



# **Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities**

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## **Volume One**

Peer Review Draft

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**Screening Level Ecological Risk Assessment  
Protocol for Hazardous Waste Combustion  
Facilities**

**Volume One**

**U.S. EPA, OFFICE OF SOLID WASTE**

**U.S. ENVIRONMENTAL PROTECTION AGENCY**

## **DISCLAIMER**

This document provides guidance to U.S. EPA Regions and States on how best to implement RCRA and U.S. EPA's regulations to facilitate permitting decisions for hazardous waste combustion facilities. It also provides guidance to the public and to the regulated community on how U.S. EPA intends to exercise its discretion in implementing its regulations. The document does not substitute for U.S. EPA's regulations, nor is it a regulation itself. Thus, it cannot impose legally-binding requirements on U.S. EPA, States, or the regulated community. It may not apply to a particular situation based upon the circumstances. U.S. EPA may change this guidance in the future, as appropriate.

## ACKNOWLEDGMENTS

Jeff Yurk (U.S. EPA Region 6), the primary author/editor of this document, would like to acknowledge that the development of this document could not have been accomplished without the support, input, and work of a multitude of U.S. EPA and support contractor personnel. The foundation for the combustion-related guidance and methodologies outlined in this document were first developed by the Office of Research and Development (ORD) and the Office of Solid Waste (OSW) in previous versions of combustion risk assessment guidance. The State of North Carolina's combustion risk assessment methodology was also evaluated in preparation of this document. The foundation for the ecological risk-related procedures and methodologies outlined in this document were based on previous guidance developed by the Office of Research and Development (ORD) and EPA's Superfund program. This version of the protocol was originally initiated in response to the desire of the Region 6 Multimedia Planning and Permitting Division to implement an up-to-date and technically sound hazardous waste combustion permitting program. The decision to incorporate guidance on a full range of national combustion risk assessment issues into the document was encouraged and supported by the Director of the Office of Solid Waste.

The development of this document was significantly enhanced by a number of capable organizations and personnel within U.S. EPA. Karen Pollard, Stephen Kroner and David Cozzie of the Economic Methods and Risk Analysis Division in conjunction with Rosemary Workman of the Permits and State Programs Division, Fred Chanania of the Hazardous Waste Minimization and Management Division, and Karen Kraus of the Office of General Council provided overall policy, technical and legal comment on this document. Anne Sergeant, Randy Bruins, David Reisman, Glenn Rice, Eletha Brady Roberts and Matthew Lorber of the National Center for Environmental Assessment (NCEA), Office of Research and Development, John Nichols of the National Health and Environmental Effects Research Laboratory, Vince Nabholz of the Office of Prevention, Pesticides and Toxic Substances, and Dorothy Canter, Science Advisor to the Assistant Administrator for the Office of Solid Waste and Emergency Response, provided key input on breaking scientific developments in the areas of ecological risk assessment, mercury speciation, the dioxin reassessment, endocrine disruptors, toxicity factors, sulfur and brominated dioxin analogs, as well as technical comment on the overall methodologies presented in the document.

Contributions by Larry Johnson of the National Exposure Research Laboratory of ORD and Jeff Ryan and Paul Lemieux of the National Risk Management Research Laboratory of ORD were significant in providing methodologies for conducting TO analysis and defining appropriate detection limits to be used in the risk assessment. Donna Schwede of the National Exposure Research Laboratory of ORD and Jawad Touma of the Office of Air Quality Planning and Standards provided technical review comments to strengthen the air modeling section of the document. Review and comment on the soil and water fate and transport models was provided by Robert Ambrose of EPA's Environmental Research Laboratory in Athens, GA.

All U.S. EPA Regional Offices contributed valuable comments which have significantly improved the usability of this document. In particular, staff from Region 4 aided in making sure guidance for conducting trial burns was consistent with this document, and staff from Region 8 provided significant input on the overall approach. The authors would be remiss if they did not acknowledge significant contributions from the Texas Natural Resource and Conservation Commission through both comments and discussions of real-world applications of risk assessment methodologies. Additionally, useful comments were received from the State of Utah. The Region 6 Superfund Division is to be commended for its valuable review of the

early document. Region 6 apologizes and bears full responsibility for any mistakes made in the incorporation of comments and input from all reviewers into the document.

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Region 6 looks forward to the insight and input yet to be provided by the public and other interested parties during the full external peer review of the document.

## REVIEWERS

Preliminary drafts of this ecological risk assessment document, as well as its companion human health risk assessment document, have received extensive internal Agency and State review. The following is a list of reviewers who have commented on these documents prior to their release as a peer review draft.

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LIST OF ACRONYMS

$\mu\text{g}$	Microgram
$\mu\text{g}/\text{kg}$	Micrograms per kilogram
$\mu\text{g}/\text{L}$	Micrograms per liter
$\mu\text{g}/\text{s}$	Micrograms per second
$\mu\text{m}$	Micrometer
$\mu\text{m}/\text{s}$	Micrometers per second
$\mu\text{m}^2$	Square micrometers
$^{\circ}\text{C}$	Degrees Celsius
$^{\circ}\text{F}$	Degrees Fahrenheit
$^{\circ}\text{K}$	Degrees Kelvin
ADOM	Acid Deposition and Oxidant Model
AET	Apparent effects threshold
APCS	Air pollution control system
$\text{atm}\cdot\text{m}^3/\text{mol}\cdot\text{K}$	Atmosphere-cubic meters per mole-degrees Kelvin
ATSDR	Agency for Toxic Substances and Disease Registry
AWFCO	Automatic waste feed cutoff
AWQC	Ambient water quality criteria
BAF	Bioaccumulation factor
BaP	Benzo(a)pyrene
BCF	Bioconcentration factor
BD	Soil bulk density
BEF	Bioaccumulation equivalency factor
BEHP	Bis(2-ethylhexyl)phthalate
BIF	Boiler and industrial furnace
BPIP	Building profile input program
BS	Benthic solids
BSAF	Sediment bioaccumulation factor
BTAG	Biological Technical Assistance Group
BW	Body weight
CARB	California Air Resources Board
CAS	Chemical Abstracts Service
CERM	Conceptual ecological risk model
CKD	Cement kiln dust
COMPDEP	COMPLEX terrain model with DEPosition
COMPLEX I	COMPLEX terrain model, Version 1
COPC	Compound of potential concern
CPF	Cumulative probability density function
CRQL	Contract required quantitation limit
CWA	Clean Water Act

LIST OF ACRONYMS (Continued)

DEHP	Diethylhexylphthalate (same as Bis(2-ethylhexyl)phthalate)
DEM	Digital Elevation Model
DNOP	Di(n)octylphthalate
DOE	U.S. Department of Energy
DQL	Data quality level
DRE	Destruction and removal efficiency
EDQL	Ecological data quality levels
EEL	Estimated exposure level
EPA	U.S. Environmental Protection Agency
EPC	Exposure point concentration
EQL	Estimated quantitation limit
EQP	Equilibrium partitioning
ERA	Ecological risk assessment
ERL	Effects range low
ERT	Environmental Research and Technology
ESP	Electrostatic precipitator
ESI	Ecological screening index
ESQ	Ecological screening quotient
FCM	Food chain multiplier
FWS	U.S. Fish and Wildlife Service
g/s	Grams per second
g/cm <sup>3</sup>	Grams per cubic centimeter
g/m <sup>3</sup>	Grams per cubic meter
GAQM	Guideline on Air Quality Models
GC	Gas chromatography
GEP	Good engineering practice
HBC	Hexachlorobenzene
HgCl <sub>2</sub>	Mercuric chloride
HQ	Hazard quotient
HSDB	Hazardous substances data base
IDL	Instrument detection limit
IEM	Indirect exposure model
IRIS	Integrated risk information system
ISCST3	Industrial source complex short-term model
ISCSTDFT	Industrial Source Complex Short Term Draft
kg	Kilogram
kg/L	Kilograms per liter

**LIST OF ACRONYMS (Continued)**

L	Liter
LC <sub>50</sub>	Lethal concentration to 50 percent of the test population
LCD	Local Climatological Data Annual Summary with Comparative Data
LD <sub>50</sub>	Lethal dose to 50 percent of the test population
LEL	Lowest effect level
LFI	Log fill-in
LOAEL	Lowest observed adverse effect level
LOD	Level of detection
LOEL	Lowest observed effect level
m	Meter
m/s	Meters per second
mg	Milligram
mg/kg	Milligrams per kilogram
mg/kg/day	Milligrams per kilogram per day
mg/L	Milligrams per liter
mg/m <sup>3</sup>	Milligrams per cubic meter
MACT	Maximum achievable control technology
MDL	Method detection limit
MLE	Maximum likelihood estimation
MPRM	Meteorological Processor for Regulatory Models
MPTER	Air quality model for multiple point source gaussian dispersion algorithm with terrain adjustments
MPTER-DS	Air quality model for multiple point source gaussian dispersion algorithm with terrain adjustments including deposition and sedimentation
NC DEHNR	North Carolina Department of Environment, Health, and Natural Resources
NCDC	National Climatic Data Center
NCEA	National Center for Environmental Assessment
NEL	No effect level
NFI	Normal fill-in
NOAA	National Oceanic and Atmospheric Administration
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
NOEL	No observed effect level
NRC	U.S. Nuclear Regulatory Commission
NTIS	National technical information service
NWS	National weather service
OAQPS	Office of Air Quality Planning and Standards
OAQPS TTN	Office of Air Quality and Planning Standards and Technology Transfer Network
OC	Organic carbon
OCDD	Octachlorodibenzodioxin
ORD	Office of Research and Development
ORNL	Oak Ridge National Laboratory
OSW	Office of Solid Waste

**LIST OF ACRONYMS (Continued)**

OV	Deposition output values
PAH	Polycyclic aromatic hydrocarbon
PCB	Polychlorinated biphenyl
PCDD	Polychlorinated dibenzo(p)dioxin
PCDF	Polychlorinated dibenzofuran
PCRAMMET	Personal computer version of the meteorological preprocessor for the old RAM program
PDF	Probability density function
PIC	Product of incomplete combustion
PM	Particulate matter
PM10	Particulate matter less than 10 micrometers in diameter
POHC	Principal organic hazardous constituent
PQL	Practical quantitation limit
PRC	PRC Environmental Management, Inc.
PU	Polyurethane
QA/QC	Quality assurance/Quality control
QAPjP	Quality assurance project plan
QSAR	Quantitative structure activity relationship
RCRA	Resource Conservation and Recovery Act
REACH	
RME	Reasonable maximum exposure
RTDM	Rough terrain diffusion model
RTDMDEP	Rough terrain diffusion model deposition
RTECS	Registry of Toxic Effects of Chemical Substances
SAMSON	Solar and Meteorological Surface Observational Network
SCRAM BBS	Support Center for Regulatory Air Models Bulletin Board System
SFB	San Francisco Bay
SMDP	Scientific management decision point
SO	Source
SQL	Sample quantitation limit
SVOC	Semivolatile organic compound
TAL	Target analyte list
TCDD	Tetrachlorodibenzo(p)dioxin
TDA	Toluene diisocyanate
TEF	Toxicity equivalent factor
TG	Terrain grid
TIC	Tentatively identified compound
TL	Trophic level
TOC	Total organic carbon
TRV	Toxicity reference value
TSS	Total suspended solids

**LIST OF ACRONYMS (Continued)**

UF	Uncertainty factor
UFI	Uniform fill-in
USGS	U.S. Geological Survey
USLE	Universal soil loss equation
UTM	Universal transverse mercator
VOC	Volatile organic compound
watts/m <sup>2</sup>	Watts per square meter
WRPLOT	Wind Rose PLOTing program

LIST OF VARIABLES

$\lambda_z$	=	Dimensionless viscous sublayer thickness (unitless)
$\mu_a$	=	Viscosity of air (g/cm-s)
$\mu_w$	=	Viscosity of water corresponding to water temperature (g/cm-s)
$\rho_a$	=	Air density (g/cm <sup>3</sup> or g/m <sup>3</sup> )
$\rho_s$	=	Bed sediment density (kg/L)
$\rho_w$	=	Density of water corresponding to water temperature (g/cm <sup>3</sup> )
$\theta$	=	Temperature correction factor (unitless)
$\theta_{bs}$	=	Bed sediment porosity (unitless)
$\theta_s$	=	Soil volumetric water content (mL/cm <sup>3</sup> soil)
$a$	=	Empirical intercept coefficient (unitless)
$A$	=	Surface area of affected area (m <sup>2</sup> )
$b$	=	Empirical slope coefficient (unitless)
$BAF_l$	=	Bioaccumulation factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
$BCF_{a/s}$	=	Aquatic-sediment bioconcentration factor (unitless)
$BCF_l$	=	Bioconcentration factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
$BCF_{Pi-H}$	=	Bioconcentration factor for plant-to-herbivore for <i>i</i> th plant food item (unitless)
$BCF_i$	=	Soil-to-soil invertebrate bioconcentration factor (unitless)
$BCF_{Pi-OM}$	=	Bioconcentration factor for plant-to-omnivore for <i>i</i> th plant food item (unitless)
$BCF_{S/BS-C}$	=	Bioconcentration factor for soil- or bed sediment-to-carnivore (unitless)
$BCF_{S/BS-H}$	=	Bioconcentration factor for soil-to-plant or bed sediment-to-plant (unitless)
$BCF_{W-C}$	=	Bioconcentration factor for water-to-carnivore (L/kg)
$BCF_{W-HM}$	=	Bioconcentration factor for water-to-herbivore (L/kg)
$BCF_{WI}$	=	Bioconcentration factor for water-to-invertebrate (L/kg)
$BCF_r$	=	Plant-soil biotransfer factor (unitless)
$BD$	=	Soil bulk density (g soil/cm <sup>3</sup> soil)
$BMF_n$	=	Biomagnification factor for <i>n</i> th trophic level
$BS$	=	Benthic solids concentration (kg/L or g/cm <sup>3</sup> )
$BSAF$	=	Sediment bioaccumulation factor (unitless)
$Bv$	=	Air-to-plant biotransfer factor ( $\mu$ g COPC/g DW plant)/( $\mu$ g COPC/g air)
$BW$	=	Body weight (kg)
$C$	=	USLE cover management factor (unitless)
$C_{Ai}$	=	COPC concentration in <i>i</i> th animal food item (mg/kg)
$C_C$	=	COPC concentration in carnivore (mg/kg)
$C_d$	=	Drag coefficient (unitless)
$C_{dw}$	=	Dissolved phase water concentration (mg/L)
$C_F$	=	COPC concentration in fish (mg/kg)
$CFO_2$	=	Correction factor for conversion to 4.5 percent O <sub>2</sub> (unitless)
$C_{gen}$	=	Generic chemical concentration (mg/kg or mg/L)
$C_H$	=	COPC concentration in herbivore (mg/kg)
$C_i$	=	Stack concentration of <i>i</i> th identified COPC (carbon basis) (mg/m <sup>3</sup> )



