{-}10^7$	Required input
Average Depth of Landfill Cell	m	None	0-20	Required input
Total Number of Cells in Landfill	unitless	None	0-10,000	Required input
Average Annual Quantity of Waste Disposed	Mg/yr	None	$0\text{-}1.2\times10^7$	Required input
Waste Characterization Information				
Dry Bulk Density of Waste in Landfill	g/cm^3	1.4	0.8-3	ERG and Abt (1992). Uses a default of 1.4 g/cm^3 for waste sludge U.S. EPA (1989). Uses sludge density of 1.01 g/cm^3
Average Molecular Weight of Oily Waste	g/gmol	147	18-400	RTI (1988). Default input for CHEMDAT8 landfill
Total Porosity of Waste	volume fraction	0.50	0-1	U.S. EPA (1991). Input used for all active landfills RTI (1988). Default input for CHEMDAT8 landfill ERG and Abt (1992). Uses default of 0.40 Schroeder et al. (1994). Halogenated Aliphatics used 0.46
Air-filled Porosity of Waste	volume fraction	0.25	0-total porosity	U.S. EPA (1991). Input used for all active landfills RTI (1988). Default input for CHEMDAT8 landfill Schroeder et al. (1994). Halogenated Aliphatics used range = 0.16 to 0.31

[a]Parameters with ranges shown as "0-x" must be greater than zero.

Table 2-2. Input Parameters for Land Application Units (LAUs)

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design and Operating Parameters				
Operating Life of LAU	years	None	0-100	Required input
Tilling Depth of LAU	m	None	0-1	Required input
Surface Area of LAU	m^2	None	$0\text{-}10^7$	Required input
Average Annual Quantity of Waste Applied	Mg/yr	None	$0\text{-}5.2\times10^7$	Required input
Number of Applications per Year	yr^{-1}	None	0-12	Required input
Waste Characterization Information				
Dry Bulk Density of Waste/Soil Mixture	g/cm^3	1.3	0.8-3	Loehr et al. (1993). Reports density = 1.39 g/cm^3 for surface soil U.S. EPA (1992). Uses a default value of 1.4 g/cm^3 for sewage sludge/soil in LAU Li and Voudrias (1994). Wet soil column density = 1.03 g/cm^3
Average Molecular Weight of Oily Waste	g/gmol	282	18-400	RTI (1988). Default input for CHEMDAT8 LAU
Total Porosity of Waste/Soil Mixture	volume fraction	0.61	0-1	U.S. EPA (1991). Default input used for all model LAU. RTI (1988). Default input for CHEMDAT8 LAU U.S. EPA (1992). Uses default of 0.4 Loehr et al. (1993). Reports porosity = 0.49 for surface soil Li and Voudrias (1994). Wet soil column porosity = 0.558
Air-filled Porosity of Waste/Soil	volume fraction	0.5	0-total porosity	U.S. EPA (1991). Default input used for all model LAU RTI (1988). Default input for CHEMDAT8 LAU

[a]Parameters with ranges shown as "0-x" must be greater tan zero.

2.2.1 Chemical-Specific Input Parameters

Chemical-specific input parameters are those parameters that relate to the physical or chemical properties of each individual chemical. The values of these parameters are different for each of the 95 chemicals covered by IWAIR. Key chemical-specific input parameters that have a significant impact on modeled emissions include: air-liquid equilibrium partitioning coefficients (vapor pressure or Henry's law constant), liquid-solid equilibrium partitioning coefficient (log octanol-water partition coefficient for organics), biodegradation rate constants, and liquid and air diffusivities. The hazardous waste identification rule (HWIR) chemical properties database (RTI, 1995) was used as the primary data source for the physical and chemical properties for the constituents being modeled. This chemical properties database provided the following chemical-specific input parameters: molecular weight, vapor pressure, Henry's law constant, solubility, liquid and air diffusivities, log octanol-water partition coefficient, and the soil biodegradation rate constants. The CHEMDAT8 chemical properties database (U.S. EPA, 1994a) was used as a secondary data source for the physical and chemical properties for the constituents being modeled. This chemical properties database provided the following chemical-specific input parameters: density, boiling point, Antoine's coefficients (for adjusting vapor pressure to

Table 2-3. Input Parameters for Wastepiles

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design and Operating Parameters				
Height of Wastepile	m	None	0-10	Required input
Surface Area of Wastepile	m^2	None	$0\text{-}1.5\times10^7$	Required input
Average Annual Quantity of Waste Added to waste pile	Mg/yr	None	$0\text{-}10^6$	Required input
Dry Bulk Density of Waste	g/cm^3	1.4	0.8-3	ERG and Abt (1992). Uses default of 1.4 g/cm^3 for waste sludge U.S. EPA (1991). Uses default of 1.8 g/cm^3 for wastepile RTI (1988). Uses "liquid in fixed waste" density of 1.16 g/cm^3 U.S. EPA (1989). Uses sludge density of 1.01 g/cm^3
Waste Characterization Information				
Average Molecular Weight of Waste	g/gmol	147	18-400	RTI (1988). Default input for CHEMDAt8
Total Porosity of Waste	volume fraction	0.5	0-1	U.S. EPA (1991). Input used for all model wastepiles RTI (1988). Default input for CHEMDAT8 wastepile
Air-filled Porosity of Waste	volume fraction	0.25	0-total porosity	U.S. EPA (1991). Input used for all model wastepiles RTI (1988). Default input for CHEMDAT8 wastepile

[a]Parameters with ranges shown as "0-x" must be greater than zero.

temperature), and biodegradation rate constants for surface impoundments. The biodegradation rate constants in the downloaded CHEMDAT8 database file were compared with the values reported in the summary report that provided the basis for the CHEMDAT8 surface impoundment biodegradation rate values (Coburn et al., 1988). Surface impoundment biodegradation rate constants for compounds with no data were assigned biodegradation rates equal to the most similar compound in the biodegradation rate database. The specific chemical properties input database used for the emission modeling is provided in Appendix A.

2.2.2 Input Parameters for LAUs, Landfills, and Wastepiles

The input parameters for land-based units are presented in Tables 2-1 through 2-3.

Unit Design and Operating Parameters. The annual waste quantity is a critical site-specific input parameter. This parameter, along with assumptions regarding the frequency of contaminant addition and the dimensions of the unit, combine to influence a number of model input parameters. Because these are so critical, and because the values of these parameters for a specific unit to be modeled should be readily available to the user, no default values are provided for these parameters.

Table 2-4. Input Parameters for Aerated and Nonaerated Surface Impoundments (SIs)

Input Parameter	Units	Default Value	Range[a]	Basis
Unit Design Data				
Depth of Liquid in SI	m	None	0-20	Required input
Surface Area of SI	m^2	None	$0\text{-}10^7$	Required input
Average Annual Flow Rate	m^3/yr	None	$0\text{-}1.6\times10^7$	Required input
Aeration Data				
Fraction of Surface Area Agitated	unitless	0.25	0-1	U.S. EPA (1991.) Input for medium sized aerated SI - model units T02I and T02J
Submerged Air Flow Rate	m^3/s	0	0-10	Default assumes mechanical aeration
Mechanical Aeration Information				
Oxygen Transfer Rate	lb O_2/h-hp	3	2.9-3.0	U.S. EPA (1991.) Range = 2.9 to 3.0 lb O_2/h-hp
Number of Aerators	unitless	1	10-150	U.S. EPA (1991.) Input for medium sized aerated SI - model units T02I and T02J
Total Power Input to All Aerators	hp	75	0-3,000	U.S. EPA (1991.) Input for medium sized aerated SI - model units T02I and T02J
Power Efficiency of Aerators	fraction	0.83	0.8-0.85	U.S. EPA (1991.) Range = 0.80 to 0.85.
Aerator Impeller Diameter	cm	61	0-300	U.S. EPA (1991.) Input used for all model SI
Aerator Impeller Rotational Speed	radians/s	130	0-1,000	U.S. EPA (1991.) Input used for all model SI
Waste Characteristic Data				
Average Molecular Weight	g/gmol	282	18-400	U.S. EPA (1994a.) CHEMDAT8 oily film model default
Active Biomass Conc. (as MLVSS) in the SI	g/L	0.05	0-15	RTI (1988.) Default value used for SI in developing biodegradation rate constants U.S. EPA (1994a.) Recommended default for quiescent SI; suggests a default for aerated SI = 0.25 g/L
Total Suspended Solids (TSS) in SI Influent	g/L	0.2	0-100	U.S. EPA (1994a.) Range = 0.11 - 0.40 for SI designed for biodegradation
Total Organics (TOC or COD) in SI Influent	mg/L	100	0-100,000	
Degradation Rate of Total Organics	mg/g biomass-h	19	0-100	U.S. EPA (1994a.) Default value recommended in CHEMDAT8

[a]Parameters with ranges shown as "o-x" must be greater than zero, except for waste characteristic parameters, which may be se to zero.

Waste Characterization. One of the most important inputs for emission estimates is whether the waste is aqueous or oily. This input tells the CHEMDAT8 model which equilibrium partitioning model to use between the liquid and gas phases. For oily (organic) wastes, the model uses Raoult's law and the liquid-to-air partition coefficient becomes proportional to the contaminant's partial vapor pressure. For aqueous wastes, the model uses Henry's law and the liquid-to-air partition coefficient becomes proportional to the contaminant's Henry's law coefficient. A useful rule of thumb for determining if a waste is aqueous or oily is to determine if the waste contains more than 10 percent organics. If it does, emissions are more accurately modeled as oily. Therefore, for forward calculations, if the total concentration of all chemicals entered exceeds 100,000 ppm (or 10 percent), IWAIR automatically considers the waste oily. However, the user can designate wastes as oily even if the chemicals being modeled do not exceed 10 percent of the waste stream. For backward calculations, IWAIR calculates both an aqueous and an oily emission rate. Section 6 describes how the model determines which of these emission rates to use.

Organic Chemicals

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

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

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

where

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

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

Meteorological Conditions. Two meteorological parameters are used as inputs to CHEMDAT8: annual average windspeed and temperature. The CHEMDAT8 model is insensitive to windspeeds for long-term emission estimates from land-based units. Temperature affects the air diffusivity, which affects the volatilization rate. Consequently, temperature is the only meteorological data input that potentially impacts the emissions results for the CHEMDAT8 model for the land-based WMU. By default, IWAIR uses the annual average temperature and

windspeed for the meteorological station identified as most representative for the site location. However, the user may override these with site-specific data.

2.2.3 Input Parameters for Surface Impoundments

The input parameters for surface impoundments are presented in Table 2-1.

Unit Design Data. The annual waste quantity (flow rate), the dimensions of the surface impoundment, and whether or not the impoundment is aerated are critical input parameters for impoundments. Because these are so critical, and because the values of these parameters for a specific unit to be modeled should be readily available to the user, no default values are provided for these parameters.

Aeration. Factors that impact the relative surface area of turbulence and the intensity of that turbulence are important in determining the rate of volatilization of the chemicals in aerated surface impoundments. The aerated surface impoundment model has several input parameters that impact the degree and intensity of the turbulence created by the aeration (or mixing). The aerated surface impoundment model is most sensitive to the fraction aerated. The total power, power per aerator (number of aerators), and impeller diameter have some impact on the emission results. The other parameters have only a slight impact on the estimated emissions. Default values are provided for these inputs, but the user is strongly encouraged to enter site-specific values if available.

Meteorological Conditions. Meteorological inputs are also important for the surface impoundment emission model. Emissions estimates for nonaerated impoundments are impacted by both temperature and windspeed. Emissions for aerated impoundments are predominantly driven by the turbulent area and associated mass transfer coefficients; therefore, the emissions from aerated impoundments are not strongly impacted by the windspeed; they are impacted by temperature. Note that, dependent on the residence time of the waste in the impoundment, the temperature of the waste is not expected to vary significantly with changing atmospheric temperatures. Therefore, annual average temperatures are used to estimate the average waste temperature in the impoundment. By default, IWAIR uses the annual average temperature and windspeed for the meteorological station identified as most representative for the site location. However, the user may override these with site-specific data.

Waste Characterization Inputs. Factors that influence the rate of biodegradation are important in determining emissions from surface impoundments. Unlike the biodegradation rate model that was used for the land-based units, the biodegradation rate model used in CHEMDAT8 for surface impoundments is dependent on the amount of active biomass in the WMU. Therefore, the active biomass concentration is a critical parameter for impoundments. A default value is provided, but the user is encouraged to enter a site-specific value if available. The total suspended solids in, total organics in, and total biorate impact the rate of biomass production and subsequently the amount of contaminant that is absorbed onto the solids. These inputs, however, have little or no impact on the estimated emission rates for most of the contaminants modeled in this analysis. Default values are provided, but the user is strongly encouraged to enter site-specific values if available.

2.3 Mathematical Development of Emissions

This section describes how the inputs described in Section 2.2 are used to calculate the inputs needed for CHEMDAT8 and how the output of CHEMDAT8 (the fraction emitted) is converted to a mass emission rate for use in IWAIR. This section does not document the CHEMDAT8 model equations used to calculate fraction emitted from the CHEMDAT8 inputs. For documentation on CHEMDAT8, refer to the model documentation, which may be downloaded from EPA's web site (http://www/epa.gov/ttn/chief/software.html) at no charge.

2.3.1 Landfills

The basic assumptions used for modeling landfills are as follows:

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

$$t_{calc} = \frac{t_{life} \times 365.25 \times 24 \times 3{,}600}{N} \qquad (2\text{-}2)$$

where

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

- The modeled waste is homogeneous with an initial concentration of 1 mg/kg for backward calculations or is user-specified for forward calculations; the landfill may also contain other wastes with different properties.
- Loading is calculated from the annual waste quantity and the size of the landfill as follows:

$$L = \frac{Q_{annual} \times t_{life}}{A_{total} \times D_{total}} \qquad (2\text{-}3)$$

where

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

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

- Landfill **cell** areas and depth are used for the model run: $Area_{cell} = Area_{total} / N$; $Depth_{cell} = Depth_{total}$.

- Biodegradation is not modeled.

CHEMDAT8 is used to calculate the emission fraction for each of the selected contaminants. The average emission rate for the landfill can be calculated as follows:

$$E = \frac{Q_{annual} \times C_{waste} \times L \times f_{emitted}}{A_{cell} \times BD \times 365.25 \times 24 \times 3{,}600} \tag{2-4}$$

where

E	=	emission rate (g/m^2 - s)
Q_{annual}	=	annual waste quantity (Mg/yr)
C_{waste}	=	concentration of chemical in waste (mg/kg = g/Mg)
L	=	loading rate ($Mg/m^3 = g/cm^3$)
$f_{emitted}$	=	emission fraction (unitless)
A_{cell}	=	area of cell (m^2)
BD	=	bulk density of waste in landfill (g/cm^3)
365.25	=	units conversion (d/yr)
24	=	units conversion (h/d)
3,600	=	units conversion (s/h).

2.3.2 Land Application Units

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

- The land treatment unit operates for t_{life} years.

- Waste application occurs N_{appl} per year.

- Emissions are calculated for one application using a time of calculation as follows:

$$t_{calc} = \frac{365.25 \times 24 \times 3{,}600}{N_{appl}} \tag{2-5}$$

where

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

- The waste is homogeneous with an initial concentration of 1 mg/kg for backward calculations or is user-specified for forward calculations.

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

$$L = \frac{Q_{annual} \times 100}{N_{appl} \times A \times d_{till}} \tag{2-6}$$

where

L	=	loading rate ($Mg/m^3 = g/cm^3$)
Q_{annual}	=	annual quantity of waste (Mg/yr)
N_{appl}	=	number of waste applicatons per year (yr^{-1})
A	=	area of unit (m^2)
d_{till}	=	tilling depth (cm)
100	=	units conversion (cm/m).

- Biodegradation is modeled.

The CHEMDAT8 model calculates the fraction emitted and biodegraded for each chemical to the time of one application. However, for the land treatment unit, additional waste is added to and mixed with the oil/waste matrix after the modeled time step. It is assumed that the volume of the land treatment unit remains constant. Therefore, as more waste is applied, it is assumed that an equal volume of waste/soil mixture becomes buried or otherwise removed from the active tilling depth. For the first application, the mass of constituent in the LAU is:

$$M_o = M_{start,1} = \frac{Q_{annual} \times C_{waste}}{N_{appl}} \tag{2-7}$$

where

M_o	=	mass of chemical in unit at time 0 (g)
$M_{start,1}$	=	mass of chemical in unit at start of time step 1 (g)
Q_{annual}	=	annual quantity of waste (Mg/yr)
C_{waste}	=	concentration of chemical in waste (mg/kg = g/Mg)
N_{appl}	=	number of waste applications per year (yr^{-1}).

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

$$M_{end,1} = M_o \times (1 - f_{emitted} - f_{bio}) \tag{2-8}$$

where

$M_{end,1}$	=	mass of chemical in unit at end of time step 1 (g)
M_o	=	mass of chemical in unit at time 0 (g)
$f_{emitted}$	=	fraction emitted (unitless).
f_{bio}	=	fraction biodegraded (unitless).

The generalized equation for the starting mass of contaminant (just after any waste application number, n) is

$$M_{start,n} = M_o + M_{end,n-1} \times \left(1 - \frac{d_{appl}}{d_{till}}\right) \tag{2-9}$$

where

$M_{start,n}$	=	mass of chemical in unit at start of time step n (g)
M_o	=	mass of chemical in unit at time 0 (g)
$M_{end,n-1}$	=	mass of chemical in unit at end of time step n-1 (g)
d_{appl}	=	depth of waste applied (cm) - see Equation 2-10.
d_{till}	=	tilling depth (cm).

Depth of waste applied is calculated as

$$d_{appl} = \frac{Q_{annual} \times 100}{N_{appl} \times BD \times A} \tag{2-10}$$

where

d_{appl}	=	depth of waste applied (cm)
Q_{annual}	=	annual quantity of waste (Mg/yr)
N_{appl}	=	number of applications per year f (yr^{-1})
BD	=	bulk density of waste ($g/cm^3 = Mg/m^3$)
A	=	area of unit (m^2)
100	=	units conversion (cm/m).

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

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

$$M_{end,n} = M_{start,n} \times (1 - f_{emitted} - f_{bio}) \tag{2-11}$$

where

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

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

$$M_{emitted,n} = M_{start,n} \times f_{emitted} \tag{2-12}$$

where

$M_{emitted,n}$	=	mass of chemical emitted in time step n (g)
$M_{start,n}$	=	mass of chemical in unit at start of time step n (g)
$f_{emitted}$	=	fraction emitted (unitless).

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

$$E_n = \frac{M_{emitted,n}}{t_{calc} \times A} \tag{2-13}$$

where

E_n	=	emission rate in time step n (g/m^2-s)
$M_{emitted,n}$	=	mass of chemical emitted in time step n (g)
t_{calc}	=	time of calculation (s) - see Equation 2-5
A	=	area of unit (m^2).

The starting, ending, and emitted mass of constituent is calculated for the life of the unit plus 30 years. For noncarcinogens, the maximum E_n is used in calculating hazard quotient. For carcinogens, IWAIR determines the highest 30-year average of the E_n values.

2.3.3 Wastepiles

The modeling assumptions used for modeling wastepiles are as follows:

- The wastepile is modeled as a batch process with the waste remaining in the wastepile for the average residence time (Res.Time). This encompasses two scenarios:

  1. The wastepile is instantaneously filled at time t=0 and remains dormant (no other waste added) for Res.Time, at which time the entire wastepile is emptied and completely filled with fresh waste.

  2. An annual quantity of waste is added to the wastepile consistently (in small quantities) throughout the year and a corresponding quantity of old waste is removed from the wastepile (so that the wastepile becomes a steady-state plug flow system).

- The waste added is homogeneous with an initial concentration of 1 mg/kg for backward calculations or is user-specified for forward calculations.

- Biodegradation is modeled.

- Loading is the bulk density of the waste material.

- Time of calculation = average Res.Time of waste in the wastepile as follows:

$$t_{calc} = \frac{A \times D \times BD \times 365.25 \times 24 \times 3{,}600}{Q_{annual}} \qquad (2\text{-}14)$$

where

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

The average emission rate for the wastepile can be calculated as follows:

$$E = \frac{Q_{annual} \times C_{waste} \times f_{emitted}}{A_{cell} \times 365.25 \times 24 \times 3{,}600} \qquad (2\text{-}15)$$

where

E	=	emission rate (g/m^2 - s)
Q_{annual}	=	annual waste quantity (Mg/yr)
C_{waste}	=	concentration of chemical in waste (mg/kg = g/Mg)
$f_{emitted}$	=	emission fraction (unitless)

A_{cell}	=	area of cell (m^2)
365.25	=	units conversion (d/yr)
24	=	units conversion (h/d)
3,600	=	units conversion (s/h).

2.3.4 Aerated or Quiescent Surface Impoundments

The basic modeling assumptions used for modeling surface impoundments include:

- The WMU operates at steady state
- The WMU is well mixed
- Waste has an influent concentration of 1 mg/L (= 1 g/m^3) for backward calculations or is user-specified for forward calculations
- Biodegradation rate is first order with respect to biomass concentrations
- Biodegradation rate follows Monod kinetics with respect to contaminant concentrations
- Hydrolysis rate is first order with respect to contaminant concentrations.

The surface area, depth, and flow rate are all directly specified by the model units. The CHEMDAT8 model is used to calculate the emission fractions for the model units, and the emission rate, in grams per square meter per second, is calculated from the fraction emitted, the flow rate, waste concentration, and the surface area as follows:

$$E = \frac{Q_{flow} \times C_{infl} \times f_{emitted}}{A} \qquad (2\text{-}16)$$

where

E	=	emission rate (g/m^2 - s)
Q_{flow}	=	flow rate (m^3/s)
C_{infl}	=	influent concentration (g/m^3)
$f_{emitted}$	=	fraction emitted (unitless)
A	=	area of unit (m^2).

3.0 Development of Dispersion Factors Using ISCST3

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

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

- 29 meteorological stations, chosen to represent the nine general climate regions of the continental U.S.
- 4 unit types
- 14 surface area sizes for landfills, land application units and surface impoundments, and 7 surface area sizes and 2 heights for waste piles
- 6 receptor distances from the unit (25, 50, 75, 150, 500, 1000 meters)
- 16 directions

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

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

The Industrial Source Complex - Short Term v.3 (ISCST3) (U.S. EPA, 1995) dispersion model was selected for development of the dispersion factors in IWAIR. ISCST3 was chosen because it can provide reasonably accurate dispersion estimates for area sources that are both ground-level and elevated. Section 3.1 describes the development of the dispersion factor database used in IWAIR. Section 3.2 describes the interpolation routine.

3.1 Development of Dispersion Factor Database

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

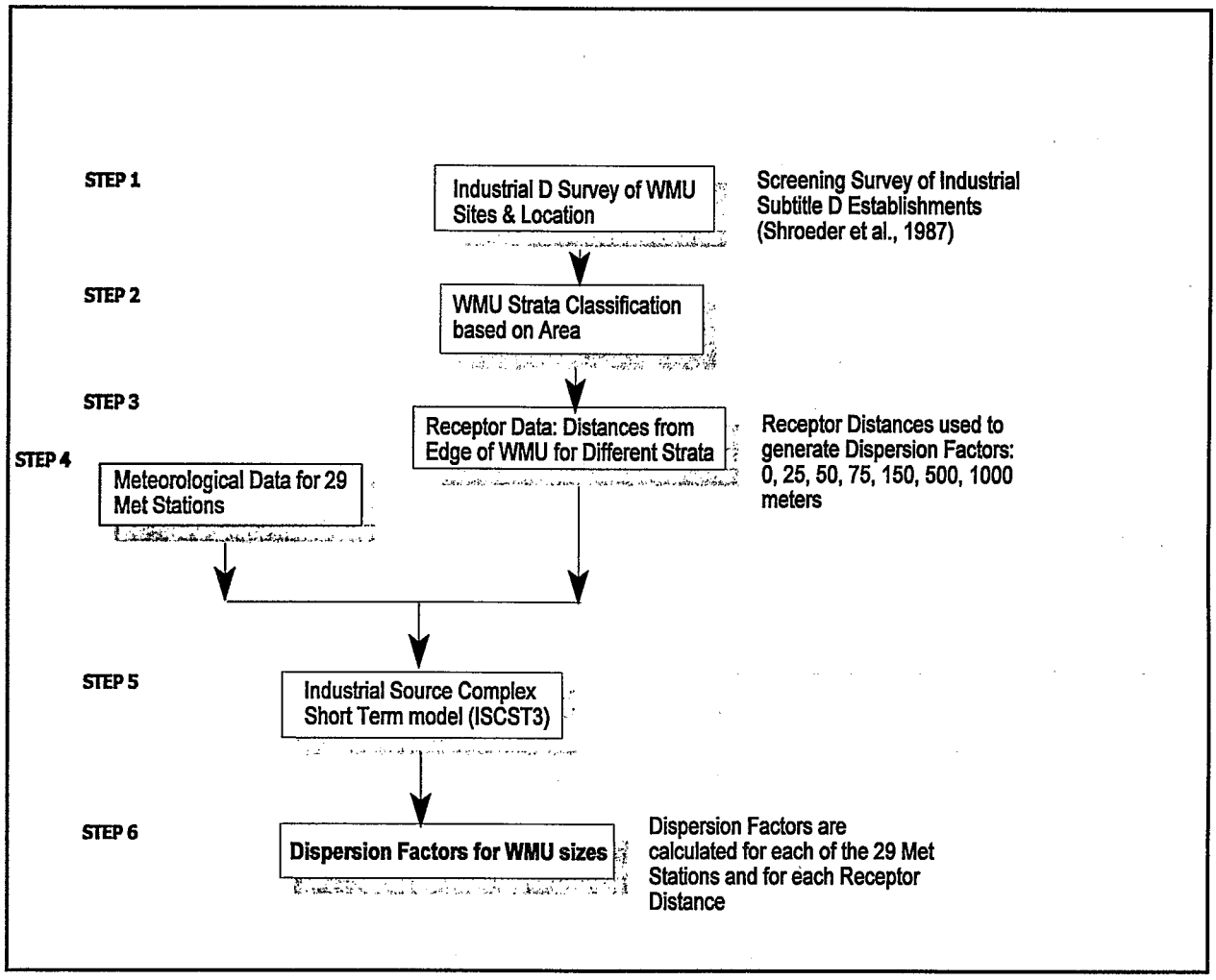


Figure 3-1. Development of ISCST3 dispersion factors.

3.1.1 Industrial D Survey of WMU Sites and Locations (Step 1)

The primary source of data used in the analysis for determining the appropriate range of WMU sizes to model is the Industrial D Screening Survey responses (Schroeder et al., 1987). These survey data provide information on the distribution of areas for nonhazardous WMUs across the continental United States.

3.1.2 WMU Strata Classification Based on Survey (Step 2)

Area of a WMU is one of the most sensitive parameters in dispersion modeling. To construct a database that contained benchmark dispersion coefficients, an appropriate set of "model" units to run had to be determined.

To develop representative cutpoints, a statistical method called the Dalenius-Hodges procedure was used as a starting point. This method attempts to break the distribution of a known variable (in this case, area) that is assumed to be highly correlated with the model output (in this case, dispersion factor) into a fixed number of strata in an optimal way. An area near the midpoint for each strata is then used to represent that stratum. Used on a highly skewed distribution, this process results in strata that tend to emphasize the tail. In this case, the distribution of WMU areas is highly skewed to the right—there is a long tail with a few very large areas. As a result, the initial results of this method yielded strata that over characterized a few very large units and inadequately characterized the smaller units that make up the bulk of the distribution. Therefore, the strata were modified to better capture these smaller areas.

Landfills, land application units, and surface impoundments are all ground-level sources, and are therefore modeled the same way using ISCST3. However, wastepiles are elevated sources and so must be modeled separately in ISCST3. Therefore, two sets of areas were developed, one for landfills, LAUs, and surface impoundments and one for wastepiles. Tables 3-1 and 3-2 show the final area strata used for IWAIR. For each stratum, the median area was modeled.

Table 3-1. Final WMU Area Strata Used for ISCST3 Model Runs for Wastepiles

Strata	Average Area (m^2)		
	Low	*Median*	*High*
1	5	20	81
2	94	162	283
3	324	486	931
4	1,010	2,100	4,860
5	5,200	10,100	44,600
6	45,200	101,000	248,000
7	251,000	1,300,000	2,020,000

Table 3-2. Final WMU Area Strata Used for ISCST3 Model Runs for Landfills, Land Application Units, and Surface Impoundments

Strata	Average Area (m^2)		
	Low	*Median*	*High*
1	14	81	293
2	310	567	789
3	809	1,551	2,293
4	2,307	4,047	7,487
5	7,588	12,546	26,980
6	27,115	40,500	59,653
7	60,300	78,957	119,000
8	120,763	161,880	210,000
9	210,444	243,000	295,000
10	303,525	376,776	546,345
11	554,439	607,000	728,460
12	753,754	906,528	999,609
13	1,007,703	1,408,356	2,430,000
14	2,521,281	8,090,000	13,500,000

3.1.3 Receptor Data Used for Dispersion Modeling (Step 3)

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

The results of the sensitivity analysis of area sources show that the maximum impacts are generally higher for a dense receptor grid (i.e., 64 or 32 receptors on each square) than for a scattered receptor grid (i.e., 16 receptors on each square). For this application, however, the differences of the maximum receptor impacts are not significant between a dense and a scattered receptor grid. Therefore, 16 evenly spaced receptor points on each square were used in the modeling. The sensitivity analysis also shows that the maximum downwind concentrations decrease sharply from the edge of the area source to about 1,000 meters from the source. Therefore, receptor points were placed at 25, 50, 75, 150, 500, and 1,000 meters so that a user could examine the areas that are most likely to have a risk.

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

3.1.4 Meteorological Data Used for 29 Meterological Stations (Step 4)

Meteorological data at over 200 meteorological stations in the United States are available on the SCRAM Bulletin Board (http://www.epa.gov/scram001) and from a number of other sources. A set of 29 meteorological stations selected in an assessment for EPA's Superfund program Soil Screening Levels (SSLs) (EQM and Pechan, 1993) as being representative of the nine general climate regions of the continental United States was used in this analysis. Summary data and windroses for the 29 meteorological stations are provided in Appendix B.

In EPA's SSL study, it was determined that 29 meteorological stations would be a sufficient sample to represent the population of 200 meteorological stations and predict mean dispersion values with a high (95 percent) degree of confidence. The 29 meteorological stations were distributed among nine climate regions based on meteorological representativeness and variability across each region.

These climate regions were:

- North Pacific Coastal
- South Pacific Coastal
- Southwest
- Northwest Mountains
- Central Plains
- Southeast
- Midwest
- Northern Atlantic
- South Florida.

Large-scale regional average conditions were used to select the actual stations (EQM and Pechan, 1993).

The 29 meteorological stations are listed in Table 3-3. To assign facilities to a meteorological station, IWAIR uses a set of polygons around each station. These polygons were constructed using a geographic information system (GIS) to construct Thiessen polygons around each station that enclose the areas closest to each station. The boundaries of these areas were then adjusted to ensure that each boundary encloses an area that is most similar in meteorological conditions to those measured at the meteorological station. To assist in this process, a GIS coverage of Bailey's ecoregion divisions and provinces (Bailey et al., 1994) was used to conflate the boundaries to correspond to physiographic features likely to influence climate or boundaries corresponding to changes in temperature or precipitation. General wind regimes were also considered in the conflation process.

Key factors considered in the conflation process include: defining coastal regimes as narrow polygons, which generally stretched about 25 to 50 miles inland, to capture regions dominated by coastal climate effects; maintaining tropical/subtropical and arid/semiarid divisions in the southwestern United States; and using the ecoregion boundaries in Washington, Oregon, and California to separate the more humid marine/redwood or Mediterranean mountain regimes from the deserts to the east. In general, Thiessen polygons were used to define the meteorological station areas for the remainder of the country.

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

Table 3-3. Meteorological Stations Used in the Air Characteristic Study

City	Met Station		Latitude		Longitude	
	State	#	Degree	Minute	Degree	Minute
Albuquerque	NM	23050	35	3	106	37
Atlanta	GA	13874	33	39	84	25
Bismarck	ND	24011	46	46	100	45
Boise	ID	24131	43	34	116	13
Casper	WY	24089	42	55	106	28
Charleston	SC	13880	32	54	80	2
Chicago	IL	94846	41	59	87	54
Cleveland	OH	14820	41	25	81	52
Denver	CO	23062	39	46	104	52
Fresno	CA	93193	36	46	119	43
Harrisburg	PA	14751	40	13	76	51
Hartford	CT	14740	41	56	72	41
Houston	TX	12960	29	58	95	21
Huntington	WV	03860	38	22	82	33
Las Vegas	NV	23169	36	5	115	10
Lincoln	NE	14939	40	51	96	45
Little Rock	AR	13963	34	44	92	14
Los Angeles	CA	23174	33	56	118	24
Miami	FL	12839	25	49	80	17
Minneapolis	MN	14922	44	53	93	13
Philadelphia	PA	13739	39	53	75	15
Phoenix	AZ	23183	33	26	112	1
Portland	ME	14764	43	39	70	19
Raleigh-Durham	NC	13722	35	52	78	47
Salem	OR	24232	44	55	123	0
Salt Lake City	UT	24127	40	47	111	57
San Francisco	CA	23234	37	37	122	23
Seattle	WA	24233	47	27	122	18
Winnemucca	NV	24128	40	54	117	48

Source: EQM and Pechan (1993).

facility's latitudinal/longitudinal coordinates. Figure 3-2 shows the final meteorological station boundaries used for the study along with the locations of the Industrial D facility sites.

The modeling analysis was conducted using 5 years of representative meteorological data from each of the 29 meteorological stations. Five-year wind roses representing the frequency of wind directions and windspeeds for the 29 meteorological stations were analyzed. These show that the 29 meteorological stations represent a variety of wind patterns.

Shape of Wind Rose for 29 Meteorological Stations

Shape of Wind Rose	No. of Stations
Narrowly distributed	10
Moderately distributed	4
Evenly distributed	6
Bimodally distributed	9

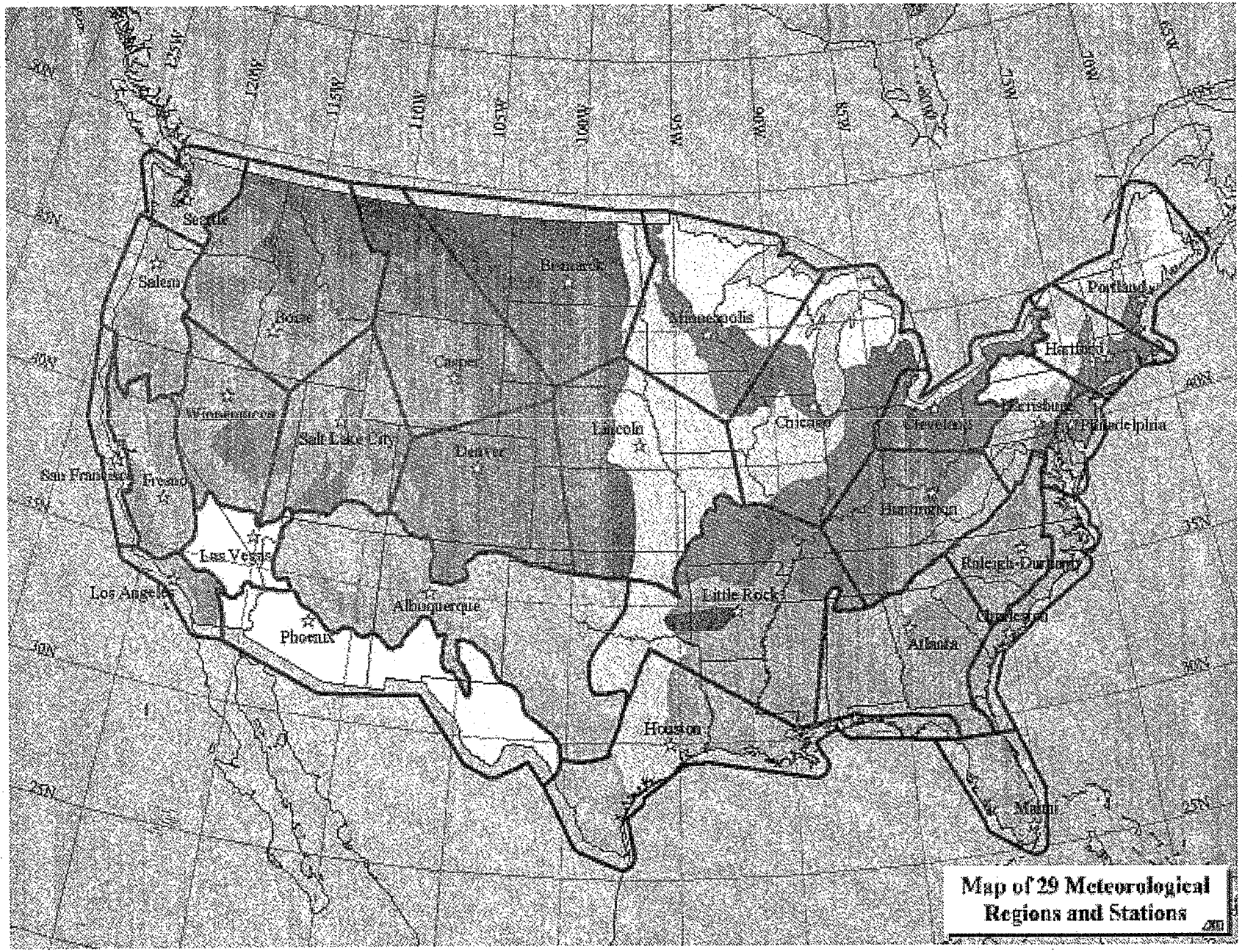


Figure 3-2. Meteorological station regions.

Meteorological Data for the ISCST3 Model without Depletion

Wind Direction (or Flow Vector)
Windspeed
Ambient Temperature
Stability Class
Mixing Height

Wind direction and windspeed are typically the most important meteorological inputs for dispersion modeling analysis. Wind direction determines the direction of the greatest impacts. Windspeed is inversely proportional to ground-level air concentrations, so that the lower the windspeed, the higher the air concentration.

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

3.1.5 Industrial Source Complex Short-term Version 3 Model (Step 5)

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

3.1.5.1 General Assumptions. This section discusses depletion, rural vs. urban, and terrain assumptions.

Assumptions Made for Dispersion Modeling

- Dry and wet depletion options were not activated in the dispersion modeling.
- The rural option was used in the dispersion modeling since the types of WMUs being assessed are typically in nonurban areas.
- Flat terrain was assumed.
- An area source was modeled for all WMUs.
- To minimize error due to site orientation, a square area source with sides parallel to X- and Y- axes was modeled.
- Receptor points were placed on 0, 25, 50, 75, 150, 500, and 1,000 m receptor squares starting from the edge of the source with 16 receptor points on each square.
- Modeling was conducted using a unit emission rate of 1 $\mu g/s\text{-}m^2$.

Depletion. Air concentrations can be calculated in ISCST3 with or without wet and dry depletion. Modeled concentrations without depletions are higher than those with depletions. A sensitivity analysis was conducted that showed that the differences in the maximum concentrations with depletion and without depletion are small at close-to-source receptors, increasing only slightly as the distance from the source increases. The sensitivity analysis also shows that the run time for calculating concentrations using the ISCST3 model with depletion options is 15 to 30 times longer than the run time without depletions for the 5th and 95th percentile of the sizes of LAUs. (The difference is greater for larger sources; see sensitivity analysis in Appendix D for details.) Therefore, concentrations were calculated without depletions in this analysis so that a greater number of meteorological locations could be modeled and included in IWAIR.

Rural vs. Urban. ISCST3 may be run in rural or urban mode, depending on land use within a 3-km radius from the source. These modes differ with respect to wind profile exponent

and potential temperature gradients. Unless the site is located in a heavily metropolitan area, the rural option is generally more appropriate. Because the types of WMUs being assessed are typically in nonurban areas, the rural option was used in this analysis.

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

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

Source Type and Elevation. All WMU types modeled in this analysis were modeled as area sources. Landfills, land application units, and surface impoundments were modeled as ground-level sources, and wastepiles were modeled as elevated sources.

Source Shape and Orientation. The ISCST3 models an area source as a rectangle or combination of rectangles. The user may also specify an angle of rotation relative to a north-south orientation. A sensitivity analysis was conducted to compare the air concentrations from a square area source, a rectangular area source oriented east to west, and a rectangular area source oriented north to south to determine what role source shape and orientation play in determining dispersion coefficients of air pollutants. The results show that the differences in unitized air concentration between the square area source and the two rectangular area sources are less than the differences between the two rectangular sources. In addition, a square area source has the least amount of impact on orientation. Because information on source shapes or orientations is not available, a square source was chosen to minimize the errors caused by source shapes and orientations. (See sensitivity analysis in Appendix D for details.)

3.1.6 Dispersion Factors Available in Program (Step 6)

Unitized air concentrations were calculated by running ISCST3 with a unit emission rate (i.e., 1 $\mu g/m^2$-s). The selected areas for each type of WMU were modeled with 29 representative meteorological locations in the continental United States to estimate UACs. The 5-year average UACs at all receptor points were calculated.

The maximum annual average UACs are presented in Tables 3-4 and 3-5 for the different types of WMUs. Typically, the location of maximum impacts with respect to the source are determined by the prevailing wind direction. For ground-level area sources (i.e., landfills, land application units, and surface impoundments), maximum annual average UACs are always located on the first receptor square (i.e., 25-m receptors). For elevated area sources, the

maximum annual average UACs are usually located on the first receptor square and occasionally located on the second or third receptor square. The results in Tables 3-4 and 3-5 show that the annual average UACs increase with the increasing area size of the sources.

Figures 3-3 through 3-5 show that maximum UACs vary with meteorological location. For landfills and LAUs, the maximum UACs at some meteorological locations can be twice as much as those at other locations. For wastepiles, the maximum UACs at some meteorological locations are more than twice those at other meteorological locations.