**LIST OF VARIABLES (Continued)**

$C_i$	=	COPC concentration in <i>i</i> th plant or animal food item (mg COPC/kg)
$C_I$	=	COPC concentration in soil or benthic invertebrate (mg/kg)
$C_{IW}$	=	COPC concentration in soil or sediment interstitial water (mg/L)
$C_M$	=	COPC concentration in media (mg COPC/kg [soil, sediment] or mg COPC/L [water])
$C_{OM}$	=	COPC concentration in omnivore (mg/kg)
$C_{Pi}$	=	COPC concentration in <i>i</i> th plant food item (mg/kg)
$C_{PREY}$	=	Concentration in prey
$C_{sed}$	=	COPC concentration in bed sediment (g COPC/cm <sup>3</sup> sediment or mg COPC/kg sediment)
$C_{s/sed}$	=	COPC concentration in soil or bed sediment (mg/kg)
$C_{TOC}$	=	Stack concentration of TOC, including speciated and unspeciated compounds (mg/m <sup>3</sup> )
$C_{TP}$	=	COPC concentration in terrestrial plants (mg COPC/kg WW)
$C_{wctot}$	=	Total COPC concentration in water column (mg/L)
$C_{wtot}$	=	Total water body COPC concentration (including water column and bed sediment) (g/m <sup>3</sup> or mg/L)
$C_{yp}$	=	Unitized yearly air concentration from particle phase (μg-s/g-m <sup>3</sup> )
$C_{yv}$	=	Unitized yearly air concentration from vapor phase (μg s/g m <sup>3</sup> )
$C_{yww}$	=	Unitized yearly watershed air concentration from vapor phase (μg-s/g-m <sup>3</sup> )
$D_1$	=	Lower bound of a particle size density for a particular filter cut size
$D_2$	=	Upper bound of a particle size density for a particular filter cut size
$D_a$	=	Diffusivity of COPC in air (cm <sup>2</sup> /s)
$d_{bs}$	=	Depth of upper benthic sediment layer (m)
$DD_{TEQ}$	=	Daily dose of 2,3,7,8-TCDD <i>TEQ</i> (μg/kg BW/d)
$DD_i$	=	Daily dose of <i>i</i> th congener (μg/kg BW/d)
$D_{mean}$	=	Mean particle size density for a particular filter cut size
$D_s$	=	Deposition term (mg/kg-yr)
$D_w$	=	Diffusivity of COPC in water (cm <sup>2</sup> /s)
$d_{wc}$	=	Depth of water column (m)
$D_{yd}$	=	Unitized yearly dry deposition rate of COPC (g/m <sup>2</sup> -yr)
$D_{ydp}$	=	Unitized yearly dry deposition from particle phase (s/m <sup>2</sup> -yr)
$D_{ytwp}$	=	Unitized yearly watershed total deposition (wet and dry) from particle phase (s/m <sup>2</sup> -yr)
$D_{ywp}$	=	Unitized yearly wet deposition from particle phase (s/m <sup>2</sup> -yr)
$D_{yww}$	=	Unitized yearly wet deposition from vapor phase (s/m <sup>2</sup> -yr)
$D_{ywww}$	=	Unitized yearly watershed wet deposition from vapor phase (s/m <sup>2</sup> -yr)
$d_z$	=	Total water body depth (m)
$E_v$	=	Average annual evapotranspiration (cm/yr)
ER	=	Soil enrichment ratio (unitless)

**LIST OF VARIABLES (Continued)**

$F_{Ai}$	=	Fraction of diet consisting of $i$ th animal food item (unitless)
$f_{bs}$	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
$FCM$	=	Trophic level-specific food-chain multiplier (unitless)
$FCM_{TLn}$	=	Food chain multiplier for $n$ th trophic level
$FCM_{TLn-Ai}$	=	Food chain multiplier for trophic level of $i$ th animal food item (unitless)
$FCM_{TL3}$	=	Food chain multiplier for trophic level 3 (unitless)
$f_{wc}$	=	Fraction of total water body COPC concentration in the water column (unitless)
$F_v$	=	Fraction of COPC air concentration in vapor phase (unitless)
$F_{OC}$	=	Fraction of organic carbon (unitless)
$F_{Pi}$	=	Fraction of diet consisting of $i$ th plant food item (unitless)
$F_W$	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$H$	=	Henry's law constant (atm-m <sup>3</sup> /mol)
$Ir_{MEDIUM}$	=	Ingestion rate of soil, surface water, or sediment
$I$	=	Average annual irrigation (cm/yr)
$IR$	=	Ingestion rate (kg/day)
$k$	=	von Karman's constant (unitless)
$K$	=	USLE erodibility factor (ton/acre)
$k_b$	=	Benthic burial rate (yr <sup>-1</sup> )
$K_G$	=	Gas phase transfer coefficient (m/yr)
$K_L$	=	Liquid phase transfer coefficient (m/yr)
$Kd_{bs}$	=	Bed sediment/sediment pore water partition coefficient (L/kg or cm <sup>3</sup> /g)
$Kd_{ij}$	=	Partition coefficient for COPC $i$ associated with sorbing material $j$ (unitless)
$Kd_s$	=	Soil-water partition coefficient (cm <sup>3</sup> /g or mg/L)
$Kd_{sw}$	=	Suspended sediments/surface water partition coefficient (L/kg)
$K_{oc}$	=	Organic carbon partition coefficient (mg/L)
$K_{ocj}$	=	Sorbing material-independent organic carbon partition coefficient for COPC $j$
$K_{ow}$	=	Octanol-water partition coefficient (unitless)
$kp$	=	Plant surface loss coefficient (yr <sup>-1</sup> )
$ks$	=	COPC soil loss constant due to all processes (yr <sup>-1</sup> )
$kse$	=	COPC loss constant due to soil erosion (yr <sup>-1</sup> )
$ksg$	=	COPC loss constant due to biotic and abiotic degradation (yr <sup>-1</sup> )
$ksl$	=	COPC loss constant due to leaching (yr <sup>-1</sup> )
$ksr$	=	COPC loss constant due to runoff (yr <sup>-1</sup> )
$ksv$	=	COPC loss constant due to volatilization (yr <sup>-1</sup> )
$k_v$	=	Water column volatilization rate constant (yr <sup>-1</sup> )
$K_v$	=	Overall transfer rate coefficient (m/yr)
$k_{wt}$	=	Overall total water body COPC dissipation rate constant (unitless)
$L$	=	Monin-Obukhov Length (m)

LIST OF VARIABLES (Continued)

$L_{DEP}$	=	Total (wet and dry) particle phase and wet vapor phase direct deposition load to water body (g/yr)
$L_{dif}$	=	Dry vapor phase diffusion load to water body (g/yr)
$L_E$	=	Soil erosion load (g/yr)
$L_R$	=	Runoff load from pervious surfaces (g/yr)
$L_{RI}$	=	Runoff load from impervious surfaces (g/yr)
$L_T$	=	Total COPC load to water body (g/yr)
$LS$	=	USLE length-slope factor (unitless)
$MW$	=	Molecular weight of COPC (g/mol)
$OC_i$	=	Organic carbon content of sorbing material $I$ (unitless)
$OV$	=	Deposition output values
$P$	=	Average annual precipitation (cm/yr)
$P_{Ai}$	=	Proportion of $i$ th animal food item in diet that is contaminated (unitless)
$P_d$	=	COPC concentration in plant due to direct deposition (mg/kg WW)
$PF$	=	USLE supporting practice factor (unitless)
$P_{Pi}$	=	Proportion of $i$ th plant food item in diet that is contaminated (unitless)
$Pr$	=	COPC concentration in plant due to root uptake (mg/kg WW)
$P_{S/BS}$	=	Proportion of soil or bed sediment in diet that is contaminated (unitless)
$P_V$	=	COPC concentration in plant due to air-to-plant transfer (mg/kg WW)
$P_W$	=	Proportion of water in diet that is contaminated (unitless)
$Q$	=	COPC emission rate (g/s)
$Q_i$	=	Emission rate of COPC ( $i$ ) (g/s)
$Q_{i(adj)}$	=	Adjusted emission rate of COPC ( $i$ ) (g/s)
$Q_f$	=	Anthropogenic heat flux ( $W/m^2$ )
$Q_*$	=	Net radiation absorbed ( $W/m^2$ )
$r$	=	Interception fraction-the fraction of material in rain intercepted by vegetation and initially retained (unitless)
$R$	=	Universal gas constant ( $atm \cdot m^3/mol \cdot K$ )
$RO$	=	Average annual runoff (cm/yr)
$RF$	=	USLE rainfall (or erosivity) factor ( $yr^{-1}$ )
$Sc$	=	Average soil concentration over exposure duration (mg/kg)
$Sc_{Tc}$	=	Soil concentration at time $Tc$ (mg/kg)
$SD$	=	Sediment delivery ratio (unitless)
$SGC$	=	COPC stack gas concentration as measured in the trial burn ( $\mu g/dscm$ )
$SGF$	=	Stack gas flow rate at 7 percent $O_2$ (dscm/s)
$T_a$	=	Ambient air temperature (K) = 298.1 K
$T_p$	=	Length of plant exposure to deposition per harvest of the edible portion of the $i$ th plant group (yr)

**LIST OF VARIABLES (Continued)**

$tD$	=	Total time period over which deposition occurs (time period of combustion) (yr)
$T_m$	=	Melting point temperature (K)
$TSS$	=	Total suspended solids concentration (mg/L)
$T_w$	=	Water body temperature (K)
$u$	=	Current velocity (m/s)
$V$	=	Volume
$V_{dv}$	=	Dry deposition velocity (cm/s)
$V_{f_x}$	=	Average volumetric flow rate through water body (m <sup>3</sup> /yr)
$VG_{ag}$	=	Empirical correction factor for aboveground produce (unitless)
$VP$	=	Vapor pressure (atm)
$W$	=	Average annual wind velocity (m/s)
$WA_I$	=	Area of impervious watershed receiving COPC deposition (m <sup>2</sup> )
$WA_L$	=	Area of watershed receiving COPC deposition (m <sup>2</sup> )
$WA_w$	=	Water body surface area (m <sup>2</sup> )
$X_e$	=	Unit soil loss (kg/m <sup>2</sup> -yr)
$Yp$	=	Standing crop biomass (productivity) (kg/m <sup>2</sup> DW)
$Z_s$	=	Soil mixing zone depth (cm)

**CONVERSIONS**

0.001	=	Units conversion factor (g/mg)
$10^6$	=	Units conversion factor ( $\mu\text{g/g}$ )
907.18	=	Units conversion factor (kg/ton)
$3.1536 \times 10^7$	=	Conversion constant (s/year)
4,047	=	Units conversion factor ( $\text{m}^2/\text{acre}$ )
100	=	Units conversion factor ( $\text{m}^2\text{-mg/cm}^2\text{-kg}$ )
$10^{-6}$	=	Units conversion factor ( $\text{g}/\mu\text{g}$ )
0.12	=	Dry weight to wet weight (plants) conversion factor (unitless)

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# Chapter 1

## Introduction

### What's Covered in Chapter 1:

- ◆ Objective and Purpose
  - ◆ Related Trial Burn Issues
  - ◆ Reference Documents
  - ◆ Overview of the Risk Assessment Process
  - ◆ Relationship to U.S. EPA HHRAP
  - ◆ Definitions
- 
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Risk assessment is a science used to evaluate the potential hazards to the environment that are attributable to emissions from hazardous waste combustion units. There is general guidance available regarding the general ecological risk assessment process including problem formulation, analysis, and risk characterization (U.S. EPA 1997c; 1998d). This document expands on that general guidance with respect to the ecological screening level procedures and provides a prescriptive tool to support permitting of hazardous waste burning combustion facilities under the Resource Conservation and Recovery Act (RCRA). It is not intended to be used to perform screening or baseline ecological risk assessments (ERA) in other areas of the RCRA program, such as corrective action.

The following definitions were adopted from *Superfund: Process for Designing and Conducting Ecological Risk Assessments. Interim Final* (U.S. EPA 1997c) and *Guidelines For Ecological Risk Assessment* (U.S. EPA 1998d), and identify key terms used throughout this guidance. Some of the terms are annotated with additional information to clarify the definition and explain its use in this protocol.

**Area Use Factor:** A ratio of an organism's home range, breeding range, or feeding and foraging range to the area of contamination of the assessment area.

**Assessment Endpoint:** An explicit expression of the environmental value that is to be protected; it includes both an ecological entity and specific attributes of that entity. The assessment endpoint in this protocol is used to link the risk assessment to management concerns and ultimately development of a protective RCRA operating permit. One or more assessment endpoints may be selected for performing a risk assessment.

**Bioaccumulation:** The net accumulation of a substance by an organism as a result of uptake directly from all environmental sources, including food. Bioaccumulation occurs through all exposure routes.

**Bioaccumulation Factor (BAF):** *BAF* represents the ratio of the concentration of a chemical to its concentration in a medium. The factor must be measured at steady-state when the rate of uptake is balanced by the rate of excretion. In this protocol a bioaccumulation factor (*BAF*) is estimated by multiplying a bioconcentration factor (*BCF*) by a food chain multiplier (*FCM*) derived based on the trophic level of the prey ingested by a measurement receptor.

**Bioconcentration:** A process by which there is a net accumulation of a chemical directly from an exposure medium into an organism.

**Bioconcentration Factor (BCF):** *BCF* represents the ratio of the concentration of a chemical in an aquatic organism to the concentration of the chemical in surface water, sediment, or soil. The factor must be measured at steady-state when the rate of uptake is balanced by the rate of excretion. *BCFs* are used in this protocol to estimate the body burden of a *COPC* in producers, primary consumers, and fish consumed by mid- or upper-trophic level measurement receptors.

**Biomagnification:** The process by which the concentration of some chemicals increase with increasing trophic level; that is, the concentration in a predator exceeds the concentration in its prey. In this protocol, a ratio of *FCM*'s are used to account for biomagnification.

**Biotransfer Factor:** *COPC* accumulation factor between a food item and its consumer. In this protocol biotransfer factors are used to evaluate transport of contaminants in plants to mammals and birds.

**Depuration:** The loss of a compound from an ecological receptor as a result of any active or passive process.

**Direct Uptake:** Direct uptake is a term applied to producers, primary consumers, and detritivores. Direct uptake includes all exposure routes for aquatic receptors, benthic receptors, soil invertebrates, and terrestrial plants. Direct uptake is used in this manner because it is difficult, given feeding and habitat niches of these receptors and limited availability of empirical information, to discern the relative importance of exposure through ingestion, respiration, dermal uptake, or root uptake. In addition, toxicity tests (used as the basis of risk assessment toxicity reference values) on these receptors (except some aquatic fauna) usually do not make a distinction between exposure routes or tend to overemphasize or isolate a particular route.

**Ecological Effects Assessment:** A portion of the analysis phase of the risk assessment that evaluates the ability of a stressor to cause adverse effects under a particular set of circumstances. Toxicity reference values identified in ecological effects assessment are used in risk characterization.

**Ecological Risk Assessment:** The process that evaluates the likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors.

**Ecological Screening Quotient (ESQ):** A quotient used to assess risk during the risk assessment in which protective assumptions are used. Generally, the numerator is the reasonable worst-case COPC concentration at the point of exposure, and the denominator is the no-adverse-effects-based toxicity reference value.

**Environmental Attribute:** Characteristic of a food web functional group (e.g., herbivorous mammal) that is relevant to the ecosystem. Examples of environmental attributes include seed dispersal, decomposition, pollination, and food source.

**Exposure Assessment:** A portion of the analysis phase of ERA that evaluates the interaction of the stressor with one or more ecological components. Exposure can be expressed as co-occurrence or contact, depending on the stressor and ecological component involved. Information from the exposure assessment is used in risk characterization.

**Exposure Pathway:** A pathway by which a compound travels from a combustion facility to an ecological receptor. A complete exposure pathway occurs when a chemical enters or makes contact with an ecological receptor through one or more exposure routes.

**Exposure Route:** A point of contact or entry of a chemical from the environment into an organism. The exposure routes for terrestrial wildlife are ingestion, dermal absorption, and inhalation. The exposure routes for aquatic fauna are ingestion, dermal absorption, and respiration. The exposure routes for terrestrial plants are root absorption or foliar uptake. Exposure routes for aquatic plants are direct contact with water and sediments.

**Food Chain:** The transfer of food energy from the source in plants through a series of organisms with repeated eating and being eaten (Odum 1971).

**Food Web:** The interlocking patterns of food chains (Odum 1971).

**Food-Chain Multiplier (FCM):** The FCM is used to account for dietary uptake of a compound by an ecological receptor. It may be used to estimate a *BAF* from a *BCF* in the absence of reliable *BAF* data. The FCM values in Table 5-1 have been adopted from *Water Quality Guidance for the Great Lakes System* (U.S. EPA 1995j).

**Guild:** A group of species occupying a particular trophic level and exploiting a common resource base in a similar fashion (Root 1967).

**Habitat:** The physical environment in which a species is distributed. Habitat location depends on several factors, such as chemical conditions, physical conditions, vegetation, species eating strategy, and species nesting strategy. By analogy, the habitat is an organism's "address."

**Measure of Effect:** A measurable ecological characteristic that is related to the valued characteristic chosen as the assessment endpoint. It is the measure used to evaluate the response of the assessment endpoint when exposed to a chemical (U.S. EPA 1998d). This protocol proposes, for each class/guild, representative receptors (measurement receptors) for characterizing risk from exposure to compounds emitted from a combustion facility.



**Measure of Effect:** A measurable ecological characteristic that is related to the valued characteristic chosen as the assessment endpoint.

**Measure of Exposure:** A measurable stressor characteristic that is used to help quantify exposure.

**Measurement Receptor:** A species, population, community, or assemblage of communities (such as “aquatic life”) used to characterize ecological risk to an assessment endpoint.

**Problem Formulation:** A systematic planning step that identifies the focus and scope of the risk assessment. Problem formulation includes ecosystem characterization, pathway analysis, assessment endpoint development, and measurement endpoint identification. Problem formulation results in the development of a problem statement that is addressed in the analysis step.

**Scientific and Management Decision Point:** A point during the risk assessment at which the risk assessor and risk manager discuss results. The risk manager determines whether the information is sufficient to arrive at a decision regarding the significance of the results and whether additional information is needed before proceeding forward in the risk assessment.

**Special Ecological Area:** Habitats and areas for which protection and special consideration has been conferred legislatively (federal or state), such as critical habitat for federally or state-designated endangered or threatened species. In characterizing media concentrations of COPCs, special emphasis is placed on estimating concentrations and, therefore, exposure potential, in sensitive areas.

**Stressor:** Any physical, chemical, or biological entity that can induce an adverse response.

**Trophic Level:** One of the successive levels of nourishment in a food web or food chain. Plant producers constitute the first (lowest) trophic level, and dominant carnivores constitute the last (highest) trophic level.

**Uncertainty Factor:** Quantitative values used to adjust toxicity values from laboratory toxicity tests to toxicity values representative of chronic no-observed-adverse-effect-levels (NOAELs). In this guidance, uncertainty factors (UF) are used to extrapolate from acute and subchronic test duration to chronic duration, and to extrapolate from point estimated (e.g., LD50) and lowest-observed-adverse-effect-level (LOAEL) endpoints to an NOAEL endpoint.

**Uptake:** Acquisition by an ecological receptor of a compound from the environment as a result of any active or passive process.

This Screening Level Ecological Risk Assessment Protocol (SLERAP) has been developed as national guidance to consolidate information presented in other risk assessment guidance and methodology documents previously prepared by U.S. EPA and state environmental agencies. In addition, this guidance also addresses issues that have been identified while conducting risk assessments for existing hazardous waste combustion units. The overall purpose of this document is to explain how ecological risk assessments should be performed at hazardous waste combustion facilities. This document is intended as

(1) guidance for personnel conducting risk assessments, and (2) an information resource for permit writers, risk managers, and community relations personnel.

The RCRA “omnibus” authority of §3005(c)(3) of RCRA, 42 U.S.C. §6925(c)(3) and 40 CFR §270.32(b)(2) gives the Agency both the authority and the responsibility to establish risk-based permit conditions on a case-by-case basis as necessary to protect human health and the environment. These risk-based site-specific permit conditions are in addition to the national technical standards required in the hazardous waste incinerator and boiler/industrial furnace regulations of 1981 and 1991, respectively. Often, the determination of whether or not a permit is sufficiently protective can be based on its conformance to the technical standards specified in the regulations. Since the time that the regulations for hazardous waste incinerators and boilers/industrial furnaces were issued, however, additional information became available which suggested that technical standards may not fully address potentially significant risks. For example, many studies (including the *Draft Health Reassessment of Dioxin-Like Compounds*, *Mercury Study Report to Congress*, *Risk Assessment Support to the Development of Technical Standards for Emissions from Combustion Units Burning Hazardous Wastes: Background Information Document*, and the *Waste Technologies Industries (WTI) Risk Assessment*) indicate that there can be significant risks from indirect exposure pathways (e.g., pathways other than direct inhalation). The food chain pathway appears to be particularly important for bioaccumulative pollutants which may be emitted from hazardous waste combustion units. In many cases, risks from indirect exposure may constitute the majority of the risk from a hazardous waste combustor. This key portion of the risk from hazardous waste combustor emissions was not directly taken into account when the hazardous waste combustion standards were developed. In addition, uncertainty remained regarding the types and quantities of non-dioxin products of incomplete combustion emitted from combustion units and the risks posed by these compounds.

As a result, until such time that the technical standards could be upgraded to more completely address potential risk from hazardous waste combustion, U.S. EPA recommended, pursuant to the “omnibus” authority, that site-specific risk assessments be performed for all combustion facilities as a part of the RCRA permitting process. Performance of a site-specific risk assessment can provide the information necessary to determine what, if any, additional permit conditions are necessary for each situation to ensure that operation of the combustion unit is protective of human health and the

environment. Under 40 C.F.R. §270.10(k), U.S. EPA may require a permit applicant to submit additional information (e.g., a site-specific risk assessment) that the Agency needs to establish permit conditions under the omnibus authority. In certain cases, the Agency may also seek additional testing or data under the authority of RCRA §3013 (where the presence or release of a hazardous waste “may present a substantial hazard to human health or the environment”) and may issue an order requiring the facility to conduct monitoring, testing, analysis, and reporting. Any decision to add permit conditions based on a site-specific risk assessment under this authority must be justified in the administrative record for each facility, and the implementing agency should explain the basis for the conditions.

U.S. EPA promulgation of the Maximum Achievable Control Technology (MACT) standards for hazardous waste incinerators, cement kilns and light-weight aggregate kilns effectively upgraded the existing national technical standards for these combustion units. U.S. EPA intends to similarly upgrade the technical standards for other types of hazardous waste combustors in a later rulemaking. Since the MACT standards are more protective than the original standards for incinerators, cement kilns and light-weight aggregate kilns, U.S. EPA revised its earlier recommendation regarding site-specific risk assessments. As discussed in the preamble to the final MACT rule, U.S. EPA recommended that the permitting authority determine if a site-specific risk assessment is needed in addition to the MACT standards in order to meet the RCRA statutory obligation of protection of human health and the environment. For hazardous waste combustors not subject to the Phase I MACT standards, U.S. EPA continues to recommend that site-specific risk assessments be conducted as part of the RCRA permitting process. If the permitting authority determines a risk assessment is warranted, it should be conducted as part of the RCRA permitting process.

The permitting agency should consider several factors in its evaluation of the need to perform a risk assessment (human health and ecological). These factors include:

- whether any proposed or final regulatory standards exist that U.S. EPA has shown to be protective for site-specific receptors
- whether the facility is exceeding any final technical standards
- the current level of hazardous constituents being emitted by a facility, particularly in comparison to proposed or final technical standards, and to levels at other facilities where risks have been estimated
- the scope of waste minimization efforts and the status of implementation of a facility waste minimization plan

- particular site-specific considerations related to the exposure setting (such as physical, land use, presence of threatened or endangered species and special subpopulation characteristics) and the impact on potential risks
- the presence of significant ecological considerations (e.g., high background levels of a particular contaminant, proximity to a particular sensitive ecosystem)
- the presence of nearby off-site sources of pollutants
- the presence of other on-site sources of pollutants
- the hazardous constituents most likely to be found and those most likely to pose significant risk
- the identity, quantity, and toxicity of possible non-dioxin PICs
- the volume and types of wastes being burned
- the level of public interest and community involvement attributable to the facility

This list is by no means exhaustive, but is meant only to suggest significant factors that have thus far been identified. Others may be equally or more important.

The companion document of the SLERAP is the Human Health Risk Assessment Protocol (HHRAP) (U.S. EPA 1998c). U.S. EPA OSW has prepared these guidance documents as a resource to be used by authorized agencies developing risk assessment reports to support permitting decisions for facilities with hazardous waste combustion units.

## 1.1 OBJECTIVE AND PURPOSE

This protocol is a multipathway screening tool based on reasonable, protective assumptions about the potential for ecological receptors to be exposed to, and to be adversely affected by, compounds of potential concern (COPC) emitted from hazardous waste combustion facilities. The U.S. EPA OSW risk assessment process is a prescriptive analysis intended to be performed expeditiously using (1) measurement receptors representing food web-specific class/guilds and communities, and (2) readily available exposure and ecological effects information. To avoid the time-intensive and resource-consuming process of collecting site-specific information on numerous constituents, this guidance provides a process to obtain and evaluate various types of technical information that will enable a risk assessor to perform a risk assessment

relatively quickly. Additionally this guidance provides: (1) example food webs; (2) example measurement receptor natural history information; (3) fate and transport data, bioconcentration factors, and toxicity reference values for 38 COPCs. In lieu of this information, a facility may substitute site-specific information where appropriate and approved by the applicable permitting authority.

U.S. EPA OSW's objective is to present a user-friendly set of procedures for performing risk assessments, including (1) a complete explanation of the basis of those procedures, and (2) a comprehensive source of data needed to complete those procedures. The first volume of this document provides the explanation (Chapters 1 through 6); and the second and third volumes (Appendices A-H) provides the data sources. Appendix A presents compound-specific information necessary to complete the risk assessment. Appendix B presents equations for calculating media concentrations. Appendices C and D provide chemical and media-specific bioconcentration factors (BCFs). Appendix E provides toxicity reference values (TRVs) for 38 compounds of potential concern (COPCs) and several possible measurement receptors. Appendix F presents equations for calculating risk. Appendix G provides contact information for obtaining site-specific species information, and Appendix H provides toxicological profiles for 38 COPCs. Figure 1-1 summarizes the steps needed to complete a screening level ecological risk assessment.