3.2 Interpolation of Dispersion Factor

Because the ISCST3 model is sensitive to the size of the area source, the relationship between air concentrations and size of the area source was analyzed. As illustrated in Figure 3-6, the results show that, for relatively small area sources, air concentrations increase significantly as the size of the area source increases. For large area sources, this increase in air concentrations is not as significant.

As described in Section 3.2.2, area strata were identified from WMU data in the Industrial D Survey. The median area size for each stratum was used in the dispersion modeling analysis. Tables 3-6 and 3-7 present the source areas and heights used in the modeling analysis.

This provided a set of UACs for use in the analysis. For any specific WMU, IWAIR estimates a dispersion factor using an interpolation routine that uses the UACs associated with modeled areas immediately above and below the actual area of the unit as follows:

$$UAC = \left(\frac{A - A_i}{A_j - A_i}\right) \times \left(UAC_j - UAC_i\right) + UAC_i \qquad (3\text{-}1)$$

where

UAC	=	unitized air concentration for specific WMU ([μg/m^3]/[μg/m^2-s])
A	=	area of specific WMU (m^2)
A_i	=	area modeled in dispersion modeling immediate below area of specific WMU (m^2)
A_j	=	area modeled in dispersion modeling immediate above area of specific WMU (m^2)
UAC_i	=	unitized air concentration developed for area i ([μg/m^3]/[μg/m^2-s])
UAC_j	=	unitized air concentration developed for area j ([μg/m^3]/[μg/m^2-s]).

If a WMU area is less than the smallest area modeled, A_j and UAC_j are set to the values for the smallest area modeled, and A_i and UAC_i are set to zero. If a WMU area is greater than the largest area modeled, the A_i, UAC_i, A_j, and UAC_j are set to correspond to the two largest areas

Table 3-4. Maximum Annual Average Unitized Air Concentrations ($\mu g/m^3$ / $\mu g/s\text{-}m^2$) for Landfills, Land Application Units, and Surface Impoundments

Met Station	Station No.	Area (m^2)													
		81	567	1,551	4,047	12,546	40,500	78,957	161,880	243,000	376,776	607,000	906,529	1,408,356	8,090,000
Albuquerque, NM	23050	3.521	5.791	7.103	8.450	10.175	12.112	13.316	14.535	15.487	16.406	17.299	18.206	19.287	25.002
Atlanta, GA	13874	3.919	6.369	7.789	9.236	11.119	13.224	14.526	15.927	16.902	17.896	18.937	19.950	21.142	27.323
Bismarck, ND	24011	3.598	5.871	7.182	8.528	10.273	12.231	13.443	14.816	15.650	16.579	17.620	18.566	19.667	25.220
Boise, ID	24131	4.806	7.739	9.458	11.251	13.543	16.138	17.770	19.508	20.710	21.978	23.311	24.550	26.052	33.867
Casper, WY	24089	3.532	5.718	6.980	8.265	9.923	11.790	12.931	14.184	15.020	15.892	16.833	17.724	18.751	24.085
Charleston, SC	13880	3.760	6.134	7.503	8.907	10.733	12.778	14.045	15.392	16.350	17.320	18.316	19.302	20.451	26.415
Chicago, IL	94846	3.678	6.011	7.356	8.726	10.505	12.493	13.712	14.980	15.944	16.871	17.797	18.741	19.843	25.626
Cleveland, OH	14820	4.163	6.639	8.064	9.519	11.415	13.527	14.833	16.268	17.227	18.232	19.308	20.341	21.564	27.959
Denver, CO	23062	5.364	8.645	10.541	12.488	15.039	17.898	19.690	21.634	22.945	24.336	25.798	27.217	28.886	37.541
Fresno, CA	93193	5.783	9.460	11.587	13.794	16.611	19.800	21.792	24.024	25.383	26.916	28.634	30.144	31.955	41.022
Harrisburg, PA	14751	4.291	6.892	8.380	9.900	11.877	14.073	15.434	16.882	17.900	18.937	20.006	21.060	22.298	28.745
Hartford, CT	14740	4.478	7.454	9.176	10.934	13.216	15.775	17.344	18.848	20.221	21.412	22.470	23.684	25.101	32.702
Houston, TX	12960	4.137	6.811	8.352	9.925	11.961	14.239	15.632	17.227	18.189	19.244	20.448	21.531	22.784	28.985
Huntington, WV	3860	5.548	9.154	11.240	13.378	16.161	19.282	21.207	23.265	24.728	26.197	27.720	29.218	30.966	39.932
Las Vegas, NV	23169	4.353	7.072	8.645	10.254	12.349	14.700	16.159	17.697	18.816	19.941	21.081	22.222	23.557	30.668
Lincoln, NE	14939	3.007	4.867	5.936	7.027	8.445	10.027	11.000	12.036	12.781	13.525	14.291	15.051	15.939	20.577
Little Rock, AR	13963	4.500	7.402	9.079	10.795	13.023	15.528	17.065	18.732	19.883	21.053	22.296	23.486	24.888	32.110
Los Angeles, CA	24174	4.492	7.480	9.269	11.100	13.457	16.112	17.745	19.332	20.709	21.944	23.083	24.311	25.753	33.445
Miami, FL	12839	3.752	6.150	7.550	8.984	10.845	12.944	14.240	15.718	16.612	17.608	18.731	19.750	20.932	26.829
Minneapolis, MN	14922	3.334	5.453	6.676	7.924	9.541	11.354	12.464	13.676	14.502	15.347	16.253	17.121	18.127	23.300
Philadelphia, PA	13739	4.359	7.076	8.643	10.243	12.317	14.644	16.076	17.596	18.689	19.784	20.908	22.021	23.317	30.083
Phoenix, AZ	23183	5.640	9.043	11.002	13.016	15.650	18.591	20.439	22.494	23.763	25.185	26.729	28.164	29.850	30.083
Portland, ME	14764	5.028	8.269	10.146	12.070	14.574	17.389	19.127	20.946	22.310	23.642	24.983	26.344	27.933	36.239
Raleigh-Durham, NC	13722	4.407	7.196	8.805	10.453	12.599	14.999	16.483	18.079	19.192	20.327	21.510	22.665	24.018	30.956
Salem, OR	24232	4.580	7.348	8.939	10.567	12.687	15.053	18.120	18.120	19.185	20.308	21.513	22.661	24.005	31.007
Salt Lake City, UT	24127	4.735	7.576	9.218	10.909	13.095	15.546	18.754	18.754	19.865	21.050	22.318	23.521	24.956	32.412
San Francisco, CA	23234	4.500	7.257	8.842	10.465	12.585	14.946	17.977	17.977	19.084	20.213	21.376	22.524	23.882	30.988
Seattle, WA	24233	4.276	6.799	8.231	9.691	11.592	13.686	16.390	16.390	17.324	18.310	19.359	20.365	21.547	27.722
Winnemucca, NV	24128	4.123	6.720	8.222	9.763	11.772	14.028	16.889	16.889	17.980	19.055	20.130	21.224	22.505	29.215

Table 3-5. Maximum Annual Average Unitized Air Concentrations ($\mu g/m^3$ / $\mu g/s\text{-}m^2$) for Wastepiles

Met Station	Station No.	Area (m^2) (2-m Height Wastepiles)							Area Strata (m^2) (5-m Height Wastepiles)						
		20	162	486	2,100	10,100	101,000	1,300,000	20	162	486	2,100	10,100	101,000	1,300,000
Albuquerque, NM	23050	0.037	0.171	0.378	0.993	2.359	5.704	11.011	0.014	0.053	0.107	0.288	0.824	2.956	7.671
Atlanta, GA	13874	0.043	0.195	0.431	1.141	2.644	6.284	12.066	0.016	0.060	0.120	0.325	0.940	3.312	8.467
Bismarck, ND	24011	0.035	0.155	0.343	0.932	2.273	5.685	11.093	0.013	0.049	0.097	0.258	0.759	2.867	7.693
Boise, ID	24131	0.056	0.235	0.520	1.389	3.183	7.621	14.732	0.021	0.072	0.143	0.384	1.132	3.996	10.383
Casper, WY	24089	0.040	0.181	0.405	1.084	2.461	5.714	10.846	0.015	0.056	0.110	0.301	0.894	3.080	7.678
Charleston, SC	13880	0.038	0.168	0.372	1.003	2.393	5.944	11.581	0.014	0.053	0.105	0.280	0.820	3.008	8.027
Chicago, IL	94846	0.038	0.170	0.380	1.030	2.431	5.897	11.340	0.014	0.053	0.106	0.285	0.845	3.049	7.929
Cleveland, OH	14820	0.049	0.214	0.479	1.251	2.897	6.712	12.611	0.018	0.064	0.128	0.353	1.038	3.634	9.059
Denver, CO	23062	0.054	0.237	0.518	1.401	3.393	8.397	16.369	0.020	0.075	0.148	0.391	1.137	4.262	11.383
Fresno, CA	93193	0.077	0.344	0.744	1.858	4.018	9.168	17.785	0.028	0.101	0.205	0.562	1.556	5.002	12.248
Harrisburg, PA	14751	0.047	0.214	0.477	1.269	2.978	6.960	13.027	0.018	0.066	0.131	0.357	1.049	3.731	9.318
Hartford, CT	14740	0.049	0.212	0.474	1.283	2.999	7.096	14.060	0.018	0.067	0.132	0.354	1.050	3.762	9.585
Houston, TX	12960	0.042	0.191	0.424	1.129	2.696	6.640	12.839	0.016	0.059	0.119	0.320	0.933	3.392	8.910
Huntington, WV	3860	0.057	0.248	0.548	1.450	3.416	8.647	17.196	0.021	0.077	0.153	0.410	1.191	4.284	11.707
Las Vegas, NV	23169	0.045	0.194	0.432	1.185	2.852	6.949	13.504	0.017	0.062	0.122	0.323	0.961	3.588	9.440
Lincoln, NE	14939	0.032	0.142	0.317	0.867	2.046	4.850	9.212	0.012	0.045	0.088	0.237	0.708	2.566	6.520
Little Rock, AR	13963	0.045	0.201	0.442	1.181	2.830	7.049	13.894	0.017	0.063	0.126	0.335	0.967	3.553	9.533
Los Angeles, CA	24174	0.055	0.255	0.564	1.466	3.232	7.230	14.069	0.020	0.076	0.153	0.465	1.263	4.022	9.655
Miami, FL	12839	0.041	0.181	0.404	1.080	2.521	6.016	11.650	0.015	0.056	0.112	0.303	0.889	3.163	8.083
Minneapolis, MN	14922	0.033	0.147	0.326	0.896	2.168	5.320	10.290	0.013	0.047	0.093	0.246	0.729	2.726	7.166
Philadelphia, PA	13739	0.045	0.198	0.439	1.200	2.876	6.962	13.365	0.017	0.063	0.124	0.330	0.978	3.610	9.369
Phoenix, AZ	23183	0.062	0.274	0.597	1.555	3.628	8.793	16.962	0.023	0.085	0.170	0.455	1.281	4.533	11.828
Portland, ME	14764	0.046	0.196	0.433	1.209	3.056	7.866	15.636	0.018	0.065	0.126	0.327	0.972	3.857	10.701
Raleigh-Durham, NC	13722	0.043	0.191	0.424	1.152	2.802	6.956	13.566	0.016	0.061	0.120	0.320	0.936	3.523	9.394
Salem, OR	24232	0.048	0.209	0.466	1.287	3.060	7.288	13.859	0.018	0.067	0.130	0.347	1.045	3.844	9.833
Salt Lake City, UT	24127	0.052	0.232	0.514	1.386	3.218	7.569	14.453	0.020	0.072	0.142	0.383	1.131	4.041	10.268
San Francisco, CA	23234	0.046	0.207	0.464	1.252	2.975	7.163	13.747	0.018	0.065	0.127	0.345	1.029	3.743	9.704
Seattle, WA	24233	0.053	0.240	0.540	1.440	3.187	7.022	12.804	0.020	0.073	0.145	0.399	1.193	3.974	9.363
Winnemucca, NV	24128	0.040	0.172	0.380	1.040	2.555	6.432	12.676	0.015	0.056	0.109	0.287	0.842	3.211	8.724

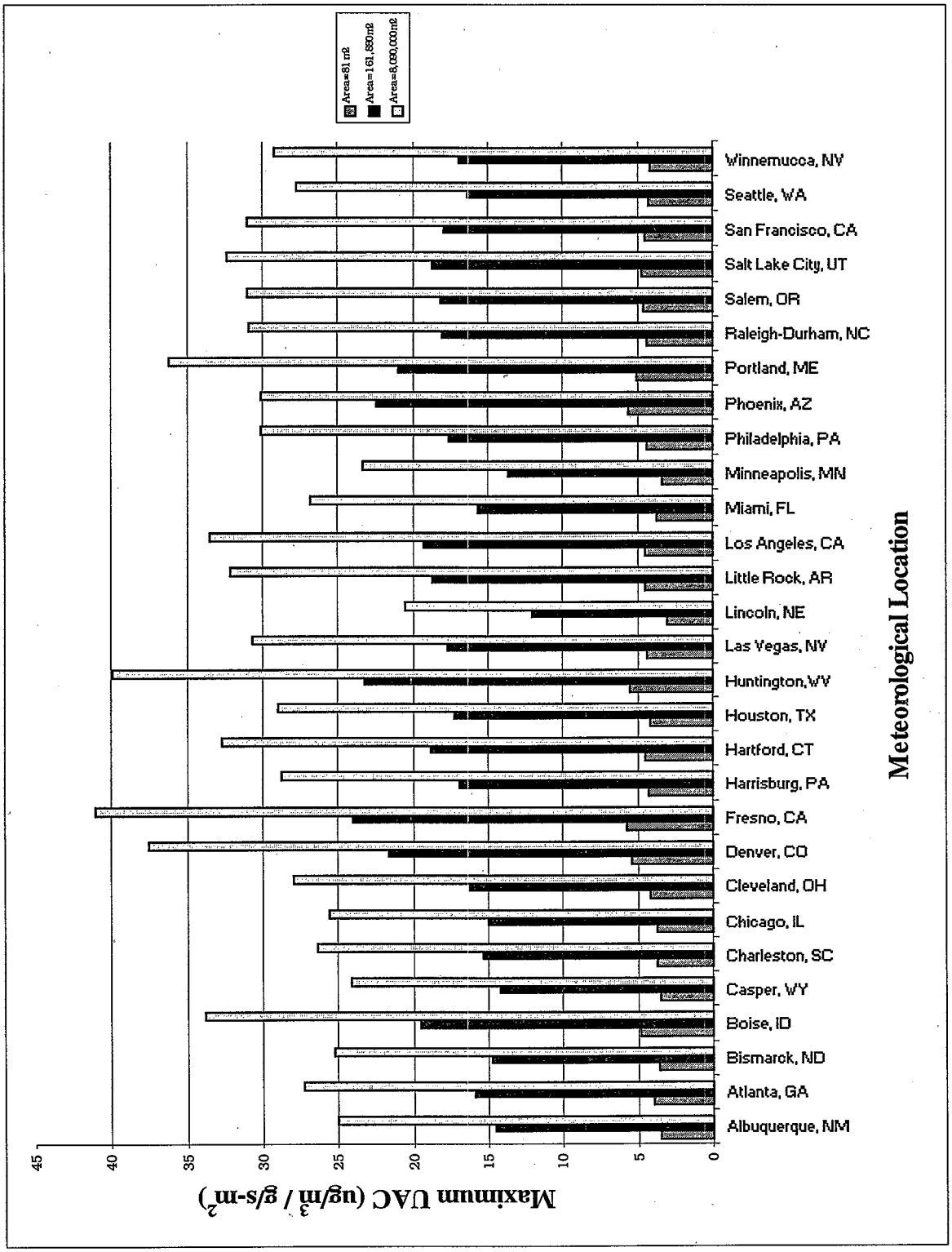


Figure 3-3. Maximum UAC by meteorological location (landfills, LAUs, and surface impoundments).

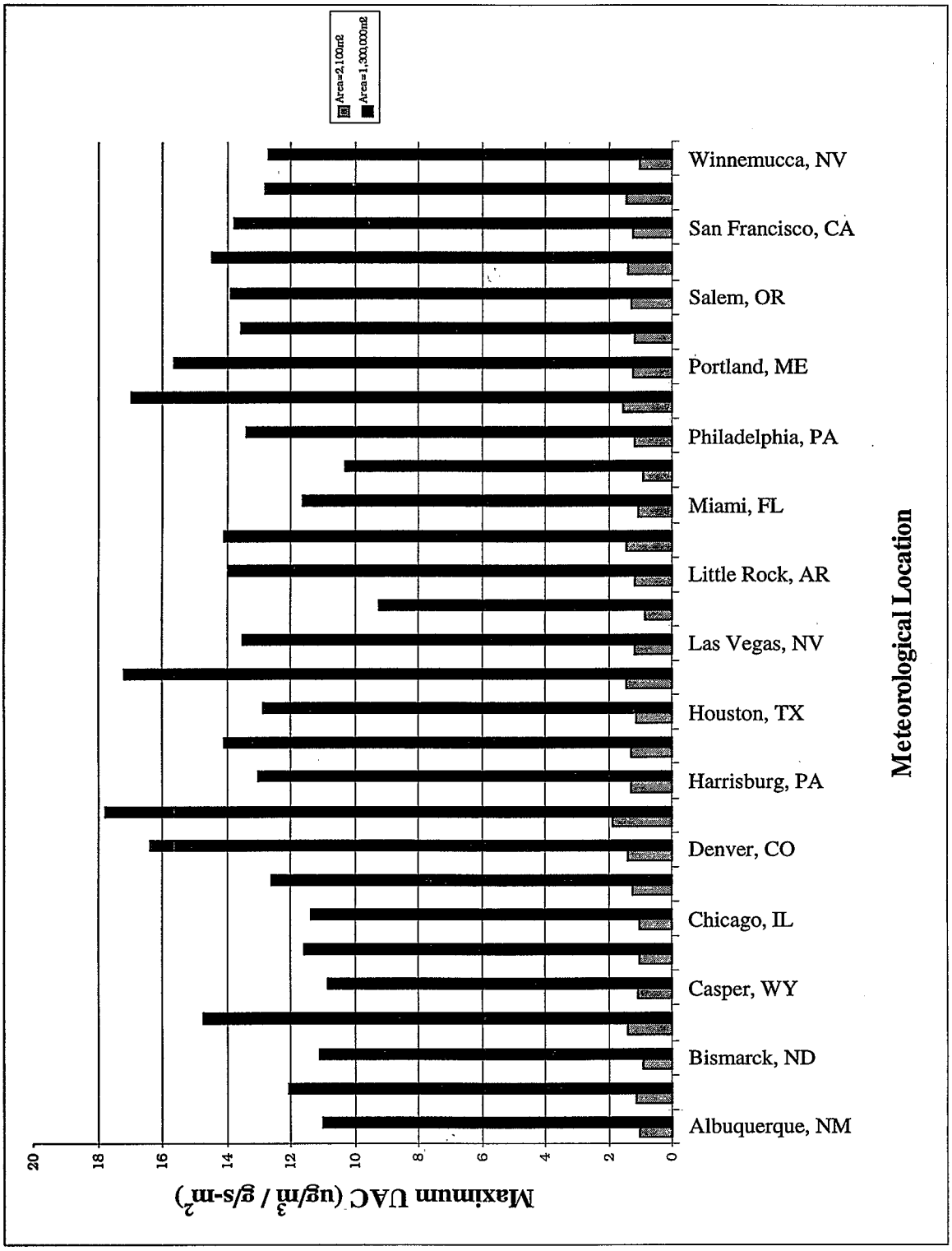


Figure 3-4. Maximum UAC by meteorological location (2-m wastepiles).

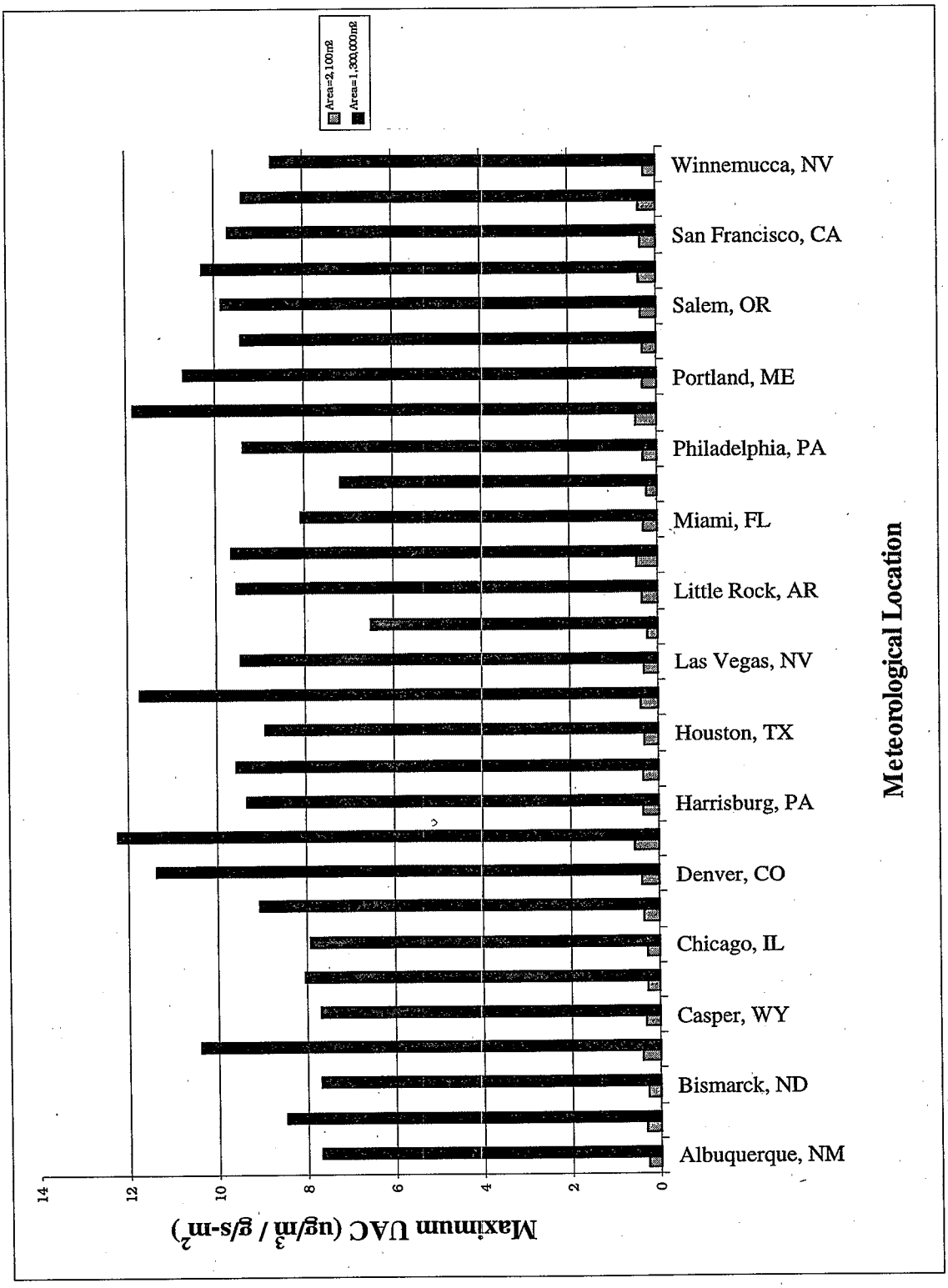
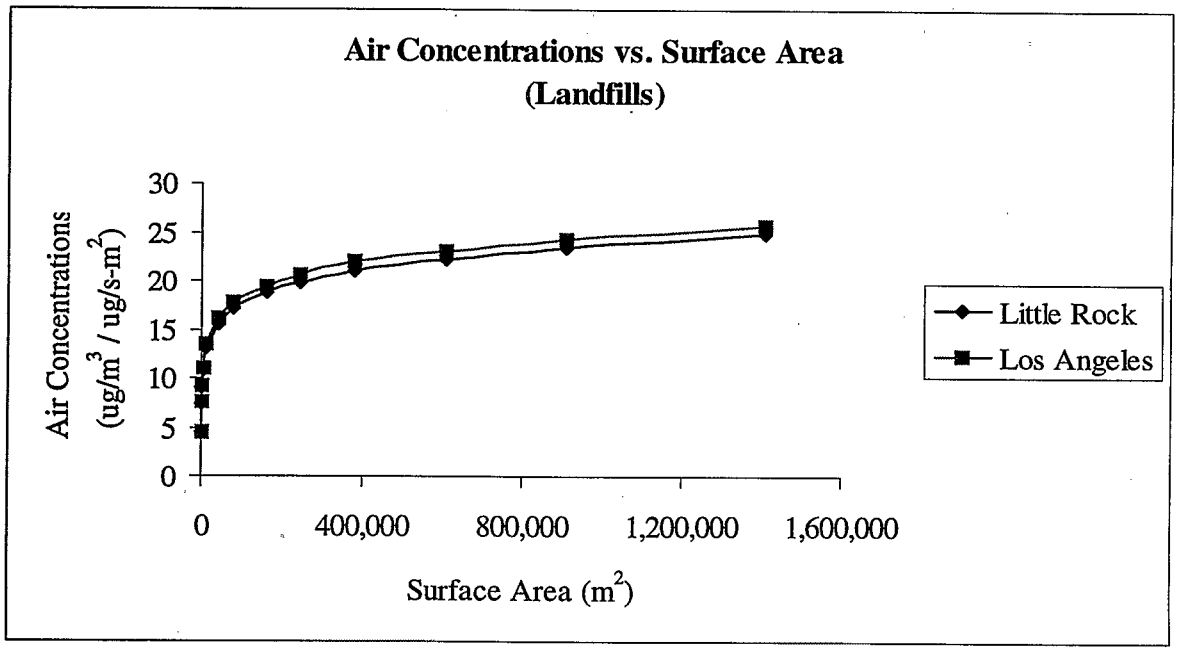
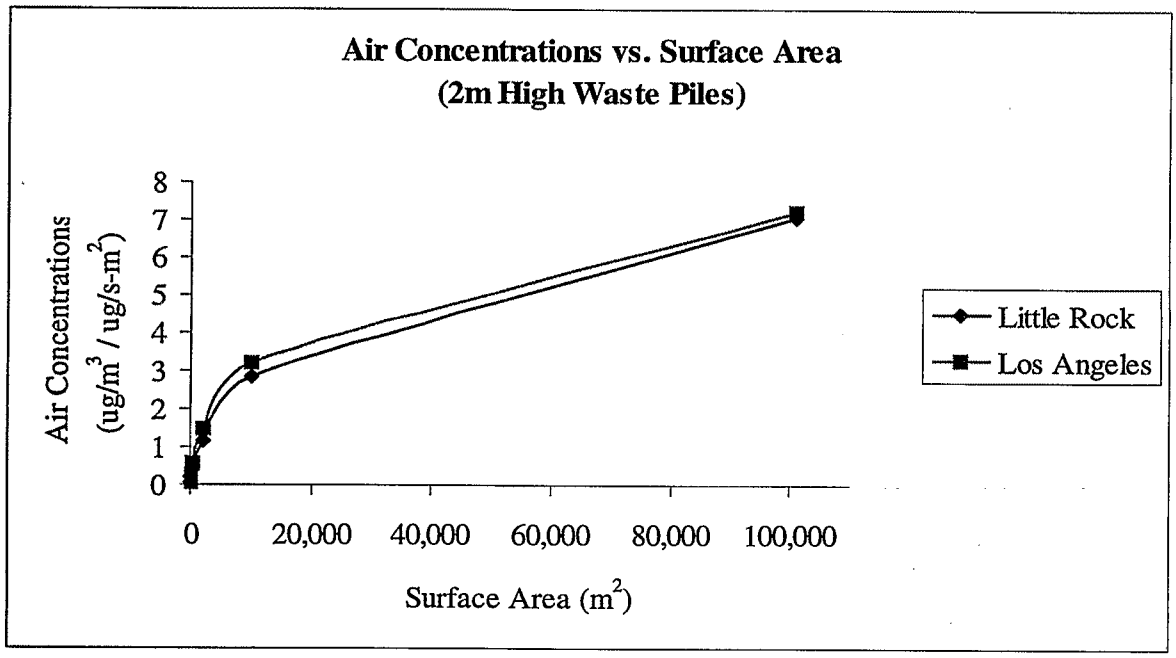


Figure 3-5. Maximum UAC by meteorological location (5-m wastepiles).





Note: Largest areas modeled for each WMU type have been omitted from the chart to improve clarity.

Figure 3-6. Air concentration vs. size of area source.

Table 3-6. Areas Modeled for Landfills, Land Application Units, and Surface Impoundments

Source Area (m^2)	Source Height (m)
81	0
567	0
1,551	0
4,047	0
12,546	0
40,500	0
78,957	0
161,880	0
243,000	0
376,776	0
607,000	0
906,528	0
1,408,356	0
8,090,000	0

Table 3-7. Areas and Source Heights Modeled for Wastepiles

Source Area (m^2)	Source Heights (m)	
20	2	5
162	2	5
486	2	5
2,100	2	5
10,100	2	5
101,000	2	5
1,300,000	2	5

modeled, based on the assumption that the UAC continues to increase with the same slope above the largest area modeled.

Dispersion factors for wastepiles were developed for two pile heights: 2 m and 5 m. If the entered wastepile height is 3.5 m or less, IWAIR uses the 2-m dispersion factors. If the entered wastepile height is greater than 3.5 m, IWAIR uses the 5-m dispersion factors.

4.0 Exposure Factors

This section describes the development of the exposure factors used in IWAIR. All data in this section are from the *Exposure Factors Handbook* (U.S. EPA, 1997a; hereafter, the EFH). These exposure factors are used only for carcinogenic chemicals (see box at right). For noncarcinogens, the hazard quotient is a ratio of air concentration to the health benchmark (a Reference Concentration) and no exposure factors are used.

All exposure factors were developed for the following subpopulations:

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

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

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

Carcinogens Modeled

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

4.1 Exposure Duration

An overall exposure duration of 30 years was selected as a high end value for residents. This was then allocated to the various age ranges modeled, based on the number of years in each age bracket. Table 4-1 shows the values used.

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

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

For workers, the typical default exposure values used in the past were an 8-h shift, 240 d/wk, for 40 years. The EFH presents data on occupational mobility that are in stark contrast to the assumed value of 40 years at a single place of employment. As presented in the EFH, the median occupational tenure of the working population (109.1 million people) ages 16 years of age and older in January 1987 was 6.6 years. This value includes full- and part-time workers. The worker modeled in IWAIR is assumed to be a full-time worker. Therefore, a value of 7.2 years, from EFH Table 15-160 and reflecting full-time male and female workers of all ages, was used.

4.2 Inhalation Rate

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

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

Table 4-3 summarizes the values for inhalation rate for workers presented in the EFH. The recommended hourly average of 1.3 m^3/h was used in IWAIR. To convert this to a daily value, an 8-h workday was assumed, yielding a daily inhalation rate for workers of 10.4 m^3/d.

Table 4-2. Recommended Inhalation Rates for Residents

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

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

Table 4-3. Recommended Inhalation Rates for Workers

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

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

4.3 Body Weight

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

The EFH presents summary data on body weight for adults in Table 7-2. The data for males and females combined are summarized here in Table 4-4. Because an adult resident aged 19-29 was desired, the weighted average of the values for ages 18-24 and 25-34 was used, weighting each by the number of years in that age range (6 in 18-24 and 5 in 25-34).

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

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

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

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

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

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

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

4.4 Exposure Frequency

Exposure frequency is the number of days per year that a receptor is exposed. A value of 350 d/yr was used for residents, and a value of 240 d/yr was used for workers. These are based, respectively, on 7 d/wk and 5 d/wk for 50 wk/yr and account for the receptor being elsewhere on vacation for 2 wk/yr.

5.0 Development of Inhalation Health Benchmarks

Chronic inhalation health benchmarks used in IWAIR include inhalation reference concentrations (RfCs) for noncarcinogens and inhalation cancer slope factors (CSFs) for carcinogens. Unit risk factors (URFs) and CSFs are used in the model for carcinogenic constituents, regardless of the availability of an RfC. Inhalation health benchmarks were identified in the IRIS and AST (U.S. EPA, 1997b, 1998a). IRIS and HEAST are maintained by EPA, and values from IRIS and HEAST were used in the model whenever available. Provisional EPA benchmarks and Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs) were used to fill in data gaps (see Section 5.1). Additional chronic inhalation health benchmarks were derived for use in this analysis for constituents lacking EPA or ATSDR values (see Section 5.2).

Figure 5-1 describes the approach used to develop the chronic inhalation health benchmarks used in this analysis. The benchmarks are summarized in Table 5-1.

5.1 Alternate Chronic Inhalation Health Benchmarks Identified

If IRIS or HEAST chronic inhalation health benchmarks were not available, benchmarks from alternative sources were sought. Provisional EPA benchmarks, ATSDR inhalation MRLs, and California EPA noncancer chronic reference exposure levels (CalEPA, 1997a) were included whenever available. Alternate RfCs were identified for

- Acetone
- Cyclohexanol
- Isophorone
- 2-Methoxyethanol acetate
- Phenol
- Pyridine
- Tetrachloroethylene
- 1,1,1-Trichloroethane
- Xylenes.

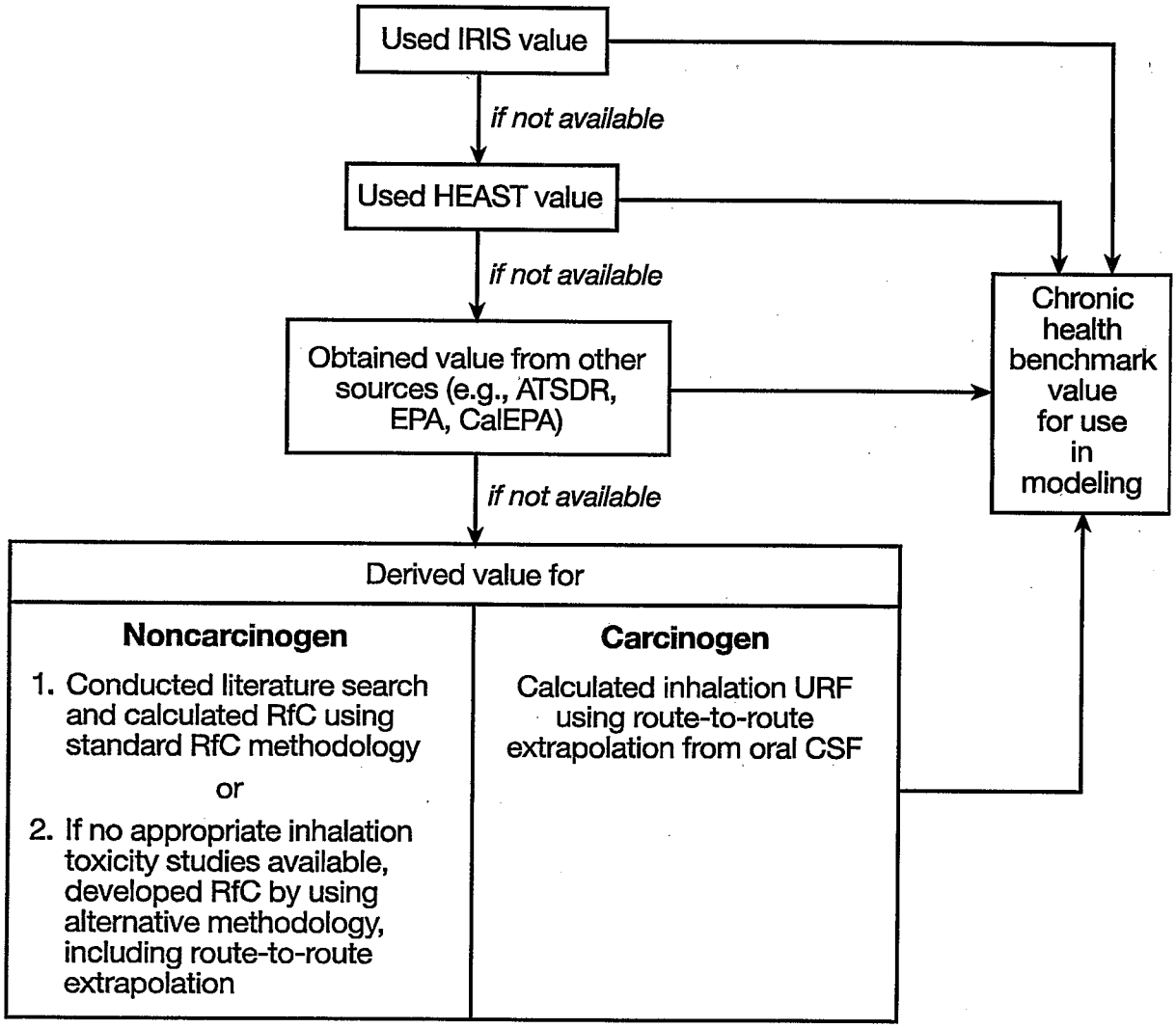


Figure 5-1. Approach used to select chronic inhalation health benchmark values.