Implementation of this guidance will demonstrate that developing defensible estimates of compound emission rates is one of the most important elements of the risk assessment. As described in Chapter 2, traditional trial burns conducted to measure destruction and removal efficiency (DRE) do not sufficiently characterize organic products of incomplete combustion (PIC) and metal emissions for use in performing risk assessments. In some instances, a facility or regulatory agency may want to perform a pretrial burn risk assessment, following the procedures outlined in this document, to ensure that sample collection times during the trial burn or risk burn are sufficient to collect the sample volumes needed to meet the detection limits required for the risk assessment. The decision to perform such an assessment should consider regulatory permitting schedules and other site-specific factors.

U.S. EPA OSW anticipates that ecological risk assessments will be completed for new and existing facilities as part of the permit application process. The SLERAP recommends a process for evaluating *reasonable*—not theoretical worst-case maximum—potential risks to receptors posed by emissions from RCRA regulated units. The use of existing and site-specific information early in, and throughout, the risk assessment process is encouraged; protective assumptions should be made only when needed to ensure that

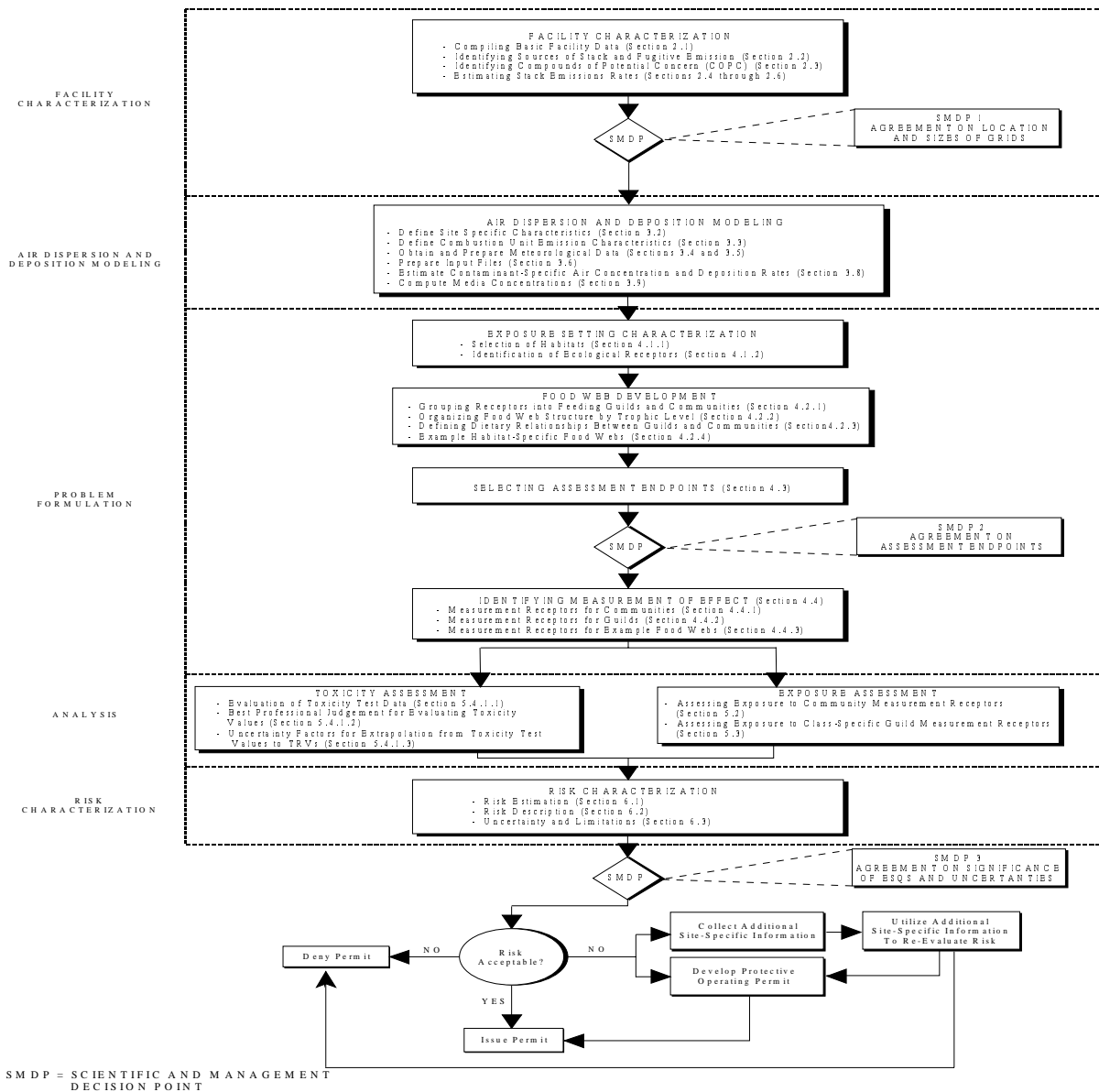
emissions from combustion units do not pose unacceptable risks. More protective assumptions may be incorporated to make the process fit a classical “screening level” approach that is more protective and may be easier to complete.

Regardless of whether theoretical worst case or more reasonable protective assumptions are used in completing the risk assessment process, every risk assessment is limited by the quantity and quality of:

- site-specific environmental data
- emission rate information
- other assumptions made during the risk estimation process (for example, fate and transport variables, exposure assumptions, and receptor characteristics)

These limitations and uncertainties are described throughout this document and the appendixes, and are summarized in Chapter 6.

FIGURE 1-1  
 SCREENING-LEVEL ECOLOGICAL RISK ASSESSMENT PROCESS



Potentially, unacceptable risks or other significant issues identified by collecting preliminary site information and completing risk assessment calculations can be addressed by the permitting process or during an iteration of the risk assessment. After the initial ecological risk assessment has been completed, it may be used by risk managers and permit writers in several ways:

- If the initial risk assessment indicates that estimated ecological risks are below regulatory levels of concern, risk managers and permit writers will likely proceed through the permitting process without adding any risk-based unit operating conditions to the permit.
- If the initial ecological risk assessment indicates potentially unacceptable risks, additional site-specific information demonstrated to be more representative of the exposure setting may be collected and additional iterations of risk assessment calculations can then be performed.
- If the initial risk assessment or subsequent iterations indicate potentially unacceptable risks, risk managers and permit writers may use the results of the risk assessment to revise tentative permit conditions (for example, waste feed limitations, process operating conditions, and expanded environmental monitoring). To determine if the subject hazardous waste combustion unit can be operated in a manner that is protective of the environment, an additional iteration of the risk assessment should be completed using the revised tentative operating conditions. If the revised conditions still indicate unacceptable risks, this process can be continued in an iterative fashion until acceptable levels are reached. In some situations, it may be possible to select target risk levels and back-calculate the risk assessment to determine the appropriate emission and waste feed rate levels. In any case, the acceptable waste feed rate and other appropriate conditions can then be incorporated as additional permit conditions.
- If the initial ecological risk assessment, or subsequent iterations, indicate potentially unacceptable risks, risk managers and permit writers may also choose to deny the permit.

This process is also outlined in Figure 1-1. As stated earlier, in some instances, a facility or regulatory agency may want to perform a pretrial burn risk assessment—following the procedures outlined in this document—to ensure that sample collection times during the trial burn or risk burn are sufficient to collect the sample volumes necessary to meet the appropriate detection limits for the risk assessment. This is expected to reduce the need for additional trial burn tests or iterations of the risk assessment due to problems caused when detection limits are not low enough to estimate risk with certainty sufficient for regulatory decision making.



## 1.2 RELATED TRIAL BURN ISSUES

In the course of developing this guidance and completing risk assessments across the country, U.S. EPA OSW has learned that developing defensible estimates of compound of potential concern (COPC) emission rates is one of the most important parts of the risk assessment process. As described in Chapter 2, traditional trial burns conducted to measure destruction and removal efficiency (DRE) *do not* sufficiently characterize organic products of incomplete combustion (PIC) and metal emissions for use in performing risk assessments.

U.S. EPA OSW considers the trial burn and risk assessment planning and implementation processes as interdependent aspects of the hazardous waste combustion unit permitting process. In addition, U.S. EPA OSW advocates that facility planning, regulatory agency review, and completion of tasks needed for both processes be conducted simultaneously to eliminate redundancy or the need to repeat activities. U.S. EPA OSW expects that the following guidance documents will typically be used as the main sources of information for developing and conducting appropriate trial burns:

- U.S. EPA. 1989f. *Handbook: Guidance on Setting Permit Conditions and Reporting Trial Burn Results. Volume II of the Hazardous Waste Incineration Guidance Series.* Office of Research and Development (ORD). EPA/625/6-89/019. January.
- U.S. EPA. 1989g. *Handbook: Hazardous Waste Incineration Measurement Guidance Manual. Volume III of the Hazardous Waste Incineration Guidance Series.* Office of Solid Waste and Emergency Response (OSWER). EPA/625/6-89/021. June.
- U.S. EPA. 1992e. *Technical Implementation Document for EPA's Boiler and Industrial Furnace Regulations.* OSWER. EPA-530-R-92-011. March.
- U.S. EPA. 1994n. *Draft Revision of Guidance on Trial Burns. Attachment B, Draft Exposure Assessment Guidance for Resource Conservation and Recovery Act (RCRA) Hazardous Waste Combustion Facilities.* OSWER. April 15.
- U.S. EPA. 1998b. *Guidance on Collection of Emissions Data to Support Site-Specific Risk Assessments at Hazardous Waste Combustion Facilities.* Prepared by EPA Region 4 and the Office of Solid Waste.
- Generic Trial Burn Plan and QAPPs developed by EPA regional offices or states.

### 1.3 REFERENCE DOCUMENTS

This section describes, in chronological order, the primary guidance documents used to prepare this guidance. Some of the guidance documents received a thorough review from EPA's Science Advisory Board, which mostly supported the work. Additional references used to prepare this guidance are listed in the References chapter of this document. These documents have been developed over a period of several years; in most cases, revisions to the original guidance documents address only the specific issues being revised rather than representing a complete revision of the original document. The following discussion lists and briefly describes each document. Overall, each of the guidance documents reflects a continual enhancing of the methodology.

This ecological assessment portion of this protocol is based on protecting the functions of ecological receptors in ecosystems and protecting special ecological areas around a hazardous waste combustion facility. It is generally consistent with current U.S. EPA guidance, including the Risk Assessment Forum's *Guidelines for Ecological Risk Assessment* (U.S. EPA 1998d), as well as the interim final *Ecological Risk Assessment Guidance for Superfund* (U.S. EPA 1997c). The most current methodology for assessing fate and transport of COPC's frequently referenced in this guidance is the U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (In Press).

The following document was the first U.S. EPA NCEA guidance document for conducting risk assessments at combustion units:

- U.S. EPA. 1990a. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Environmental Criteria and Assessment Office. ORD. EPA-600-90-003. January.

This document outlined and explained a set of general procedures recommended in this guidance for determining media concentrations utilized in ecological risk assessments. This document was subsequently revised by the following:

- U.S. EPA. 1993h. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Office of Health and Environmental Assessment. ORD. EPA-600-AP-93-003. November 10.

U.S. EPA (1993h) outlined recommended revisions to previous U.S. EPA guidance (1990a), which have been used by the risk assessment community since the release of the document; however, these recommended revisions were never formally incorporated into the original document.

Finally, U.S. EPA Region 5 contracted for development of a *Screening Ecological Risk Assessment of Waste Technologies Industries (WTI) Hazardous Waste Incinerator*, in Liverpool, Ohio (U.S. EPA 1995l). This document was extensively peer reviewed and represents the most current application of ecological risk assessment guidance at a combustion facility. The WTI screening ecological risk assessment was reviewed and considered throughout the development of the approach presented in this guidance document.

U.S. EPA. 1998d. *Proposed Guidance for Ecological Risk Assessment*. Risk Assessment Forum, Washington, D.C. EPA/630/R-95/002B. August.

U.S. EPA. 1997c. *Ecological Risk Assessment Guidance for Superfund: Process for Designing and Conducting Ecological Risk Assessments*. Interim Final. Environmental Response Team, Office of Emergency and Remedial Response, Edison, New Jersey. June 5.

Root, R.B. 1967. "The Niche Exploitation Pattern of the Blue-Gray Gnatcatcher." *Ecological Monographs*. Volume 37, Pages 317-350.

Odum, E.P. 1971. *Fundamentals of Ecology*. Third Edition. W.B. Saunders Company, Philadelphia. 574 pp.

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# Chapter 2

## Facility Characterization

### What's Covered in Chapter 2:

- ◆ [Compiling Basic Facility Information](#)
  - ◆ [Identifying Emission Sources](#)
  - ◆ [Estimating Emission Rates](#)
  - ◆ [Identifying Compounds of Potential Concern \(COPCs\)](#)
  - ◆ [Estimating COPC Concentrations for Non-Detects](#)
  - ◆ [Evaluating Contamination In Blanks](#)
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This chapter provides guidance on characterizing the nature and magnitude of emissions released from facility sources. The characterization includes (1) compiling basic facility information, (2) identifying emission sources, (3) estimating emission rates, (4) identifying COPCs, (5) estimating COPC concentrations for non-detects, and (6) evaluating contamination in blanks.