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

		Noncarcinogens			Carcinogens		
CAS#	Name	RfC (mg/m³)	RfC Target Organ	Ref[a]	Inhal URF (µg/m³)⁻¹	Inhal CSF (mg/kg/d)⁻¹	Ref[a]
75-07-0	Acetaldehyde	9.0E-03	Respiratory	I	2.2E-06	7.7E-03	I
67-64-1	Acetone	3.1E+01	Neurological	A	NA	NA	
75-05-8	Acetonitrile	5.0E-02	Liver	H	NA	NA	
107-02-8	Acrolein	2.0E-05	Respiratory	I	NA	NA	
79-06-1	Acrylamide	NA			1.3E-03	4.6E+00	I
79-10-7	Acrylic acid	1.0E-03	Respiratory	I	NA	NA	
107-13-1	Acrylonitrile	2.0E-03	Respiratory	I	6.8E-05	2.4E-01	I
107-05-1	Allyl chloride	1.0E-03	Neurological	I	NA	NA	
62-53-3	Aniline	1.0E-03	Spleen	I	NA	NA	
71-43-2	Benzene	NA			8.3E-06	2.9E-02	I
92-87-5	Benzidine	NA			6.7E-02	2.3E+02	I
50-32-8	Benzo(*a*)pyrene	NA			1.7E-03	6.0E+00	
75-27-4	Bromodichloromethane	NA			1.8E-05	6.2E-02	D
75-25-2	Bromoform (Tribromomethane)	NA			1.1E-06	3.9E-03	I
106-99-0	Butadiene, 1,3-	NA			2.8E-04	9.8E-01	I
75-15-0	Carbon disulfide	7.0E-01	Reproductive	I	NA	NA	
56-23-5	Carbon tetrachloride	NA			1.5E-05	5.3E-02	I
126-99-8	Chloro-1,3-butadiene, 2- (Chloroprene)	7.0E-03	Respiratory	H	NA	NA	
108-90-7	Chlorobenzene	2.0E-02	Kidney and liver	H	NA	NA	
124-48-1	Chlorodibromomethane	NA			2.4E-05	8.4E-02	D
67-66-3	Chloroform	NA			2.3E-05	8.1E-02	I
95-57-8	Chlorophenol, 2-	1.4E-03	Repro/developmental	D	NA	NA	
1319-77-3	Cresols (total)	4.0E-04	Hematological	D	NA	NA	
98-82-8	Cumene	4.0E-01	Kidney and adrenal	I	NA	NA	
108-93-0	Cyclohexanol	2.0E-05	NA	S	NA	NA	
96-12-8	Dibromo-3-chloropropane, 1,2-	2.0E-04	Reproductive	I	6.9E-07	2.4E-03	H
95-50-1	Dichlorobenzene, 1,2-	2.0E-01	Body weight	H	NA	NA	
106-46-7	Dichlorobenzene, 1,4-	8.0E-01	Reproductive	I	NA	NA	
75-71-8	Dichlorodifluoromethane	2.0E-01	Liver	H	NA	NA	
107-06-2	Dichloroethane, 1,2-	NA			2.6E-05	9.1E-02	I
75-35-4	Dichloroethylene, 1,1-	NA			5.0E-05	1.8E-01	I
78-87-5	Dichloropropane, 1,2-	4.0E-03	Respiratory	I	NA	NA	
10061-01-5	Dichloropropene, cis-1,3-	2.0E-02	Respiratory	I	3.7E-05	1.3E-01	H
10061-02-6	Dichloropropene, trans-1,3-	2.0E-02	Respiratory	I	3.7E-05	1.3E-01	H
57-97-6	Dimethylbenz(*a*)anthracene, 7,12-	NA			2.4E-02	8.4E+01	D
68-12-2	Dimethylformamide, *N,N*-	3.0E-02	Liver	I	NA	NA	
95-65-8	Dimethylphenol, 3,4-	NA	NA		NA	NA	
121-14-2	Dinitrotoluene, 2,4-	NA			1.9E-04	6.8E-01	D
123-91-1	Dioxane, 1,4-	8.0E-01	No liver, kidney, or hemato effects	D	NA	NA	

(continued)

Table 5-1. (continued)

CAS#	Name	Noncarcinogens			Carcinogens		
		RfC (mg/m³)	RfC Target Organ	Ref[a]	Inhal URF (µg/m³)⁻¹	Inhal CSF (mg/kg/d)⁻¹	Ref[a]
122-66-7	Diphenylhydrazine, 1,2-	NA			2.2E-04	7.7E-01	I
106-89-8	Epichlorohydrin	1.0E-03	Respiratory	I	1.2E-06	4.2E-03	I
106-88-7	Epoxybutane, 1,2-	2.0E-02	Respiratory	I	NA	NA	
111-15-9	Ethoxyethanol acetate, 2-	7.0E-02	NA	S	NA	NA	
110-80-5	Ethoxyethanol, 2-	2.0E-01	Reproductive	I	NA	NA	
100-41-4	Ethylbenzene	1.0E+00	Developmental	I	NA	NA	
106-93-4	Ethylene dibromide	2.0E-04	Reproductive	H	2.2E-04	7.7E-01	I
107-21-1	Ethylene glycol	6.0E-01	Respiratory	D	NA	NA	
75-21-8	Ethylene oxide	NA			1.0E-04	3.5E-01	H
50-00-0	Formaldehyde	NA			1.3E-05	4.6E-02	I
98-01-1	Furfural	5.0E-02	Respiratory	H	NA	NA	
87-68-3	Hexachloro-1,3-butadiene	NA			2.2E-05	7.7E-02	I
118-74-1	Hexachlorobenzene	NA			4.6E-04	1.6E+00	I
77-47-4	Hexachlorocyclopentadiene	7.0E-05	Respiratory	H	NA	NA	
67-72-1	Hexachloroethane	NA			4.0E-06	1.4E-02	I
110-54-3	Hexane, n–	2.0E-01	Respiratory and neurological	I	NA	NA	
78-59-1	Isophorone	1.2E-02	NA	S	NA	NA	
7439-97-6	Mercury	3.0E-04	Neurological	I	NA	NA	
67-56-1	Methanol	1.3E+01	Developmental	D	NA	NA	
110-49-6	Methoxyethanol acetate, 2-	2.6E+01	NA	S	NA	NA	
109-86-4	Methoxyethanol, 2-	2.0E-02	Reproductive	I	NA	NA	
74-83-9	Methyl bromide (bromomethane)	5.0E-03	Respiratory	I	NA	NA	
74-87-3	Methyl chloride (chloromethane)	NA			1.8E-06	6.3E-03	H
78-93-3	Methyl ethyl ketone	1.0E+00	Developmental	I	NA	NA	
108-10-1	Methyl isobutyl ketone	8.0E-02	Kidney and liver	H	NA	NA	
80-62-6	Methyl methacrylate	7.0E-01	Respiratory	I	NA	NA	
1634-04-4	Methyl *tert*-butyl ether	3.0E+00	Kidney and liver	I	NA	NA	
56-49-5	Methylcholanthrene, 3-	NA			2.1E-03	7.4E+00	D
75-09-2	Methylene chloride	3.0E+00	Liver	H	4.7E-07	1.6E-03	I
91-20-3	Naphthalene	3.0E-03	Respiratory	I	NA	NA	
98-95-3	Nitrobenzene	2.0E-03	Kidney, liver, hematological, adrenal	H	NA	NA	
79-46-9	Nitropropane, 2-	2.0E-02	Liver	I	2.7E-03	9.4E+00	H
55-18-5	Nitrosodiethylamine	NA			4.30E-02	1.5E+02	I
924-16-3	Nitrosodi-*n*-butylamine	NA			1.60E-03	5.6E+00	I
930-55-2	*n*-Nitrosopyrrolidine	NA			6.10E-04	2.1E+00	I
108-95-2	Phenol	6.0E-03	NA	S	NA	NA	
85-44-9	Phthalic anhydride	1.2E-01	Respiratory	H	NA	NA	
75-56-9	Propylene oxide	3.0E-02	Respiratory	I	3.7E-06	1.3E-02	I

(continued)

Table 5-1. (continued)

CAS#	Name	Noncarcinogens			Carcinogens		
		RfC (mg/m³)	RfC Target Organ	Ref[a]	Inhal URF (µg/m³)⁻¹	Inhal CSF (mg/kg/d)⁻¹	Ref[a]
110-86-1	Pyridine	7.0E-03	Liver	O	NA	NA	
100-42-5	Styrene	1.0E+00	Neurological	I	NA	NA	
1746-01-6	TCDD, 2,3,7,8-	NA			NA	1.6E+05	H
630-20-6	Tetrachloroethane, 1,1,1,2-	NA			7.4E-06	2.6E-02	I
127-18-4	Tetrachloroethylene	3.0E-01	Neurological	A	NA	NA	
79-34-5	Tetrachloroethane, 1,1,2,2-	NA			5.8E-05	2.0E-01	I
108-88-3	Toluene	4.0E-01	Respiratory and neurological	I	NA	NA	
95-53-4	Toluidine, o-	NA			6.9E-05	2.4E-01	D
76-13-1	Trichloro-1,2,2-trifluoroethane, 1,1,2-	3.0E+01	Body weight	H	NA	NA	
120-82-1	Trichlorobenzene, 1,2,4-	2.0E-01	Liver	H	NA	NA	
71-55-6	Trichloroethane, 1,1,1-	1.0E+00	Neurological	SF	NA	NA	
79-00-5	Trichloroethane, 1,1,2-	NA			1.6E-05	5.6E-02	I
79-01-6	Trichloroethylene	NA			1.7E-06	6.0E-03	SF
75-69-4	Trichlorofluoromethane	7.0E-01	Kidney and respiratory	H	NA	NA	
121-44-8	Triethylamine	7.0E-03	No respiratory effects	I	NA	NA	
108-05-4	Vinyl acetate	2.0E-01	Respiratory	I	NA	NA	
75-01-4	Vinyl chloride	NA			8.4E-05	3.0E-01	H
1330-20-7	Xylenes (total)	3.0E-01	Neurological	A	NA	NA	

CAS = Chemical Abstract Service.
CSF = Cancer slope factor.
NA = Not available.
RfC = Reference concentration.
URF = Unit risk factor.

[a] Sources:
I = IRIS (U.S. EPA, 1998a)
H = HEAST (U.S. EPA, 1997b)
A = Agency for Toxic Substances Disease Registry (ATSDR) minimal risk levels (MRLs)
SF = Superfund Risk Issue Paper (U.S. EPA, 1996b; U.S. EPA, n.d.)
FR = 61 FR 42317-354 (U.S. EPA, 1996a)
D = Developed for this study.
O = Other source (see Sections 5.1 and 5.2).
S = Solvents listing, 63FR 64371-402 (U.S. EPA, 1998b)

For acetone, naphthalene, tetrachloroethylene, and total xylenes, ATSDR's chronic inhalation MRLs were used. Naphthalene is currently undergoing review by EPA's IRIS pilot program (future publication date not known) and a new RfC may be available soon. Provisional RfCs were identified for cyclohexanol, isophorone, and phenol in a *Federal Register* notice (61 FR 42317) concerning solvents listings (U.S. EPA, 1996b). An inhalation acceptable daily intake (ADI) was identified for pyridine (U.S. EPA, 1986). An RfC for 1,1,1-trichloroethane

was identified in a Superfund risk issue paper (U.S. EPA, 1996c). Table 5-2 summarizes the alternate RfCs identified as well as the target organs, sources, and critical studies.

Table 5-2. Alternate Chronic Inhalation Health Benchmarks

CAS #	Chemical Name	Inhalation Benchmark and Benchmark Value	Target Organ	Source
67-64-1	Acetone (2-propanone)	RfC = 13 ppm (31 mg/m^3)	Neurological	ATSDR chronic inhalation MRL based on Stewart et al. (1975) *Acetone: Development of a Biological Standard for the Industrial Worker by Breath Analysis*, Cincinnati, OH: NIOSH. NTIS PB82-172917
108-93-0	Cyclohexanol	Provisional RfC = 0.00002 mg/m^3	NA	63 FR 64371 (U.S. EPA, 1998b)
111-15-9	2-Ethoxyethanol Acute	Provisional RfC = 0.07 mg/m^3	NA	63 FR 64371 (U.S. EPA, 1998b)
78-59-1	Isophorone	Provisional RfC= 0.012 mg/m^3	NA	63 FR 64371 (U.S. EPA, 1998b)
110-49-6	2-Methoxyethanol acetate	Provisional RfC = 26 mg/m^3	NA	63 FR 64371 (U.S. EPA, 1998b)
108-95-2	Phenol	Provisional RfC = 0.006 mg/m^3	NA	63 FR 64371 (U.S. EPA, 1998b)
110-86-1	Pyridine	Inhalation ADI= 0.002 mg/kg/d; converts to 0.007 mg/m^3	Liver	Cited in Health and Environmental Effects Profile (HEEP) for Pyridine (EPA/600/x-86-168)
127-18-4	Tetrachloroethylene	RfC = 0.04 ppm (0.3 mg/m^3)	Neurological	ATSDR chronic inhalation MRL based on Ferroni et al. (1992) Neurobehavioral and neuroendocrine effects of occupational exposure to perchloroethylene. *Neurotoxicology* 12:243-247
71-55-6	1,1,1-Trichloroethane	RfC= 1.0 mg/m^3	Neurological	Superfund risk issue paper (U.S. EPA 1996b)
1330-20-7	Xylenes (total)	RfC = 0.1 ppm (0.3 mg/m^3)	Neurological	ATSDR chronic inhalation MRL based on Uchida et al. (1993) Symptoms and signs in workers exposed predominantly to xylenes. *Int Arch Occup Environ Health* 64:597-605.

5.2 Chronic Inhalation Health Benchmarks Derived for IWAIR

Chronic inhalation health benchmarks for constituents lacking IRIS, HEAST, alternative EPA, or ATSDR values were developed for IWAIR. RfCs were developed for

- 2-Chlorophenol
- Cresols
- 1,4-Dioxane
- Ethylene glycol
- Methanol.

For cresols, 1,4-dioxane, ethylene glycol, and methanol, appropriate inhalation studies were identified and RfCs were developed using EPA's standard RfC methodology as detailed in *Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry* (U.S. EPA, 1994b). For 2-chlorophenol, an RfC was developed using route-to-route extrapolation of the oral RfD for 2-chlorophenol (U.S. EPA, 1998a).

Inhalation cancer slope factors were developed for

- Bromodichloromethane
- Chlorodibromomethane
- 7,12-Dimethylbenz[*a*]anthracene
- 2,4-Dinitrotoluene
- 3-Methylcholanthrene
- o-Toluidine.

For bromodichloromethane, chlorodibromomethane, 2,4-dinitrotoluene, and o-toluidine, the oral CSFs (U.S. EPA, 1997b, 1998a) were used to develop inhalation CSFs for the compounds. For 7,12-dimethylbenz[*a*]anthracene and 3-methylcholanthrene, inhalation URFs developed by California's EPA (CalEPA,1997b) were used as the cancer benchmarks.

Table 5-3 summarizes the RfCs, inhalation unit risk factors, and inhalation cancer slope factors that were derived; the method of development and critical studies used; and the target organs identified. Details on the derivation of these inhalation benchmark values are provided in Appendix C.

Table 5-3. Chronic Inhalation Health Benchmarks Derived for IWAIR

CAS #	Chemical Name	Inhalation Benchmark and Benchmark Value	RfC Target Organ	Method of Derivation
75-27-4	Bromodichloromethane (dichlorobromomethane)	Inhal CSF = 6.2E-02 per mg/kg/d Inhal URF = 1.8E-05 per $\mu g/m^3$		Inhal CSF and URF based on IRIS oral CSF (renal)
124-48-1	Chlorodibromomethane (dibromochloromethane)	Inhal CSF = 8.4E-02 per mg/kg/d Inhal URF = 2.4E-05 per $\mu g/m^3$		Inhal CSF and URF based on IRIS oral CSF (hepatocellular adenoma/carcinoma)
95-57-8	2-Chlorophenol (o-)	RfC = 0.0014 mg/m^3	Repro/ developmental	Route-to-route extrapolation of IRIS RfD (0.005 mg/kg/d for reproductive effects)
1319-77-3	Cresols, total	RfC = 0.0004 mg/m^3	Hematological	Standard RfC derivation based on: Uzhdavini et al. (1972)
57-97-6	7,12-Dimethylbenz[*a*]anthracene	Inhal CSF = 8.4E+01 per mg/kg/d Inhal URF = 2.4E-02 per $\mu g/m^3$		Inhal CSF and URF derived by CalEPA (1997b) based on TD_{50} approach
95-65-8	3,4-Dimethylphenol	NA - RfC derivation is inappropriate		
121-14-2	2,4-Dinitrotoluene	Inhal CSF = 6.8E-01 per mg/kg/d Inhal URF= 1.9E-04 per $\mu g/m^3$		Inhal CSF and URF based on IRIS oral CSF (liver, mammary gland)
123-91-1	1,4-Dioxane (1,4-diethyleneoxide)	RfC = 0.8 mg/m^3	Liver, kidney, hematological	Standard RfC derivation based on Torkelson et al. (1974)
107-21-1	Ethylene glycol	RfC= 0.6 mg/m^3	Respiratory	Derived using standard RfC methodology
67-56-1	Methanol	RfC = 13 mg/m^3	Developmental	Standard RfC derivation based on Rogers et al. (1993)
56-49-5	3-Methylcholanthrene	Inhal CSF = 7.4E+00 per mg/kg/d Inhal URF = 2.1E-03 per $\mu g/m^3$		Inhal CSF and URF derived by CalEPA (1997b) based on TD_{50} approach
95-53-4	o-Toluidine	Inhal CSF = 2.4E-01 per mg/kg/d Inhal URF = 6.9E-05 per $\mu g/m^3$		Inhal CSF and URF based on HEAST oral CSF (skin fibroma)

6.0 Calculation of Risk/Hazard Quotient or Waste Concentration

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

6.1 Forward Calculation of Risk or Hazard Quotient

To calculate risk, the air concentration must first be calculated from the WMU emission rate and the dispersion factor, as follows:

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

where

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

The risk or hazard quotient is calculated based on the calculated air concentration and the exposure factors.

Risk for carcinogens is calculated as follows:

$$Risk_j = \frac{C_{air,j} \times 10^{-3}\ mg/\mu g \times CSF_j \times EF}{AT \times 365\ d/yr} \times \sum_{i=1}^{4} \frac{IR_i \times ED_i}{BW_i} \qquad (6\text{-}2)$$

where

$Risk_j$ = individual risk for chemical j (unitless)
$C_{air,j}$ = air concentration for chemical j ([$\mu g/m^3$])
CSF_j = cancer slope factor for chemical j (per mg/kg-d)
i = index on age group (e.g., <1 yr, 1-5 yr, 6-11 yr, 12-19 yr, adult)
IR_i = inhalation rate for age group i (m^3/d)
ED_i = exposure duration for age group i (yr)
EF = exposure frequency (d/yr)
BW_i = body weight for age group i (kg)
AT = averaging time (yr) = 70.

Averaging time is a fixed input to this equation because it must be consistent with the averaging time used to develop the cancer slope factor. For workers, only exposure factors for adult workers are used.

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

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

where

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

The hazard quotient for noncarcinogens was calculated as follows:

$$\text{HQ}_j = \frac{C_{air,j} \times 10^{-3} \text{mg/}\mu\text{g}}{\text{RfC}_j} \tag{6-4}$$

where

HQ_j	=	hazard quotient for chemical j (unitless)
$C_{air,j}$	=	air concentration for chemical j ([μg/m^3])
RfC_j	=	reference concentration for chemical j (mg/m^3).

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

6.2 Backward Calculation of Waste Concentration

The backward calculation of protective waste concentration from a target risk or hazard quotient is somewhat more complex than a forward calculation of risk, because care must be taken to ensure that a physically impossible result is not achieved. To ensure that result, an iterative forward calculation methodology adapted from the Newton-Raphson method was used in IWAIR. The following subsections describe the constraints on backcalculated waste concentrations to reflect physical limitations, the calculation of air concentration for the backcalculation, the Newton-Raphson method, and the application of that method in IWAIR.

6.2.1 Constraints on Backcalculated Waste Concentrations to Reflect Physical Limitations

Wastes are typically assumed to be aqueous phase (i.e., dilute wastes that partition primarily to water within the soil). However, aqueous phase wastes can only occur in land-based units up to the soil saturation limit. At concentrations above the soil saturation limit, wastes can only occur in oily phase. The soil saturation limit is calculated as follows:

$$C_{sat} = \frac{S}{\rho_b} (K_d \times \rho_b + \theta_w + H' \times \theta_a) \qquad (6\text{-}5)$$

where

C_{sat} = soil saturation limit (mg/kg)
S = solubility limit (mg/L)
ρ_b = bulk density of soil / waste matrix (kg/L)
K_d = soil-water partition coefficient (L/kg)
θ_w = water-filled soil porosity (unitless)
H' = dimensionless Henry's law constant (unitless = H/RT)
θ_a = air-filled soil porosity (unitless).

Wastes can also occur in the oily phase at concentrations below the soil saturation limit, but, for most chemicals, the aqueous phase produces greater emissions than the organic phase for the same concentration and, therefore, greater risk. A few chemicals (most notably formaldehyde) have greater emissions (and therefore greater risk) from the oily phase than the aqueous phase.

For surface impoundments, the concentration limit for the aqueous phase is the solubility of the chemical in water.

Regardless of whether the chemical is in the aqueous or oily phase, the concentration can not exceed 1,000,000 mg/kg or mg/L (ppm) by definition.

6.2.2 General Newton-Raphson Method

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

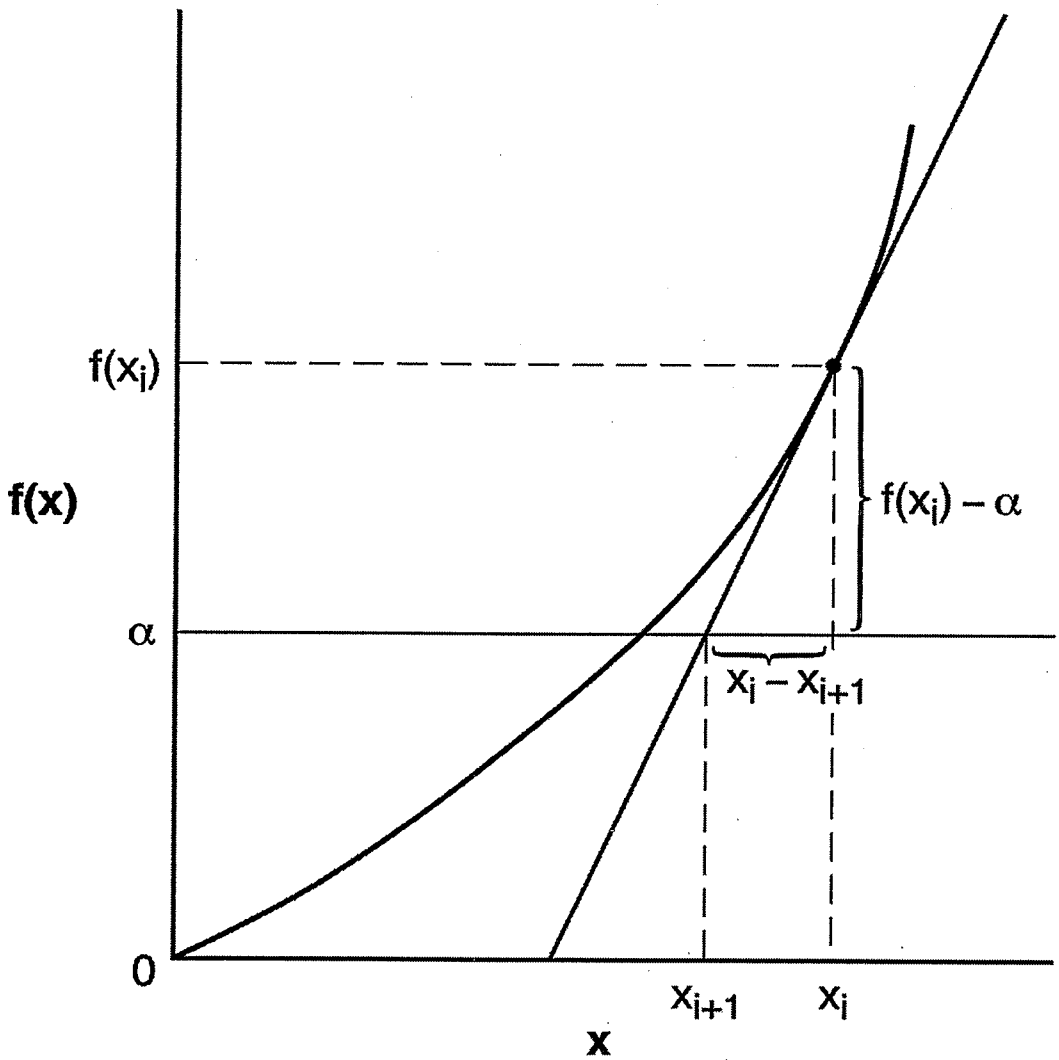


Figure 6-1. Graphical interpretation of the Newton-Raphson Method.

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

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

where

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

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

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

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

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

where

$f'(x_i)$	=	the slope of f(x) at x_i
$f(x_i + \epsilon)$	=	the value of f(x) at $x_i + \epsilon$
x_i	=	the initial guess for x
ϵ	=	a small value relative to x_i.

For IWAIR, ϵ was set to $0.1x_i$.

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

6.2.3 Application of Newton-Raphson Method to Account for Aqueous vs. Oily Phase

The variable x in the general Newton-Raphson method is waste concentation, and the function f(x) is the calculation of either risk or hazard quotient presented in Equations 6-2 and 6-4. However, the air concentration used in those equations differs slightly from Equation 6-1 because the emission rate is normalized to a unit concentration in the WMU rather than an actual emission rate associated with a specific concentration. For the backcalculation, air concentration is calculated as follows:

$$C_{air} = (C_w \times E_{unit} \times 10^6 \ \mu g/g) \times DF \tag{6-9}$$

where

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

Due to the difference in emission rates in the aqueous and oily phases, f(x) is actually a discontinuous function, with a break at the soil saturation limit or the solubility. To account for this, IWAIR first checks the maximum possible concentration in each phase (the soil saturation

limit or solubility for the aqueous phase and 1 million ppm for the oily phase) to see if the target risk or hazard quotient is achievable in that phase. If it is, the Newton-Raphson method is applied to that phase. If it is not, the waste concentration for that phase is set to the maximum, and the risk or hazard quotient associated with that concentration is saved as the maximum risk or hazard quotient achievable in that phase. Finally, IWAIR compares the results for the two phases and outputs the smallest concentration that achieves the target risk or hazard quotient. If the target risk or hazard quotient cannot be achieved in one or both phases, IWAIR outputs the concentration that maximizes risk or hazard quotient.

7.0 References

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Appendix A

Chemical-Specific Data Used in Emission Modeling

A. Chemical-Specific Data Used in Emission Modeling

Key chemical-specific input parameters include: air-liquid equilibrium partitioning coefficient (vapor pressure or Henry's law constant), liquid-solid equilibrium partitioning coefficient (log octanol-water partition coefficient for organics), biodegradation rate constants, and liquid and air diffusivities. The HWIR chemical properties database (RTI, 1995) was used as the primary data source for the physical and chemical properties for the constituents being modeled. This chemical properties database provided the following chemical-specific input parameters: molecular weight, vapor pressure, Henry's law constant, solubility, liquid and air diffusivities, log octanol-water partition coefficient, and the soil biodegradation rate constants. The CHEMDAT8 chemical properties database (U.S. EPA, 1994) was used as a secondary data source for the physical and chemical properties not included in the HWIR data base. The CHEMDAT8 chemical properties database primarily provided the following chemical-specific input parameters: density, boiling point, Antoine's coefficients (for adjusting vapor pressure to temperature), and biodegradation rate constants for surface impoundments. Hydrolysis rates were taken from Kollig et al. (1993). The biodegradation rate constants in the downloaded CHEMDAT8 data base file were compared with the values reported in the summary report that provided the basis for the CHEMDAT8 surface impoundment biodegradation rate values (Coburn et al., 1988). Tank biodegradation rates constants for compounds with no data were assigned biodegradation rates equal to the most similar compound in the biodegradation rate data base. The chemical specific input parameters used for the emission model estimates are presented in Table A-1.

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Table A-1. Chemical Specific Input Parameters

CAS #	COMPOUND NAME	Mol. Wt. (g/mol)	Density (g/cc)	VAP. Press. (mmHg)	H Law Const. (atm-m3/mol)	Diffusivity in Water (cm2/sec)	Diffusivity in Air (cm2/sec)	Antoines' Vapor Pressure Coefficients A	B	C	log Oct Water Part. Coeff.	Kmax mgVO/g-hr.	K1 L/g-hr.	Hydrol. Rate sec-1	Soil Biodeg. Rate sec-1	Solubility mg/L
50000	Formaldehyde	30.03	0.97	5240	3.4E-07	1.98E-05	1.78E-01	7.195	971	244	-0.05	5	0.25	0	6.08E-10	5.50E+05
50328	Benzo(a)pyrene	252.32	1.11	5.5E-09	1.1E-06	9.00E-06	4.30E-02	9.246	3724	273	6.11	0.001	0.31	0	4.61E-08	2.50E-02
55185	N-Nitrosodiethylamine	102.14		0.86	3.6E-06	8.00E-06	8.00E-02			273	0.48	4.4	0.45		1.56E-08	9.30E+04
56235	Carbon tetrachloride	153.82	1.59	115	0.0304	8.80E-06	7.80E-02	6.934	1242	230	2.73	1.5	1.50	0	3.13E-08	7.93E+02
56495	3-Methylcholanthrene	268.36	1.02	7.7E-09	9.4E-07	5.36E-06	2.09E-02	8.164	3364	273	6.42	0.001	0.31	0	1.22E-07	3.23E-03
57976	7,12-Dimethylbenz[a]anthracene	256.35	1.02	5.6E-09	3.1E-08	4.98E-06	4.61E-02	6.955	2163	171	6.62	0.001	0.31	0	2.43E-09	2.50E-02
62533	Aniline	93.13	1.02	0.49	1.9E-06	8.30E-06	7.00E-02	6.950	1467	177	0.98	7.1	21.00	0	6.95E-10	3.61E+04
67561	Methanol	32.04	0.79	126	4.6E-06	1.64E-05	1.50E-01	7.897	1474	229	-0.71	18	0.20	0	6.08E-10	1.00E+06
67641	Acetone	58.08	0.79	230	3.9E-05	1.14E-05	1.24E-01	7.117	1211	230	-0.24	1.3	1.15	0	6.08E-10	1.00E+06
67663	Chloroform	119.38	1.49	197	0.00367	1.00E-05	1.04E-01	6.493	929	196	1.92	28	0.79	0	2.43E-09	7.92E+03
67721	Hexachloroethane	236.74	2.09	0.21	0.00389	6.80E-06	2.49E-03	7.228	1348	133	4	0.001	0.03	0	1.56E-08	5.00E+01
68122	N,N-Dimethyl formamide	73.09	0.9445	4	1.9E-07	1.92E-05	9.39E-02	6.928	1401	196	-1.01	9.7	0.13	0	1.00E-20	1.00E+06
71432	Benzene	78.11	0.87	95	0.00558	9.80E-06	8.80E-02	6.905	1211	221	2.13	19	1.40	0	1.39E-09	1.75E+03
71556	1,1,1-Trichloroethane	133.4	1.33	124	0.0172	8.80E-06	7.80E-02	6.827	1147	219	2.48	3.5	0.74	2E-08	2.37E-08	1.33E+03
74839	Methyl bromide	94.94	1.41	1620	0.00624	1.21E-05	7.28E-02	7.566	1301	273	1.19	10.76	0.35	0	2.43E-09	1.52E+04
74873	Methyl chloride	50.49	0.95	4300	0.00882	6.50E-06	1.26E-01	7.093	949	249	0.91	10.76	0.72	0	2.43E-09	5.33E+03
75014	Vinyl chloride	62.5	0.91	2980	0.027	1.23E-05	1.06E-01	6.991	969	251	1.5	10.76	0.14	0	1.56E-08	2.76E+03
75058	Acetonitrile	41.05	0.78	91.1	3.5E-05	1.66E-05	1.28E-01	7.119	1314	230	-0.34	9.7	0.10	0	2.43E-09	1.00E+06
75070	Acetaldehyde	44.05	0.788	902	7.9E-05	1.41E-05	1.24E-01	8.005	1600	292	1.25	82.42	0.20	0	1.00E-20	1.00E+06
75092	Methylene chloride	84.93	1.34	433	0.00219	1.17E-05	1.01E-01	6.968	1074	223	1.25	18	0.38	0	2.43E-09	1.30E+04
75150	Carbon disulfide	76.14	1.26	359	0.03022	1.00E-05	1.04E-01	6.942	1169	242	2	15.3	0.89	0	1.00E-20	1.19E+03
75218	Ethylene oxide	44.06	0.87	1094	0.00012	1.45E-05	1.04E-01	7.128	1055	238	-0.3	4.2	0.91	0	1.00E-20	3.83E+05
75252	Tribromomethane	252.73	2.89	5.51	0.00054	1.03E-05	1.49E-02	7.988	2159	273	2.35	10.76	1.01	0	1.56E-08	3.10E+03
75274	Bromodichloromethane	163.83	1.97	50	0.0016	1.06E-05	2.98E-02	7.966	1847	273	2.1	10.76	0.70	0	1.00E-20	6.74E+03
75354	1,1-Dichloroethylene	96.94	1.213	600	0.0261	1.04E-05	9.00E-02	6.972	1099	237	2.13	10.76	0.90	0	1.56E-08	2.25E+03
75569	Propylene oxide	58.08	0.83	532.1	8.5E-05	1.00E-05	1.04E-01	7.067	1133	236	0.03	17.56	0.17	0	1.00E-20	4.76E+05
75694	Trichlorofluoromethane	137.37	1.49	803	0.097	9.70E-06	8.70E-02	6.884	1043	237	2.53	1.076	0.12	0	3.13E-08	1.10E+03
75718	Dichlorodifluoromethane	120.91	1.41	4850	0.343	8.00E-06	8.00E-02	7.590	1329	273	2.16	1.076	0.07	0	1.56E-08	2.80E+02
76131	1,1,2-Trichloro-1,2,2-trifluoroethane	187.38	1.41	332	0.4815	8.20E-06	7.80E-02	8.784	1894	273	3.16	0.001	0.03	0	1.00E-20	1.70E+02
77474	Hexachlorocyclopentadiene	272.77	1.7	0.0596	0.027	6.16E-06	5.61E-02	8.415	2835	273	5.39	0.001	0.03	0	2.43E-09	1.80E+00
78591	Isophorone	138.21	0.92	0.438	6.6E-06	6.76E-06	6.23E-02	7.963	2481	273	1.7	15.3	0.60	0	2.43E-09	1.20E+04
78875	1,2-Dichloropropane	112.99	1.156	52	0.0028	8.73E-06	7.82E-02	6.980	1380	223	1.97	17	1.40	0	1.12E-07	2.80E+03

(continued)

Table A-1. Chemical Specific Input Parameters

CAS #	COMPOUND NAME	Mol. Wt. (g/mol)	Density (g/cc)	VAP. Press. (mmHg)	H Law Const. (atm-m3/mol)	Diffusivity in Water (cm2/sec)	Diffusivity in Air (cm2/sec)	Antoines' Vapor Pressure Coefficients A	B	C	log Oct Water Part. Coeff.	Kmax mgVO/g-hr.	K1 L/g-hr.	Hydrol. Rate sec-1	Soil Biodeg. Rate sec-1	Solubility mg/L
78933	Methyl ethyl ketone	72.11	0.82	95.3	5.6E-05	9.80E-06	8.08E-02	7.112	1305	229	0.28	2	0.20	0	6.08E-10	2.23E+05
79005	1,1,2-Trichloroethane	133.4	1.435	23.3	0.00091	8.80E-06	7.80E-02	7.192	1480	229	2.05	3.5	0.74	0	3.17E-08	4.42E+03
79016	Trichloroethylene	131.39	1.4	73.5	0.0103	9.10E-06	7.90E-02	6.518	1019	193	2.71	3.9	0.88	0	3.13E-08	1.10E+03
79061	Acrylamide	71.08	0.84	0.007	1E-09	1.06E-05	9.70E-02	11.293	3940	273	-0.96	9.7	0.27	0	6.52E-11	6.40E+05
79107	Acrylic acid	72.06	1.12	4	1.2E-07	1.06E-05	9.60E-02	5.652	649	155	0.35	17.56	0.18	0	1.00E-20	1.00E+06
79345	1,1,2,2-Tetrachloroethane	167.85	1.59	4.62	0.00035	7.90E-06	7.10E-02	6.894	1355	192	2.39	6.2	0.68	0	3.82E-09	2.97E+03
79469	2-Nitropropane	89.09	0.9876	18	0.00012	1.01E-05	9.23E-02	7.272	1531	229	0.87	9.7	0.42	0	1.56E-08	1.70E+04
80626	Methyl methacrylate	100.12	0.95	38.4	0.00034	8.60E-06	7.70E-02	6.517	1052	188	1.38	17.56	4.30	0	2.43E-09	1.50E+04
85449	Phthalic anhydride	148.12	1.33	0.00052	1.6E-08	9.60E-06	7.10E-02	8.022	2869	273	-0.62	17.56	0.08	0.0155	1.00E-20	6.20E+03
87683	Hexachloro-1,3-butadiene	260.76	1.67	0.221	0.00815	6.16E-06	5.61E-02	7.485	1956	215	4.81	0.001	0.03	0	1.56E-08	3.23E+00
91203	Naphthalene	128.17	1.14	0.085	0.00048	7.50E-06	5.90E-02	7.373	1968	223	3.36	42.47	1.00	0	4.17E-09	3.10E+01
92875	Benzidine	184.24	1.02	8E-09	3.9E-11	1.50E-05	8.00E-02	7.542	2626	163	1.66	31.1	0.66	0	6.95E-10	5.00E+02
95501	o-Dichlorobenzene	147	1.31	1.36	0.0019	7.90E-06	6.90E-02	6.883	1538	205	3.43	2.5	0.58	0	1.56E-08	1.56E+02
95534	o-Toluidine	107.16	0.989	0.32	2.7E-06	9.12E-06	7.14E-02	7.197	1683	191	1.34	31.1	0.86	0	6.08E-10	1.66E+04
95578	2-Chlorophenol	128.56	1.26	2.34	0.00039	9.46E-06	5.01E-02	6.877	1472	193	2.15	15	0.89	0	1.00E-20	2.20E+04
95658	3,4-Dimethylphenol	122.17	0.97	0.05836	2.3E-07	8.33E-06	6.02E-02	7.504	1940	197	2.23	5.5	1.05	0	1.00E-20	4.00E+04
96128	1,2-Dibromo-3-chloropropane	236.33	1.41	0.58	0.00015	7.02E-06	2.12E-02	8.073	2436	273	2.34	10.76	0.16	0	1.56E-08	1.23E+03
98011	Furfural	96.09	1.16	2.21	4E-06	1.04E-05	6.72E-02	6.575	1199	163	0.41	17.56	0.54	0	1.00E-20	1.10E+05
98828	Cumene	120.19	0.86	4.5	1.16	7.10E-06	8.60E-02	6.963	1461	208	3.58	31.1	2.88	0	6.95E-10	6.13E+01
98953	Nitrobenzene	123.11	1.2	0.245	2.4E-05	8.60E-06	7.60E-02	7.115	1747	202	1.84	11	2.30	0	1.71E-08	2.09E+03
100414	Ethylbenzene	106.17	0.87	9.6	0.00788	7.80E-06	7.50E-02	6.975	1424	213	3.14	6.8	2.10	0	8.69E-10	1.69E+02
100425	Styrene	104.15	0.9	6.12	0.00275	8.00E-06	7.10E-02	6.945	1437	208	2.94	31.1	0.11	0	2.43E-09	3.10E+02
106467	p-Dichlorobenzene	147	1.29	1	0.0024	7.90E-06	6.90E-02	7.199	1690	218	3.42	6.4	2.30	0	1.00E-20	7.38E+01
106887	1,2-Epoxybutane	72.11	0.826	207.912	0.00046	1.03E-05	1.35E-01	6.832	1141	228	1.441	10.76	0.48	0	1.00E-20	4.28E+04
106898	Epichlorohydrin	92.53	1.18	16.4	3E-05	9.80E-06	8.60E-02	8.229	2087	273	0.25	10.76	0.14	0	2.43E-09	6.59E+04
106934	Ethylene dibromide	187.86	2.7	13.3	0.00074	1.19E-05	2.17E-02	7.345	1675	245	1.96	10.76	0.55	0	1.56E-08	4.18E+03
106990	1,3-Butadiene	54.09	0.76	2110	0.0736	1.08E-05	2.49E-01	7.217	1145	269	1.99	15.3	0.69	0	1.00E-20	7.35E+02
107028	Acrolein	56.06	0.84	274	0.00012	1.22E-05	1.05E-01	7.213	1297	247	-0.01	7.8	0.34	0	2.43E-09	2.13E+05
107051	Allyl chloride	76.53	0.94	368	0.011	1.08E-05	1.17E-01	7.576	1494	273	1.45	10.76	0.31	0	1.21E-09	3.37E+03
107062	1,2-Dichloroethane	98.96	1.26	78.9	0.00098	9.90E-06	1.04E-01	7.068	1293	225	1.47	2.1	0.98	0	1.56E-08	8.52E+03
107131	Acrylonitrile	53.06	0.97	109	0.0001	1.34E-05	1.22E-01	7.110	1336	238	0.25	18	0.75	0	2.00E-09	7.40E+04
107211	Ethylene glycol	62.07	1.11	0.092	6E-08	1.22E-05	1.08E-01	8.091	2089	204	-1.36	17.56	0.06	0	1.00E-20	1.00E+06

(continued)

Table A-1. Chemical Specific Input Parameters

CAS #	COMPOUND NAME	Mol. Wt. (g/mol)	Density (g/cc)	VAP. Press. (mmHg)	H Law Const. (atm-m3/mol)	Diffusivity in Water (cm2/sec)	Diffusivity in Air (cm2/sec)	Antoines' Vapor Pressure Coefficients A	B	C	log Oct Water Part. Coeff.	Kmax mgVO/g-hr.	K1 L/g-hr.	Hydrol. Rate sec-1	Soil Biodeg. Rate sec-1	Solubility mg/L
108054	Vinyl acetate	86.09	0.93	90.2	0.00051	9.20E-06	8.50E-02	7.210	1296	227	0.73	17.56	0.30	0	1.00E-20	2.00E+04
108101	Methyl isobutyl ketone	100.16	0.8	19.9	0.00014	7.80E-06	7.50E-02	6.672	1168	192	1.19	0.74	0.45	0	6.08E-10	1.90E+04
108883	Toluene	92.14	0.87	28.4	0.00664	8.60E-06	8.70E-02	6.954	1345	219	2.75	6.7	2.40	0	1.91E-09	5.26E+02
108907	Chlorobenzene	112.56	1.11	12	0.0037	8.70E-06	7.30E-02	6.978	1431	218	2.86	0.39	10.00	0	1.30E-08	4.72E+02
108930	Cyclohexanol	100.2	0.95	1.22	4.5E-06	8.31E-06	2.14E-01	6.255	913	109	1.577	17.56	0.54	0	1.00E-20	3.60E+04
108952	Phenol	94.11	1.07	0.276	4E-07	9.10E-06	8.20E-02	7.133	1517	175	1.48	97	13.00	0	8.69E-10	8.28E+04
109864	2-Methoxyethanol	76.09		2.55697	2.6E-07	8.00E-06	8.00E-02			273	-0.77	19.8	1.00		1.00E-20	1.00E+06
110496	2-Methoxyethanol acetate	130.15		9.28503	1.6E-06	8.00E-06	8.00E-02			273	0	19.8	1.00		1.00E-20	1.00E+06
110543	n-Hexane	86.18	0.66	151	0.0143	7.77E-06	2.00E-01	6.876	1171	224	4	15.3	1.47	0	1.00E-20	1.24E+01
110805	2-Ethoxyethanol	90.12	0.9	5.31	3.5E-07	9.57E-06	9.47E-02	7.874	1844	234	-0.1	19.8	1.00	0	2.43E-09	1.00E+06
110861	Pyridine	79.1	0.98	20.8	8.9E-06	7.60E-06	9.10E-02	7.041	1374	215	0.67	35.03	0.24	0	6.08E-10	1.00E+06
111159	2-Ethoxyethanol acetate	143.01		11.6912	2.2E-06	8.00E-06	8.00E-02			273	0	19.8	1.00		1.00E-20	1.00E+06
118741	Hexachlorobenzene	284.78	2.04	1.8E-05	0.00132	5.91E-06	5.42E-02	9.554	3249	203	5.89	0.001	0.03	0	1.82E-07	6.20E+00
120821	1,2,4-Trichlorobenzene	181.45	1.41	0.431	0.00142	8.23E-06	3.00E-02	7.706	2243	253	4.01	1.076	0.44	0	1.56E-08	3.00E+02
121142	2,4-Dinitrotoluene	182.14	1.31	0.00015	9.3E-08	7.06E-06	2.03E-01	7.981	3074	280	2.01	9.7	0.78	0	1.56E-08	2.70E+02
121448	Triethylamine	101.19	0.7326	57.07	0.00014	7.88E-06	8.81E-02	6.959	1272	223	1.45	9.7	1.06	0	1.00E-20	5.50E+04
122667	1,2-Diphenylhydrazine	184.24	1.19	0.00043	1.5E-06	7.36E-06	3.17E-02	13.836	5403	273	2.94	19	1.91	0	1.00E-20	6.80E+01
123911	1,4-Dioxane	88.11	1.03	38.1	4.8E-06	1.02E-05	2.29E-01	7.351	1518	238	-0.39	17.56	0.39	0	1.56E-08	1.00E+06
124481	Chlorodibromomethane	208.28	2.451	4.9	0.00078	1.05E-05	1.96E-02	8.220	2100	273	2.17	10.76	0.04	0	1.56E-08	2.60E+03
126998	Chloroprene	88.54	0.958	213.658	0.0143	1.00E-05	1.04E-01	6.161	783	180	2.08	10.76	0.22	0	1.56E-08	1.74E+03
127184	Tetrachloroethylene	165.83	1.624	18.6	0.0184	8.20E-06	7.20E-02	6.976	1387	218	2.67	6.2	0.68	0	3.13E-08	2.00E+02
630206	1,1,1,2-Tetrachloroethane	167.85	1.59	12.03	0.00242	7.90E-06	7.10E-02	6.894	1355	192	2.63	6.2	0.68	0	5.81E-09	1.10E+03
924163	N-Nitrosodi-n-butylamine	158.24		0.03	0.00032	8.00E-06	8.00E-02			273	2.41	0.0001	1.00		1.00E-20	1.27E+03
930552	N-Nitrosopyrrolidine	100.12		0.092	1.2E-08	1.04E-05	7.36E-02			273	-0.19	0.0001	1.00		1.56E-08	1.00E+06
1319773	Cresols (total)	108.1	1.03	0.3	1.6E-06	9.30E-06	6.94E-02	8.850	2795	273	0	23	17.00	0	1.00E-20	2.20E+04
1330207	Xylenes	106.17	0.86	8.04178	0.00604	9.34E-06	7.14E-02	7.940	2090	273	3.17	40.8	1.80	0	2.43E-09	1.86E+02
1634044	Methyl tert-butyl ether	88	0.97	185.949	0.00056	1.05E-05	1.02E-01	6.852	1104	223	1.901	17.56	0.71	0	1.00E-20	3.88E+04
1746016	2,3,7,8-TCDD	322	1.41	7.4E-10	1.6E-05	8.00E-06	4.70E-02	6.977	2377	159	6.64	0.001	0.03	0	1.00E-20	1.90E-05
7439976	Mercury	200.59		0.00196	0.0092	6.30E-06	3.07E-02			273	4.978				1.00E-20	5.62E-02
10061015	cis-1,3-Dichloropropylene	110.97	1.2	32.8	0.00176	1.10E-05	5.85E-02	6.807	1328	230	2	10.76	0.76	0	9.81E-10	2.72E+03
10061026	trans-1,3-Dichloropropylene	110.97	1.2	23.3	0.00125	1.10E-05	5.85E-02	6.807	1328	230	2	10.76	0.76	0	9.81E-10	2.72E+03

Appendix B

Summary Data for 29 Meteorological Stations

Table B-1. Meteorological Data for 29 Meteorological Locations Used

	Prevailing Wind Direction	Precipitation cm/yr	Precipitation d/yr	Temperature (°C)	Windspeed (m/s)	Frequency of windspeed >5.4 m/s (%)
Albuquerque	N	21	58	14	4.1	22
Atlanta	NW	126	116	17	4.6	21
Bismark	SSE	39	96	6	6.2	33.2
Boise	ESE	30	91	11	4.6	21
Casper	SW	30	95	8	7.2	47.3
Charleston	NE	132	113	18	4.1	19.1
Chicago	SW	90	125	9	4.6	31.7
Cleveland	SW	94	157	10	5.1	33.6
Denver	S	39	89	11	4.1	20.9
Fresno	WNW	27	89	17	3.6	7.4
Harrisburg	W	99	125	12	4.6	16.6
Hartford	S	112	126	10	4.1	21.9
Houston	SE	119	101	21	4.1	16.3
Huntington	SW	105	142	13	3.6	8.2
Las Vegas	SW	10	27	19	5.1	25.9
Lincoln	S	75	91	11	5.1	31.1
Little Rock	SW	129	104	17	3.6	14.4
Los Angeles	WSW	29	33	17	4.1	14.7
Miami	E	145	128	24	4.6	25.5
Minneapolis	SE	69	113	7	5.7	35.2
Philadelphia	SW	105	117	13	4.6	25.6
Phoenix	E	19	37	22	3.1	6.8
Portland	S	110	129	8	4.6	23
Raleigh-Durham	SSW	107	110	16	4.1	14.5
Salem	S	102	146	11	4.6	15.2
Salt Lake City	SE	40	92	11	4.6	20.1
San Francisco	WNW	49	63	14	6.2	37.4
Seattle	S	98	157	11	5.1	22.1
Winnemucca	S	21	67	9	4.1	17.2

Appendix C

Derivation of Chronic Inhalation Noncancer and Cancer Health Benchmark Values

C.1 Derivation of Inhalation Reference Concentrations

This section contains derivations of Reference Concentrations for:

- 2-Chlorophenol
- Cresols
- 3,4-Dimethylphenol
- 1,4-Dioxane
- Ethylene glycol
- Methanol

2-Chlorophenol
CAS #95-57-8

RfC:	0.0014 mg/m^3
Basis for RfC:	Route-to-route extrapolation from the RfD
Critical Study:	Exon, J.H., and L.D. Koller. 1982. Effects of transplacental exposure to chlorinated phenols. *Environ Health Perspect* 46:137-140 (as cited in U.S. EPA, 1998).
Critical Dose:	5 mg/kg/d [X] NOAEL [ ] LOAEL
Critical Effect:	Increase in conception rate and number of stillbirths and decrease in size of litters
Species:	Rat
Route of Exposure:	Drinking water
Duration:	10 weeks
Uncertainty Factor:	1000: 10 for extrapolation from animals to humans 10 for protection of sensitive human subpopulations 10 for use of a subchronic study
Modifying Factor:	1

Calculations:
RfC = RfD x 1/70 kg x 20 m^3/d = 0.005 mg/kg/d x 1/70 kg x 20 m^3/d = 0.0014 mg/m^3

where:
70 kg = default adult human body weight
20 m^3/d = default human daily rate of inhalation
Calculations assume 100% absorption.

Summary of Study:
The RfD is based on a NOAEL of 5 mg/kg/d with a LOAEL of 50 mg/kg/d for reproductive effects in a subchronic drinking water study in rats (Exon and Koller, 1982, as cited in U.S. EPA, 1998). In this study, groups of 12 to 20 weanling female Sprague-Dawley rats were exposed to 0, 5, 50, or 500 ppm of 2-chlorophenol in the drinking water and bred after 10 weeks of 2-chlorophenol treatment. Treatment was continued during breeding, gestation, and weaning. The weanling rats were evaluated for percent conception, litter size, birth weight, weaning weight, number of stillbirths, and hematology (hematocrit, hemoglobin levels, red and white cell counts, and mean corpuscular volume). The evaluations revealed an increase in the conception rate and in the number of stillborns as well as a decrease in the size of the litters in the rats exposed to 500 ppm, which can be converted to a dosage of 50 mg/kg/d–the LOAEL. No effects

were observed at 50 ppm, which can be converted to a dosage of 5 mg/kg/d. Dividing the NOAEL of 5 mg/kg/d by an uncertainty factor of 1,000 (10 factors each for animal to human extrapolation, interspecies variability, and the use of subchronic data), yields the RfD of 0.005 mg/kg/d (EPA, 1998).

Rationale for Route-to-Route Extrapolation:
A first pass in the liver or respiratory tract is not expected to contribute to the toxicity of 2-chlorophenol because it has been demonstrated that the toxic action of the lower chlorinated phenols is due to the undissociated molecule. In studies with rats, it was observed that the toxicity of chlorophenols administered via subcutaneous and intraperitoneal routes is similar to that which is observed in orally administered chlorophenols (Deichmann and Keplinger, 1981). Since the dermal irritation index for 2-chlorophenol is low, no significant portal of entry effect is expected from inhalation exposure to 2-chlorophenol (HSDB, 1998).

Consequently, route-specific difference in toxicity is not expected for 2-chlorophenol. Therefore, in accordance with EPA guidelines (U.S. EPA, 1994), the oral toxicity data for 2-chlorophenol are adequate for use in the calculation of an inhalation RfC for the substance.

Strengths and Uncertainties:
The strength of the RfC is that it is based on an RfD on IRIS that has undergone rigorous EPA peer review.

The major uncertainty of the RfC is the lack of inhalation toxicity studies in humans or animals and the use of default values in the route-to-route extrapolation.

References:
Deichmann, W.B., and M.L. Keplinger. 1981. Aromatic Hydrocarbons. In: G.D. Clayton and F.E. Clayton (eds). *Patty's Industrial Hygiene and Toxicology*. 3rd revised edition. Volume 2A: Toxicology. New York: John Wiley and Sons, pp. 3325-3415.

Exon, J.H., and L.D. Koller. 1982. Effects of transplacental exposure to chlorinated phenols. *Environ Health Perspect* 46:137-140 (as cited in U.S. EPA, 1998).

Hazardous Substances Databank (HSDB): 2-Chlorophenol. 1998. Online database. National Library of Medicine, Bethesda, MD.

U.S. Environmental Protection Agency. 1994. Methods for derivation of inhalation reference concentrations and application of inhalation dosimetry. Research Triangle Park, NC: Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Office of Research and Development, U.S. EPA. EPA/600/8-90-066F.

U.S. Environmental Protection Agency. 1998. Integrated Risk Information System (IRIS). 2-Chlorophenol. Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH.

Cresols
CAS #1319-77-3

RfC: 0.0004 mg/m^3

Critical Study: Uzhdavini, E.R., K. Astaf'yeva, A.A. Mamayeva, and G.Z. Bakhtizina. 1972. [Inhalation toxicity of o-cresol]. Trudy Ufimskogo Nauchno-Isseldovatel'skogo Instituto Gigiyeny Profzabolevaniya, 7:115-9. (Russian) [as cited in CalEPA, 1997, and U.S. EPA 1985, 1986]

Critical Dose: 9 mg/m^3
[ ] NOAEL [X] LOAEL

Critical Effect: Alterations in bone marrow cellularity

Species: Rat

Route of Exposure: Inhalation

Duration: 4 months

Uncertainty Factor: 3000:
10 for use of a LOAEL
10 for extrapolation from animals to humans
10 for protection of sensitive human subpopulations
3 for extrapolation from subchronic to chronic exposure

Modifying Factor: 1

Calculations:
$RfC = LOAEL_{HEC} \div UF = 1.3\ mg/m^3 \div 3000 = 0.0004\ mg/m^3$

Summary of Study:
Male and female rats were exposed to 0 or 9.0 mg/m^3 o-cresol via inhalation, first for 2 months (6 h/d, 5 d/wk) and then for 2 more months (4 h/d, 5 d/wk) (Uzhdavini et al., 1972, as cited in CalEPA, 1997). The following endpoints were examined: elemental conditioned defensive reflex, white blood cell levels, bone marrow elements, and liver function (as indicated indirectly by hexobarbital narcosis). Both exposed and control animals showed some loss of the defensive reflex, with the effect occurring in all exposed animals before the end of the second month and in control animals at later times. White blood cell counts were elevated in male animals, peaking at the end of the exposure period and returning to normal 1 month after cessation of exposure. Exposed animals also showed a statistically significant change in the leukoid-to-erythroid ratio in the bone marrow. Liver toxicity was suggested by an extension of hexobarbital narcosis duration in treated animals. A LOAEL of 9 mg/m^3 for hematological effects was identified.

The LOAEL of 9 mg/m^3 was adjusted for continuous exposure (1.3 mg/m^3). A $LOAEL_{HEC}$ was calculated as per EPA's inhalation dosimetry methodology (1994), using equation 4-48a (category 3 - extrarespiratory effects). An uncertainty factor of 3000 was applied: 10 for use of a

LOAEL, 10 for extrapolation from humans to animals, 10 for human variability, and 3 for extrapolation from subchronic to chronic exposure.

Conversion Factors:

$LOAEL_{ADJ} = 9\ mg/m^3 \times (5/24\ h) \times (5/7\ d) = 1.3\ mg/m^3$

$LOAEL_{HEC} = LOAEL_{ADJ} \times RGDR$

$LOAEL_{HEC} = LOAEL_{ADJ} \times (H_{b/g})_A/(H_{b/g})_H$

$LOAEL_{HEC} = 1.3\ mg/m^3 \times 1 = 1.3\ mg/m^3$

where

$LOAEL_{ADJ}$ is the adjusted LOAEL, RGDR is the regional gas dose ratio (animal:human), and $(H_{b/g})_A/(H_{b/g})_H$ is the ratio of blood:gas partition coefficient; $(H_{b/g})_A/(H_{b/g})_H$ defaults to 1 where $H_{b/g}$ values are not known.

Additional Information:

In humans, inhalation exposure is reported to cause respiratory effects, including the development of pneumonia, pulmonary edema, and hemorrhage (Clayton and Clayton, 1981). Irritation of the nose and throat, nasal constriction, and dryness was reported in 8 of 10 individuals briefly exposed to 6 mg/m^3 (Uzhdavini et al., 1972, as cited in CalEPA 1997).

Signs of respiratory irritation (as indicated by increased paratid gland secretions) were observed in cats exposed to 5 to 9 mg/m^3 o-cresol for 30 minutes (Uzhdavini et al., 1972, as cited in CalEPA 1997). Exposure of mice to 50 mg/m^3 o-cresol for 2 h/d for 1 month did not affect mortality; however, heart muscle degeneration and degeneration of nerve cells and glial elements were reported (Uzhdavini et al., 1972, as cited in CalEPA, 1997, U.S. EPA, 1985).

Strengths and Uncertainties:

Major areas of uncertainty are the lack of human data, the scarcity of animal inhalation data, and the lack of a NOAEL for this study. Also, the data presented were incomplete, the number of animals used is not known, exposure and control conditions were not described, statistical analyses were not provided, and the purity of the compound tested could not be ascertained.

References:

California Environmental Protection Agency (CalEPA). 1997. Technical support document for the determination of noncancer chronic reference exposure levels, Draft for Public Review. Office of Environmental Health Hazard Assessment, Air Toxicology and Epidemiology Section, Berkeley, CA.

Clayton, G.D., and F.E. Clayton (eds). 1981. *Patty's Industrial Hygiene and Toxicology*. 3rd revised edition. Volume 2A: Toxicology. New York: John Wiley and Sons, pp. 2597-2601.

U.S. Environmental Protection Agency. 1985. Health and environmental effects profile for cresols. Cincinnati, OH: Environmental Criteria and Assessment Office, Office of Research and Development, U.S. EPA. EPA/600/x-85-358.

U.S. Environmental Protection Agency. 1986. Health effects assessment for cresols. Cincinnati, OH: Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Office of Research and Development, U.S. EPA. EPA/540/1-86-050.

U.S. Environmental Protection Agency. 1994. Methods for derivation of inhalation reference concentrations and application of inhalation dosimetry. Research Triangle Park, NC: Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Office of Research and Development, U.S. EPA. EPA/600/8-90-066F.

Uzhdavini, E.R., K. Astaf'yeva, A.A. Mamayeva, and G.Z. Bakhtizina. 1972. [Inhalation toxicity of o-cresol]. Trudy Ufimskogo Nauchno-Isseldovatel'skogo Instituto Gigiyeny Profzabolevaniya, 7:115-9. [as cited in CalEPA, 1997, and U.S. EPA 1985, 1986]

3,4-Dimethylphenol
CAS # 95-65-8

RfC: Data are inadequate to support the derivation of an RfC at this time.

Supporting Data:
An RfD of 0.001 mg/kg/d is listed in IRIS (U.S. EPA, 1998), based on a subchronic feeding study in rats. Changes in blood pressure and body weight and histopathological changes in liver, kidney and spleen were reported (Veldre and Janes, 1979). Route-to-route extrapolation of an RfC from the RfD is not recommended because of the potential for respiratory tract effects following inhalation exposure and first-pass effects following ingestion exposure.

Although dimethylphenols have been detected in tobacco smoke, automobile exhausts, and exhausts from stationary sources, they have not been detected in ambient air (U.S. EPA, 1986). 3,4-Dimethylphenol is not likely to occur at detectable concentrations in ambient air because it is a solid at ambient temperatures and has a low vapor pressure. Consequently, inhalation exposures are unlikely to be important for the general population. Skin absorption and ingestion, which can be evaluated by the RfD, are likely to be the predominant exposure pathways.

Very little toxicity or metabolism data specific to 3,4-dimethylphenol are available. Dimethylphenols and related compounds (phenol and methylphenols [cresols]) are rapidly absorbed following ingestion, inhalation, or skin contact and are corrosive to skin, eyes, mucous membranes, and the respiratory tract. Therefore, portal-of-entry effects are likely to be important and cannot be addressed from route-to-route extrapolation. First-pass effects also may be important. These compounds are metabolized predominantly to glucuronide and sulfate conjugates and excreted in the urine (U.S. EPA, 1986). Skowronski et al. (1994) suggested that a lack of first-pass metabolism in the liver may contribute to the toxicity of phenol following skin absorption; therefore, differences in metabolism following ingestion and inhalation exposures also could affect toxicity.

References:
Skowronski, G.A., A.M. Kadry, R.M. Turkall, et al. 1994. Soil decreases the dermal penetration of phenol in male pig in vitro. *J Toxicol Environ Health* 41:467-479.

U.S. Environmental Protection Agency. 1986. Health and environmental effects profile for dimethylphenols. Environmental Criteria and Assessment Office, Cincinnati, OH. EPA/600/x-86/256.

U.S. Environmental Protection Agency. 1994. Methods for derivation of inhalation reference concentrations and application of inhalation dosimetry. Research Triangle Park, NC: Environmental Criteria and Assessment Office, Office of Health and Environmental Assesment, Office of Research and Development, U.S. EPA. EPA /600//8-90-066F.

U.S. Environmental Protection Agency. 1998. Integrated Risk Information System (IRIS). 3,4-Dimethylphenol. Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH.

Veldre, I.A., and H.J. Janes. 1979. Toxicological studies of shale oils, some of their components and commercial products. *Environ Health Perspect* 30:141-146 (as cited in U.S. EPA, 1998).

1,4-Dioxane
CAS # 123-91-1

RfC: 0.8 mg/m^3

Critical Study: Torkelson, T.R., B.K.J. Leong, R.J. Kociba, et al. 1974. 1,4-Dioxane. II. Results of a 2-year inhalation study in rats. *Toxicol Appl Pharmacol* 30:287-298.

Critical Dose: 400 mg/m^3
[X] NOAEL [ ] LOAEL

Critical Effect: No effect on liver, kidney, or hematological endpoints

Species: Rat

Route of Exposure: Inhalation

Duration: 2 years

Uncertainty Factor: 100:
10 for extrapolation from animals to humans
10 for protection of sensitive human subpopulations

Modifying Factor: 1

Calculations:
$RfC = NOAEL_{HEC} \div UF = 83.3\ mg/m^3 \div 100 = 0.8\ mg/m^3$ (0.2 ppm)

Summary of Study:
Groups of Wistar rats were exposed to 0 or 111 ppm (0 or 400 mg/m^3) 1,4-dioxane 7 h/d, 5 d/wk for 2 years (Torkelson et al., 1974). Animals were observed for signs of toxicity, including behavioral changes, eye and nasal irritation, respiratory distress, and skin condition. Body weight was measured weekly. Hematological measurements were made at 16 and 23 months and included serum glutamic-pyruvic transaminase (SGPT) activity, blood urea nitrogen (BUN), alkaline phosphatase (AP) activity, and total protein determinations. At sacrifice, gross necropsy of all animals was performed, and organs were examined for tumors. Histological examination of tissues was conducted.

No significant differences in survival, body weight, general appearance, or behavior were reported. Packed cell volume (PCV), red blood cells, and hemoglobin were slightly, but significantly ($p<0.05$), increased and white blood cells were significantly decreased in exposed males; however, the study authors note that these differences were within normal physiological levels and not considered of toxic importance. Slightly decreased BUN and AP values observed in exposed males were not considered to be biologically significant by the investigators based on the fact that an increase, not a decrease, in these parameters would indicate kidney or liver damage. Increased total protein in exposed males was also reported but not considered to be biologically significant. No significant differences in liver, kidney, or spleen weights, or gross or

microscopic alterations were observed. Tumor incidence (including hepatic and nasal) was not significantly different in any of the organs examined.

The NOAEL of 400 mg/m^3 was adjusted for continuous exposure (83.3 mg/m^3). A $NOAEL_{HEC}$ was calculated as per EPA's inhalation dosimetry methodology (1994), using equation 4-48a (category 3 - extrarespiratory effects). An uncertainty factor of 100 was applied: 10 for extrapolation from humans to animals and 10 for human variability.

Conversion Factors:
0.4 mg/L x 1,000 L/m^3 = 400 mg/m^3

$NOAEL_{ADJ}$ = 400 mg/m^3 x (7/24 hr) x (5/7 d) = 83.3 mg/m^3
$NOAEL_{HEC}$ = $NOAEL_{ADJ}$ x RGDR
$NOAEL_{HEC}$ = $NOAEL_{ADJ}$ x $(H_{b/g})_A/(H_{b/g})_H$
$NOAEL_{HEC}$ = 83.3 mg/m^3 x 1 = 83.3 mg/m^3

where

$NOAEL_{ADJ}$ is the adjusted NOAEL, RGDR is the regional gas dose ratio (animal:human), and $(H_{b/g})_A/(H_{b/g})_H$ is the ratio of blood:gas partition coefficient; $(H_{b/g})_A/(H_{b/g})_H$ defaults to 1 where $H_{b/g}$ values are not known.

Additional Information:
The major metabolite of 1,4-dioxane in rats is beta-hydroxyethoxyacetic acid (HEAA), which is excreted in the urine (Braun and Young, 1977). Results from a study by Young et al. (1978) show that the fate of 1,4-dioxane in rats is markedly dose-dependent due to a limited capacity to metabolize dioxane to HEAA. Exposure to 1,4-dioxane by ingestion results in saturation of metabolism above a single dose of 100 mg/kg, or as low as 10 mg/kg when administered in multiple doses. When rats were exposed to 50 ppm for 6 hours, nearly all the inhaled 1,4-dioxane was also metabolized to HEAA (99%); the plasma half-life was 1.1 hours (Young et al., 1978). The correlation of the dose-dependent fate of 1,4-dioxane with the results of toxicological studies in rats supports the conclusion that there is an apparent threshold for the toxic effects of dioxane that coincides with saturation of the metabolic pathway for its detoxification (Young et al., 1978). 1,4-Dioxane and HEAA were also found in the urine of dioxane plant workers exposed to an average concentration of 1.6 ppm (TWA) for 7.5 hours (Young et al., 1976, 1977).

In a study by Kociba et al. (1974), Sherman rats were exposed to 0, 0.01, 0.1, or 1.0% 1,4-dioxane in drinking water for up to 2 years. No hematologic changes were reported. Histopathologic examination revealed hepatocellular and renal tubular degenerative changes, accompanied by regenerative activity, in rats exposed to the two highest dose levels, but not at the low dose (Kociba et al., 1974). The lack of hematological effects observed in the ingestion study suggests that the toxicity of 1,4-dioxane may be route-specific. Studies suggest that the inhalation of 1,4-dioxane may lead to adverse effects, but good dose-response data are not available. The toxicity of 1,4-dioxane may be a function of the saturation of the mechanism of metabolism (Young et al., 1978).

Strengths and Uncertainties:
The strengths of the RfC are that it is based on a lifetime study, with a large number of toxic endpoints examined and a large sample size (n=192-288). The weaknesses of the inhalation benchmark value include the use of a free-standing NOAEL, that only one exposure level was used in the Torkelson et al. (1974) study, the limited human data, the limited inhalation data in animals, and the lack of developmental and reproductive studies.

References:
Braun, W.H., and J.D. Young. 1977. Identification of beta-hydoxyethoxyacetic acid the major urinary metabolite of 1,4-dioxane in the rat. *Toxicol Appl Pharmacol* 39:33-38.

California Environmental Protection Agency (CalEPA). 1997. Technical support document for the determination of noncancer chronic reference exposure levels, Draft for Public Review. Office of Environmental Health Hazard Assessment, Air Toxicology and Epidemiology Section, Berkeley, CA.

Kociba, R.J., S.B. McCollister, C. Park, et al. 1974. 1,4-Dioxane. I. Results of a 2-year ingestion study in rats. *Toxicol Appl Pharmacol* 30:275-286.

Torkelson, T.R., B.K.J. Leong, R.J. Kociba, et al. 1974. 1,4-Dioxane. II. Results of a 2-year inhalation study in rats. *Toxicol Appl Pharmacol* 30:287-298.

U.S. Environmental Protection Agency. 1994. Methods for derivation of inhalation reference concentrations and application of inhalation dosimetry. Research Triangle Park, NC: Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Office of Research and Development, U.S. EPA. EPA/600/8-90-066F.

Young, J.D., W.H. Braun, and P.J. Gehring. 1978. Dose-dependent fate of 1,4-dioxane in rats. *J Toxicol Environ Health* 4:709-726.

Young, J.D., W.H. Braun, P.J. Gehring, et al. 1976. 1,4-Dioxane and beta-hydroxyethoxyacetic acid excretion in urine of humans exposed to dioxane vapors. *Toxicol Appl Pharmacol* 38:643-646.

Young, J.D., W.H. Braun, L.W. Rampy, et al. 1977. Pharmacokinetics of 1,4-dioxane in humans. *J Toxicol Environ Health* 3:507-520.

Ethylene glycol
CAS # 107-21-1

RfC:	0.6 mg/m^3
Critical Study:	Wills, J.H., F. Coulston, E.S. Harris, et al. 1974. Inhalation of aerosolized ethylene glycol by man. *Clin Toxicol* 7:463-476.
Critical Dose:	67 mg/m^3 [X] NOAEL [ ] LOAEL
Critical Effect:	Throat and upper respiratory tract irritation
Species:	Humans
Route of Exposure:	Inhalation
Duration:	30 days
Uncertainty Factor:	100: 10 for protection of sensitive human subpopulations 10 for use of a subchronic study
Modifying Factor:	1

Calculations:
$RfC = NOAEL_{ADJ} \div UF = 55.8\ mg/m^3 \div 100 = 0.6\ mg/m^3$

Summary of Study:
Twenty volunteer male prisoners were exposed to ethylene glycol in mean daily concentrations between 3 and 67 mg/m^3 for 30 days, 20 h/d, without effect (Wills et al., 1974). Irritation was noted after 15 minutes at an exposure concentration of 188 mg/m^3 and was judged intolerable at 244 mg/m^3. No effects were observed in clinical serum enzyme levels for liver and kidney toxicity, hematotoxicity, or psychological responses. The irritation resolved soon after exposure with no effects noted after a 6-week followup period.

A NOAEL of 67 mg/m^3 was selected and adjusted for continuous exposure (55.8 mg/m^3). An uncertainty factor of 100 was applied: 10 for use of a subchronic study (30 day-duration) and 10 for protection of sensitive human subpopulations.

Conversion Factors:
$NOAEL_{ADJ} = 67\ mg/m^3 \times 20/24\ h = 55.8\ mg/m^3$

Additional Information:.
Animal studies are inconclusive regarding the respiratory effects of ethylene glycol. Suber et al. (1989, as cited in ATSDR, 1997) report thickened respiratory epithelium with enlarged goblet cells in rats that inhaled ethylene glycol over 90 days. Another study in rhesus monkeys and rats showed no respiratory effects from continuous exposure to propylene glycol for 13 to 18 months

(Robertson et al., 1947, as cited in ATSDR, 1997). Developmental effects have been seen in animal studies. Tyl et al. (1995a, 1995b, as cited in CalEPA, 1997) reported reduced ossification in humerus, zygmotatic arch, and the metatarsals in fetuses of rats and mice exposed to ethylene glycol on days 6 through 15 of gestation.

Strengths and Uncertainties:
The major strength of the RfC is that it was based on human data with controlled inhalation exposures and the observation of a NOAEL. The major uncertainty to the RfC is the lack of chronic inhalation studies in humans and confirming studies in animals.

References:
Agency for Toxic Substances and Disease Registry. 1997. Toxicological profile for ethylene glycol and propylene glycol. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service.

California Environmental Protection Agency (CalEPA). 1997. Technical support document for the determination of noncancer chronic exposure levels, Draft for Public Review. Office of Environmental Health Hazard Assessment, Air Toxicology and Epidemiology Section, Berkeley, CA.

Robertson, O.H., C.G. Loosli, and T.T. Puck. 1947. Test for chronic toxicity of propylene glycol and triethylene glycol on monkeys and rats by vapor inhalation and oral administration. *J Pharmacol Exper Therap* 91:52-76 (as cited in ATSDR 1997).

Suber, R.L., R.D. Deskin, I. Nikiforov, et al. 1989. Subchronic nose-only inhalation study of propylene glycol in Sprague-Dawley rats. *Food Chem Toxicol* 27(9):573-584 (as cited in ATSDR, 1997).

Tyl, R.W., B. Ballantyne, L.C. Fisher, et al. 1995a. Evaluation of the developmental toxicity of ethylene glycol aerosol in CD-1 mice by nose-only exposure. *Fundam Appl Toxicol* 27:49-62 (as cited in CalEPA, 1997).

Tyl, R.W., B. Ballantyne, L.C. Fisher, et al. 1995b. Evaluation of the developmental toxicity of ethylene glycol aerosol in CD rat and CD-1 mouse by whole-body exposure. *Fundam Appl Toxicol* 24:57-75 (as cited in CalEPA, 1997).

U.S. Environmental Protection Agency. 1994. Methods for derivation of inhalation reference concentrations and application of inhalation dosimetry. Research Triangle Park, NC: Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Office of Research and Development, U.S. EPA. EPA/600/8-90-066F.

Wills, J.H., F. Coulston, E.S. Harris, et al. 1974. Inhalation of aerosolized ethylene glycol by man. *Clin Toxicol* 7:463-476.

Methanol
CAS # 67-56-1

RfC: 13 mg/m^3

Critical Study: Rogers, J.M., M.L. Mole, N. Chernoff, et al. 1993. The developmental toxicity of inhaled methanol in the CD-1 mouse, with quantitative dose-response modeling for estimation of benchmark doses. *Teratology* 47(3):175-188.

Critical Dose: 1,310 mg/m^3
[X] NOAEL [ ] LOAEL

Critical Effects: Developmental malformations (increased cervical ribs, exencephaly, and cleft palate)

Species: Mouse

Route of Exposure: Inhalation

Duration: Gd 6-15

Uncertainty Factor: 100:
10 for extrapolation from animals to humans
10 for protection of sensitive human subpopulations

Modifying Factor: 1

Calculations:
$RfC = NOAEL_{HEC} \div UF = 1310\ mg/m^3 \div 100 = 13\ mg/m^3$ (10 ppm)

Summary of Study:
Groups of pregnant CD-1 mice were exposed to 1,000, 2,000, 5,000, 7,500, 10,000, or 15,000 ppm methanol (1,310, 2,620, 6,552, 9,828, 13,104, or 19,656 mg/m^3) for 7 h/d on days 6 through 15 of gestation (Rogers et al., 1993). Three groups of controls were used. Sham-exposed controls were exposed to filtered air. Additional control groups remained in their cages and received food and water ad libitum or were food-deprived for 7 h/d (to match the food deprivation experienced by the exposed mice). Dams were observed twice daily and weighed on alternate days during the exposure period. Blood methanol concentrations were determined in three mice per exposure level on gestation days 6, 10, and 15. On day 17, the remaining mice were weighed and sacrificed and the gravid uteri removed. Implantation sites, live and dead fetuses, and resorptions were counted, and fetuses were examined externally and weighed as a litter. Half of each litter were examined for skeletal morphology and the other half of each litter were examined for internal soft tissue anomalies.

One dam died in each of the three highest exposure groups, but no dose-response relationship was evident for maternal death. The sham-exposed and food-deprived controls, as well as all methanol-exposed dams, gained less weight than did unexposed dams fed ad libitum, but methanol did not exacerbate this effect. Significant increases in the incidence of exencephaly

and cleft palate were observed at 6,552 mg/m^3 and above, increased embryo/fetal death at 9,828 mg/m^3 and above (including an increasing incidence of full-litter resorptions), and reduced fetal weight at 13,104 mg/m^3 and above. A dose-related increase in cervical ribs (small ossification sites lateral to the seventh cervical vertebra) was significant at 2,620 mg/m^3 and above. Therefore, a NOAEL of 1,310 mg/m^3 for developmental toxicity in mice was identified in this study.

Because this is a developmental study, the NOAEL of 1,310 mg/m^3 was not adjusted for continuous exposure. A $NOAEL_{HEC}$ was calculated as per EPA's inhalation dosimetry methodology (1994), using equation 4-48a (category 3 - extrarespiratory effects). An uncertainty factor of 100 was applied: 10 for extrapolation from humans to animals and 10 for human variability.

Conversion Factors:
Dose levels are:
(1,000 ppm x 32.04)/ 24.45 = 1,310 mg/m^3; 2,000 ppm = 2,620 mg/m^3; 5,000 ppm = 6,552 mg/m^3; 7,500 ppm = 9,828 mg/m^3; 10,000 ppm = 13,104 mg/m^3; 15,000 ppm = 19,656 mg/m^3

$NOAEL_{HEC} = NOAEL \times RGDR$
$NOAEL_{HEC} = NOAEL \times (H_{b/g})_A/(H_{b/g})_H$
$NOAEL_{HEC} = 1310\ mg/m^3 \times 1 = 1310\ mg/m^3$

where

RGDR is the regional gas dose ratio (animal:human) and $(H_{b/g})_A/(H_{b/g})_H$ is the ratio of blood:gas partition coefficient; $(H_{b/g})_A/(H_{b/g})_H$ defaults to 1 where $H_{b/g}$ values are not known.

Additional Information:
Developmental effects were also reported in a study by Nelson et al. (1985). Pregnant Sprague-Dawley rats were exposed to methanol at concentrations of 0, 5,000, 10,000, and 20,000 ppm (0, 6,552, 13,104, and 26,208 mg/m^3) 7 h/d on days 1 through 19 of gestation (high dose rats were exposed on Gd 7-15 only). Dams were sacrificed on Day 20. Half of the fetuses were examined for visceral defects, and the other half were examined for skeletal defects. No effect on the numbers of corpora lutea or implantations or the percentage of dead or resorbed fetuses was observed. At the two highest concentrations, a dose-related decrease in fetal weights was reported. The highest concentration of methanol produced slight maternal toxicity and a high incidence of congenital malformations ($p<0.001$), predominantly extra or rudimentary cervical ribs and urinary or cardiovascular defects. Similar malformations were seen in the 10,000 ppm group, but the incidence was not significantly different from controls. No adverse effects were noted in the 6552 mg/m^3 group (Nelson et al., 1985).

Strengths and Uncertainties:
The major strengths of the Rogers et al. (1993) study are the identification of a NOAEL and the demonstration of a dose-response relationship. The study was well performed, large numbers of animals were used (n=20-44 per group), and effects at six exposure concentrations were examined. The results are also supported by an additional developmental study (Nelson et al., 1985).

The major uncertainties of the RfC are the lack of human data for chronic inhalation exposure and the lack of comprehensive, long-term muliple dose studies.

References:

California Environmental Protection Agency (CalEPA). 1997. Technical support document for the determination of noncancer chronic reference exposure levels, Draft for Public Review. Office of Environmental Health Hazard Assessment, Air Toxicology and Epidemiology Section, Berkeley, CA.

Nelson, B.K., W.S. Brightwell, D.R. MacKenzie, et al. 1985. Teratological assessment of methanol and ethanol at high inhalation levels in rats. *Fundam Appl Toxicol* 5:727-736.

Rogers, J.M., M.L. Mole, N. Chernoff, et al. 1993. The developmental toxicity of inhaled methanol in the CD-1 mouse, with quantitative dose-response modeling for estimation of benchmark doses. *Teratology* 47(3):175-188.

U.S. Environmental Protection Agency. 1994. Methods for derivation of inhalation reference concentrations and application of inhalation dosimetry. Research Triangle Park, NC: Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Office of Research and Development, U.S. EPA. EPA/600/8-90-066F.

C.2 Derivation of Inhalation Unit Risk Factors and Cancer Slope Factors

This section contains the derivations of inhalation unit risk factors and cancer slope factors for:

- Bromodichloromethane
- Chlorodibromomethane
- 7,12-Dimethylbenz[*a*]anthracene
- 2,4-Dinitrotoluene
- 3-Methylcholanthrene
- o-Toluidine (2-Methylaniline)

Bromodichloromethane
CAS #75-27-4

Inhalation Unit Risk Factor:	1.8E-05 $(\mu g/m^3)^{-1}$
Slope Factor:	6.2E-02 $(mg/kg/d)^{-1}$
Critical Effects:	Tubular cell adenoma and tubular cell adenocarcinoma
Species:	Mice
Route of Exposure:	Gavage, corn oil
Duration:	2 years

Basis for Toxicity Values:
EPA has not developed an inhalation reference concentration (RfC) for bromodichloromethane. An oral reference dose (RfD) value of 0.02 mg/kg/d, based on a chronic gavage study in mice for renal cytomegaly is available on IRIS for bromodichloromethane (U.S. EPA, 1998).

Based on inadequate human data and sufficient evidence of carcinogenicity in animals, EPA considers bromodichloromethane a probable human carcinogen (Class B2) by the oral route and has calculated an oral cancer slope factor (CSF) of 0.062 $(mg/kg/d)^{-1}$ for the substance. In a National Toxicology Program (NTP) study, 2-year gavage administration of bromodichloromethane to both sexes of F344/N rats and B6C3F1 resulted in compound-related statistically significant increases in tumors of the kidney in male mice, the liver in female mice, and the kidney and large intestine in male and female rats (NTP, 1987, as cited in U.S. EPA, 1998).

In male mice, the incidences of tubular cell adenomas and the combined incidence of tubular cell adenomas and adenocarcinomas of the kidneys were significantly increased in the high-dose animals. In female mice, there were significant increases of hepatocellular adenomas and hepatocellular carcinomas. The combined incidence of hepatocellular adenomas or carcinomas in vehicle control, low-dose, and high-dose groups were 3/50, 18/48, and 29/50, respectively.

In male and female rats, the incidences of tubular cell adenomas, adenocarcinomas, and the combined incidence of adenomas and adenocarcinomas of the kidneys were statistically significantly increased only in the high-dose groups. The combined incidence of tubular cell adenomas or adenocarcinomas in vehicle control, low-dose, and high-dose groups were 0/50, 1/49, and 13/50 for males and 0/50, 1/50, and 15/50 for females, respectively.

Tumors of the large intestines, namely adenocarcinomas and adenomatous polyps, were significantly increased in male rats in a dose-dependent manner. These large intestinal tumors, however, were observed only in high-dose female rats (adenocarcinomas 0/46, 0/50, 6/47; adenomatous polyps 0/46, 0/50, 7/47 in the vehicle control, low-dose and high-dose groups, respectively). The combined incidence of large intestine adenocarcinomas and/or adenomatous polyps in vehicle control, low-dose, and high-dose groups were 0/50, 13/49, and 45/50 for males and 0/46, 0/50, and 12/47 for females. The combined tumor incidences in the large intestine and

kidney in male and female rats at control, low dose, and high dose were 0/50, 13/49, 46/50 and 0/46, 1/50, 24/48, respectively. Under the conditions of this bioassay, the NTP concluded there was clear evidence of carcinogenicity of bromodichloromethane in male and female F344/N rats and B6C3F1 mice (U.S. EPA, 1998).

The mechanism for the carcinogenicity of bromodichloromethane appears to be genotoxic carcinogenesis, independent of liver activation and, hence, route-independent. In one genotoxicity assay, bromodichloromethane was mutagenic in *Salmonella typhimurium* strain TA100 in the absence of liver homogenate in a vapor phase test performed in a desiccator. Positive results for mutagenicity were reported for bromodichloromethane in other *S. typhimurium* assays in which the TA100 and TA1537 strains were used without rat liver homogenate activation. Bromodichloromethane also induced weak mutagenic effects in *Saccharomyces cerevisiae* strains D7 and XV185-14C in the absence of liver homogenate (U.S. EPA, 1998; HSDB, 1998).

Thus, inhalation exposure to bromodichloromethane is likely to lead to carcinogenic consequences not dissimilar from that from oral exposure. Therefore, in accordance with current EPA guidelines, it is considered appropriate to calculate an inhalation unit risk factor for bromodichloromethane from the oral CSF listed for that substance in IRIS (U.S. EPA, 1994, 1996).

Calculations:

URF = CSF x 1 mg/1,000 μg x 1/70 kg x 20 m^3/day =
0.062 $(mg/kg/d)^{-1}$ x 1 mg/1,000 μg x 1/70 kg x 20 m^3/d = 1.8E-05$(\mu g/m^3)^{-1}$

where
70 kg = default adult human body weight
20 m^3 = default adult human daily rate of inhalation
Calculations assume 100% absorption.

Additional Information:

Inhalation CSFs are often derived from oral data. Of the 51 chemicals currently listed in IRIS (U.S. EPA, 1998) and HEAST (U.S. EPA, 1997) that have both an oral and inhalation CSF, about 60% of the inhalation CSFs were derived from oral studies and are identical or essentially identical to the oral CSF (see Table C-1, Figure C-1). In at least one case (benzene), the oral CSF was based on inhalation data resulting in identical values for both routes of exposure. In most cases (>75%) where an inhalation CSF was derived from an inhalation study, the inhalation CSF was lower than the corresponding oral CSF. Therefore, use of an oral CSF as an interim inhalation CSF appears reasonable and is unlikely to result in underestimating risk.

References:

Hazardous Substances Databank (HSDB): Bromodichloromethane. 1998. Online database. National Library of Medicine, Bethesda, MD.

National Toxicology Program (NTP). 1987. NTP Technical Report on the Toxicology and Carcinogenesis Studies of Bromodichloromethane (CAS no. 75-27-4) in F344/N Rats and B6C3F1 Mice (gavage studies). NTP Tech. Report Series No.321. U.S. Dept. Health and Human Services, Public Health Service, National Institute of Health (as cited in U.S. EPA, 1998).

U.S. Environmental Protection Agency. 1994. Provisional Guidance for the Qualitative Risk Assessment of Polycyclic Aromatic Hydrocarbons. Prepared by the Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH, for the Office of Research and Development, Cincinnati, OH. EPA/600/R-93.

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U.S. Environmental Protection Agency. 1997. Health Effects Assessment Summary Tables (HEAST), FY 1997 Update. Office of Emergency and Remedial Response, Washington, DC. EPA-540-R-97-036.