### 2.1 COMPILING BASIC FACILITY INFORMATION

Basic facility information should be considered in conducting the risk evaluation, and provided to enable reviewers to establish a contextual sense of the facility regarding how it relates to other facilities and other hazardous waste combustion units. At a minimum, the basic facility information listed in the highlighted box at the end of this and other sections should be considered in the risk evaluation. The following sections and chapters describe the collection of this information in more detail; however, users may want to consult these discussions so that all site-specific information needed to complete the risk assessment can be collected simultaneously, when appropriate, for up front consideration. The risk assessor is also referred to *Briefing the BTAG: Initial Description of Setting, History, and Ecology of a Site* (U.S. EPA 1992a) (see web site [www.epa.gov/superfund/program/risk/tooleco.htm](http://www.epa.gov/superfund/program/risk/tooleco.htm)) for more guidance on compiling basic facility information.

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**RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT**

- Principal business and primary production processes
  - Normal and maximum production rates
  - Types of waste storage and treatment facilities
  - Type and quantity of wastes stored and treated
  - Process flow diagrams showing both mass and energy inputs and outputs
  - Type of air pollution control system (APCS) associated with each unit
- 

## 2.2 IDENTIFYING EMISSION SOURCES

Combustion of a hazardous waste generally results in combustion by-products being emitted from a stack. In addition to emissions from the combustion stack, additional types of emissions of concern that may be associated with the combustion of hazardous waste include (1) process upsets, (2) general RCRA fugitive emissions, (3) cement kiln dust (CKD) fugitive emissions, and (4) accidental releases. Each of these emission source types are defined below with regards to the context and scope of this guidance.

***Stack Emissions*** - Release of compounds or pollutants from a hazardous waste combustion unit into the ambient air while the unit is operated as intended by the facility and in compliance with a permit and/or regulation (for interim status).

***Process Upset Emissions*** - Release of compounds or pollutants from a hazardous waste combustion unit into the ambient air while the unit is not being operated as intended, or during periods of startup or shutdown. Upset emissions usually result from an upset in the hazardous waste combustion process and are often known as process upset emissions. Upset emissions are generally expected to be greater than stack emissions because the process upset results in incomplete destruction of the wastes or other physical or chemical conditions within the combustion system that promote the formation and/or release of hazardous compounds from combustion stacks. Upset emissions usually occur during events and times when the hazardous waste combustion unit is not operating within the limits specified in a permit or regulation.

***RCRA Fugitive Emissions*** - Release of compounds or pollutants into the ambient air from RCRA regulated sources other than hazardous waste combustion stacks. RCRA fugitive emissions are typically associated with the release of compounds or pollutants from leaks in the combustion

chamber (e.g., “puffs”); tanks, valves, flanges, and other material handling equipment used in the storage and handling of RCRA hazardous wastes; residues from the combustion process such as ash or quench water; and other RCRA treatment, storage, or disposal units (e.g., landfills).

***CKD Fugitive Emissions*** - Release of compounds or pollutants into the ambient air caused by the handling, storage, and disposal of cement kiln dust.

***Accidental Release*** - Accidental release is defined in Section 112(r) of the Clean Air Act as an unanticipated emission of a regulated substance or other extremely hazardous substance into the ambient air from a stationary source. Accidental releases are typically associated with non-routine emissions from RCRA facilities; such as the failure of tanks or other material storage and handling equipment, or transportation accidents.

Consistent with previous U.S. EPA guidance (U.S. EPA 1994d), U.S. EPA OSW recommends that, with the exception of accidental releases, all of these emission source types be addressed in the risk assessment, as applicable. Accidental releases are not considered within the scope of this guidance, and should be evaluated as recommended in Section 112(r) of the CAA and current U.S. EPA guidance (U.S. EPA 1996k) or the *RMP Offsite Consequence Analysis Guidance*, dated May 24, 1996. A decision to consider accidental releases in risk assessments for hazardous waste combustion facilities should be made on a site specific basis by the relevant permitting authority.

The following subsections contain guidance for estimating emissions for the source types specified for inclusion in the risk assessment. Guidance on air dispersion modeling of stack and fugitive emissions is presented in Chapter 3.

### **2.2.1 Estimating Stack Emission Rates for Existing Facilities**

Stack emission rates (in grams per second) need to be determined for every compound of potential concern (COPC) identified using the procedures outlined in Section 2.3. U.S. EPA OSW expects that emission rates used to complete the risk assessment will be (1) long-term average emission rates adjusted for upsets, or (2) reasonable maximum emission rates measured during trial burn conditions in order to assure that risk assessments are conservative. Maximum emission rates measured during trial burn conditions (see Section 2.2.1.1) represent reasonable maximum emission rates. These emission rates can be controlled by hourly rolling average permit limits traditionally found in combustion unit operating permits, and are more conservative than emission estimates that are based on long-term average emission rates. Long-term

average emission rates (see Section 2.2.1.2) are based on tests of the combustion unit burning worst-case wastes at operating conditions that are representative of normal operating conditions over a long-term period. If long-term average emission rate estimates are used in the risk assessment, the final permit will likely specify limitations in addition to any hourly rolling average limit typically used to regulate hazardous waste combustion facilities.

A permitting agency's decision to allow a facility to use emission rate data developed from either normal or maximum operating conditions will be made on a case-by-case basis. Some facilities may be required to use emission rate data developed from maximum operating conditions because the variability in waste feed and operating conditions is too great to make permit decisions based on emission data collected during normal operating conditions, or because the emissions from combustion of the waste feed material are anticipated to be highly toxic and only a conservative risk assessment can adequately ensure protection.

#### **2.2.1.1 Estimates from Trial Burns**

For existing facilities (such as those built and operational), emission rate information will generally be determined by direct stack measurements during pretrial burn or trial burn tests, because trial burn tests are generally part of the permitting process to burn hazardous wastes. This policy is consistent with U.S. EPA 1998 *Guidance on Collection of Emissions Data to Support Site-Specific Risk Assessments at Hazardous Waste Combustion Facilities*, prepared by U.S. EPA Region 4 and OSW (U.S. EPA 1998b). For new facilities (see Section 2.2.3), estimated emission rates used to complete pretrial burn risk assessments should be compared to the emission rates estimated from actual trial burns completed after the new facility receives a permit and is constructed. Trial burn tests are designed to produce emission rates higher than those anticipated under normal operating conditions. U.S. EPA OSW recommends that sampling be conducted, in accordance with U.S. EPA guidance on conducting trial burns, by using compound-specific stack sampling, analytical, and quality assurance/quality control (QA/QC) protocols and procedures approved by the permitting authority. An alternative to a trial burn test is the submittal of data "in lieu of" a trial burn. U.S. EPA OSW will consider this type of data for on-site units on a case-by-case basis. U.S. EPA OSW expects that this data to be based on recent stack test measurements from a similar type of combustion unit with similar waste feed, capacity, operating conditions, and air pollution control systems (APCSs) to ensure comparable emission rates and destruction and removal efficiencies (DREs).

U.S. EPA OSW expects that using data from a trial burn as a basis for estimating COPC emission rates will tend to overestimate risk. COPC emission rates measured during trial burns are expected to be greater than emission rates during normal unit operations, because a facility “challenges” its combustion unit during a trial burn to develop a wide range of conditions for automatic waste feed cutoff (AWFCO) systems. Trial burn tests are usually conducted under two conditions: (1) a high-temperature test, in which the emission rate of metals is maximized, and (2) a low-temperature test, in which the ability of the combustion unit to destroy principal organic hazardous constituents (POHCs) in the waste feed is challenged. The lesser of the 95th percentile of the mean or maximum stack gas concentration from the three trial burn runs should be used to develop the emission rate estimate used in the risk assessment.

High POHC feed rates and extreme operating conditions tested during the low-temperature trial burn test are usually expected to result in greater product of incomplete combustion (PIC) emission rates. However, this is not true in all cases. For example, the formation of PCDDs and PCDFs does not necessarily depend on “POHC incinerability” low temperature conditions. Polychlorinated dibenzo(p)dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs) can be formed as a result of (1) catalytic formation in the low-temperature regions of the combustion unit or APCS during the low temperature test, or (2) catalytic formation that is dependent on high APCS temperatures typically experienced during the high temperature test.

Because the amount of testing required to develop estimates of COPC emission rates is so extensive and time consuming, U.S. EPA OSW places the responsibility for selecting the test conditions first on the facility and then on the permit writer. If a facility desires to receive a permit with no limits other than those traditionally based on hourly rolling average data gathered during a trial burn, then risk testing should be conducted during trial burn or “worst case” conditions. Whether the permit writer requires testing to be conducted at low, high, or both temperature conditions is a decision that must be made by the permit writer based on the characteristics of the facility and policy set forth by the senior management of the appropriate regulatory agency.



### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- All (current and historical) stack sampling information regarding rates of emissions from the combustion unit during normal or trial burn conditions
- Description of the waste feed streams burned during the stack sampling, including chemical composition and physical properties, which demonstrate that the waste feeds are representative of worst case site-specific "real" wastes

**\*\*\* NOTICE \*\*\***

Although U.S. EPA OSW will not require a risk assessment for every possible metal or PIC from a combustion unit, this does not imply that U.S. EPA OSW will allow only targeted sampling for COPCs during trial burn tests. Based on regional permitting experience and discussions with regional analytical laboratories, U.S. EPA OSW maintains that complete target analyte list analyses conducted when using U.S. EPA standard sampling methods (e.g., 0010 or 0030), do not subject facilities to significant additional costs or burdens during the trial burn process. Facilities conducting stack emission sampling should strive to collect as much information as possible which characterizes the stack gases generated from the combustion of hazardous waste. Therefore, every trial burn or "risk burn" should include, at a minimum, the following tests: Method 0010, Method 0030 or 0031 (as appropriate), total organic compounds (using the Guidance for Total Organics, including Method 0040), Method 23A, and the multiple metals train. Other test methods may be approved by the permitting authority for use in the trial burn to address detection limit or other site-specific issues.

#### 2.2.1.2 Normal Operation Emission Rate Data

Facilities with limited waste feed characteristics and operational variability may be allowed to conduct risk testing at normal operational conditions (U.S. EPA 1994c). The collection of COPC data during normal operating conditions is referred to as a "risk burn" throughout the remainder of this guidance. It is important to note, however, that a risk burn does not replace a traditional trial burn conducted to measure DRE. Instead, U.S. EPA OSW considers a risk burn as an additional operating condition of the trial burn during which data is collected for the purpose of completing a risk assessment.

Because operational data collected during the risk burn would not normally be extrapolated to hourly rolling average AWFCO limits specified in an operating permit; the regulatory agency permit writer should

craft the permit with conditions designed to ensure that the facility does not operate at conditions in “excess” of the normal conditions over the long-term operation of the facility (for example, waste feed rate or stack gas flowrate). These additional permit limits are anticipated to take the form of quarterly or annual mass feed limitations on the waste feed, quarterly or annual average temperatures or stack gas flow rates, and other appropriate limitations.

It may also be necessary for the permit to contain appropriate reporting requirements to ensure that the regulatory agency can verify that the facility does not normally operate at conditions in excess of those tested during the risk burn. Monthly, quarterly, or annual reports which document long-term operations will likely be required of the facility. If a facility violates a long-term permit condition, the permit writer may also include language that requires the facility to cease waste burning immediately until a new test, risk assessment, and/or revised permit are completed. More detailed guidance on the development of permit limits can be found in U.S. EPA Region 6's *Hazardous Waste Combustion Permitting Manual*; which can be obtained from the U.S. EPA Region 6 web page ([www.epa.gov/region06/](http://www.epa.gov/region06/)).

One of the most important criteria which should be evaluated when considering the collection of data during a risk burn rather than a trial burn is the ability of the facility to document that the test is conducted with “worst case” waste. Worst case waste should be the waste feed material or combination of materials that are most likely to result in significant emissions of COPCs. The potential for both PIC and metal emissions should be considered in the selection of the worst case waste. For example, if a facility burns two types of waste—one waste with a high chlorine content and a significant concentration of aromatic organic compounds and a second with a low chlorine content and a significant concentration of alkanes—the former waste should be considered to be the “worst case” for PIC formation and should be used during the risk burn. A similar evaluation should be considered when selecting the worst case waste for metal emissions.

If a facility chooses to develop—and the appropriate regulatory agency allows the use of—emission rate estimates from a risk burn rather than a trial burn, the data set for each COPC should be the 95th percentile of the mean COPC emission rate over all the acceptable test runs *or* the maximum COPC emission rate value from all acceptable test runs, whichever value is lower. U.S. EPA OSW does not believe that it is reasonable to perform a risk assessment with the 95th percentile of the mean emission rate

if the maximum rate is less than this value. U.S. EPA OSW also recommends that, where possible, the COPC emission rate value from the trial burn test and the risk burn test be compared in the risk assessment report along with a comparison of the operational conditions at these two test conditions. For example, if the POHC used for the DRE test in the trial burn is a semivolatile organic compound (SVOC), the facility should analyze for all SVOCs (Method 0010) during the trial burn, and compare these values to those reported for the risk burn. The difference between the emission rates from the trial burn and risk burn should be evaluated in the uncertainty section of the risk assessment.

#### **RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT**

- Sampling and analytical data for trial burn and risk burn (if the risk assessment is completed by using risk burn data) operating conditions
- Description of the operating conditions, under which each set of emission rate data being used was developed
- Complete evaluation of the differences between trial burn and risk burn operating conditions, with an explanation of the expected resultant risk differences

#### **2.2.1.3 Estimates of the Total Organic Emission (TOE) Rate**

Organic compounds that cannot be identified by laboratory analysis will not be treated as COPC's in the risk calculations. However, these compounds still may contribute significantly to the overall risk, and therefore, should be considered in the risk assessment (DeCicco 1995; U.S. EPA 1994d). U.S. EPA developed the total organic emissions (TOE) test to account for unidentified organic compounds because existing methods, such as total hydrocarbon analyzers, do not fully determine the total mass of organics present in stack gas emissions (Johnson 1996). U.S. EPA OSW anticipates that trial and risk burns will include sampling for TOE in order to provide permitting authorities with the information needed to address concerns about the unknown fraction organic emissions. The TOE can be used in conjunction with the identified organic compounds to calculate a TOE factor which can then be used to facilitate a evaluation of potential risks from the unidentified fraction of organic compounds in the stack gas.