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Chlorodibromomethane
CAS #124-48-1

Inhalation Unit Risk Factor:	2.4E-05 $(\mu g/m^3)^{-1}$
Slope Factor:	8.4E-02 $(mg/kg/d)^{-1}$
Critical Effects:	Hepatocellular adenoma or carcinoma
Species:	Mice
Route of Exposure:	Gavage
Duration:	2 years

Basis for Toxicity Values:
EPA has not developed an inhalation reference concentration (RfC) for chlorodibromomethane. An oral reference dose (RfD) value of 0.02 mg/kg/d, based on a subchronic gavage study in rats for hepatic lesions is available on IRIS for chlorodibromomethane (U.S. EPA, 1998)

Based on inadequate human data and limited evidence of carcinogenicity in animals, EPA considers chlorodibromomethane a possible human carcinogen (Class C) by the oral route and has calculated an oral cancer slope factor (CSF) of 0.084 $(mg/kg/d)^{-1}$ for the substance. In the study, 2-year gavage administration of chlorodibromomethane to both sexes of B6C3F1 mice caused increased incidence of adenomas and carcinomas in female mice and a significantly increased incidence of hepatocellular carcinomas in high-dose male mice (NTP, 1985, as cited in U.S. EPA, 1998). Drinking water administration of chlorodibromomethane to both sexes of CBAxC57B1/6 mice also resulted in significantly increased incidence of tumors (U.S. EPA, 1998).

The mechanism for the carcinogenicity of chlorodibromomethane appears to be genotoxic carcinogenesis, independent of liver activation and, hence, route-independent. In one genotoxicity assay, chlorodibromomethane produced reverse mutations in *Salmonella typhimurium* strain TA100 in a vapor-phase test performed in a desiccator. Positive results for gene conversion in *Saccharomyces cerevisiae* strain D4 without, but not with, hepatic homogenates, and negative results for mutation in strain XV185-14C both with and without hepatic homogenates have been reported for chlorodibromomethane. In others tests, chlorodibromomethane produced sister chromatid exchange in cultured human lymphocytes and in bone marrow cells of mice treated orally (U.S. EPA, 1998; HSDB, 1998).

Thus, inhalation exposure to chlorodibromomethane is likely to lead to carcinogenic consequences not dissimilar from that from oral exposure. Therefore, in accordance with current EPA guidelines, it is considered appropriate to calculate an inhalation unit risk factor for chlorodibromomethane from the oral CSF listed for that substance in IRIS (U.S. EPA, 1994, 1996).

Calculations:
URF = CSF x 1 mg/1,000 μg x 1/70 kg x 20 m^3/d =
0.084 $(mg/kg/d)^{-1}$ x 1 mg/1,000 μg x 1/70 kg x 20 m^3/d = 2.4E-05$(\mu g/m^3)^{-1}$

where
70 kg = default adult human body weight
20 m^3 = default adult human daily rate of inhalation
Calculations assume 100% absorption.

Additional Information:
Inhalation CSFs are often derived from oral data. Of the 51 chemicals currently listed in IRIS (EPA, 1998) and HEAST (U.S. EPA, 1997) that have both an oral and inhalation CSF, about 60% of the inhalation CSFs were derived from oral studies and are identical or essentially identical to the oral CSF (see Table C-1, Figure C-1). In at least one case (benzene), the oral CSF was based on inhalation data resulting in identical values for both routes of exposure. In most cases (>75%) where an inhalation CSF was derived from an inhalation study, the inhalation CSF was lower than the corresponding oral CSF. Therefore, use of an oral CSF as an interim inhalation CSF appears reasonable and is unlikely to result in underestimating risk.

References:
Hazardous Substances Databank (HSDB): Chlorodibromomethane. 1998. Online database. National Library of Medicine, Bethesda, MD.

National Toxicology Program (NTP). 1985. Toxicology and Carcinogenesis Studies of Chlorodibromomethane in F344/N Rats and B6C3F1 Mice (gavage studies). NTP TR282 (as cited in U.S. EPA, 1998).

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U.S. Environmental Protection Agency. 1996. Proposed Guidelines for Carcinogen Risk Assessment. Office of Research and Development. Washington, DC. EPA/600/P-92/003C.

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7,12-Dimethylbenz[*a*]anthracene
CAS # 57-97-6

Unit Risk Factor: 2.4E-02 $(\mu g/m^3)^{-1}$

Slope Factor: 8.4E+01 $(mg/kg/d)^{-1}$

Critical Effects: Malignant angioendothelioma of the mesenteric intestine

Species: Mouse (albino)

Route of Exposure: Diet

Duration: 60 weeks

Basis for Toxicity Values:
There are no human data available that may be used to address the carcinogenicity of 7,12-dimethylbenz[*a*]anthracene (DMBA). However, DMBA belongs to a class of chemicals known as polycyclic aromatic hydrocarbons (PAHs), which are components of coal tar and incomplete combustion. Many of the PAHs have been demonstrated to be carcinogenic to rats and mice following oral exposure, skin painting, intrapulmonary injection, inhalation, subcutaneous injection, and intraperitoneal injection; however, most of these studies are not considered suitable for quantitative risk assessment. Nevertheless, the data do indicate that the carcinogenic potencies vary and that DMBA is considered one of the most potent PAHs (Pitot and Dragan, 1996).

DMBA is not listed in EPA's IRIS (U.S. EPA, 1998) or HEAST (U.S. EPA, 1997) databases and was not included in EPA's (1993) *Provisional Guidance for Quantitative Risk Assessment of PAHs*. However, the California Environmental Protection Agency (CalEPA) has developed a unit risk factor (URF) and cancer slope factor (CSF) for DMBA in support of the Air Toxics Hot Spots Program (CalEPA, 1994a, 1994b, 1997). The CalEPA URF and inhalation CSF are listed above and are recommended as interim values.

The CalEPA developed an "expedited" approach for deriving cancer potency values in order to implement Proposition 65 (Hoover et al., 1995). The expedited approach was used for DMBA. Under the expedited approach, instead of conducting a comprehensive literature review, cancer dose response data are taken from the Carcinogenic Potency Database (CPDB) (Gold and Zeiger, 1997). The linearized multistage model is automatically used to derive cancer potency estimates for low-dose exposures, and pharmacokinetic adjustments are not made.

Only one study was listed in the CPDB (Chouroulinkov et al., 1967). Female albino mice were fed DMBA for 60 weeks at a dose rate of 0.39 mg/kg/d. No tumors were reported in 40 control mice. Malignant angioendotheliomas of the intestine were reported in 49 of 75 test animals. Twenty test animals also had nonmalignant forestomach papillomas.

Additional Information:
The CPDB summarizes the results of 5,152 cancer tests on 1,298 chemicals. Carcinogenic potency estimates are presented as TD_{50} values. TD_{50} is defined as *that dose-rate in mg/kg body wt/d which, if administered chronically for the standard lifespan of the species, will halve the probability of remaining tumorless throughout that period* (Gold and Zeiger, 1997). The TD_{50} is analogous to the dose that is lethal to 50 percent of test animals (LD_{50}). A low TD_{50} indicates high potency, just as a low LD_{50} indicates high acute toxicity.

Some studies have reported high correlations between various measures of cancer potency and the maximum tolerated dose or maximum dose tested in the carcinogenicity studies (Gaylor, 1989; Krewski et al., 1993). The correlation of TD_{50} values as reported in the CPDB and inhalation CSFs derived from IRIS or HEAST was evaluated as a possible means to estimate the CSF from the TD_{50}. Forty-five chemicals were identified that had both a TD_{50} and an inhalation CSF (see Table C-2, Figure C-2). The correlation coefficient for the regression is 0.95. The TD_{50} reported for DMBA is 0.084 mg/kg/d (Gold and Zeiger, 1997). Based on a linear regression of log TD_{50} as the independent variable and log (1/CSF) as the dependent variable, an inhalation CSF of 55 $(mg/kg/d)^{-1}$ and a URF of 1.6E-02 $(\mu g/m^3)^{-1}$ are predicted. These values are in close agreement with the CalEPA values of 84 $(mg/kg/d)^{-1}$ and 2.4E-02$(\mu g/m^3)^{-1}$, respectively.

References:
California Environmental Protection Agency (CalEPA). 1994a. Benzo[a]pyrene as a Toxic Air Contaminant. Executive Summary. California Air Resources Board, Office of Environmental Health Hazard Assessment, Berkeley, CA.

California Environmental Protection Agency (CalEPA). 1994b. Benzo[a]pyrene as a Toxic Air Contaminant. Part B Health Effects of Benzo(a)pyrene. California Air Resources Board, Office of Environmental Health Hazard Assessment, Berkeley, CA.

California Environmental Protection Agency (CalEPA). 1997. Air Toxics Hot Spots Program Risk Assessment Guidelines: Technical Support Document for Determining Cancer Potency Factors. Draft for Public Comment. Office of Environmental Health Hazard Assessment.

Chouroulinkov, I., A. Gentil, and M. Guerin. 1967. Étude de l'activité carcinogène du 9,10-diméthyl-benzanthracène et du 3,4-benzopyrène administrés par voie digestive. *Bull Cancer* 54:67-78 (as cited in Gold and Zeiger, 1997).

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U.S. Environmental Protection Agency. 1993. Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons. Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH. EPA/600/R-93/089.

U.S. Environmental Protection Agency. 1997. Health Effects Assessment Summary Tables (HEAST), FY 1997 Update. Office of Emergency and Remedial Response, Washington, DC. EPA-540-R-97-036.

U.S. Environmental Protection Agency. 1998. Integrated Risk Information System (IRIS). Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH.

2,4-Dinitrotoluene
CAS #121-14-2

Unit Risk Factor: 1.9E-04 $(\mu g/m^3)^{-1}$

Slope Factor: 6.8E-01 $(mg/kg/d)^{-1}$

Critical Effects: Hepatocellular carcinoma, liver neoplastic nodules, benign and malignant mammary gland tumors.

Species: Female Sprague-Dawley rats

Route of exposure: Diet

Duration: 2 years

Basis for Toxicity Values:
There are no human data available that may be used to address the carcinogenicity of 2,4-dinitrotoluene. 2,4-Dinitrotoluene is not listed in EPA's IRIS (U.S. EPA,1998) or HEAST (U.S. EPA, 1997) databases. However, an oral CSF of 0.68 $(mg/kg/d)^{-1}$ is available in IRIS for a mixture of 2,4-and 2,6-dinitrotoluene. The mixture was 98% 2,4-dinitrotoluene and 2% 2,6-dinitrotoluene. The oral CSF for the mixture is proposed as an interim value for the inhalation CSF for 2,4-dinitrotoluene.

Inhalation CSFs are often derived from oral data. Of the 51 chemicals currently listed in IRIS and HEAST that have both an oral and inhalation CSF, about 60% of the inhalation CSFs were derived from oral studies and are identical or essentially identical to the oral CSF (see Table E-1, Figure C-1). In at least one case (benzene), the oral CSF was based on inhalation data resulting in identical values for both routes of exposure. In most cases (>75%) where an inhalation CSF was derived from an inhalation study, the inhalation CSF was lower than the corresponding oral CSF. Therefore, use of an oral CSF as an interim inhalation CSF appears reasonable and is unlikely to result in underestimating risk.

Dose-Response Data:
The oral CSF listed in HEAST was based on a study by Ellis et al. (1979). Sprague-Dawley rats were fed dietary concentrations of 0, 15, 100, and 700 ppm and Swiss mice were fed 0, 100, 700, and 5,000 ppm for 2 years. Mortality was high in all treatment groups. A statistically significant increase in liver tumors was observed in both male and female rats and a statistically significant increase in benign mammary gland tumors was observed in female rats. In addition, an increased incidence of kidney tumors was observed in the mid-dose male mice. Data used to derive the CSF were based on liver and mammary tumors in female rats and are presented below as reported in IRIS.

Administered Dose (ppm)	Human Equivalent Dose (mg/kg/d)	Tumor Incidence
0	0	11/23
15	0.129	12/35
100	0.927	17/27
700	7.557	34/35

Calculations:
URF = CSF x 1 mg/1,000 µg x 1/70 kg x 20 m^3/d =
0.68 $(mg/kg/d)^{-1}$ x 1 mg/1,000 µg x 1/70 kg x 20 m^3/d = 1.9E-04$(\mu g/m^3)^{-1}$

where
70 kg = default adult human body weight
20 m^3 = default adult human daily rate of inhalation
Calculations assume 100% absorption.

Additional Information:
The California Environmental Protection Agency (CalEPA) adopted a URF of 8.9E-05 $(\mu g/m^3)^{-1}$ and an inhalation CSF of 3.1E-01 $(mg/kg/d)^{-1}$ for practical grade 2,4-dinitrotoluene based on a potency factor derived by EPA (U.S. EPA, 1987) (CalEPA, 1997). These values were based on a feeding study using Sprague-Dawley rats (Lee et al., 1978). Liver and mammary tumors in female rats were used to develop the CSF and results were very similar to the Ellis et al. (1979) study discussed above.

The Carcinogenic Potency Database (CPDB) summarizes the results of 5,152 cancer tests on 1,298 chemicals (Gold and Zeiger, 1997). Carcinogenic potency estimates are presented as TD_{50} values. TD_{50} values are defined as *that dose-rate in mg/kg body wt/day which, if administered chronically for the standard lifespan of the species, will halve the probability of remaining tumorless throughout that period* (Gold and Zeiger, 1997). The TD_{50} is analogous to the dose that is lethal to 50% of test animals (LD_{50}). A low TD_{50} indicates high potency, just as a low LD_{50} indicates high acute toxicity.

Some studies have reported high correlations between various measures of cancer potency and the maximum tolerated dose or maximum dose tested in the carcinogenicity studies (Gaylor, 1989; Krewski et al., 1993). The correlation of TD_{50}s as reported in the CPDB and inhalation CSFs derived from IRIS or HEAST was evaluated as a possible means to estimate the CSF from the TD_{50}. Forty-five chemicals were identified that had both a TD_{50} and an inhalation CSF (see Table C-2, Figure C-2). The correlation coefficient for the regression is 0.95. The reported TD_{50} is 9.35 mg/kg/d (Gold and Zeiger, 1997). Based on a linear regression of log TD_{50} as the independent variable and log (1/CSF) as the dependent variable, an inhalation CSF of 0.53 $(mg/kg/d)^{-1}$ and a URF of 1.5E-04 $(\mu g/m^3)^{-1}$ are predicted. These values are in close agreement with the oral CSF listed in IRIS for a mixture of 2,4- and 2,6-dinitrotoluene and the CalEPA values.

References:

California Environmental Protection Agency (CalEPA). 1997. Air Toxics Hot Spots Program Risk Assessment Guidelines: Technical Support Document for Determining Cancer Potency Factors. Draft for Public Comment. Office of Environmental Health Hazard Assessment.

Ellis, H.V., III, J.H. Hagensen, J.R. Hodgson, et al. 1979. Mammalian toxicity of munitions compounds. Phase III: Effects of life-time exposure. Part I: 2,4-dinitrotoluene. Final report No. 7. U.S. Army Medical Bioengineering Research and Development Laboratory. Midwest Research Institute. Report Order No. AD-A077692.

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Lee, C.C., H.V. Ellis, J.J. Kowalski, et al. 1978. Mammalian toxicity of munition compounds. Phase II. Effects of multiple doses and Phase III. Effects of lifetime exposure. Part II. 2,4-Dinitrotoluene. U.S. Army Medical Bioengineering Research and Development Laboratory. Midwest Research Institute, Kansas City, MO. NTIS ADA 061715.

U.S. Environmental Protection Agency. 1987. Health Effects Assessment for 2,4- and 2,6-Dinitrotoluene. Office of Health and Environmental Assessment, Cincinnati, OH. EPA/600/8-88/032.

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U.S. Environmental Protection Agency. 1998. Integrated Risk Information System (IRIS). Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH.

3-Methylcholanthrene
CAS # 56-49-5

Unit Risk Factor: 2.1E-03 $(\mu g/m^3)^{-1}$

Slope Factor: 7.4E+00 $(mg/kg/day)^{-1}$

Critical Effects: Mammary gland adenocarcinomas

Species: Wistar rats

Route of Exposure: Gavage

Duration: 26 to 52 weeks

Basis for Toxicity Values:
There are no human data available that may be used to address the carcinogenicity of 3-methylcholanthrene (3-MC). However, 3-MC belongs to a class of chemicals known as polycyclic aromatic hydrocarbons (PAHs), which are components of coal tar and incomplete combustion. Many of the PAHs have been demonstrated to be carcinogenic to rats and mice following oral exposure, skin painting, intrapulmonary injection, inhalation, subcutaneous injection, and intraperitoneal injection; however, most of these studies are not considered suitable for quantitative risk assessment. Nevertheless, the data do indicate that the carcinogenic potencies vary and that 3-MC is considered one of the most potent PAHs (Pitot and Dragan, 1996).

3-MC is not listed in EPA's IRIS (U.S. EPA, 1998) or HEAST (U.S. EPA, 1997) databases and was not included in EPA's (1993) *Provisional Guidance for Quantitative Risk Assessment of PAHs*. However, the California Environmental Protection Agency (CalEPA) has developed a unit risk factor (URF) and cancer slope factor (CSF) for 3-MC in support of the Air Toxics Hot Spots Program (CalEPA, 1994a, 1994b, 1997). The CalEPA URF and inhalation CSF are listed above and recommended as interim values.

The CalEPA developed an "expedited" approach for deriving cancer potency values in order to implement Proposition 65 (Hoover et al., 1995). The expedited approach was used for 3-MC. Under the expedited approach, instead of conducting a comprehensive literature review, cancer dose response data are taken from the Carcinogenic Potency Database (CPDB) (Gold and Zeiger, 1997). The linearized multistage model is automatically used to derive cancer potency estimates for low-dose exposures, and pharmacokinetic adjustments are not made.

Fifteen studies (4 diet and 11 gavage) were listed in the CPDB (Gold and Zeiger, 1997). All of the studies included a control group and one treatment group. No tumors were reported in any of the dietary studies; however, a significant increase in tumors was reported in all of the gavage studies. Doses for the gavage studies ranged from 2.46 mg/kg/d to 12.2 mg/kg/d. Adenocarcinomas of the mammary gland were reported in nine studies and two studies identified unspecified mammary tissue tumors. Tumor incidence ranged from 67% to 100%.

Additional Information:
The CPDB summarizes the results of 5,152 cancer tests on 1,298 chemicals. Carcinogenic potency estimates are presented as TD_{50}s. TD_{50}s are defined as *that dose-rate in mg/kg body wt/day which, if administered chronically for the standard lifespan of the species, will halve the probability of remaining tumorless throughout that period* (Gold and Zeiger, 1997). The TD_{50} is analogous to the dose that is lethal to 50% of test animals (LD_{50}). A low TD_{50} indicates high potency, just as a low LD_{50} indicates high acute toxicity.

Some studies have reported high correlations between various measures of cancer potency and the maximum tolerated dose or maximum dose tested in the carcinogenicity studies (Gaylor, 1989; Krewski et al., 1993). The correlation of TD_{50}s as reported in the CPDB and inhalation CSFs derived from IRIS or HEAST was evaluated as a possible means to estimate the CSF from the TD_{50}. Forty-five chemicals were identified that had both a TD_{50} and an inhalation CSF (see Table C-2, Figure C-2). The correlation coefficient for the regression is 0.95. The TD_{50} reported for 3-MC is 0.491 mg/kg/d (Gold and Zeiger, 1997). Based on a linear regression of log TD_{50} as the independent variable and log (1/CSF) as the dependent variable, an inhalation CSF of 9.6 $(mg/kg/d)^{-1}$ and a URF of 2.7E-03 $(\mu g/m^3)^{-1}$ are predicted. These values are in close agreement with the CalEPA values of 7.4 $(mg/kg/d)^{-1}$ and 2.1E-03 $(\mu g/m^3)^{-1}$, respectively.

References:
California Environmental Protection Agency (CalEPA). 1994a. Benzo[a]pyrene as a Toxic Air Contaminant. Executive Summary. California Air Resources Board, Office of Environmental Health Hazard Assessment, Berkeley, CA.

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U.S. Environmental Protection Agency. 1997. Health Effects Assessment Summary Tables, FY 1997 Update. Office of Emergency and Remedial Response, Washington, DC. EPA-540-R-97-036.

U.S. Environmental Protection Agency. 1998. Integrated Risk Information System (IRIS). Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH.

o-Toluidine (2-Methylaniline)
CAS # 95-53-4

Unit Risk Factor: 6.9E-05 $(\mu g/m^3)^{-1}$

Slope Factor: 2.4E-01 $(mg/kg/d)^{-1}$

Critical Effects: Skin fibromas - also increased incidence of other tumor types including sarcomas, mesotheliomas, carcinomas, hemangiosarcomas, and hepatocellular carcinomas of various tissues.

Species: F-344 rats and B6C3F1 mice

Route of Exposure: Diet

Duration: 2 years

Basis for Toxicity Values:
There is limited evidence that o-toluidine is carcinogenic in humans; however, data are inadequate for a quantitative risk assessment (U.S. EPA, 1987). o-Toluidine is not listed in EPA's IRIS (U.S. EPA, 1998) but an oral CSF is included in HEAST (U.S. EPA, 1997). The oral CSF of 2.4E-01 mg/kg/d is proposed as an interim value for the inhalation CSF.

Inhalation CSFs are often derived from oral data. Of the 51 chemicals currently listed in IRIS and HEAST that have both an oral and inhalation CSF, about 60% of the inhalation CSFs were derived from oral studies and are identical or essentially identical to the oral CSF (see Table E-1, Figure C-1). In at least one case (benzene), the oral CSF was based on inhalation data resulting in identical values for both routes of exposure. In most cases (>75%) where an inhalation CSF was derived from an inhalation study, the inhalation CSF was lower than the corresponding oral CSF. Therefore, use of an oral CSF as an interim inhalation CSF appears reasonable and is unlikely to result in underestimating risk.

Dose-Response Data:
The oral CSF listed in HEAST was based on a study by Hecht et al. (1982). Groups of 30 male F344 rats were fed dietary concentrations of 0 or 4,000 ppm o-toluidine hydrochloride for 73 weeks followed by 20 weeks of observation. An increased incidence of skin fibromas, mammary fibroadenomas, spleen fibromas, and peritoneal sarcomas was reported. Skin fibromas gave the greatest response and were used to derive the CSF. The data are summarized below as reported in U.S. EPA (1987).

Experimental Dose o-Toluidine•HCl (mg/rat/d)	Transformed Dose o-Toluidine (mg/kg/d)	Incidence
0	0	1/27
62	80	25/30

Calculations:
URF = CSF x 1 mg/1,000 μg x 1/70 kg x 20 m^3/d =
0.24 $(mg/kg/d)^{-1}$ x 1 mg/1,000 μg x 1/70 kg x 20 m^3/d = 6.9E-05$(\mu g/m^3)^{-1}$

where
70 kg = default adult human body weight
20 m^3 = default adult human daily rate of inhalation
Calculations assume 100% absorption.

Additional Information:
The National Cancer Institute (NCI) also has conducted a cancer bioassay of o-toluidine hydrochloride (NCI, 1979). F344 rats were fed diets containing 0, 3,000, and 6,000 ppm and $B6C3F_1$ mice were fed diets containing 0, 1,000, and 3,000 ppm for 2 years. Multiple site sarcomas, subcutaneous fibromas, and multiple site mesotheliomas were observed in male rats. Female rats had multiple site sarcomas, mammary fibroadenomas, splenic sarcomas, and urinary bladder carcinomas. Multiple site hemangiosarcomas were seen in male mice and hepatocellular carcinomas and adenomas were seen in female mice. U.S. EPA (1987) reported that the Hecht et al. (1982) study was selected over the NCI (1979) study because the former resulted in a higher cancer potency estimate.

References:
Hecht, S.S., K. El-Bayoumy, A. Rivenson, and E. Fiala. 1982. Comparative carcinogenicity of o-toluidine hydrochloride and o-nitrosotoluene in F-344 Rats. *Cancer Letters* 16:103-108.

National Cancer Institute (NCI). 1979. Bioassay of o-Toluidine Hydrochloride for Possible Carcinogenicity. TR-153. Bethesda, MD.

U.S. Environmental Protection Agency. 1987. Health and Environmental Effects Profile for 2-Methylaniline and 2-Methylaniline Hydrochloride. Office of Health and Envrionmental Assessment, Cincinnati, OH. EPA/600/X-87/092.

U.S. Environmental Protection Agency. 1997. Health Effects Assessment Summary Tables (HEAST), FY 1997 Update. Office of Emergency and Remedial Response, Washington, DC. EPA-540-R-97-036.

U.S. Environmental Protection Agency. 1998. Integrated Risk Information System (IRIS). Environmental Criteria and Assessment Office, Office of Health and Environmental Assessment, Cincinnati, OH.

Table C-1. Correlation of Oral and Inhalation Cancer Slope Factors Reported in IRIS and HEAST

CAS #	Chemical	Oral CSF	Inh CSF	log Oral CSF	log Inh. CSF
79-06-1	Acrylamide	4.5	4.5	0.6532	0.6532
107-13-1	Acrylonitrile	0.54	0.24	-0.2676	-0.6198
309-00-2	Aldrin	17	17	1.2304	1.2304
140-57-8	Aramite	0.025	0.025	-1.6021	-1.6021
7440-38-2	Arsenic	1.5	15	0.1761	1.1761
103-33-3	Azobenzene	0.11	0.11	-0.9586	-0.9586
71-43-2	Benzene	0.029	0.029	-1.5376	-1.5376
92-87-5	Benzidine	230	235	2.3617	2.3711
7440-41-7	Beryllium	4.3	8.4	0.6335	0.9243
111-44-4	Bis(2-chloroethyl)ether	1.1	1.16	0.0414	0.0645
542-88-1	Bis(chloromethyl)ether	220	217	2.3424	2.3365
108-60-1	Bis(2-chloro-1-methylethyl)ether	0.07	0.035	-1.1549	-1.4559
75-25-2	Bromoform	0.0079	0.0039	-2.1024	-2.4145
56-23-5	Carbon tetrachloride	0.13	0.053	-0.8861	-1.2757
57-74-9	Chlordane	1.3	1.3	0.1139	0.1139
510-15-6	Chlorobenzilate	0.27	0.27	-0.5686	-0.5686
67-66-3	Chloroform	0.0061	0.08	-2.2147	-1.0969
74-87-3	Chloromethane	0.013	0.0063	-1.8861	-2.2007
50-29-3	DDT	0.34	0.34	-0.4685	-0.4685
96-12-8	1,2-Dibromo-3-chloropropane	1.4	0.0024	0.1461	-2.6162
106-93-4	1,2-Dibromoethane	85	0.77	1.9294	-0.1135
107-06-2	1,2-Dichloroethane	0.091	0.091	-1.0410	-1.0410
75-35-4	1,1-Dichloroethylene	0.6	0.175	-0.2218	-0.7570
542-75-6	1,3-Dichloropropene	0.18	0.13	-0.7447	-0.8861
60-57-1	Dieldrin	16	16	1.2041	1.2041
122-66-7	1,2-Diphenylhydrazine	0.8	0.77	-0.0969	-0.1135
106-89-8	Epichlorohydrin	0.0099	0.0042	-2.0044	-2.3768
75-21-8	Ethylene oxide	1.02	0.35	0.0086	-0.4559
319-84-6	HCH alpha	6.3	6.3	0.7993	0.7993
319-85-7	HCH beta	1.8	1.8	0.2553	0.2553
608-73-1	HCH tech.	1.8	1.8	0.2553	0.2553
76-44-8	Heptachlor	4.5	4.5	0.6532	0.6532
1024-57-3	Heptachlor epoxide	9.1	9.1	0.9590	0.9590
118-74-1	Hexachlorobenzene	1.6	1.6	0.2041	0.2041
87-68-3	Hexachlorobutadiene	0.078	0.077	-1.1079	-1.1135
67-72-1	Hexachloroethane	0.014	0.014	-1.8539	-1.8539

(continued)

Table C-1. (continued)

CAS #	Chemical	Oral CSF	Inh CSF	log Oral CSF	log Inh. CSF
302-01-2	Hydrazine	3	17.1	0.4771	1.2330
75-09-2	Methylene chloride	0.0075	0.0016	-2.1249	-2.7959
101-14-4	4,4'-Methylenebis(2-chloroaniline)	0.13	0.13	-0.8861	-0.8861
924-16-3	*N*-Nitrosodi-n-butylamine	5.4	5.6	0.7324	0.7482
55-18-5	*N*-Nitrosodiethylamine	150	151	2.1761	2.1790
62-75-9	*N*-Nitrosodimethylamine	51	49	1.7076	1.6902
930-55-2	*N*-Nitrosopyrrolidine	2.1	2.13	0.3222	0.3284
1336-36-3	PCBs	2	0.4	0.3010	-0.3979
75-56-9	Propylene oxide	0.24	0.013	-0.6198	-1.8861
630-20-6	1,1,1,2,-Tetrachloroethane	0.026	0.026	-1.5850	-1.5850
79-34-5	1,1,2,2,-Tetrachloroethane	0.2	0.2	-0.6990	-0.6990
8001-35-2	Toxaphene	1.1	1.1	0.0414	0.0414
79-00-5	1,1,2-Trichloroethane	0.057	0.056	-1.2441	-1.2518
88-06-2	2,4,6,-Trichlorophenol	0.011	0.011	-1.9586	-1.9586
75-01-4	Vinyl chloride	1.9	0.3	0.2788	-0.5229

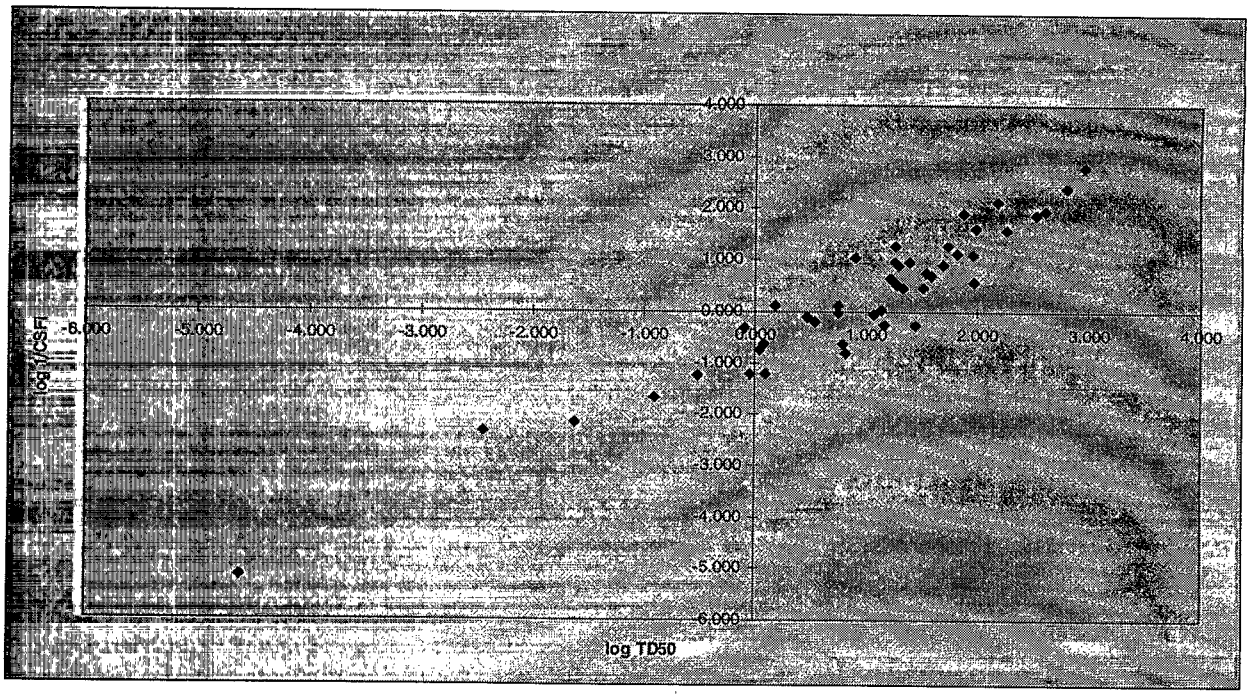


Figure C-1. Correlation of Oral and Inhalation Cancer Slope Factors.

Table C-2. Correlation of TD_{50s} Reported in the Cancer Potency Database and Inhalation Cancer Slope Factors Reported in IRIS and HEAST.

Chemical	CAS #	TD_{50}[a] Rat	TD_{50}[a] Mouse	TD_{50} Geo Mean[b]	Inh CSF[c]	CSF test species[d]	1/CSF	log TD_{50}[e] (X)	log 1/CSF (Y)
Carbon tetrachloride	56-23-5	2.29	150	18.53	0.053	b	18.87	1.268	1.276
DDT	50-29-3	84.7	12.3	32.28	0.34	b	2.94	1.509	0.469
Aldrin	309-00-2	-	1.27	*	17	m	0.059	0.104	-1.230
Bis(2-chloroethyl)ether	111-44-4	-	11.7	*	1.16	m	0.86	1.068	-0.064
1,3-Butadiene	106-99-0	261	13.9	*	0.98	m	1.020	1.143	0.009
Chlordane	57-74-9	-	2.99	*	1.3	m	0.77	0.476	-0.114
Chlorobenzilate	510-15-6	-	93.9	*	0.27	m	3.70	1.973	0.569
Chloroform	67-66-3	262	90.3	*	0.08	m	12.50	1.956	1.097
1,1-Dichloroethylene	75-35-4	-	34.6	*	0.175	m	5.71	1.539	0.757
1,3-Dichloropropene	542-75-6	94	49.6	*	0.13	m	7.692	1.695	0.886
Dieldrin	60-57-1	-	0.912	*	16	m	0.0625	-0.040	-1.204
HCH alpha	319-84-6	11.2	6.62	*	6.3	m	0.159	0.821	-0.799
HCH beta	319-85-7	-	27.8	*	1.8	m	0.556	1.444	-0.255
HCH tech.	608-73-1	-	14.8	*	1.8	m	0.556	1.170	-0.255
Heptachlor	76-44-8	-	1.21	*	4.5	m	0.222	0.083	-0.653
Hexachloroethane	67-72-1	55.4	338	*	0.014	m	71.429	2.529	1.854
Methylene chloride	75-09-2	724	918	*	0.0016	m	625.000	2.963	2.796
N-Nitrosodi-n-butylamine	924-16-3	0.691	1.09	*	5.6	m	0.179	0.037	-0.748
1,1,1,2,-Tetrachloroethane	630-20-6	-	182	*	0.026	m	38.4615	2.260	1.585
1,1,2,2,-Tetrachloroethane	79-34-5	-	38.3	*	0.2	m	5	1.583	0.699
Toxaphene	8001-35-2	-	5.57	*	1.1	m	0.909	0.746	-0.041
1,1,2-Trichloroethane	79-00-5	-	55	*	0.056	m	17.857	1.740	1.252
Acetaldehyde	75-07-0	153	-	*	0.0077	r	129.870	2.185	2.114
Acrylamide	79-06-1	6.15	-	*	4.5	r	0.222	0.789	-0.653
Acrylonitrile	107-13-1	16.9	-	*	0.24	r	4.167	1.228	0.620
Aramite	140-57-8	96.7	158	*	0.025	r	40	1.985	1.602
Azobenzene	103-33-3	24.1	-	*	0.11	r	9.09	1.382	0.959
Bis(Chloromethyl)ether	542-88-1	0.004	0.182	*	217	r	0.00	-2.447	-2.336
Bromoethene	593-60-2	18.5	-	*	0.11	r	9.091	1.267	0.959
Bromoform	75-25-2	648	-	*	0.004	r	250.00	2.812	2.398
1,2-Dibromoethane	106-93-4	1.52	7.45	*	0.77	r	1.299	0.182	0.114
1,2-Dichloroethane	107-06-2	8.04	101	*	0.091	r	10.99	0.905	1.041
1,2-Diphenylhydrazine	122-66-7	5.59	26	*	0.77	r	1.298701	0.747	0.114
Ethylene oxide	75-21-8	21.3	63.7	*	0.35	r	2.857	1.328	0.456
Hexachlorobenzene	118-74-1	3.51	65.1	*	1.6	r	0.625	0.545	-0.204
Hexachlorobutadiene	87-68-3	65.8	-	*	0.077	r	12.987	1.818	1.114
Hydrazine	302-01-2	0.309	2.93	*	17.1	r	0.058	-0.510	-1.233
4,4'-Methylenebis(2-chloroaniline)	101-14-4	19.3	-	*	0.13	r	7.692	1.286	0.886
N-Nitrosodiethylamine	55-18-5	0.024	-	*	151	r	0.007	-1.625	-2.179
N-Nitrosodimethylamine	62-75-9	0.124	0.189	*	49	r	0.020	-0.907	-1.690
N-Nitrosopyrrolidine	930-55-2	0.799	0.679	*	2.13	r	0.469	-0.097	-0.328
Propylene oxide	75-56-9	74.4	912	*	0.013	r	76.9231	1.872	1.886
2,3,7,8-TCDD	1746-01-6	2E-05	2E-04	*	150000	r	0.000	-4.629	-5.176
2,4,6,-Trichlorophenol	88-06-2	405	1070	*	0.011	r	90.909	2.607	1.959
Vinyl chloride	75-01-4	19.1	20.9	*	0.3	r	3.333	1.281	0.523
								n	45
								r^2	0.949
								slope	0.983
								intercept	-0.679

a Gold and Zeiger, 1997
b Geometric mean of the TD_{50} reported for mice and rats (only used when the CSF was derived from both species).
c IRIS, 1998 or HEAST, 1997.
d Test species reported as the basis for the CSF derivation ("b" is both rats and mice, "m" is mice, and "r" is rats).
e Selected to correspond with the CSF test species.
n Number of chemicals with a TD50 and inhalation CSF.
r^2 Correlation coefficient.
\- No data available.
* Not calculated because the CSF was based on a single species.

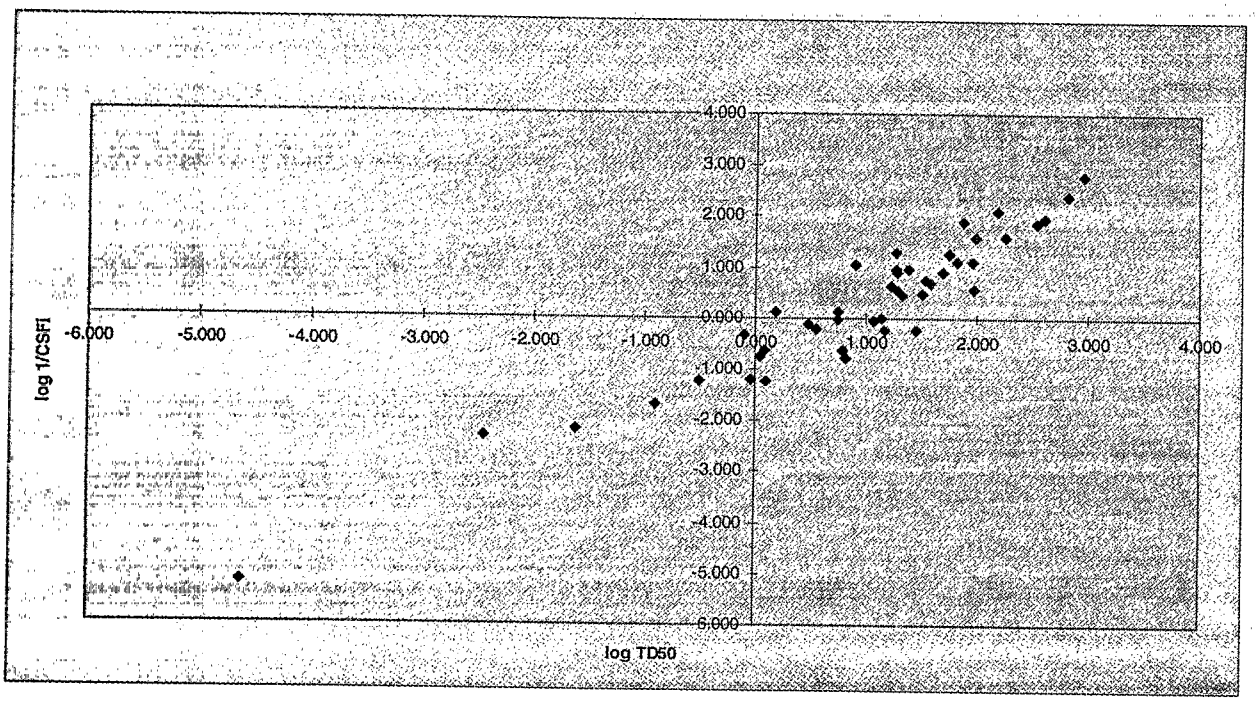


Figure C-2. Correlation of TD_{50} and inhalation cancer slope factors.

Appendix D

Sensitivity Analysis of ISC Air Model

D. Sensitivity Analysis of ISC Air Dispersion Model

This appendix describes sensitivity analysis on depletion options, source shape and orientation and receptor location and spacing.

D.1 Options With and Without Depletions

A sensitivity analysis was conducted using the ISCST3 model to determine whether dry and wet depletion options should be used in the risk analysis for five types of waste management units. A discussion of the analysis follows.

The depletion options (dry depletion and wet depletion) may be used with concentrations and depositions in the ISCST3 model runs. The model concentrations/depositions without depletion are higher than those with depletion. Because it takes much longer to run the ISCST3 model with depletions than without depletions, a sensitivity analysis was performed to investigate the differences of model outputs with and without selecting depletion options.

In this investigation, the 5th and the 95th percentile of sizes of LAUs were used to determine the relationship between concentrations with depletions and sizes of units.

For dry depletion, two meteorological stations (Little Rock, Arkansas, and Winnemucca, Nevada) were selected for the sensitivity analysis. The average particle sizes used in the sensitivity analysis are 20 μm and 5 μm with corresponding mass fraction of 50 percent each. The roughness length at application site was assumed as 0.4 meters.

For wet depletion, two meteorological stations were selected for the sensitivity analysis: Atlanta, Georgia, with 49.8 inches precipitation per year (4th highest annual precipitation rate among the 29 meteorological stations to be modeled), and Winnemucca, Nevada, with 8.1 inches precipitation per year (3rd lowest annual precipitation rate). The reason for selecting a wet site and a dry site was to examine (1) whether wet depletion has a more significant impact for a wet site than a dry site; and (2) the differences of ambient concentrations that a very wet site can make with and without selecting wet depletion.

Five-year average concentrations with and without dry depletion were calculated using meteorological data from Little Rock and Winnemucca for the 5th and the 95th percentile of sizes of LAUs. The results show that the differences of the maximum concentrations with and without dry depletion are very small at close-to-source receptors. As the distance from the source increases, the differences between the dry depletion option and without dry depletion increase only slightly. The differences of concentrations are about 10 percent of the concentrations for the 95th percentile and are less than 2 percent of the concentrations for the 5th percentile at 50 meters from the edge of the LAU. The larger the area source, the larger the differences of the maximum concentrations. The results are shown in Figures D-1a through D-1d.

Five-year average concentrations with and without wet depletion also were calculated using meteorological data from Atlanta and Winnemucca for the 5th and 95th percentile of sizes of LAUs. The results show that the differences of the maximum concentrations with and without wet depletion are small for both Atlanta and Winnemucca sites. However, the differences in the maximum concentrations between the wet depletion option and without wet depletion are about 5 to 10 times greater for the Atlanta site than the Winnemucca site. Tables D-1a and D-1b show that for the 95th percentile unit size, at 50 meters from the edge of the unit, the differences in the maximum concentrations are only 0.03% and 0.37% for Winnemucca and Atlanta, respectively. This means that model concentrations with and without wet depletion are about the same.

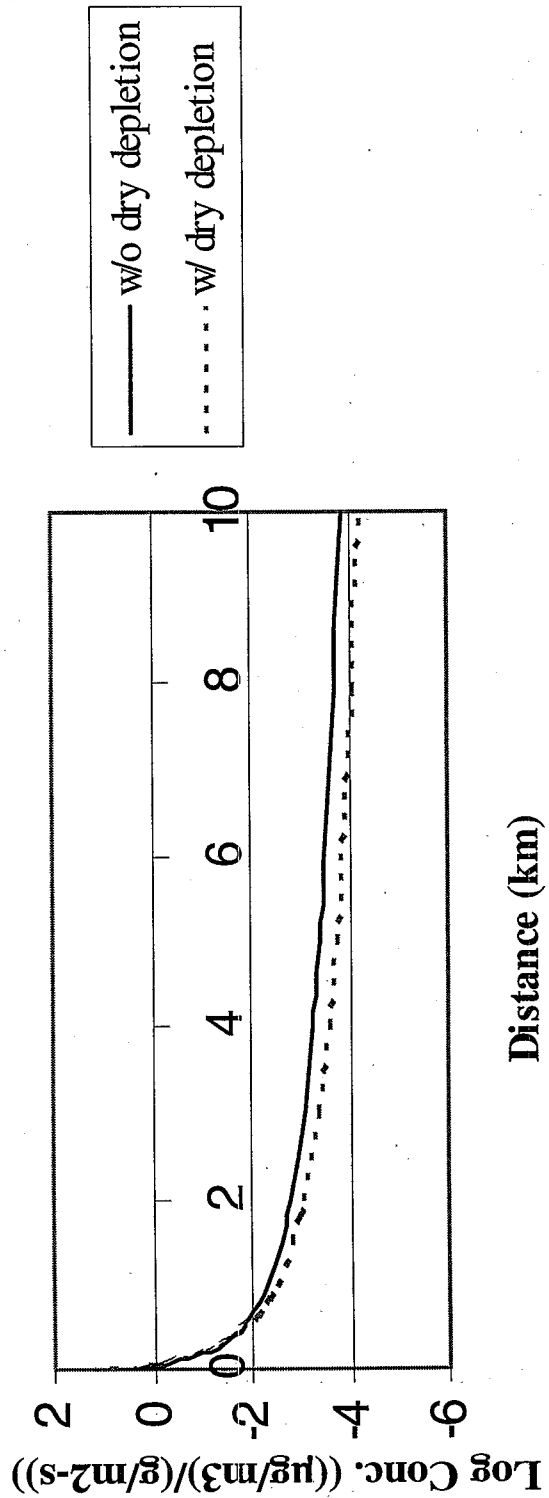


Figure D-1a. Air Concentrations of Particles (LAU, 5th Percentile, Little Rock, AR)

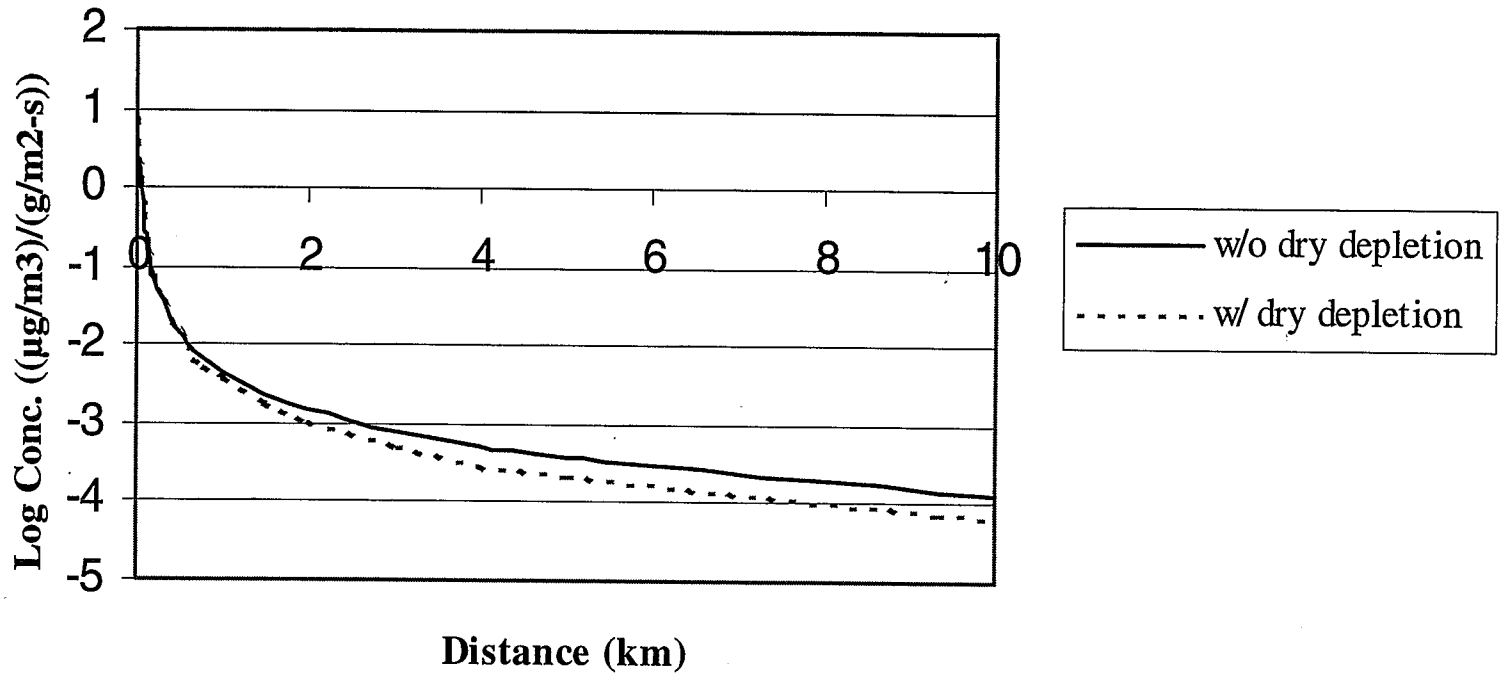


Figure D-1b. Air Concentrations of Particles (LAU, 5th Percentile, Winnemucca, NV)

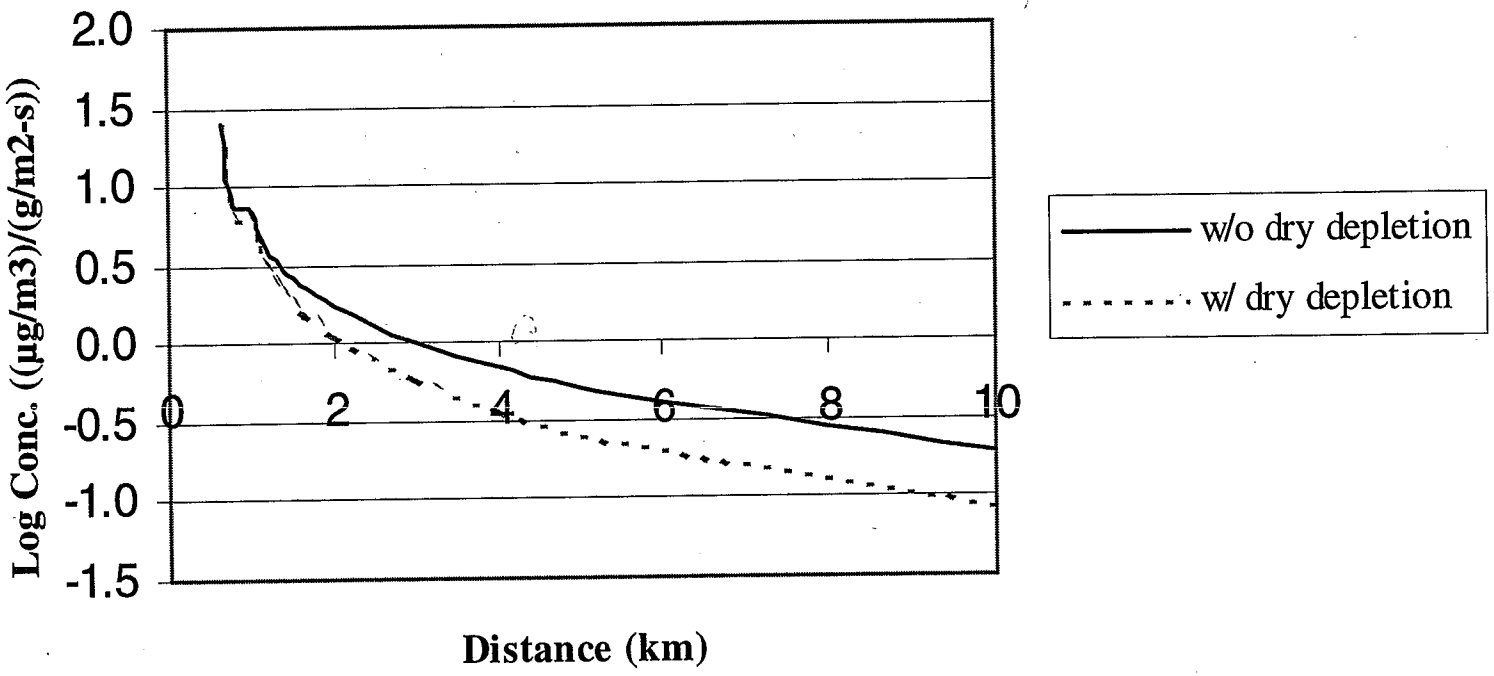


Figure D-1c. Air Concentrations of Particles (LAU, 95th Percentile, Little Rock, AR)

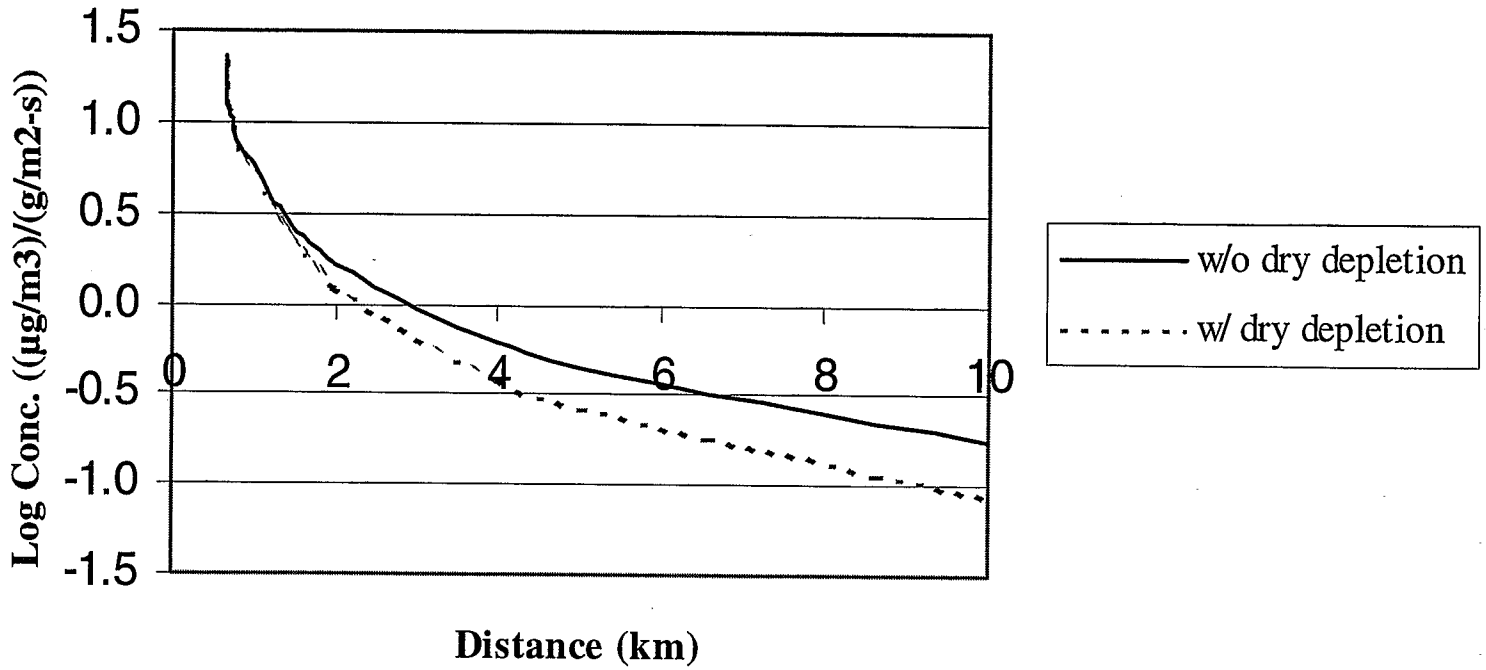


Figure D-1d. Air Concentrations of Particles (LAU, 95th Percentile, Winnemucca, NV)

Table D-1a. Differences of Air Concentrations for Vapors Between Wet Depletion Option and Without Wet Depletion

(Atlanta, GA Site)

5th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
19.3 (1)	7.40752	7.40716	0.00036	0.005%
47.3 (1)	0.93175	0.93159	0.00016	0.017%
75.2 (1)	0.38178	0.38168	0.00010	0.026%
100	0.25129	0.25121	0.00008	0.032%
103.2 (1)	0.21003	0.20996	0.00007	0.033%
187.0 (1)	0.06886	0.06882	0.00004	0.058%
200	0.07091	0.07086	0.00005	0.071%
300	0.03390	0.03387	0.00003	0.088%
400	0.02026	0.02024	0.00002	0.099%
500	0.01359	0.01357	0.00002	0.147%
600	0.00981	0.00979	0.00002	0.204%
800	0.00590	0.00589	0.00001	0.169%
1000	0.00400	0.00399	0.00001	0.250%
1500	0.00205	0.00205	0.00000	0.000%
2000	0.00128	0.00128	0.00000	0.000%
3000	0.00068	0.00067	0.00001	1.471%
4000	0.00044	0.00043	0.00001	2.273%
5000	0.00031	0.00031	0.00000	0.000%
10000	0.00011	0.00011	0.00000	0.000%

95th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
651.9 (1)	0.00614	0.00612	0.00002	0.33%
676.9 (1)	0.00574	0.00573	0.00001	0.17%
701.9 (1)	0.00539	0.00537	0.00002	0.37%
726.9 (1)	0.00507	0.00505	0.00002	0.39%
801.9 (1)	0.00427	0.00426	0.00001	0.23%
1000	0.00400	0.00399	0.00001	0.25%
1100	0.00342	0.00341	0.00001	0.29%
1200	0.00296	0.00295	0.00001	0.34%
1300	0.00260	0.00259	0.00001	0.38%
1400	0.00230	0.00229	0.00001	0.43%
1500	0.00205	0.00205	0.00000	0.00%
1600	0.00185	0.00184	0.00001	0.54%
1800	0.00152	0.00152	0.00000	0.00%
2000	0.00128	0.00128	0.00000	0.00%
3000	0.00068	0.00067	0.00001	1.47%
4000	0.00044	0.00043	0.00001	2.27%
5000	0.00031	0.00031	0.00000	0.00%
10000	0.00011	0.00011	0.00000	0.00%

(1) These refer to the distances from the center of emission source to the maximum concentration points along 0, 25, 50, 75, and 150 meter receptor squares, respectively.

Table D-1b. Differences of Air Concentrations for Vapors Between Wet Depletion Option and Without Wet Depletion

(Winnemucca, NV Site)

5th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
17.3 (1)	7.79132	7.79125	0.00007	0.001%
42.3 (1)	1.08468	1.08464	0.00004	0.004%
67.3 (1)	0.48369	0.48367	0.00002	0.004%
92.3 (1)	0.27965	0.27963	0.00002	0.007%
100	0.24315	0.24313	0.00002	0.008%
167.3 (1)	0.09949	0.09948	0.00001	0.010%
200	0.07296	0.07295	0.00001	0.014%
300	0.03600	0.03599	0.00001	0.028%
400	0.02181	0.02180	0.00001	0.046%
500	0.01475	0.01474	0.00001	0.068%
600	0.01070	0.01070	0.00000	0.000%
800	0.00649	0.00648	0.00001	0.154%
1000	0.00443	0.00443	0.00000	0.000%
1500	0.00229	0.00229	0.00000	0.000%
2000	0.00144	0.00144	0.00000	0.000%
3000	0.00077	0.00077	0.00000	0.000%
4000	0.00050	0.00050	0.00000	0.000%
5000	0.00036	0.00036	0.00000	0.000%
10000	0.00013	0.00013	0.00000	0.000%

95th Percentile

Distance (m)	w/o wet depletion Concentrations (ug/m^3 / g/m^2-s)	w/ wet depletion Concentrations (ug/m^3 / g/m^2-s)	Difference (ug/m^3 / g/m^2-s)	Difference in Percentage
651.9 (1)	23.14326	23.13885	0.00441	0.02%
676.9 (1)	13.86979	13.86551	0.00428	0.03%
701.9 (1)	11.62889	11.62486	0.00403	0.03%
726.9 (1)	10.25373	10.24985	0.00388	0.04%
801.9 (1)	7.84900	7.84548	0.00352	0.04%
1000	5.85241	5.84988	0.00253	0.04%
1100	4.69239	4.68991	0.00248	0.05%
1200	3.98357	3.98130	0.00227	0.06%
1300	3.43255	3.43045	0.00210	0.06%
1400	2.99083	2.98887	0.00196	0.07%
1500	2.63019	2.62837	0.00182	0.07%
1600	2.33211	2.33042	0.00169	0.07%
1800	1.93762	1.93554	0.00208	0.11%
2000	1.65686	1.65487	0.00199	0.12%
3000	0.91889	0.91727	0.00162	0.18%
4000	0.61160	0.61020	0.00140	0.23%
5000	0.45013	0.44890	0.00123	0.27%
10000	0.17843	0.17767	0.00076	0.43%

(1) These refer to the distances from the center of emission source to the maximum concentration points along 0, 25, 50, 75, and 150 meter receptor squares, respectively.

D.2 Source Shape and Orientation

A sensitivity analysis was conducted using the ISCST3 air model to determine what role source shape and orientation play in determining dispersion coefficients of air pollutants. A discussion of this analysis follows.

Three different sources were chosen for this analysis. The sources were a square (source No. 1), a rectangle oriented east to west (source No. 2), and a rectangle oriented north to south (source No. 3). All three sources had an area of 400 m^2 in order to ensure that equal emission rates were compared. The rectangles were selected to be exactly two times longer and half as wide as the square (see Figure D-2).

Two meteorological stations at Little Rock, Arkansas, and Los Angeles, California, were selected for this modeling analysis in order to compare two different meteorological regimes. Little Rock was selected because of its evenly distributed wind directions and Los Angeles was selected because it has a predominantly southwest wind direction (see Figure D-3). Five years of meteorological data were used for this analysis.

Each area source was modeled with similar receptor grids to ensure consistency. Sixteen receptors were placed on the edge of each of the area sources and another 16 were placed 25 meters out from the edge. Each of these two receptor groups were modeled as a Cartesian receptor grid. Two receptor rings were also placed at 50 and 100 meters out from the center of the source. This polar receptor grid consisted of 16 receptors with a 22.5 degree interval between receptors. See Figures D-4a through D-4c for receptor locations.

The ISCST3 model was run using the meteorological data from Little Rock, Arkansas, and Los Angeles, California, and the results are shown in Tables D-2a and D-2b. The results indicated that the standard deviation of the differences in air concentrations is greatest between source No. 2 and source No. 3. This difference is due to the orientation of the source. This occurs for both the Cartesian receptor grid and the polar receptor grid at both meteorological locations. This shows that the model is sensitive to the orientation of the rectangular area source.

Standard deviations are significantly smaller when source No. 1 is compared to source Nos. 2 or 3. This shows that the differences in Unitized Air Concentration (UAC) between the square source and the two rectangular sources are less than the differences between the two rectangular sources. A square area source also contributes the least amount of impact of orientation. Since no information on source shape or orientation is available, a square source will minimize the errors caused by different source shapes and orientations.

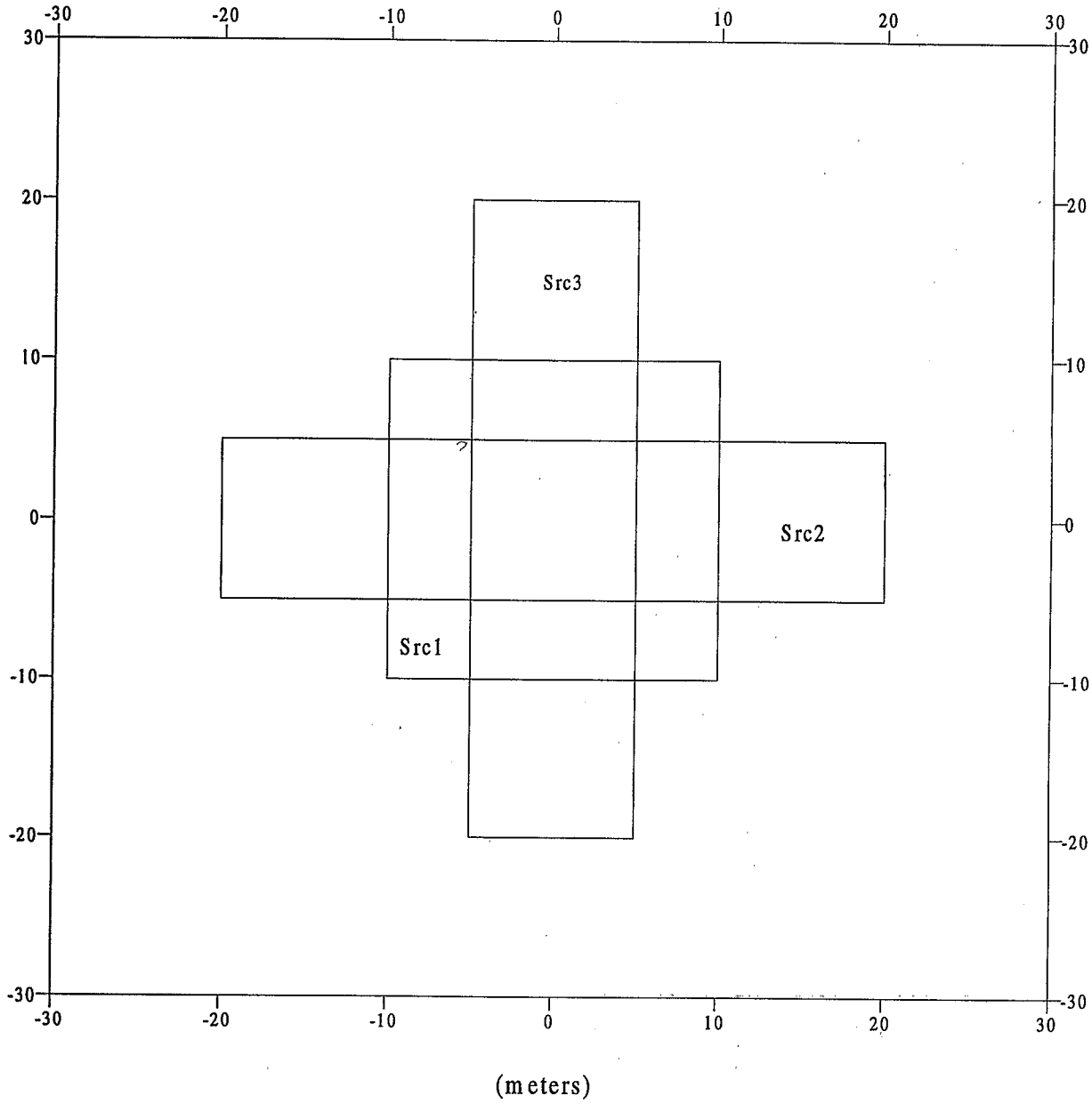
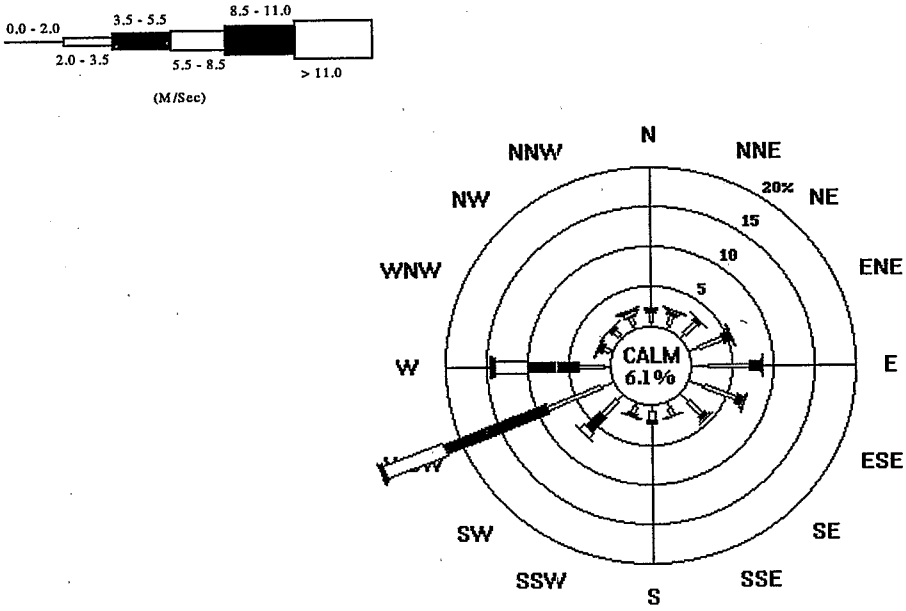


Figure D-2. Source Shapes and Orientations

Los Angeles, California



Little Rock, Arkansas

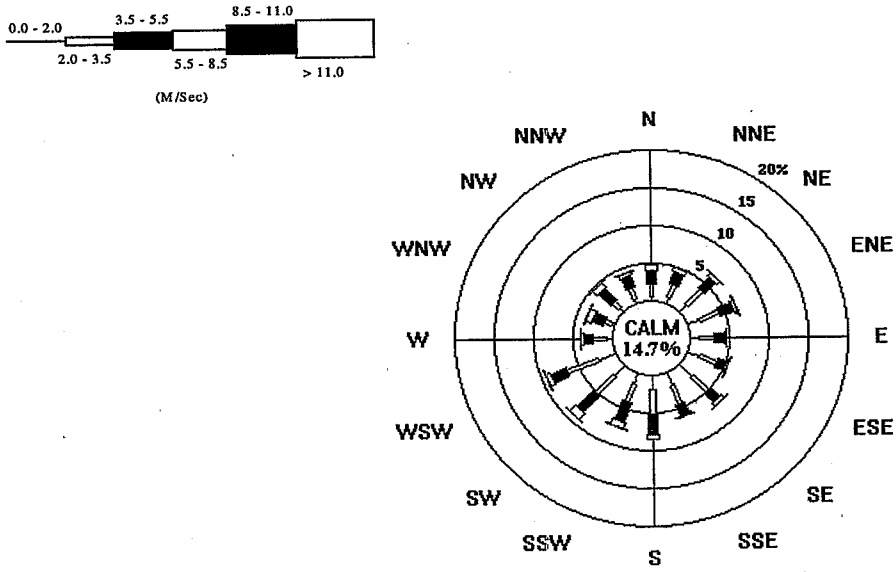


Figure D-3. Wind Roses

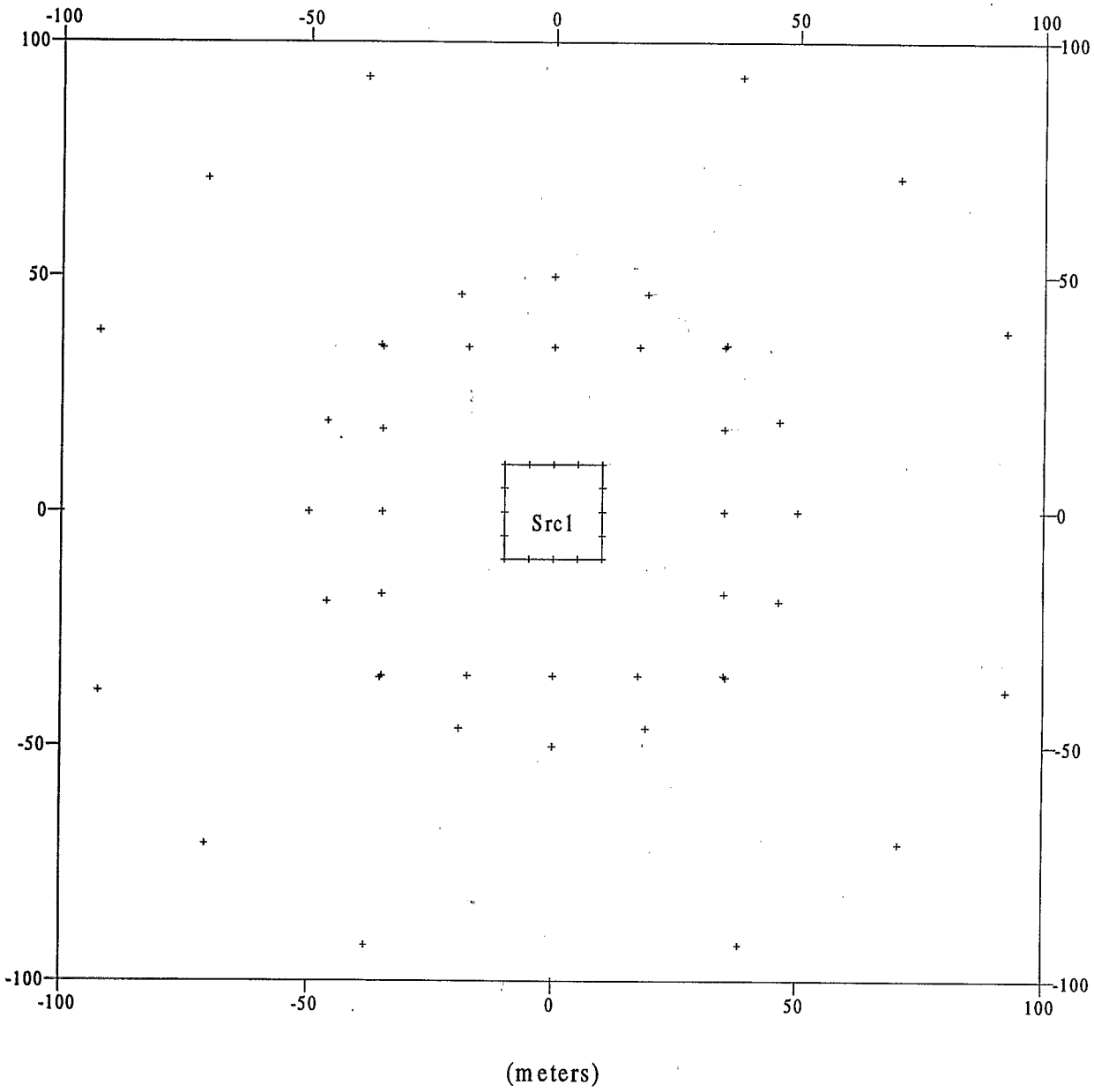


Figure D-4a. Receptor Locations (Source No. 1)

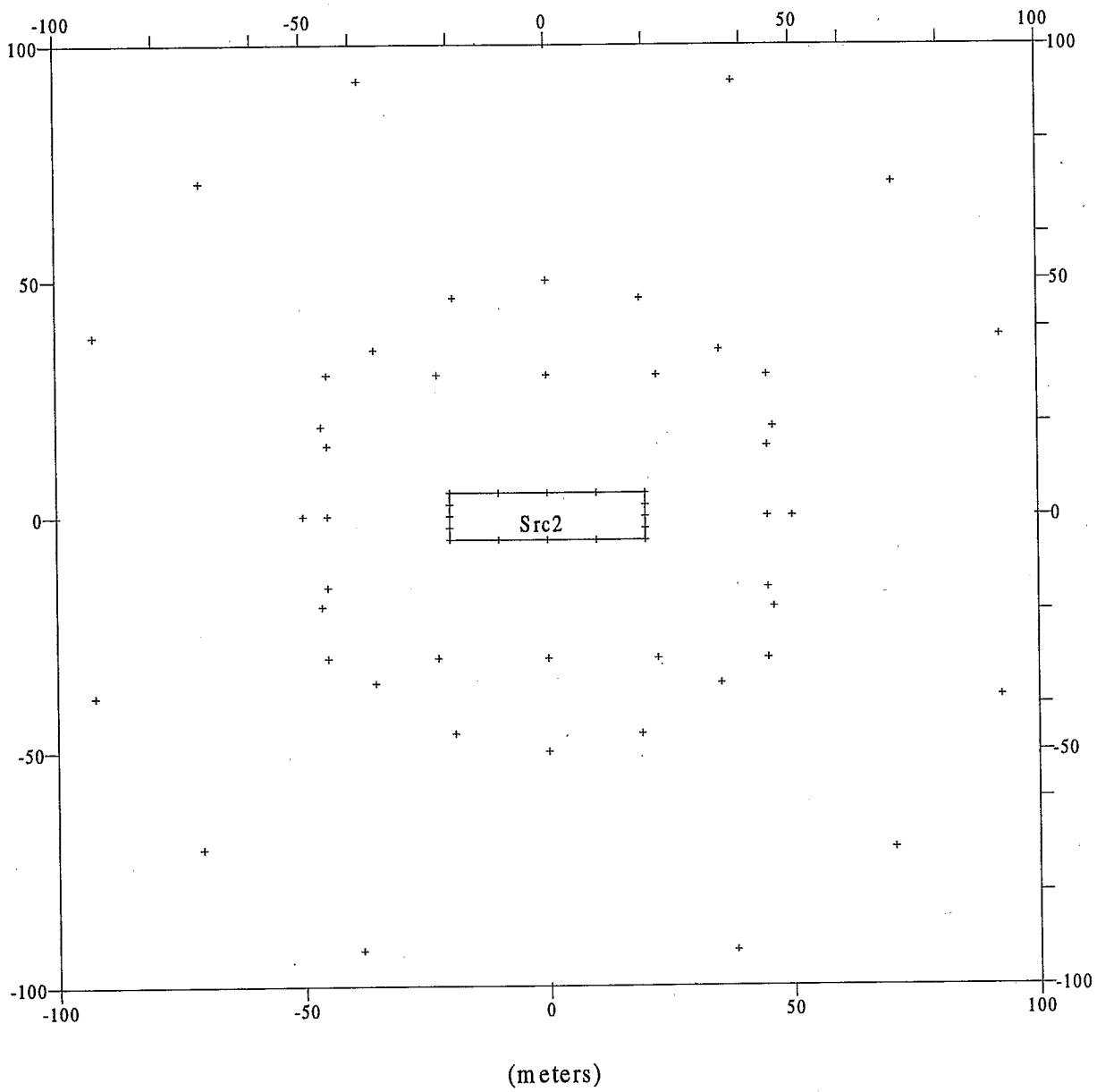


Figure D-4b. Receptor Locations (Source No. 2)

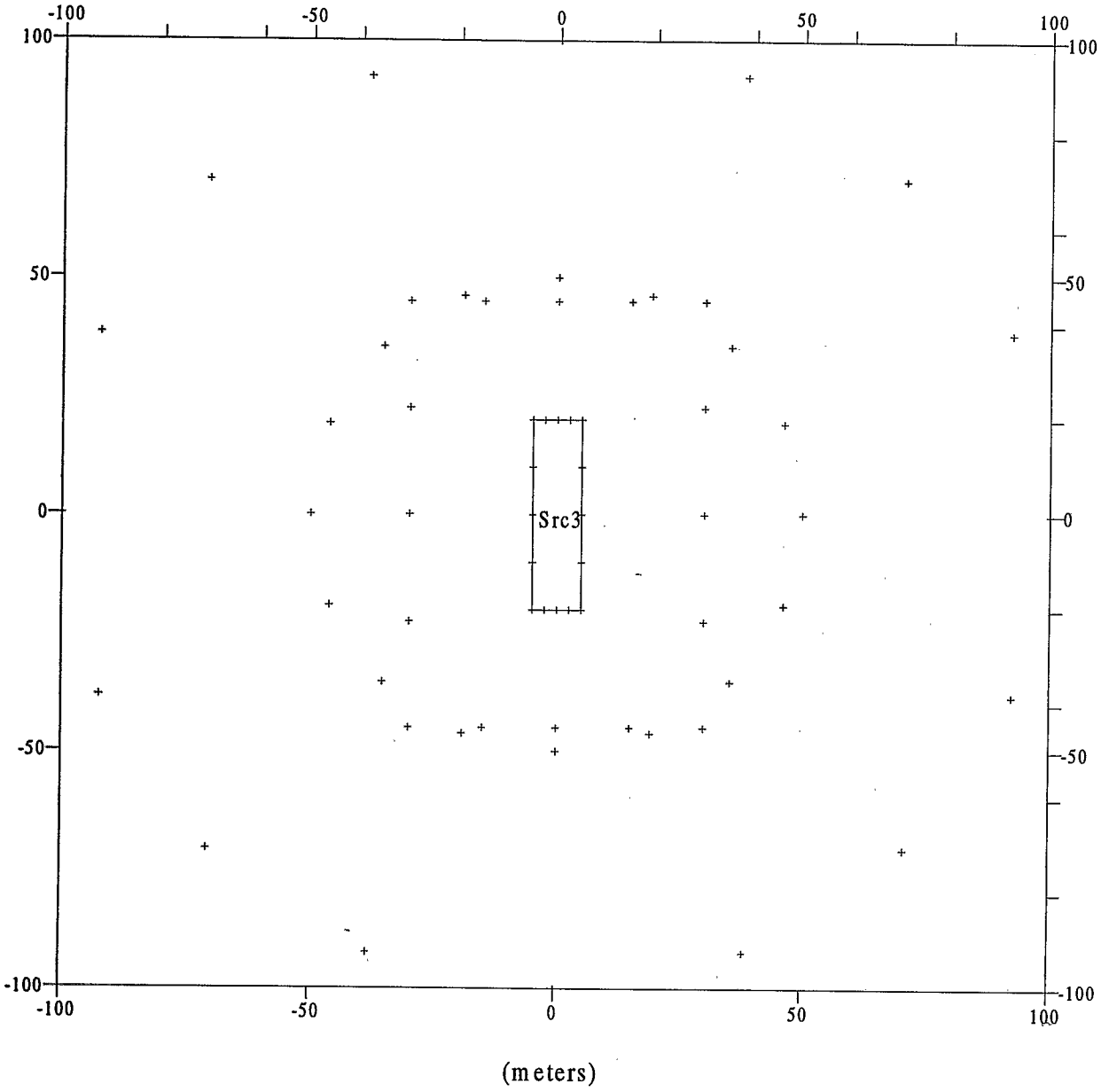


Figure D-4c. Receptor Locations (Source No. 3)