The TOE test is the subject of other guidance; see the *Guidance for Total Organics* (U.S. EPA 1996b). Use of the TOE data is dependent on a good understanding of the test method and how the data is reported. The TOE method defines total organics as the sum of three fractions:

**Fraction 1: Total Volatile Organic Compounds (TO<sub>VOC</sub>) (referred to as Field GC Component in the TO Guidance)** - TO<sub>VOC</sub> is defined as the fraction of organic compounds having a boiling point less than 100°C. This VOC fraction is collected using U.S. EPA Method 0040. U.S. EPA Method 0040 allows for quantification of the total mass of organic compounds with boiling points less than 100°C, determined by summing the gas chromatograph/flame ionization detector results as described in the TO Guidance.

**Fraction 2: Total Chromatographical Semivolatiles (TO<sub>SVOC</sub>) (referred to as Total Chromatographical Organics Component in the TO Guidance)** - TO<sub>SVOC</sub> is defined as the fraction of organic compounds having boiling points between 100°C and 300°C. This VOC fraction is collected using modified U.S. EPA Method 0010 procedures as defined by U.S. EPA (1996b). The total mass of organic compounds with boiling points 100°C to 300°C is determined by summing the total gas chromatograph/flame ionization detector results as described in the TO Guidance.

**Fraction 3: Total Gravimetric Compounds (TO<sub>GRAV</sub>) (referred to as Gravimetric component in the TO Guidance)** - TO<sub>GRAV</sub> is defined as the fraction of organic compounds having boiling points greater than 300°C. This fraction includes two types of compounds: (1) Identified SVOCs collected using U.S. EPA Method 0010 having boiling points greater than 300°C and (2) unidentified nonvolatile organics having boiling points greater than 300°C. This fraction is determined by using modified U.S. EPA Method 0010 procedures defined by U.S. EPA (1996b), which quantifies the mass, above this fractions boiling point, by measuring the total mass by evaporation and gravimetry (weighing) for nonvolatile total organics.

It should be noted that the TO total (TO<sub>TOTAL</sub>) is the sum of the sums of each fraction. The sum of the TO fractions are described as follows:

$$TO_{TOTAL} = TO_{VOC} + TO_{SVOC} + TO_{GRAV} \quad \text{Equation 2-1}$$

where

$TO_{TOTAL}$  = stack concentration of TO, including identified and unidentified compounds (mg/m<sup>3</sup>)  
 $TO_{VOC}$  = stack concentration of volatile TO, including identified and unidentified compounds (mg/m<sup>3</sup>)

$TO_{SVOC}$	=	stack concentration of SVOC TO, including identified and unidentified compounds (mg/m <sup>3</sup> )
$TO_{GRAV}$	=	stack concentration of GRAV TO, including identified and unidentified compounds (mg/m <sup>3</sup> )

The TOE data is used in conjunction with the identified data to compute a TOE factor. TOE factors have been computed which range from 2 to 40. The TOE factor is defined by this guidance as the ratio of the  $TO_{TOTAL}$  mass to the mass of identified organic compounds and calculated by the following equation:

$$F_{TOE} = \frac{TO_{TOTAL}}{\sum_i C_i} \quad \text{Equation 2-2}$$

where

$F_{TOE}$	=	TOE factor (unitless)
$TO_{TOTAL}$	=	total organic emission (mg/m <sup>3</sup> )
$C_i$	=	stack concentration of the <i>i</i> th identified COPC (mg/m <sup>3</sup> )

One of the most critical components of the TOE factor is the identification of the organic compounds in the denominator of Equation 2-2. Although the permitting authority may not require a facility to analyze the organic compounds with all possible analytical methods, facilities should consider the effects that gaps in compound specific identification may have on the computation of the TOE factor. For example, hazardous waste burning cement kilns have expressed concern about the amount of light hydrocarbons that may be evolved from the raw materials processed in the cement kilns because these light hydrocarbons have not typically been identified in trial burns. If such concerns are significant, permitting authorities and facilities may choose to use additional test methods in the trial burn in order to speciate the maximum number of organic compounds.

U.S. EPA OSW also recommends that permitting authorities include tentatively identified compounds (TICs) in the denominator when computing the TOE factor to ensure that appropriate credit is given to defensible efforts at identifying the maximum number of organic compounds. Finally, U.S. EPA OSW recommends that non-detect compounds of potential concern be treated consistently between the risk assessment and TOE evaluation. That is, if a non-detected constituent is deleted as a compound of

potential concern (See Section 2.3), then it would not be included in the identified fraction of the TOE equation. Compounds of potential concern identified as per Section 2.3, but not detected, should be included in the TOE factor equation at the reliable detection limit (non-isotope dilution methods) or the estimated detection limit (isotope dilution methods).

The results of the gravimetric fraction should also be carefully evaluated when using the TOE factor. Both regulated industry and U.S. EPA scientists have expressed some concern that the gravimetric fraction of TOE test may contain materials that are not organic. U.S. EPA Office of Research and Development National Risk Management Research Laboratory (NRMRL) recently completed a study conducted to identify products of incomplete combustion (U.S. EPA 1997a). U.S. EPA NRMRL suggested in the study report that the gravimetric fraction of the TOE test may consist of organic and/or inorganic mass not directly attributable to organic incinerator emissions. U.S. EPA NRMRL theorized that these artifacts could consist of inorganic salts, super-fine particulate, or fractured XAD-2 resin. U.S. EPA NRMRL also concluded in this study report that the vast majority of the non-target semivolatile organic compounds detected, but not fully identified, were alkanes with more than 10 carbon atoms, esters of high molecular weight carboxylic acids, and phthlates. Most problems associated with accurately determining the gravimetric fraction attributable to incinerator emissions can be minimized; see the U.S. EPA 1998 *Guidance on Collection of Emissions Data to Support Site-Specific Risk Assessments at Hazardous Waste Combustion Facilities* (U.S. EPA 1998b) for minimizing sample errors.

The TOE factor is used in the uncertainty section of the risk assessment report to evaluate the risks from the unknown fraction of organics. Permitting authorities can evaluate the TOE factor and assess to what extent actual risks may be greater than estimated risks. For example, if the risk from the known portion of the emissions show that risks may be borderline and/or the TOE method shows that the unknowns are a significant portion of the emission profile, the permitting authority may decide to do any or all of the following:

1. Describe in a narrative form what is known of the unknown portion of the emissions.
2. Attribute a risk to the unknown portion of the emissions. An example was presented as a preferred option in U.S. EPA (1994d) which assumed that the unknown compounds are similar in toxicity and chemical properties to the known compounds taken as a whole. The referenced equation is as follows:

$$Q_{i,adj} = Q_i \cdot \frac{TO_{TOTAL}}{\sum_i C_i} \quad \text{Equation 2-2A}$$

where

$$\begin{aligned} Q_{i,adj} &= \text{adjusted emission rate of compound } i \text{ (g/s)} \\ Q_i &= \text{emission rate of compound } i \text{ (g/s)} \\ TO_{TOTAL} &= \text{total organic emission (mg/m}^3\text{)} \\ C_i &= \text{stack concentration of the } i\text{th identified COPC (mg/m}^3\text{)} \end{aligned}$$

3. Require additional testing to identify a greater fraction of the organic compounds.
4. Specify permit conditions that further control total organic emissions or that further control the risks associated with known emissions.

Permitting authorities may use variations of the TOE factor to address site-specific concerns. For example, some permitting authorities may compute three separate TOE factors based on the apportioning provided by the TOE test (i.e.,  $TO_{VOC}$ ,  $TO_{SVOC}$ , and  $TO_{GRAV}$ ). The unknowns associated with each separate fraction of unidentified organic compounds can then be evaluated separately.

### 2.2.2 Estimating Emission Rates for Facilities with Multiple Stacks

Emissions from all combustion units burning hazardous waste at a facility, not just the unit currently undergoing the permitting process, should be considered in the risk assessment. As discussed further in Chapter 3, air dispersion modeling for each combustion unit (source) should be conducted separate from the other combustion units, to allow evaluation of risk on a stack or source-specific basis. A case example is where a chemical manufacturing facility may operate both an on-site incinerator and several hazardous waste burning boilers. Whether it is the incinerator or the boilers undergoing the permitting process, the risk assessment should consider the emissions from all the combustion units in the estimate of facility risk. In addition to RCRA combustion units, emissions from other RCRA treatment, storage, or disposal units (e.g., open burning/open detonation and thermal desorption) may also be included in the risk evaluation in some cases.

### 2.2.3 Estimating Stack Emission Rates for Facilities Not Yet Operational

New hazardous waste combustion facilities should submit a Part B permit application, go through an extensive permitting process, and, if successful, receive a final permit to commencement of operation. The permitting process requires submittal of sufficiently detailed information for the regulatory authorities to evaluate compliance with existing regulations, guidance, and protectiveness. Stack (source) locations and dimensions, design flow and emission rate estimates, waste feed characteristics, surrounding building dimension data, facility plot plans, and terrain data should be reviewed and used in a pre-operation risk assessment. This will assist in decision-making and designing permit requirements.

The design emission rates, waste feed characteristics, and other design data should be reviewed along with supplementing documentation to assure they are representative, accurate, and comprehensive. Good engineering practice dictates a check of, and comparison with, data from similar existing units. Stack test reports for facilities of similar technology, design, operation, capacity, auxiliary fuels, waste feed types, and APCs should be used to estimate COPC emission rates for new facilities that have not been constructed.

If the preferred option of using surrogate data from similar facilities is not available, some state environmental agencies enforce emission rate limits based on state laws. Since these limits cannot be exceeded, they can be used to develop emission rate estimates for the risk assessment. The facility will demonstrate that its emissions are less than the those considered in the permit and risk assessment during the trial or risk burn.

Other data which may cause problems when performing risk assessments for new facilities is particle size distribution. A default particle size distribution is presented in Chapter 3 for use if particle size distribution data from a similar type of facility are not available.

### 2.2.4 Estimating Stack Emission Rates for Facilities Previously Operated

Emissions from the historical operation of combustion units burning hazardous waste at a facility, not just the unit currently undergoing the permitting process, may also be considered in the risk assessment on a



case-by-case basis as determined by the permitting authority. Such a case may be when the emissions from historical operation of a source or sources may have already resulted in potential risk concerns at or surrounding the facility. Emissions from historical operations could be taken into consideration by modeling as a separate source or, if applicable, in the fate and transport equations by adding the previous years of operation to the anticipated time period of combustion for a new or existing operating source. In addition to RCRA combustion units, historical emissions from other RCRA treatment, storage, or disposal units (e.g., open burning/open detonation and thermal desorption) at the facility under evaluation may also be included in the risk assessment in some cases.

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- All stack test reports for combustion units used to develop emission rate estimates
- If using surrogate data for a new facility, descriptions of how the combustion data used represent similar technology, design, operation, capacity, auxiliary fuels, waste feed types, and APCSs
- Demonstration that the data used to develop the emission rate estimates were collected by using appropriate U.S. EPA sampling and analysis procedures
- The range of data obtained, and values used, in completing the risk assessment

**\*\*\* NOTICE \*\*\***

Facilities may use estimated emission rate data from other combustion units only to determine whether the construction of a new combustion unit should be completed. After a combustion unit has been constructed, U.S. EPA OSW will require an additional risk assessment using emission rates collected during actual trial burn conditions.

#### 2.2.5 Emissions From Process Upsets

Uncombusted hazardous waste can be emitted through the stack as a result of various process upsets, such as start-ups, shutdowns, and malfunctions of the combustion unit or APCS. Emissions can also be caused by operating upsets in other areas of the facility (e.g., an upset in a reactor which vents gases to a boiler burning hazardous waste could trigger a process upset in the boiler, resulting in increased emissions). U.S.

EPA (1994d) indicates that upsets are not generally expected to significantly increase stack emissions over the lifetime of the facility.

Process upsets occur when the hazardous waste combustion unit is not being operated as intended, or during periods of startup or shutdown. Upset emissions are generally expected to be greater than stack emissions (over short periods of time) because the process upset results in incomplete destruction of the wastes or other physical or chemical conditions within the combustion system that promote the formation and/or release of hazardous compounds from combustion stacks. Upset emissions usually occur during events and times when the hazardous waste combustion unit is not operating within the limits specified in a permit or regulation.

To account for the increased emissions associated with process upsets, the stack emission rate estimated from trial burn data (upset factor is not applied to non-PIC emission rate estimates where the total mass of a constituent in the waste feed is assumed to be emitted) is multiplied by an upset factor. When available, facilities should use site specific emissions or process data to estimate the upset factor. The following types of data may be considered and evaluated to derive the upset factor:

- Data for continuous emissions monitoring systems that measure stack carbon monoxide, oxygen, total hydrocarbon (if required), or opacity (if appropriate)
- Data on combustion chamber, APCS, or stack gas temperature
- Frequency and causes of automatic waste feed cutoffs (AWFCO)
- Ratio of AWFCO frequency and duration to operating time
- APCS operating variables, such as baghouse pressure drop, liquid scrubber flow rate, or electrostatic precipitator voltage
- Stack test collected while the combustion unit was operated under upset conditions

This information may be analyzed with the objective of estimating the magnitude of the increase in emissions and the percentage of time on an annual basis that the unit operates at upset conditions.

When site specific data are not available or are inappropriate for deriving an upset factor, consistent with previous guidance (U.S. EPA 1993h), U.S. EPA OSW recommends that upset emissions be estimated by using a procedure based on work by the California Air Resources Board (CARB) (1990).