Table D-2a. Comparisons of Unitized Air Concentrations (ug/m^3 / ug/s-m^2) for Different Source Shapes and Orientations (Littte Rock, Arkansas)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Polar Receptor Grid														
X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.
19	46	0.190	19	46	0.199	19	46	0.211	0.010	5%	0.021	11%	0.012	6%
38	92	0.050	38	92	0.051	38	92	0.051	0.001	1%	0.001	2%	0.000	1%
35	35	0.249	35	35	0.243	35	35	0.278	-0.007	-3%	0.028	11%	0.035	14%
71	71	0.067	71	71	0.067	71	71	0.069	-0.001	-1%	0.001	2%	0.002	3%
46	19	0.321	46	19	0.361	46	19	0.256	0.041	13%	-0.065	-20%	-0.105	-29%
92	38	0.095	92	38	0.098	92	38	0.088	0.003	3%	-0.007	-7%	-0.010	-10%
50	0	0.124	50	0	0.128	50	0	0.147	0.004	3%	0.023	19%	0.020	15%
100	0	0.030	100	0	0.030	100	0	0.033	0.000	-1%	0.003	9%	0.003	11%
46	-19	0.085	46	-19	0.096	46	-19	0.084	0.011	12%	-0.001	-1%	-0.011	-12%
92	-38	0.023	92	-38	0.024	92	-38	0.023	0.001	2%	-0.001	-2%	-0.001	-5%
35	-35	0.106	35	-35	0.109	35	-35	0.103	0.003	3%	-0.003	-3%	-0.006	-6%
71	-71	0.030	71	-71	0.030	71	-71	0.029	0.000	0%	0.000	-1%	-0.001	-2%
19	-46	0.117	19	-46	0.113	19	-46	0.128	-0.005	-4%	0.011	9%	0.016	14%
38	-92	0.033	38	-92	0.032	38	-92	0.034	-0.001	-4%	0.001	2%	0.002	7%
0	-50	0.122	0	-50	0.117	0	-50	0.143	-0.005	-4%	0.021	17%	0.026	22%
0	-100	0.035	0	-100	0.033	0	-100	0.037	-0.002	-5%	0.002	5%	0.004	11%
-19	-46	0.134	-19	-46	0.128	-19	-46	0.150	-0.006	-4%	0.016	12%	0.022	17%
-38	-92	0.038	-38	-92	0.036	-38	-92	0.038	-0.002	-4%	0.001	2%	0.002	6%
-35	-35	0.161	-35	-35	0.158	-35	-35	0.170	-0.003	-2%	0.009	6%	0.012	8%
-71	-71	0.043	-71	-71	0.043	-71	-71	0.045	0.000	1%	0.001	3%	0.001	3%
-46	-19	0.159	-46	-19	0.185	-46	-19	0.140	0.026	16%	-0.019	-12%	-0.045	-24%
-92	-38	0.044	-92	-38	0.046	-92	-38	0.043	0.002	4%	-0.002	-4%	-0.004	-8%
-50	0	0.103	-50	0	0.114	-50	0	0.107	0.011	11%	0.004	4%	-0.007	-6%
-100	0	0.027	-100	0	0.027	-100	0	0.027	0.000	2%	0.000	1%	0.000	0%
-46	19	0.126	-46	19	0.145	-46	19	0.118	0.019	15%	-0.008	-6%	-0.027	-18%
-92	38	0.035	-92	38	0.036	-92	38	0.034	0.001	4%	-0.001	-4%	-0.003	-7%
-35	35	0.152	-35	35	0.160	-35	35	0.153	0.008	5%	0.001	0%	-0.007	-5%
-71	71	0.041	-71	71	0.042	-71	71	0.041	0.001	3%	0.001	2%	-0.001	-2%
-19	46	0.173	-19	46	0.179	-19	46	0.187	0.007	4%	0.014	8%	0.008	4%
-38	92	0.047	-38	92	0.047	-38	92	0.048	0.000	0%	0.001	3%	0.001	3%
0	50	0.224	0	50	0.191	0	50	0.276	-0.032	-14%	0.052	23%	0.085	44%
0	100	0.068	0	100	0.061	0	100	0.074	-0.008	-11%	0.006	9%	0.014	22%
								Standard Deviation:	**0.012**	**7%**	**0.018**	**9%**	**0.028**	**14%**

(continued)

Table D-2a (Cont.). Comparisons of Unitized Air Concentrations (ug/m^3 / ug/s-m^2) for Different Source Shapes and Orientations (Littte Rock, Arkansas)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Cartesion Receptor Grid														
X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.
-10	-10	3.014	-20	-5	2.675	-5	-20	2.673	-0.339	-11%	-0.341	-11%	-0.002	0%
-5	-10	4.266	-10	-5	4.219	-2.5	-20	3.451	-0.047	-1%	-0.815	-19%	-0.769	-18%
0	-10	4.354	0	-5	4.307	0	-20	3.526	-0.047	-1%	-0.827	-19%	-0.781	-18%
5	-10	3.961	10	-5	4.069	2.5	-20	3.152	0.109	3%	-0.809	-20%	-0.918	-23%
10	-10	2.175	20	-5	1.899	5	-20	2.011	-0.276	-13%	-0.164	-8%	0.112	6%
10	-5	5.211	20	-2.5	3.875	5	-10	5.567	-1.337	-26%	0.355	7%	1.692	44%
10	0	5.968	20	0	4.704	5	0	5.913	-1.264	-21%	-0.055	-1%	1.209	26%
10	5	6.012	20	2.5	4.918	5	10	5.834	-1.094	-18%	-0.178	-3%	0.916	19%
10	10	4.946	20	5	4.468	5	20	4.344	-0.477	-10%	-0.602	-12%	-0.125	-3%
5	10	6.804	10	5	6.758	2.5	20	5.550	-0.047	-1%	-1.254	-18%	-1.208	-18%
0	10	6.846	0	5	6.830	0	20	5.604	-0.016	0%	-1.242	-18%	-1.226	-18%
-5	10	6.157	-10	5	6.353	-2.5	20	4.954	0.196	3%	-1.203	-20%	-1.399	-22%
-10	10	3.245	-20	5	2.793	-5	20	3.052	-0.451	-14%	-0.193	-6%	0.259	9%
-10	5	4.923	-20	2.5	3.801	-5	10	5.166	-1.121	-23%	0.244	5%	1.365	36%
-10	0	5.169	-20	0	4.032	-5	0	5.287	-1.137	-22%	0.118	2%	1.255	31%
-10	-5	4.809	-20	-2.5	3.727	-5	-10	4.991	-1.081	-22%	0.182	4%	1.264	34%
-35	-35	0.164	-45	-30	0.158	-30	-45	0.132	-0.006	-4%	-0.032	-19%	-0.026	-16%
-17.5	-35	0.219	-22.5	-30	0.247	-15	-45	0.167	0.027	12%	-0.052	-24%	-0.079	-32%
0	-35	0.243	0	-30	0.284	0	-45	0.179	0.041	17%	-0.063	-26%	-0.104	-37%
17.5	-35	0.186	22.5	-30	0.192	15	-45	0.147	0.006	3%	-0.039	-21%	-0.045	-23%
35	-35	0.108	45	-30	0.088	30	-45	0.100	-0.020	-19%	-0.008	-7%	0.012	14%
35	-17.5	0.141	45	-15	0.105	30	-22.5	0.160	-0.036	-25%	0.019	14%	0.055	52%
35	0	0.277	45	0	0.164	30	0	0.401	-0.113	-41%	0.124	45%	0.236	144%
35	17.5	0.503	45	15	0.396	30	22.5	0.466	-0.107	-21%	-0.037	-7%	0.070	18%
35	35	0.254	45	30	0.263	30	45	0.200	0.009	3%	-0.054	-21%	-0.063	-24%
17.5	35	0.315	22.5	30	0.373	15	45	0.234	0.058	18%	-0.081	-26%	-0.139	-37%
0	35	0.417	0	30	0.445	0	45	0.341	0.028	7%	-0.076	-18%	-0.104	-23%
-17.5	35	0.272	-22.5	30	0.286	-15	45	0.214	0.014	5%	-0.057	-21%	-0.071	-25%
-35	35	0.155	-45	30	0.131	-30	45	0.146	-0.024	-15%	-0.009	-6%	0.015	11%
-35	17.5	0.211	-45	15	0.155	-30	22.5	0.232	-0.056	-27%	0.022	10%	0.078	50%
-35	0	0.213	-45	0	0.145	-30	0	0.298	-0.068	-32%	0.084	40%	0.153	106%
-35	-17.5	0.265	-45	-15	0.193	-30	-22.5	0.264	-0.073	-27%	-0.002	-1%	0.071	37%
								Standard Deviation:	0.463	15%	0.435	17%	0.747	41%

(continued)

Table D-2b. Comparisons of Unitized Air Concentrations (ug/m^3 / ug/s-m^2) for Different Source Shapes and Orientations (Los Angeles, California)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Polar Receptor Grid														
X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.
19	46	0.059	19	46	0.065	19	46	0.069	0.006	9%	0.010	17%	0.005	7%
38	92	0.016	38	92	0.016	38	92	0.016	0.000	-1%	0.000	3%	0.001	4%
35	35	0.188	35	35	0.168	35	35	0.284	-0.020	-11%	0.096	51%	0.116	69%
71	71	0.046	71	71	0.045	71	71	0.052	-0.001	-3%	0.006	13%	0.007	16%
46	19	0.582	46	19	0.607	46	19	0.461	0.025	4%	-0.121	-21%	-0.146	-24%
92	38	0.172	92	38	0.174	92	38	0.161	0.003	2%	-0.011	-6%	-0.014	-8%
50	0	0.278	50	0	0.293	50	0	0.293	0.014	5%	0.015	5%	0.001	0%
100	0	0.068	100	0	0.067	100	0	0.074	-0.001	-2%	0.005	8%	0.007	10%
46	-19	0.061	46	-19	0.062	46	-19	0.087	0.002	3%	0.026	43%	0.025	40%
92	-38	0.015	92	-38	0.015	92	-38	0.016	0.000	0%	0.002	10%	0.002	11%
35	-35	0.062	35	-35	0.068	35	-35	0.062	0.006	10%	0.000	0%	-0.006	-9%
71	-71	0.016	71	-71	0.017	71	-71	0.017	0.001	4%	0.001	3%	0.000	-1%
19	-46	0.080	19	-46	0.076	19	-46	0.087	-0.004	-4%	0.007	9%	0.011	14%
38	-92	0.023	38	-92	0.022	38	-92	0.024	-0.001	-5%	0.001	3%	0.002	8%
0	-50	0.086	0	-50	0.084	0	-50	0.096	-0.003	-3%	0.009	11%	0.012	15%
0	-100	0.023	0	-100	0.024	0	-100	0.024	0.000	1%	0.001	3%	0.000	2%
-19	-46	0.099	-19	-46	0.092	-19	-46	0.108	-0.006	-7%	0.009	9%	0.016	17%
-38	-92	0.028	-38	-92	0.027	-38	-92	0.028	-0.001	-2%	0.000	1%	0.001	3%
-35	-35	0.122	-35	-35	0.119	-35	-35	0.143	-0.003	-2%	0.021	18%	0.024	20%
-71	-71	0.033	-71	-71	0.032	-71	-71	0.034	0.000	-1%	0.001	4%	0.002	5%
-46	-19	0.218	-46	-19	0.223	-46	-19	0.226	0.005	2%	0.008	4%	0.003	2%
-92	-38	0.060	-92	-38	0.061	-92	-38	0.061	0.001	1%	0.001	1%	0.000	0%
-50	0	0.320	-50	0	0.378	-50	0	0.278	0.057	18%	-0.042	-13%	-0.099	-26%
-100	0	0.093	-100	0	0.098	-100	0	0.087	0.005	6%	-0.006	-6%	-0.011	-11%
-46	19	0.264	-46	19	0.273	-46	19	0.260	0.009	3%	-0.005	-2%	-0.013	-5%
-92	38	0.074	-92	38	0.075	-92	38	0.073	0.001	1%	-0.001	-2%	-0.002	-2%
-35	35	0.137	-35	35	0.123	-35	35	0.164	-0.014	-10%	0.027	20%	0.041	33%
-71	71	0.037	-71	71	0.035	-71	71	0.039	-0.002	-5%	0.002	4%	0.003	9%
-19	46	0.063	-19	46	0.066	-19	46	0.073	0.003	4%	0.010	15%	0.007	11%
-38	92	0.017	-38	92	0.017	-38	92	0.018	0.000	-2%	0.001	3%	0.001	5%
0	50	0.067	0	50	0.058	0	50	0.080	-0.008	-12%	0.014	21%	0.022	37%
0	100	0.020	0	100	0.018	0	100	0.021	-0.002	-9%	0.001	6%	0.003	15%
								Standard Deviation:	**0.013**	**6%**	**0.030**	**14%**	**0.040**	**18%**

(continued)

Table D-2b (Cont.). Comparisons of Unitized Air Concentrations (ug/m^3 / ug/s-m^2) for Different Source Shapes and Orientations (Los Angeles, California)

Source No. 1 (20m x 20m)			Source No. 2 (40m x 10m)			Source No. 3 (10m x 40m)			Differences in UACs Sources No. 1 and No. 2		Differences in UACs Sources No. 1 and No. 3		Differences in UACs Sources No. 2 and No. 3	
Cartesion Receptor Grid														
X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	X (m)	Y (m)	UAC	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.	Diff. In UAC	% of Diff.
-10	-10	3.225	-20	-5	3.241	-5	-20	2.674	0.016	1%	-0.551	-17%	-0.567	-17%
-5	-10	4.025	-10	-5	4.333	-2.5	-20	3.119	0.308	8%	-0.906	-23%	-1.214	-28%
0	-10	3.952	0	-5	4.297	0	-20	3.050	0.345	9%	-0.902	-23%	-1.247	-29%
5	-10	3.431	10	-5	3.871	2.5	-20	2.564	0.440	13%	-0.867	-25%	-1.307	-34%
10	-10	1.683	20	-5	1.592	5	-20	1.511	-0.091	-5%	-0.172	-10%	-0.081	-5%
10	-5	5.931	20	-2.5	4.787	5	-10	5.570	-1.143	-19%	-0.360	-6%	0.783	16%
10	0	6.636	20	0	5.882	5	0	5.644	-0.754	-11%	-0.992	-15%	-0.238	-4%
10	5	6.640	20	2.5	6.294	5	10	5.524	-0.346	-5%	-1.116	-17%	-0.770	-12%
10	10	5.600	20	5	5.866	5	20	4.325	0.266	5%	-1.275	-23%	-1.541	-26%
5	10	6.893	10	5	8.126	2.5	20	4.939	1.232	18%	-1.955	-28%	-3.187	-39%
0	10	6.860	0	5	8.285	0	20	4.913	1.424	21%	-1.947	-28%	-3.371	-41%
-5	10	6.031	-10	5	7.442	-2.5	20	4.156	1.411	23%	-1.875	-31%	-3.286	-44%
-10	10	3.393	-20	5	3.497	-5	20	2.702	0.103	3%	-0.691	-20%	-0.794	-23%
-10	5	5.649	-20	2.5	5.102	-5	10	5.015	-0.547	-10%	-0.634	-11%	-0.088	-2%
-10	0	5.944	-20	0	5.373	-5	0	5.167	-0.572	-10%	-0.777	-13%	-0.205	-4%
-10	-5	5.663	-20	-2.5	5.028	-5	-10	5.104	-0.635	-11%	-0.559	-10%	0.076	2%
-35	-35	0.124	-45	-30	0.139	-30	-45	0.095	0.014	11%	-0.029	-23%	-0.043	-31%
-17.5	-35	0.158	-22.5	-30	0.183	-15	-45	0.123	0.025	16%	-0.035	-22%	-0.060	-33%
0	-35	0.172	0	-30	0.199	0	-45	0.121	0.028	16%	-0.050	-29%	-0.078	-39%
17.5	-35	0.123	22.5	-30	0.124	15	-45	0.100	0.001	0%	-0.024	-19%	-0.024	-20%
35	-35	0.064	45	-30	0.053	30	-45	0.063	-0.011	-17%	-0.001	-2%	0.010	19%
35	-17.5	0.095	45	-15	0.076	30	-22.5	0.119	-0.019	-20%	0.024	25%	0.043	57%
35	0	0.592	45	0	0.377	30	0	0.696	-0.215	-36%	0.104	18%	0.319	85%
35	17.5	0.829	45	15	0.739	30	22.5	0.683	-0.090	-11%	-0.146	-18%	-0.055	-7%
35	35	0.192	45	30	0.304	30	45	0.101	0.112	58%	-0.091	-47%	-0.203	-67%
17.5	35	0.109	22.5	30	0.195	15	45	0.072	0.086	78%	-0.037	-34%	-0.122	-63%
0	35	0.125	0	30	0.144	0	45	0.100	0.019	15%	-0.025	-20%	-0.044	-31%
-17.5	35	0.113	-22.5	30	0.160	-15	45	0.077	0.047	42%	-0.035	-31%	-0.082	-52%
-35	35	0.139	-45	30	0.166	-30	45	0.089	0.026	19%	-0.050	-36%	-0.077	-46%
-35	17.5	0.387	-45	15	0.335	-30	22.5	0.370	-0.053	-14%	-0.017	-4%	0.036	11%
-35	0	0.603	-45	0	0.472	-30	0	0.603	-0.131	-22%	0.000	0%	0.131	28%
-35	-17.5	0.318	-45	-15	0.275	-30	-22.5	0.316	-0.043	-13%	-0.002	-1%	0.041	15%
								Standard Deviation:	**0.542**	**24%**	**0.614**	**15%**	**1.026**	**33%**

D.3 Receptor Locations and Spacings

A sensitivity analysis was conducted using the ISCST3 model to determine what receptor locations and spacings should be used in the risk analysis for five types of waste management units (WMUs). A discussion of the analysis follows.

Because it takes a substantial amount of time for the ISCST3 model to execute, it was necessary to choose a limited number of receptors to be used in the dispersion modeling analysis,. The larger the number of receptor points, the longer the run time. However, modeling fewer receptors may result in the omission of the maximum point for assessing exposure impacts. Therefore, a sensitivity analysis was conducted to determine the number of receptors needed for the model run and to locate ideal receptor placements.

A wind rose was plotted for each of the 29 meteorological stations to be used in the risk analysis for a 5-year time period in order to choose two meteorological stations for this sensitivity analysis. Little Rock, Arkansas, and Los Angeles, California, meteorological stations were selected for the sensitivity analysis. The wind roses show that Little Rock has very evenly distributed wind directions, and Los Angeles has a predominant southwest to west wind (Figure D-3). Little Rock and Los Angeles were chosen to determine if a higher density of receptors should be placed downwind of a site near Los Angeles, as compared to a site near Little Rock. Similarly, the 5th, 50th, and 95th percentile of sizes of LAUs were used in the sensitivity analysis to determine whether sizes of units can affect receptor locations and spacings. The areas of the 5th, 50th, and 95th percentile of sizes of LAUs are 1,200 m^2, 100,000 m^2, and 1,700,000 m^2, respectively.

The dispersion modeling was conducted using two sets of receptor grids. The first set of receptor points (Cartesian receptor grid) was placed around the modeled source with distances of 0, 25, 50, 75, and 150 meters from the edge of the unit. Square-shaped ground-level area sources were used in the modeling. Therefore, these receptors are located on five squares surrounding the source. The second set of receptor points (polar receptor grid) was placed outside of the first set of receptors to 10 kilometers from the center of the source. Since the ISCST3 model's area source algorithm does not consider elevated terrain, receptor elevations were not input in the modeling.

In this sensitivity analysis, both downwind and lateral receptor spacings were investigated for three unit sizes using 5 years of meteorological data from Little Rock and Los Angeles. For the first set of receptor points (i.e., Cartesian receptor grid), five downwind distances of 0, 25, 50, 75, and 150 meters from the edge of the source were used. For lateral receptor spacing, choices of 64, 32, and 16 equally spaced receptor points for each square were used in the modeling to determine the number of receptors needed to catch the maximum impacts. (See Figures D-5a through D-5c for Cartesian receptor locations and spacings [50th percentile]). For the second set of receptor points (i.e., polar receptor grid), about 20 downwind distances (i.e., receptor rings) were used. Receptor lateral intervals of 22.5° and 10° were used to determine whether 22.5° spacing can catch the maximum impacts. With a 22.5° interval, there are 16 receptors on each ring. There are 36 receptors on each ring for the 10° interval. See Figures D-6a and D-6b for polar receptor locations (5th percentile).

The results (Figures D-7a through D-7f) show that the maximum downwind concentrations decrease sharply from the edge of the area source to 150 meters from the source. The maximum concentrations decrease more sharply for a smaller area source than for a larger one. This means that more close-to-source receptors are generally needed for a small area source than for a large one.

The results also show that the maximum impacts are generally higher for a dense receptor grid (i.e., 64 or 32 receptors on each square) than for a scattered receptor grid (i.e., 16 receptors on each square). However, the differences of the maximum receptor impacts are not significant between a dense and a scattered receptor grid (Figures D-7a through D-7f). It should be noted that the above conclusions apply to both Little Rock and Los Angeles. This means that the distribution of wind directions does not play an important role in determining receptor lateral spacings.

Figures D-8a through D-8f compare the maximum concentrations at each ring for 22.5° and 10° intervals. The results show that the differences of the maximum concentrations are greater for close-to-source receptors than for further out receptors, and the differences are greater for larger area sources than for smaller area sources. The differences of the maximum concentrations for 22.5° and 10° intervals are generally small, and the concentrations tend to be the same at 10 kilometers. The conclusions were drawn from both Little Rock and Los Angeles meteorological data.

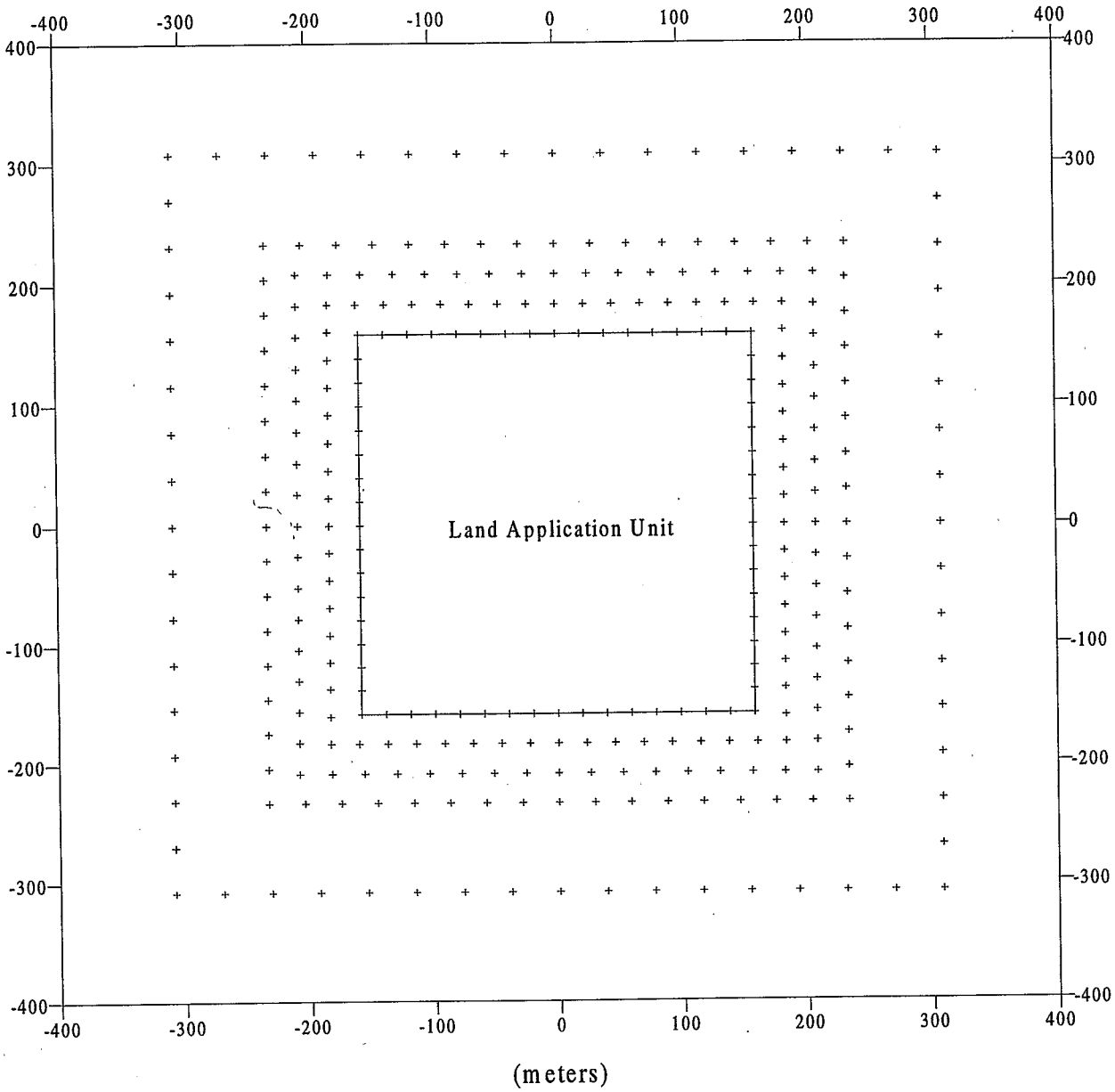


Figure D-5a. Cartesian Receptor Grid (64 receptors each square)

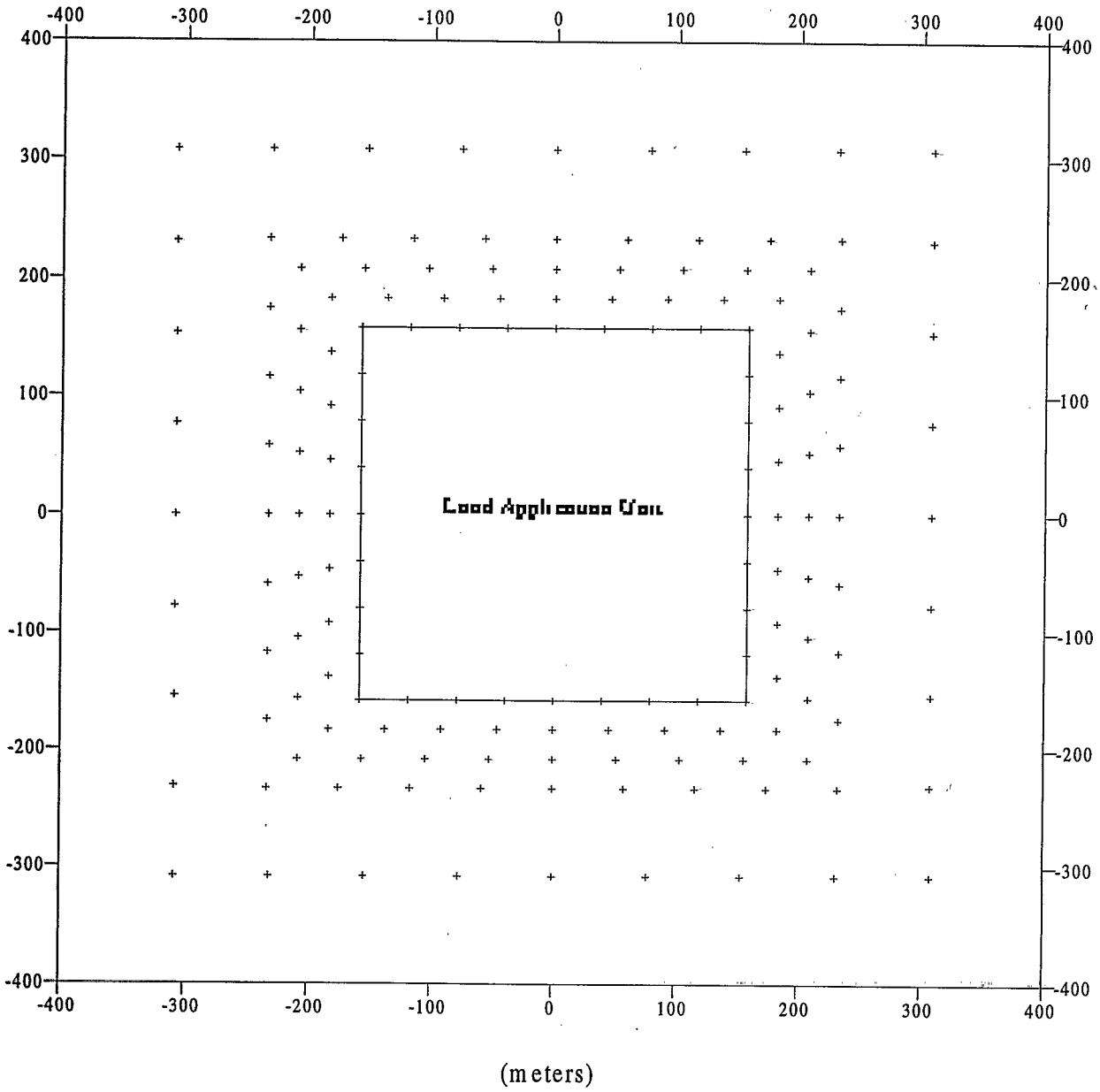


Figure D-5b. Cartesian Receptor Grid (32 receptors each square)

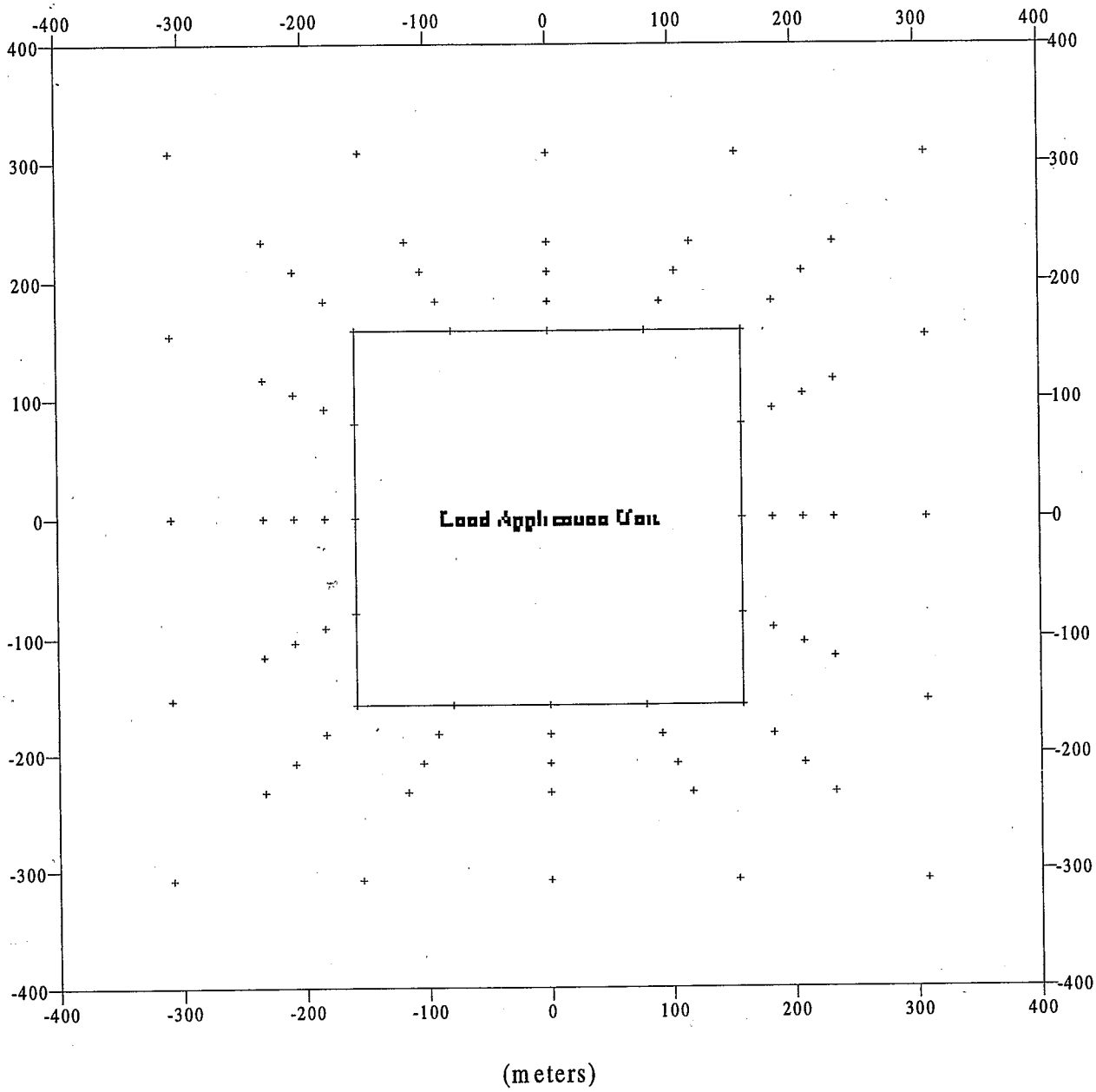


Figure D-5c. Cartesian Receptor Grid (16 receptors each square)

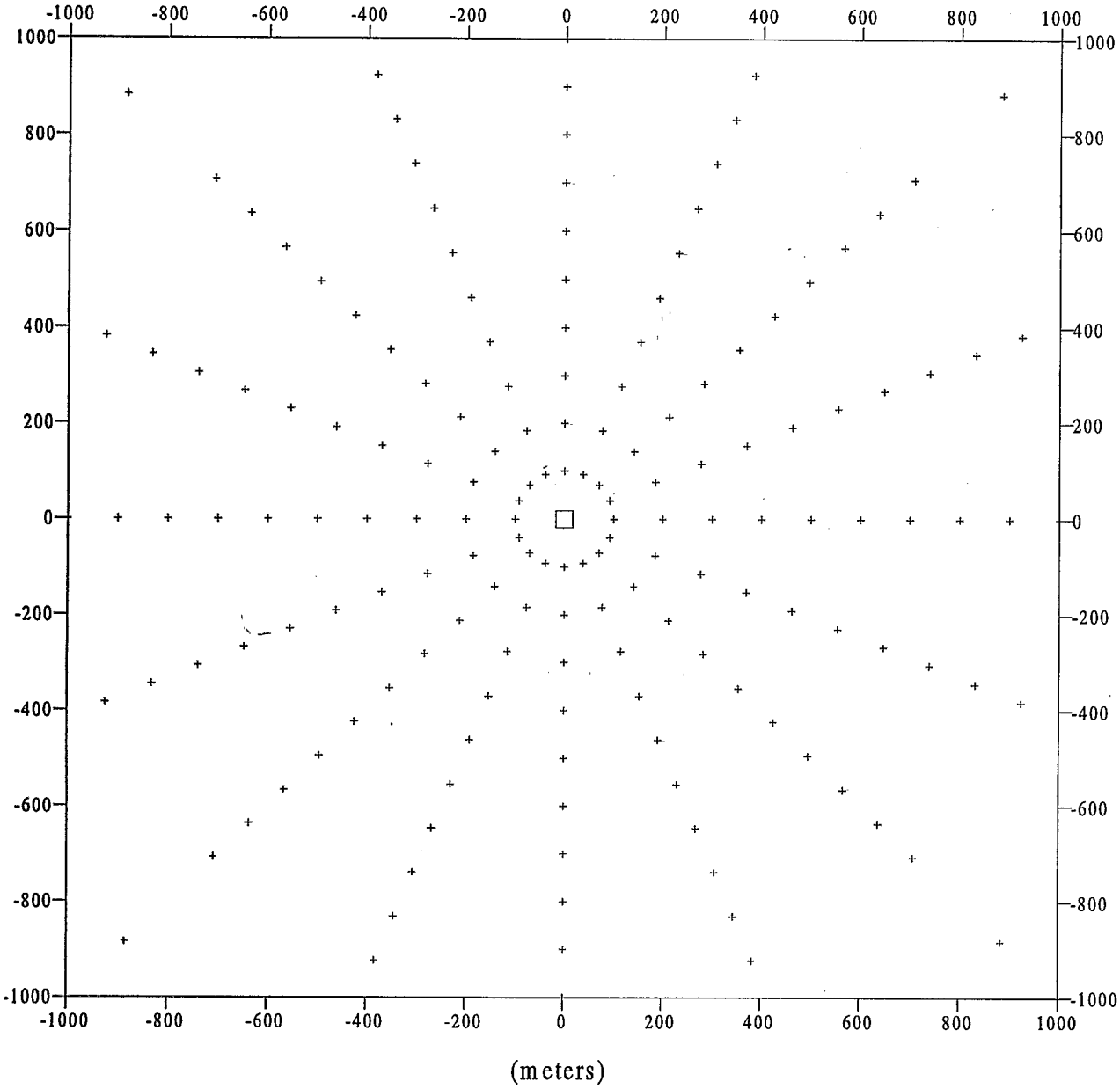


Figure D-6a. Polar Receptor Grid (22.5 degree)

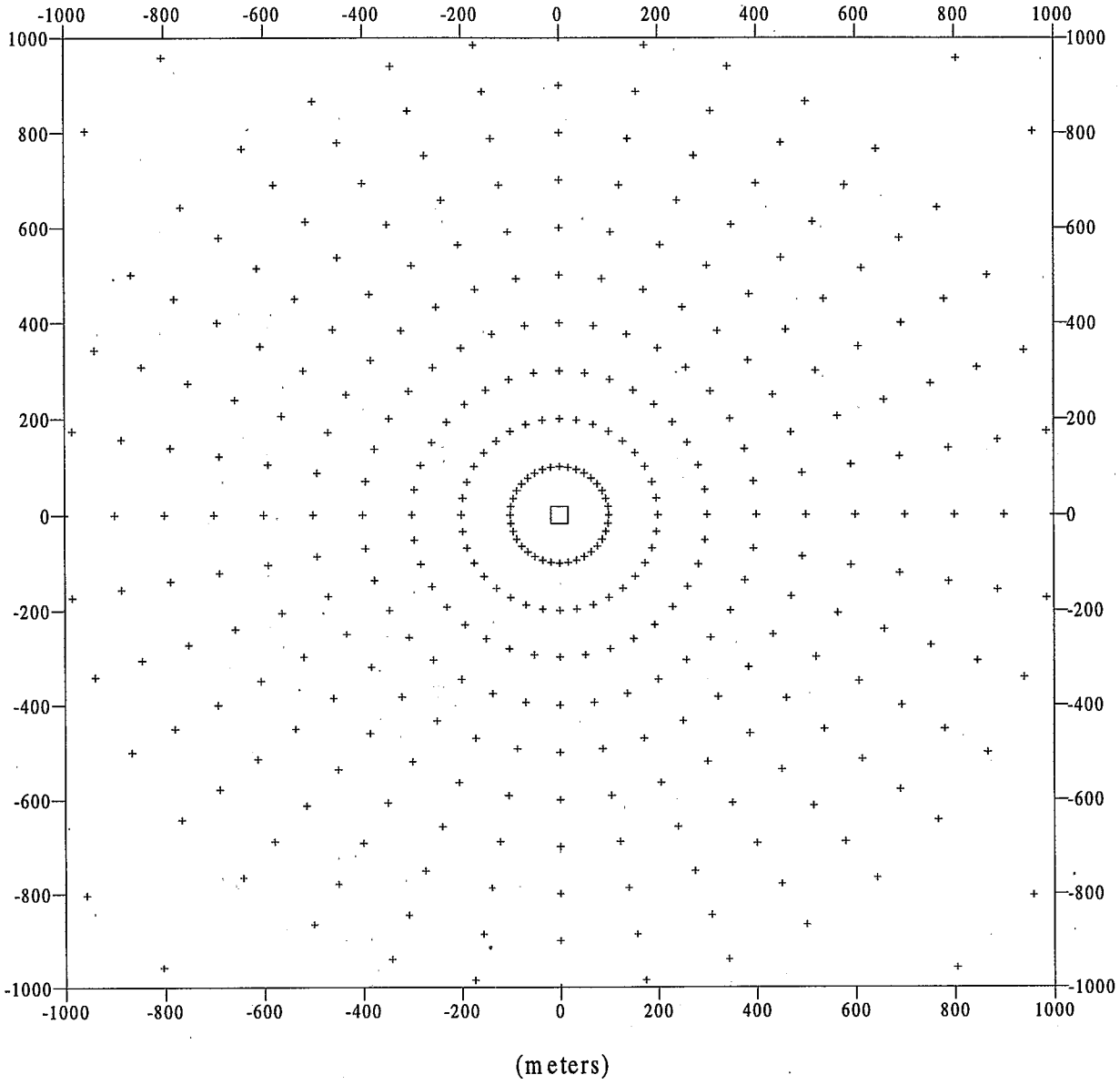


Figure D-6b. Polar Receptor Grid (10 degree)

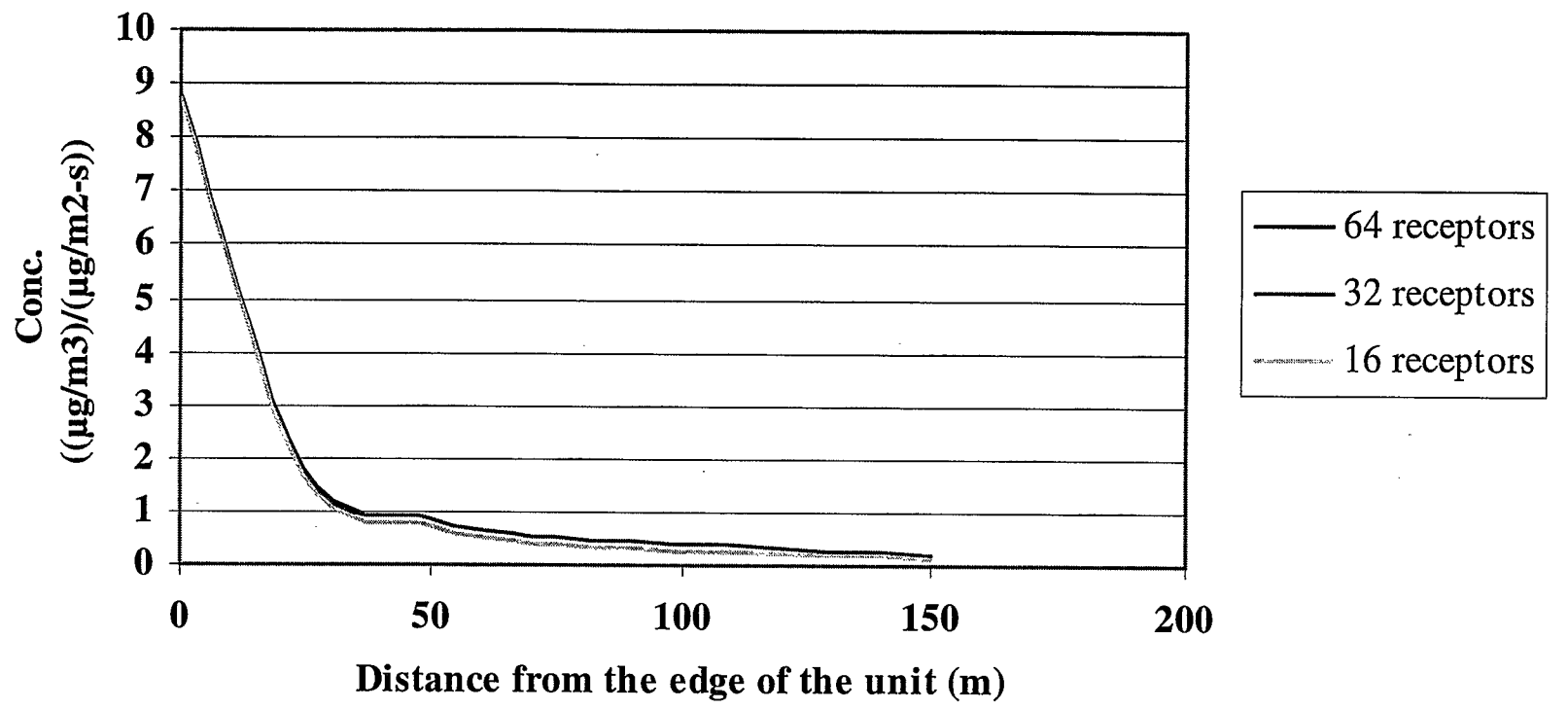


Figure D-7a. Maximum Concentrations (5th Percentile, LAU, Los Angeles, CA)

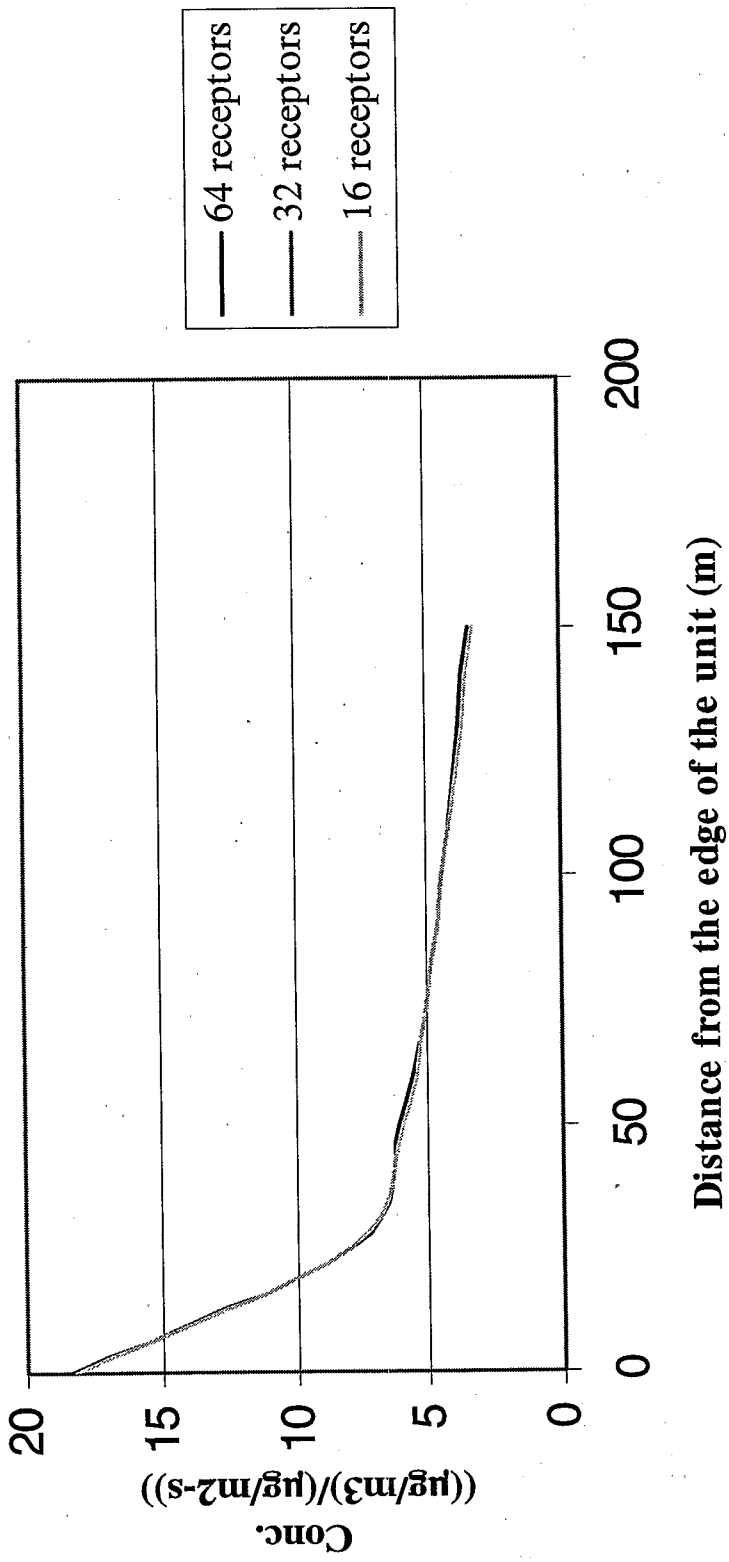


Figure D-7b. Maximum Concentrations (50th Percentile, LAU, Los Angeles, CA)

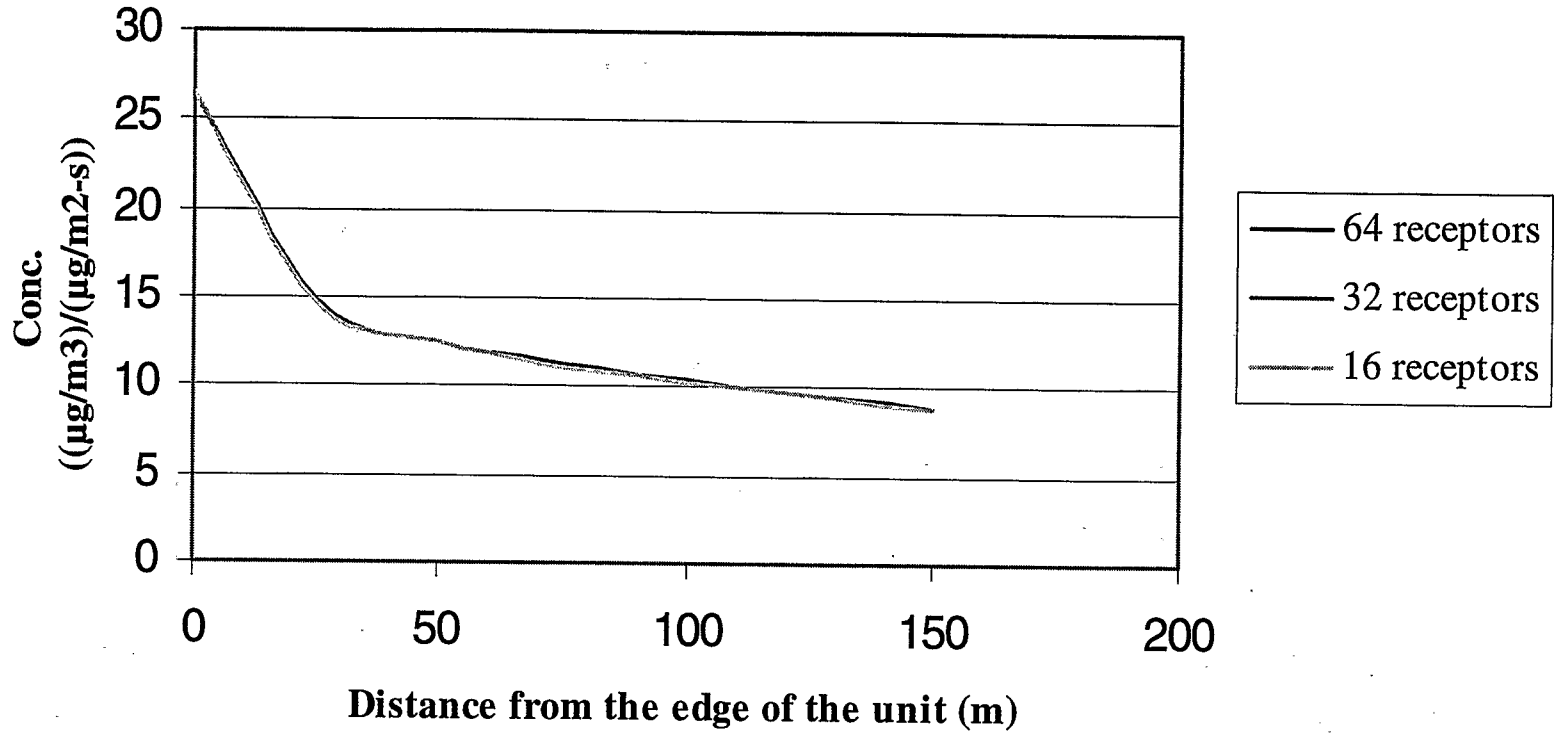


Figure D-7c. Maximum Concentrations (95th Percentile, LAU, Los Angeles, CA)

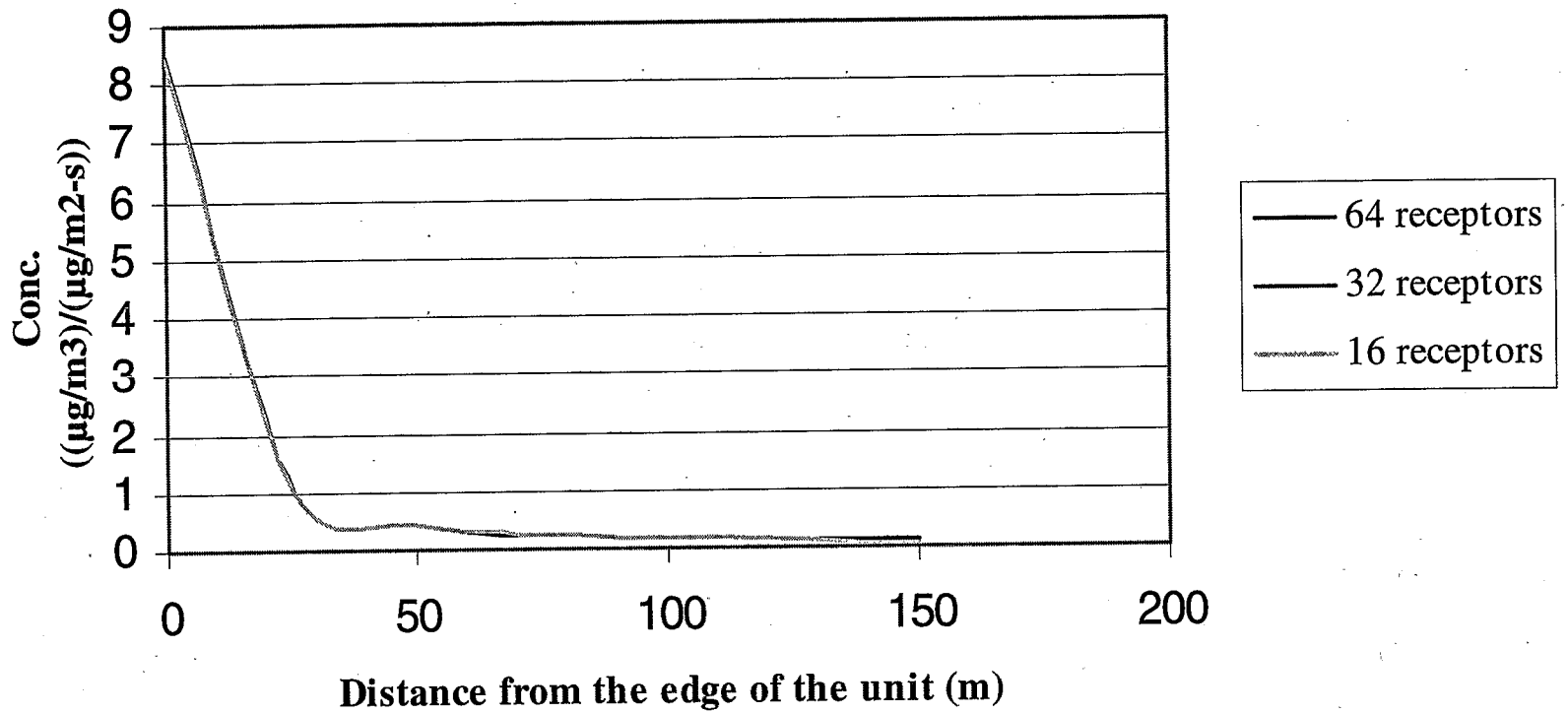


Figure D-7d. Maximum Concentrations (5th Percentile, LAU, Little Rock, AR)

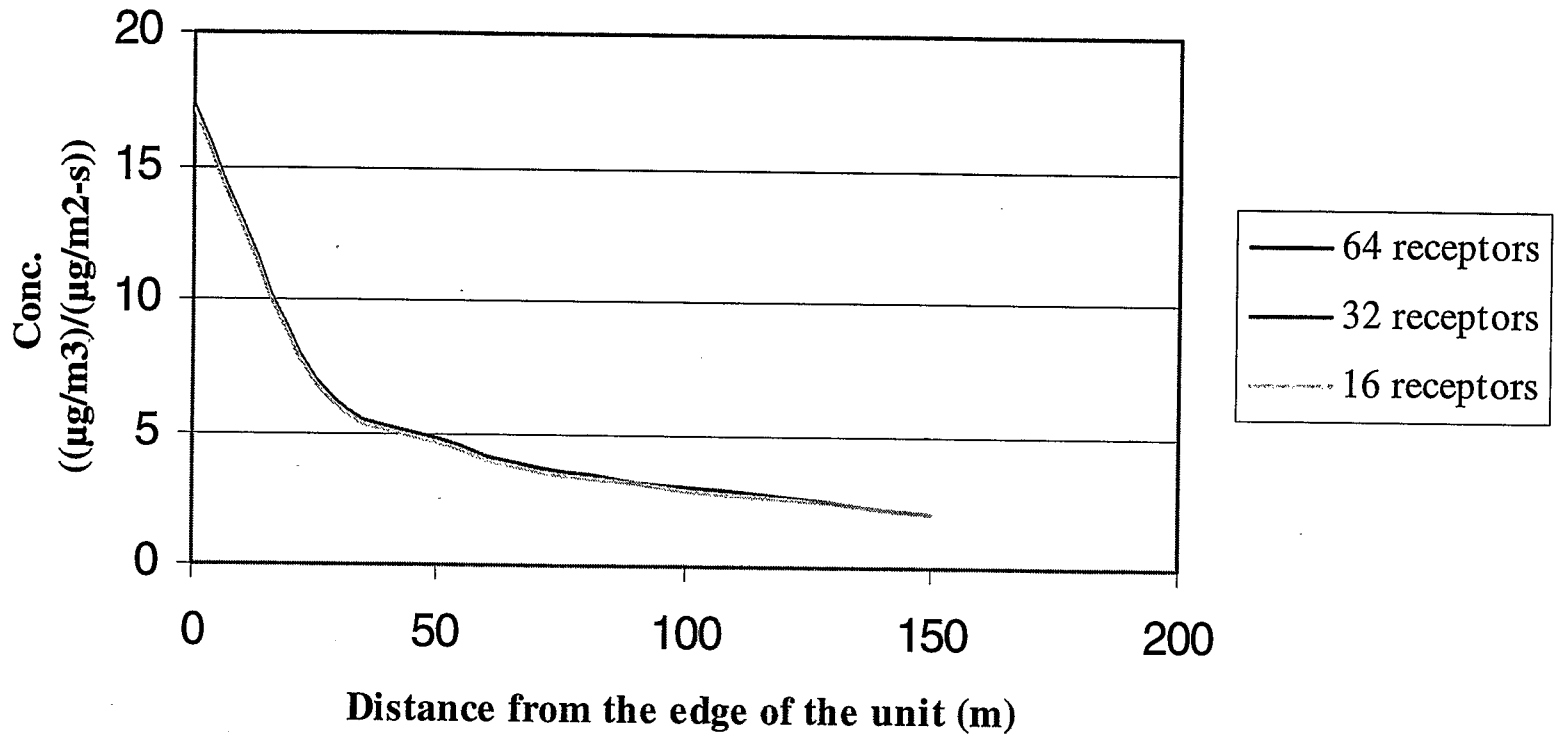


Figure D-7e. Maximum Concentrations (50th Percentile, LAU, Little Rock, AR)

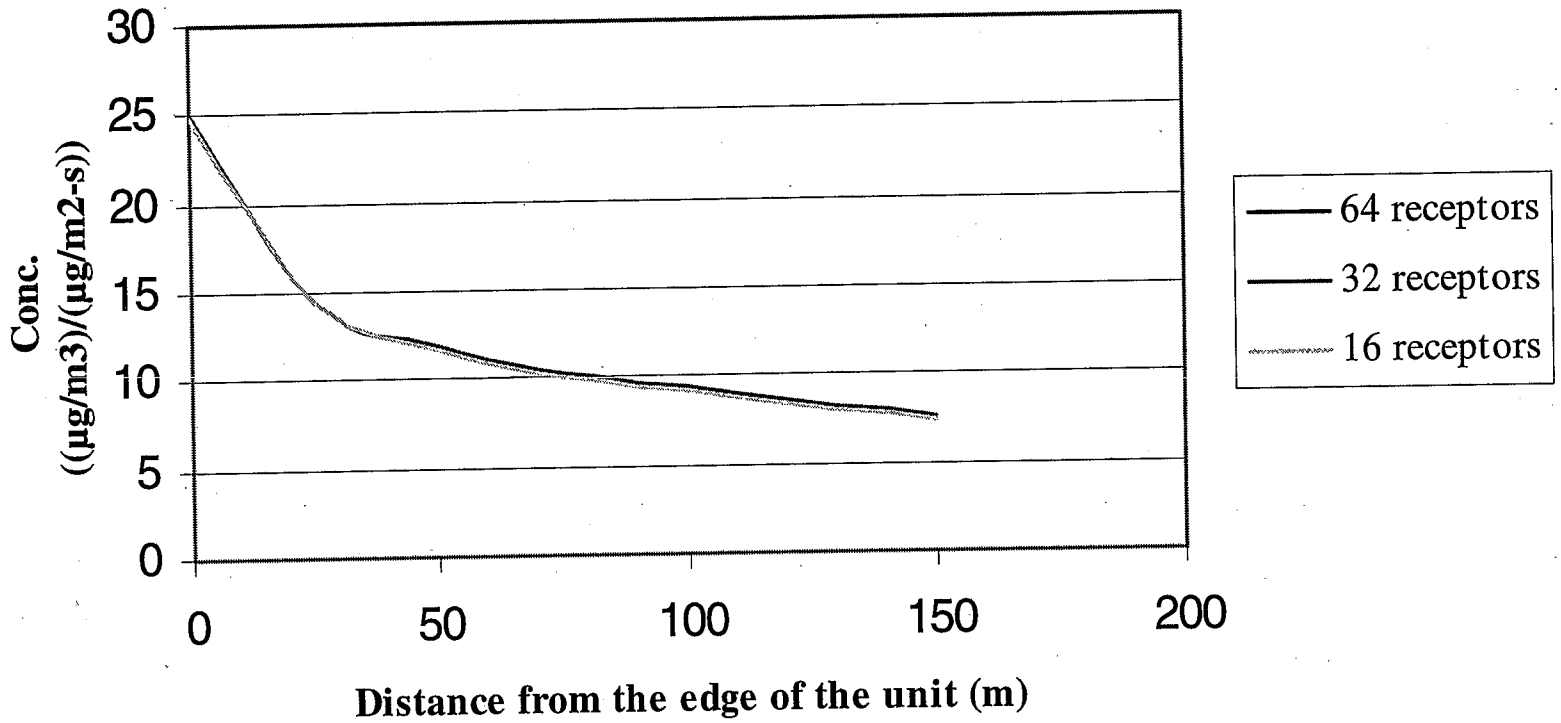


Figure D-7f. Maximum Concentrations (95th Percentile, LAU, Little Rock, AR)

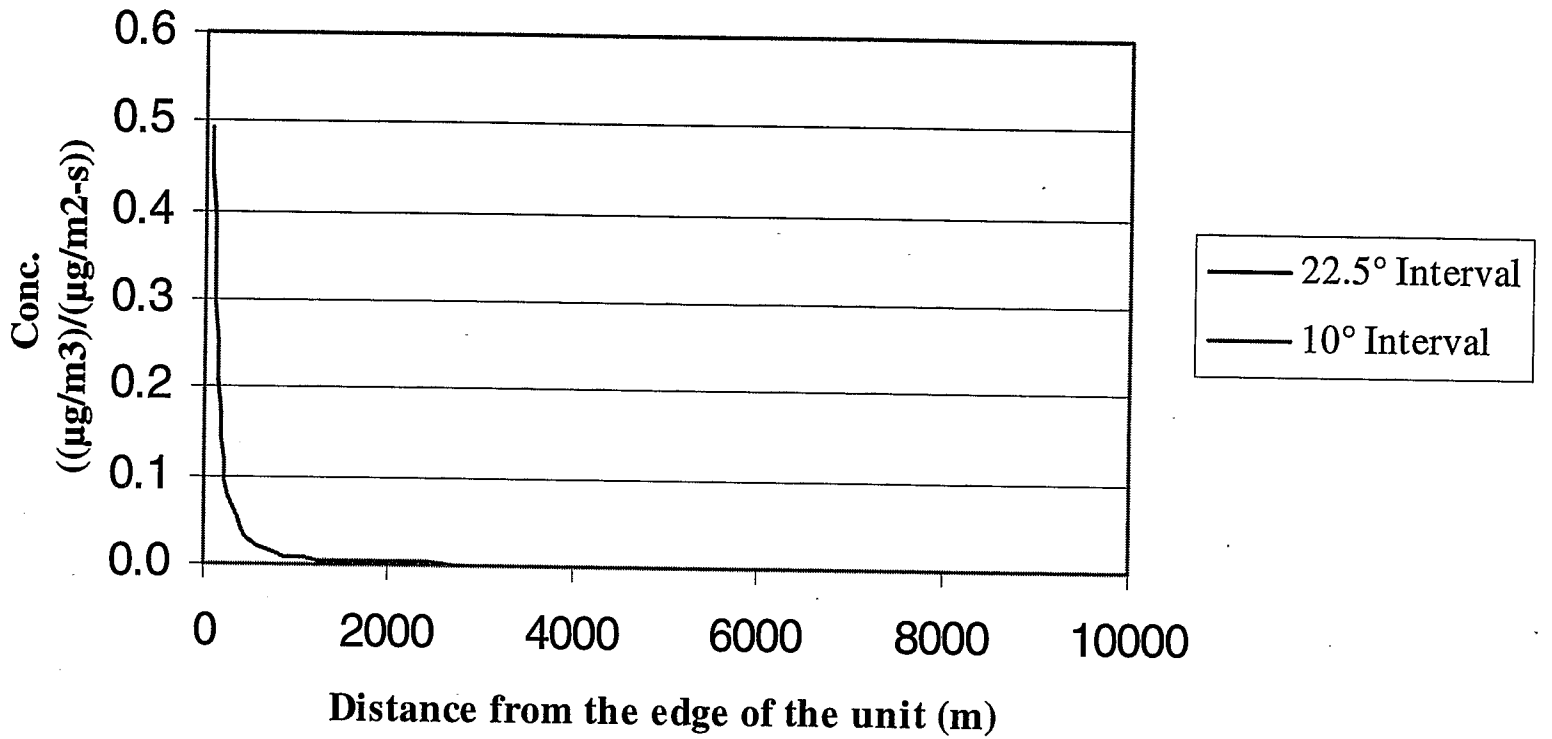


Figure D-8a. Maximum Concentrations (5th Percentile, LAU, Los Angeles, CA)

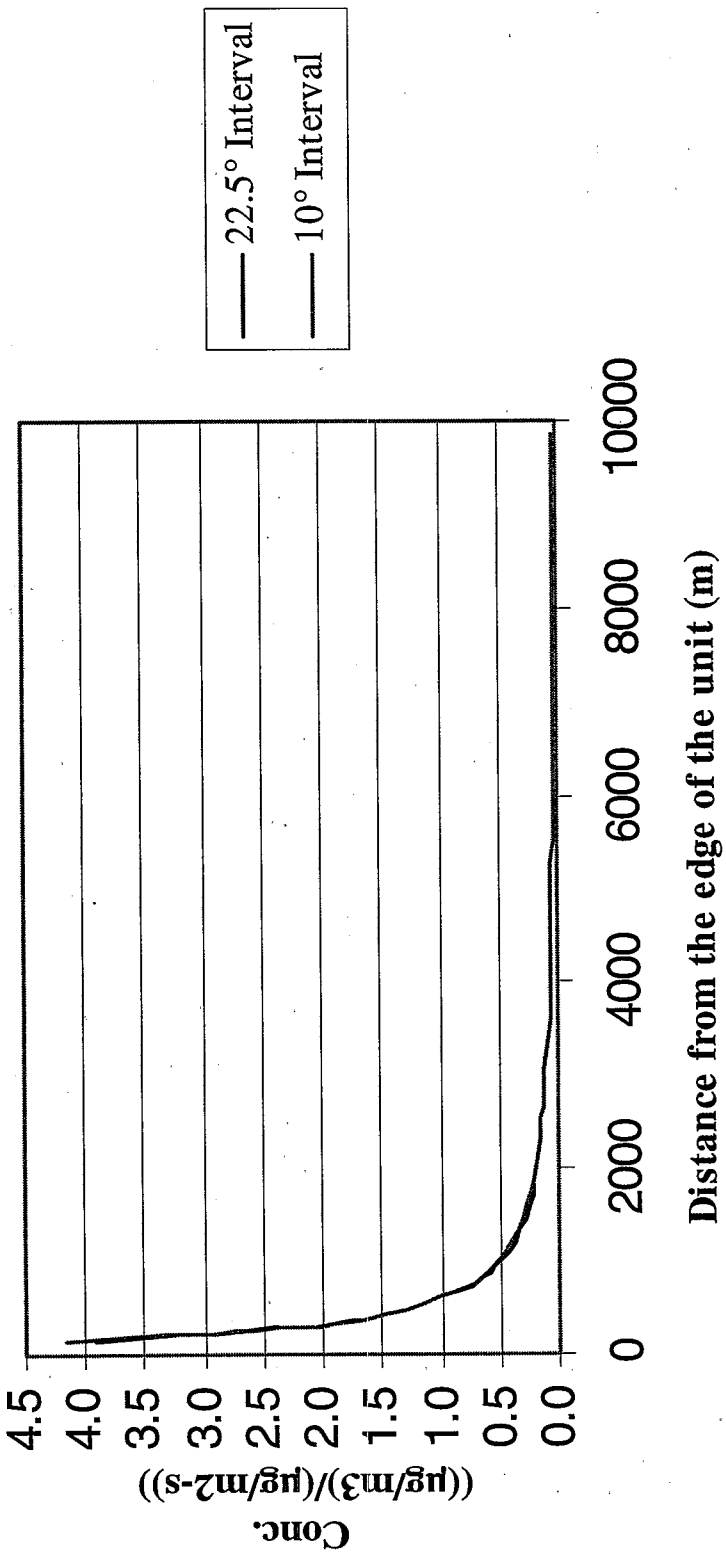


Figure D-8b. Maximum Concentrations (50th Percentile, LAU, Los Angeles, CA)

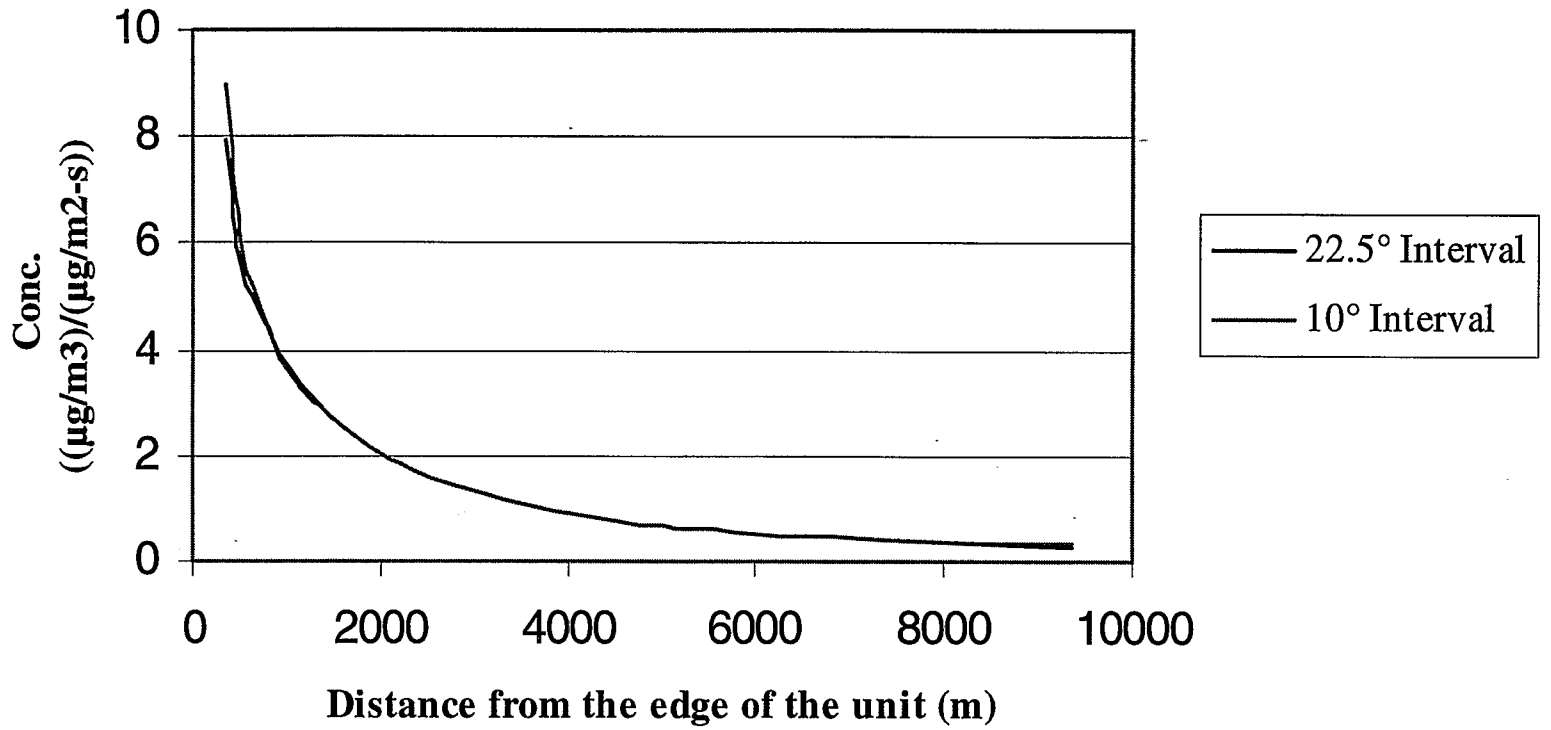


Figure D-8c. Maximum Concentrations (95th Percentile, LAU, Los Angeles, CA)

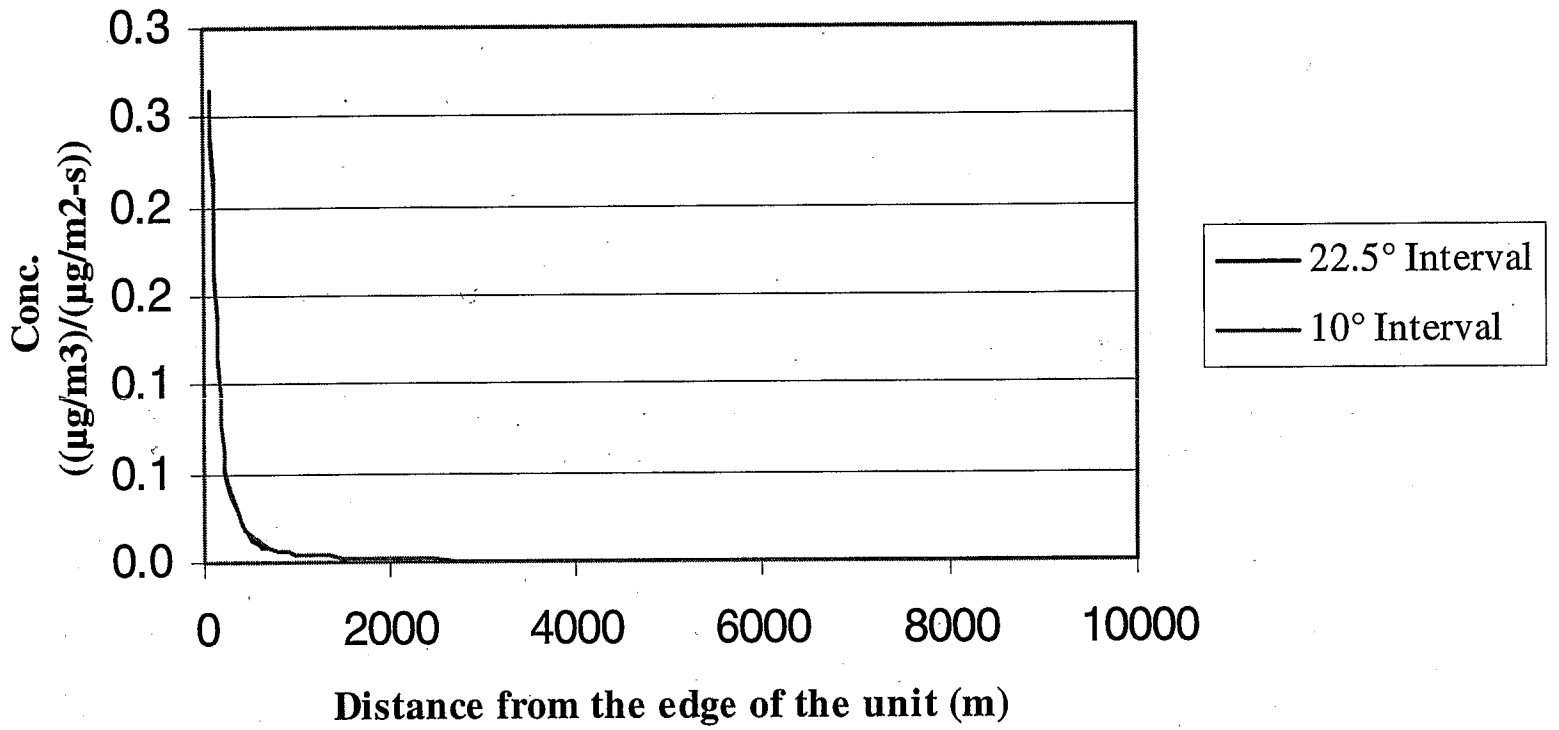


Figure D-8d. Maximum Concentrations (5th Percentile, LAU, Little Rock, AR)

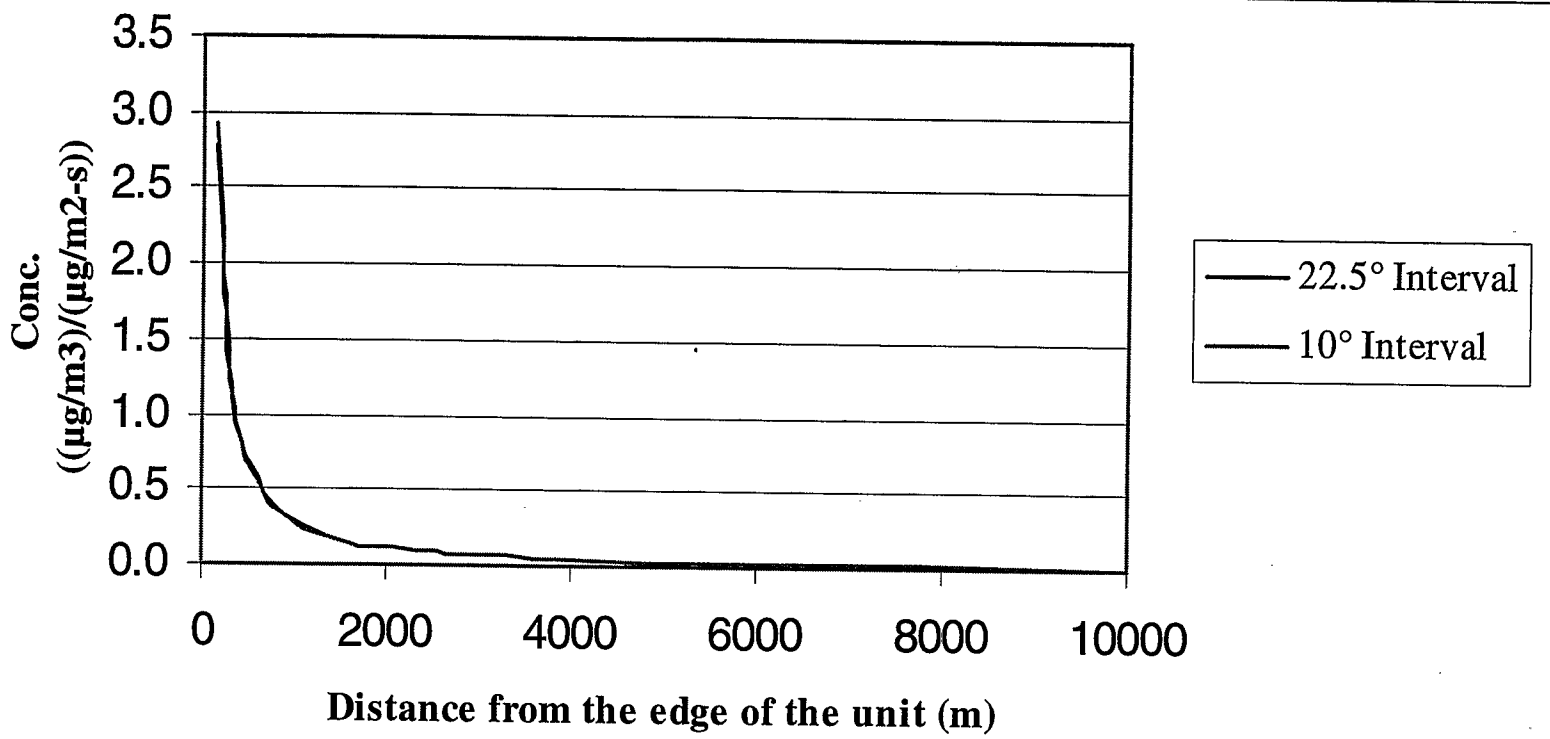


Figure D-8e. Maximum Concentrations (50th Percentile, LAU, Little Rock, AR)

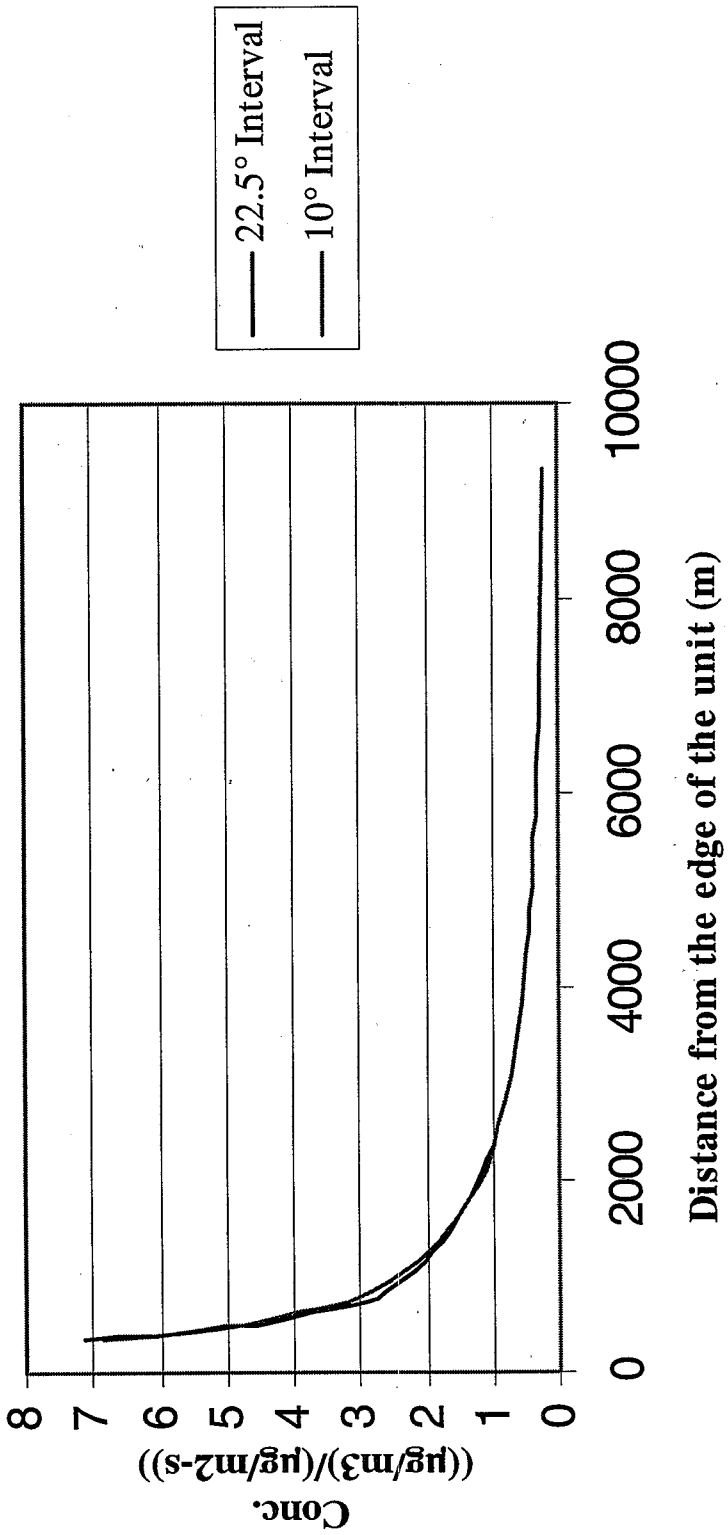


Figure D-8f. Maximum Concentrations (95th Percentile, LAU, Little Rock, AR)