***Estimating Emissions from Process Upsets:*** To represent stack emission rates during process upsets, multiply the emission rate developed from the trial burn data by 2.8 for organics and 1.45 for metals. These factors are derived by assuming that emissions during process upsets are 10 times greater than emissions measured during the trial burn. Since the unit does not operate under upset conditions continually, the factor must be adjusted to account for only the period of time, on an annual basis, that the units operates under upset conditions. For organic compounds, the facility is assumed to operate as measured during the trial burn 80 percent of the year and operate under upset conditions 20 percent of the year  $[(0.80)(1)+(0.20)(10)=2.8]$ . For metals, the combustion unit is assumed to operate as measured during the trial burn 95 percent of the year and operate under upset conditions the remaining 5 percent of the year  $[(0.95)(1)+(0.05)(10)=1.45]$ .

Catastrophic process upsets brought about by complete failure of combustion and air pollution control systems resulting from non-routine events such as explosions, fires, and power failures are considered accidental releases and are not addressed by this guidance.

#### **RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT**

- Historical operating data demonstrating the frequency and duration of process upsets
- A discussion on the potential cause of the process upsets
- Estimates of upset magnitude or emissions
- Calculations which describe the derivation of the upset factor.

#### **2.2.6 RCRA Fugitive Emissions**

RCRA fugitive emission sources that should be evaluated in the risk assessment include waste storage tanks; process equipment ancillary to the combustion unit; and the handling and disposal of combustion system residues such as ash. Fugitive emissions from other RCRA treatment, storage, or disposal units (e.g., landfills) may also require evaluation in some cases.

This section contains guidance for quantitatively estimating fugitive emissions on the basis of procedures outlined by other U.S. EPA guidance. Guidance regarding air dispersion modeling of fugitive emissions is presented in Chapter 3.

### 2.2.6.1 Quantitative Estimation of RCRA Fugitive Emissions from Process Equipment

Quantitative estimation of RCRA fugitive emissions includes (1) identifying equipment to be evaluated as fugitive emission source(s), (2) grouping equipment, as appropriate, into a combined source, and (3) estimating compound specific emission rates for each source. Figure 2-1 is an example of a facility plot plan that includes one RCRA combustion unit (CU-1), two hazardous waste feed storage tanks (WST-1 and WST-2), and ancillary equipment identified in a RCRA Part B permit application for a hypothetical example facility. This figure, as well as Tables 2-1 and 2-2, have been provided as an example to facilitate understanding of each of the steps presented for estimating fugitive emissions.

**Step 1: Identifying Fugitive Emission Sources** - Generally, RCRA fugitive emission sources to be evaluated in the risk assessment should include waste storage tanks and process equipment that comes in contact with a RCRA hazardous waste such as equipment specified in Title 40, Code of Federal Regulations (40 CFR) Part 265, Subpart BB. Equipment covered under Subpart BB includes the following:

**TABLE 2-1  
EXAMPLE CALCULATION  
TOTAL FUGITIVE EMISSION RATES  
FOR EQUIPMENT IN WASTE FEED STORAGE AREA**

1	2	3	4	5	6		7	8	9	10
Fugitive Emission Source	Waste Stream	Type of Waste Stream In Service	Equipment Type	Number of Each Equipment Type Per Waste Stream	Equipment Emission Factors		Total VOC Weight Fraction	Operational Time Period of Equipment (days)	Total VOC Emissions Rate by Equipment (g/sec)	Total Fugitive Emission Rate (g/sec)
					(kg/hr)	(g/sec)				
Waste Feed Storage Area	Process A Wastes	Light Liquid	Pumps	3	0.01990	0.00553	0.9	180	0.01493	0.14926
		Light Liquid	Valves	70	0.00403	0.00112	0.9	180	0.07056	
		Light Liquid	Connectors	30	0.00183	0.00051	0.9	180	0.01377	
		Light Liquid	Tank WST-1	1	--	--	0.9	180	0.02	
		Light Liquid	Tank WST-2	1	--	--	0.9	180	0.03	
	Process B Wastes	Heavy Liquid	Pumps	2	0.00862	0.00239	0.6	180	0.00287	0.06857
		Heavy Liquid	Valves	75	0.00023	0.00112	0.6	180	0.0504	
		Heavy Liquid	Connector	50	0.00183	0.00051	0.6	180	0.0153	
		Heavy Liquid	Tank WST-1	1	--	--	0.6	0	0	
		Heavy Liquid	Tank WST-2	1	--	--	0.6	0	0	

Notes:

- Column 1 Equipment in the Waste Feed Storage Area was identified and grouped as a combined RCRA fugitive emission source with an area extent defined by UTM coordinates (NAD83).
- Column 2 The waste streams serviced by equipment in the Waste Feed Storage Area can be determined through review of the facility's RCRA Part B Permit Application, Air Emission Standards.
- Column 3 The type of waste stream in service, defined as light or heavy for determination of equipment specific emission factors, can be determined from review of waste stream vapor pressure.
- Column 4 Similar types of equipment can be grouped according to the most applicable equipment specific emission factor and type of waste stream service (light or heavy) provided in U.S. EPA (1995f).
- Column 5 The number of equipment per type at the source was multiplied by the equipment specific emission factor (Column 6) to obtain equipment specific emission rate for that respective type of equipment (Column 7).
- Column 6 Emission factors specific to each type of equipment can be obtained from U.S. EPA (1995f), with the exception of storage tanks.
- Column 7 Weight fraction of total volatile organic compounds was obtained from dividing the concentration of VOCs (mg/L) by the density of the waste stream (mg/L).
- Column 8 Assumed the equipment is operational for 180 days a year.
- Column 9 Equipment specific fugitive emission rates were determined by multiplying Columns 5, 6, and 7. Emission rates for tanks were obtained from Title V air permit application. In the absence of such data, emission rates for tanks can be calculated using U.S. EPA's TANKS Program or by following the procedures outlined in U.S. EPA (1995a).
- Column 10 The total fugitive emission rate for each waste stream is determined by summing emission rates for all the equipment. Table 2-2 presents calculations for estimating speciated fugitive emissions.
-

**TABLE 2-2**  
**EXAMPLE CALCULATION**  
**SPECIATED FUGITIVE EMISSIONS**  
**FOR EQUIPMENT IN WASTE FEED STORAGE AREA**

1	2	3	4	5	6
Fugitive Emission Source	Waste Stream	Waste Stream Composition	Weight Fraction of Each VOC In Waste Stream (%)	Total Fugitive Emission Rate (g/sec)	Speciated Fugitive Emissions (g/sec)
Waste Feed Storage Area	Process A Wastes	Acetaldehyde	0.20	0.14926	0.0030
		Acetonitrile	0.25		0.0037
		2-Nitropropane	0.25		0.0037
		Nitromethane	0.20		0.0030
	Process B Wastes	Acetaldehyde	0.20	0.06857	0.0137
		Acetonitrile	0.10		0.0069
		Methanol	0.20		0.0137
		Propionitrile	0.05		0.0034

Notes:

- Column 1      Equipment in the Waste Feed Storage Area was identified and grouped as a combined RCRA fugitive emission source with an aerial extent defined by UTM coordinates (NAD83).
- Column 2      The waste streams serviced by equipment in the Waste Feed Storage Area can be determined through review of the facility's RCRA Part B Permit Application, Air Emission Standards.
- Column 3      The waste stream composition can be determined from analytical data
- Column 4      Weight fraction of compounds in the waste stream can be determined from analytical data or review of the facility's Title V Air Permit Application, Emissions Inventory Questionnaire (EIQ) for Air Pollutants (see example in Figure 2-2).
- Column 5      The total fugitive emission rate for each waste stream was obtained from Column 10, Table 2-1.
- Column 6      Speciated fugitive emissions were obtained by multiplying Column 4 and 5.

- Pumps
- Valves
- Connectors (flanges, unions, tees, etc.)
- Compressors
- Pressure-relief devices
- Open-ended lines
- Product accumulator vessels
- Sampling connecting systems
- Closed vent systems
- Agitators

Each fugitive emission source should be identified on a facility plot map with a descriptor and the location denoted with Universal Transverse Mercator (UTM) coordinates (specify if North American Datum [NAD] of 27 or NAD83).

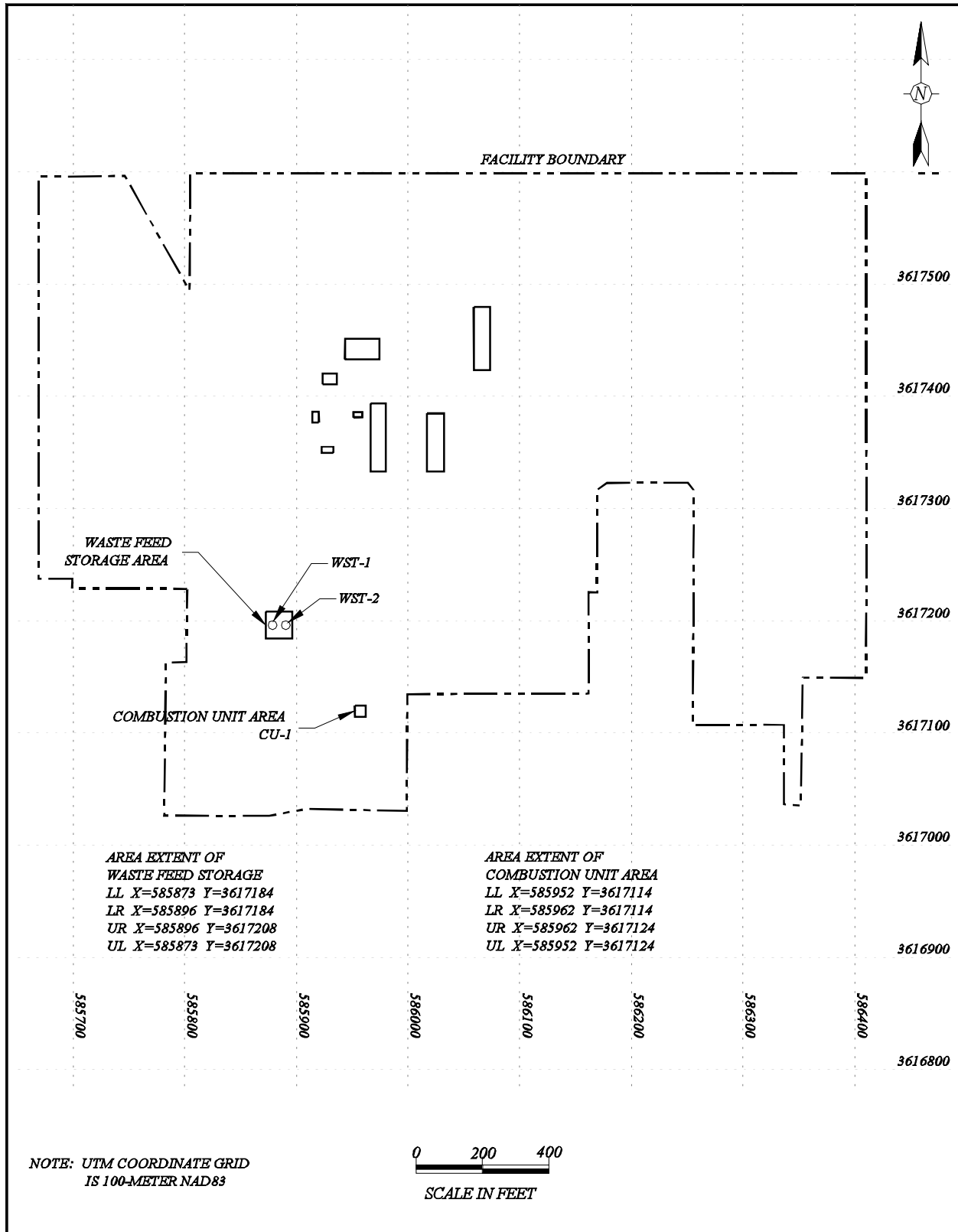
**Step 2: Grouping Equipment Into a Combined Source** - To significantly reduce the effort required to complete air dispersion modeling and subsequent risk assessment, equipment in close proximity may be grouped and evaluated as a single combined source with the speciated emission rates for each piece of equipment summed. The area extent of the grouped or combined source, as defined by UTM coordinates (specify if NAD27 or NAD83), should be clearly denoted on a facility plot map. The area extent of the combined source should be defined by the actual locations of the equipment being grouped, without exaggeration to cover areas without fugitive sources. Consideration should also be made for how fugitive emission sources are to be defined when conducting the air dispersion modeling (see Chapter 3).

As shown in Figure 2-1, equipment in two areas at the hypothetical facility have been grouped into combined sources; these consist of the Waste Feed Storage Area and the RCRA Combustion Unit Area.

**Step 3: Estimating Fugitive Emissions from Tanks** - Fugitive emission rates for waste storage tanks can be obtained from the facility's emission inventory or Title V air permit application prepared in compliance with Clean Air Act Amendments of 1990 (see example provided as Figure 2-2). If the facility does not have such information available, fugitive emissions from storage tanks can be calculated using U.S. EPA's TANKS Program or by following the procedures outlined in U.S. EPA guidance document (1995a), "*Compilation of Air Pollution Emission Factors, January 1995.*"



**FIGURE 2-1**  
**EXAMPLE FACILITY PLOT MAP**



**FIGURE 2-2**  
**EXAMPLE EMISSIONS INVENTORY**

Department of Environmental Quality Air Quality Division P. O. Box 82135 Baton Rouge, LA 70884-2135 (504) 765-0219		<b>LOUISIANA</b> <b>SINGLE POINT SOURCE / AREA SOURCE</b> <b>Emission Inventory Questionnaire (EIQ)</b> <b>for Air Pollutants</b>					LA DEQ			
Company Name Hypothetical Chemical Company			Plant location and name (if any) Baton Rouge, LA Plant			Date of submittal February 1996				
Source ID Number WST - 1	Descriptive name of the equipment served by this stack or vent Waste Feed Tank				Location of stack or vent (see instructions on how to determine location of area sources) Horizontal Coordinate 589100 m E Vertical coordinate 3616200 m N UTM zone no. 15					
STACK and DISCHARGE PHYSICAL CHARACTERISTICS Change [ ] yes [x] no	Height of stack above grade [ft] 8	Diameter or stack discharge area 0.167 ft	Stack gas exit temperature (°F) 125	Stack gas flow at process conditions, not at standard (cfm) 24.27		Stack gas exit velocity (ft/sec) 18.32		For tanks, list volume (gals) 800 Date of construction		
Fuel a b c	Type of fuel used and heat input (see instructions)		Operating Characteristics	Percent of annual throughput of pollutants through this emission point				Normal operating time of this point		Normal operating rate
	Type of Fuel	Heat input (MMBtu/hr)		Dec-Feb	Mar-May	Jun-Aug	Sep-Nov	hrs/ days/ weeks/ day week year		100%
				25	25	25	25	24.00 7 52.0		
<b>Air Pollutant Specific Information</b>										
Pollutant			Control equipment code	Control equipment efficiency	Emission Rate			Emission estimation method	Add, change, delete code	Concentration in gases exiting at stack
2-Nitropropane			000	0.0000	0.0023	0.3463	0.01	3	c	N/A ppm by vol
Acetaldehyde			000	0.0000	0.0041	125.00	0.081	3	c	N/A ppm by vol
Acetanitrile			000	0.0000	0.0023	21.1266	0.01	3	c	N/A ppm by vol
Methanol			000	0.0000	0.0023	4.502	0.01	3	c	N/A ppm by vol
Non-Toxic Voc			000	0.0000	0.0062	195.3347	0.028	3	c	N/A ppm by vol

The information required for estimating fugitive emission rates from storage tanks includes, but is not limited to, the following:

- Dimensions of the tanks
  - Shell height and diameter
- Characteristics of the tank roof
  - Color and shade
  - Condition (e.g., poor, good)
  - Type (e.g., cone, dome)
  - Height
  - Radius or slope
  - Fixed or floating
- Characteristics of the shell
  - Color and shade
  - Condition (e.g., poor, good)
  - Heated
- Settings on breathe vents
  - Vacuum setting
  - Pressure setting
- Characteristics of the stored liquids
  - Maximum and annual average liquid height
  - Working volume
  - Turnovers per year
  - Net throughput
  - Average annual temperature
  - Vapor pressures of speciated constituents (at annual average temperature)

**Step 4: Estimating Fugitive Emissions from Process Equipment** - Based on guidelines provided in U.S. EPA (1995f), "*Protocol for Equipment Leak Emission Estimates, EPA-453/R-93-017*," fugitive emissions for each equipment listed under 40 CFR Part 265, Subpart BB can be estimated by the following four approaches, in order of increasing refinement and data requirements:

- Average Emission Factor Approach (AEFA)
- Screening Ranges Approach (SRA)
- U.S. EPA Correlation Approach (EPACA)
- Unit-Specific Correlation Approach (USCA)

These four approaches can be used at any facility to estimate fugitive emission rates of volatile organic compounds (VOCs) from equipment. Except for the AEFA method, all of the approaches require screening data collected by using a portable monitoring device (PMD). Because data on fugitive emissions at a facility is generally limited, the AEFA method will apply in most cases, and therefore, has been selected for use in the example demonstrated in Figure 2-1, and Tables 2-1 and 2-2. However, U.S. EPA OSW recommends that facilities use more refined approaches such as SRA, EPACA, or USCA, if sufficient data is available. U.S. EPA (1995f) provides a detailed discussion on these three approaches.

### *An Example Calculation Using the AEFA Method*

Information for estimating fugitive emission rates using the AEFA method is as follows:

- Type of waste stream associated with each equipment type (Columns 2 and 3, Table 2-1)
  - light liquids are those in which the sum of the concentration of individual constituents with a vapor pressure over 0.3 kilopascals (kPa) at 20°C is greater than or equal to 20 weight percent
  - heavy liquids are all others liquids not meeting the definition of light liquids as specified above
- Number of each equipment type associated with each waste stream (Columns 4 and 5, Table 2-1)
- Total VOC weight fraction of each waste stream (Column 7, Table 2-1)
- Weight fraction of each VOC in each waste stream (Columns 3 and 4, Table 2-2)
- Operational time period of equipment (Column 8, Table 2-1)

When this approach is used, equipment can be grouped by waste streams of similar characteristics and VOC composition (Columns 1 and 2, Table 2-1). However, the AEFA approach does not account for different site-specific conditions such as temperature, vapor pressure, or screening values, among process units within a source category. Site-specific factors can significantly influence fugitive emission rates of leaks from equipment.

The average emission factors for synthetic organic chemicals manufacturing industry process units, refineries, and natural gas plants are presented in U.S. EPA (1995f) (Column 6, Table 2-1). The following

table is an excerpt from this guidance document. These emission factors are most valid for estimating rates of emissions from a grouping of equipment over a long time period.

SOCMI AVERAGE EMISSION FACTORS		
Equipment type	Service	Emission factor (kg/hr/source)
Valves	Gas	0.00597
	Light liquid	0.00403
	Heavy liquid	0.00023
Pump seals	Light liquid	0.0199
	Heavy liquid	0.00862
Compressor seals	Gas	0.228
Pressure relief valves	Gas	0.104
Connectors	All	0.00183
Open-ended lines	All	0.0017
Sampling connectors	All	0.0150

Source: U.S. EPA (1993e)

The total VOC emissions rate for a specified equipment type can be calculated by multiplying the equipment emission factor by the total VOC weight fraction and the number of each equipment type per waste stream (Column 9, Table 2-1 = Column 6 x Column 7 x Column 5).

The total VOC emission rates for each equipment type are summed to generate the total fugitive emission rate for the waste stream by (Column 10, Table 2-1). Speciated fugitive emissions can then be calculated by multiplying the weight fraction of each VOC in the waste stream and the total fugitive emission rate for the waste stream (Column 6, Table 2-2 = Column 4 x Column 5). This speciated emission rate is the emission rate used in the risk assessment.

### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Summary of the step-by-step process conducted to evaluate fugitive emissions
- Facility plot map clearly identifying each fugitive emission source with a descriptor and the location denoted with UTM coordinates (specify if NAD27 or NAD83).
- Speciated emission rate estimates for each waste stream serviced by each source, with supporting documentation
- Applicable discussion of monitoring and control measures used to mitigate fugitive emissions

#### 2.2.6.2 Fugitive Emissions from Combustion Unit Leaks

Fugitive emissions that result from the construction, design, or operation of a combustion unit burning hazardous waste should be evaluated, as appropriate. Examples of fugitive emissions from combustion unit leaks include the following:

- Combustion units that operate under negative pressure may experience temporary positive pressures (“puffing”) that cause fugitive emissions. This condition can occur when a slug of high BTU waste is combusted, causing a rapid expansion in the volume of combustion gases that exceeds the volume of the combustion chamber.
- Fugitive emissions resulting from the day-to-day operation of the combustion unit and APCS. These emissions will typically include (1) leaks that occur due to a positive pressure in the APCS, and (2) routine maintenance activities such as replacement of baghouse collection bags.

Currently, U.S. EPA OSW does not offer any specific quantitative guidance on how to estimate fugitive emissions from hazardous waste combustion units. However, risks associated with emissions from hazardous waste combustion unit leaks can be addressed in the uncertainty section of the risk assessment if no site specific quantitative methods are available. Specifically, the permitting authority can review facility specific data to determine whether or not the design addresses equipment leaks and whether the operational data indicates that equipment leaks may be a problem.

### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Process design information and drawings (if necessary)
- Past operating data indicating the frequency, duration, and magnitude of combustion unit leaks
- Information regarding the probable cause of combustion unit leaks
- Summary of procedures in place to monitor or minimize fugitive emissions resulting from combustion unit leaks

#### 2.2.7 RCRA Fugitive Ash Emissions

The combustion of hazardous waste materials may result in the production of flyash. Fugitive particle emissions may result from the subsequent collection, handling, and disposal of the flyash. Typically, fugitive emissions of flyash, collected from an air pollution control device (APCD) will occur during transfer into covered trucks or other conveyance mechanisms prior to disposal. Emissions generated during the loading process can be controlled by APCDs or other types equipment, however, a fraction of the flyash may still escape into the atmosphere as fugitive emissions.

##### 2.2.7.1 Quantitative Estimation of RCRA Fugitive Ash Emissions

Steps for the quantitative estimation of RCRA fugitive ash emissions include (1) determining an empirical emission factor, (2) estimating the flyash generation rate, and (3) accounting for air pollution control equipment, if applicable. As demonstrated in the example calculation below, the fugitive ash emission rate can then be estimated by multiplying the empirical emission factor by the flyash generation rate and the control deficiency of the air pollution control equipment, if applicable.

**Step 1: Determining an Empirical Emission Factor** - Particle emissions associated with flyash loading and unloading can be estimated using an empirical emission factor of 1.07 lb per ton flyash. This factor is based on a field testing program conducted at a coal fired power plant equipped with an electrostatic precipitator (ESP) (Muleski and Pendleton 1986). Because the combustion of coal and hazardous wastes are similar activities, flyash generated from similar control devices is expected to behave similarly under the same conditions, with respect to fugitive emissions. In general, particle behavior is dependent more on the physical form of the flyash than on the feed (or waste) stream being combusted. The emission factor determined during the empirical study (0.107 lb per ton flyash) can be adjusted by a factor (e.g., 10) to account for the fact that the flyash

from the combustion of coal (as in the study) was wetted. Flyash from the hazardous waste combustion facility may not be wetted depending on the facility.

**Step 2: Estimating the Flyash Generation Rate** - The flyash generation rate from the APCD can be obtained from the Part B Permit Application and the total ash content of the “generic” waste streams created from the waste profile. Both values should be approximately the same. Since a major portion of ash fed to the combustor is converted to bottom ash, it is likely that this value is a conservatively high estimate of the actual flyash generation rate.

**Step 3: Accounting for Air Pollution Control Equipment** - If an APCD is used for controlling emissions during flyash handling operations, an efficiency factor (e.g., 99.5 percent) can be applied to the emission rate. An efficiency factor of 99.5 percent is based on U.S. EPA (1995a) for typical collection efficiencies of particulate matter control devices, for the particle sizes in the range of 2.5 to 10  $\mu\text{m}$ .

### **Example Calculation**

The fugitive ash emission rate is calculated by multiplying the empirical emission factor (Step 1) times the estimated flyash generation rate (Step 2) [(1.07 lb per ton) \* (5,000 tons per year) = 5,350 lbs per year].

Accounting for the air pollution control equipment, the product of Steps 1 and 2 is multiplied times one minus the fabric filter efficiency (Step 3) to obtain the final RCRA fugitive ash emission rate for use in the risk assessment [(5,350 lbs per year) \* (1 - 0.995) = 26.75 lbs per year].

### **2.2.8 Cement Kiln Dust (CKD) Fugitive Emissions**

CKD is the particulate matter (PM) that is removed from combustion gas leaving a cement kiln. This PM is typically collected by an APCS—such as a cyclone, baghouse, ESP—or a combination of APCSs.

Many facilities recycle a part of the CKD back into the kiln. Current and applicable guidance on evaluating CKD includes (1) the *Technical Background Document for the Report to Congress* (U.S. EPA 1993g), and (2) the more recent regulatory determination of CKD (60 FR 7366, February 7, 1995).

Most CKD constituents (for example, metals) are not volatile but could be released to air through fugitive dust emissions as a volatile or semivolatile organic that can be released in gaseous form and present in relatively low concentrations, if at all (U.S. EPA 1993a). Dust particles may be suspended in the air by either wind erosion or mechanical disturbances. The extent to which dust is blown into the air by wind erosion depends on several site-specific characteristics, including (1) the texture (particle size distribution)



and moisture content of the CKD on the surface of piles, (2) nonerodible elements, such as clumps of grass or stones on the pile, (3) a surface crust, and (4) wind speeds. Mechanical disturbances that can suspend CKD constituents in the air include (1) vehicular traffic on and around CKD piles, (2) CKD dumping and loading operations, and (3) transportation of CKD around a plant site in uncovered trucks. Cement plants may use various control measures to limit the release of CKD to the air. For example, CKD may be pelletized in a pug mill, compacted, wetted, and covered to make the material less susceptible to wind erosion.

To keep the dust down, many facilities add water to CKD, before disposal, to agglomerate individual particles. In addition, as CKD sits in a pile exposed to the elements, occasional wetting by rainfall may form a thin surface crust in inactive areas of the pile. This acts to mitigate air entrainment of particles. However, based on field observations by U.S. EPA (1993g), neither surface wetting nor natural surface crusting eliminates the potential for CKD to be blown into the air. Wetting the dust before disposal provides incomplete and temporary control, because (1) infrequent application of water, and (2) the dust ultimately dries and returns to a fine particulate that is available for suspension and transport. Similarly, a surface crust may develop, but (1) the crust breaks when vehicles or people move on the pile, and (2) fresh dust is regularly added to the pile, providing a continual, exposed reservoir of fine particles. It should be noted that a crust does not always form for a variety of reasons such as weather and chemistry of the CKD.

CKD constituents that are released to the air are transported and dispersed by the winds, and are ultimately deposited onto land or water, either by settling in a dry form or by being entrained in precipitation.

#### **2.2.8.1 Composition and Characteristics of CKD**

U.S. EPA (1993g) highlighted the limited amount of available information regarding the variation in chemical constituents of CKD generated by facilities burning hazardous waste as fuel and by facilities burning only fossil or nonhazardous waste fuels. There may also be differences in composition between the “as-generated” CKD that is recycled back into the system and the “as-managed” CKD that is disposed on or offsite.

Transport in air is of concern for CKD, because the dust is a fine PM that is readily suspendable, transportable, and respirable in air. In general, particles that are  $\leq 100$  micrometers may be suspended in

the wind and transported. Within this range, particles that are  $\leq 30$  micrometers can be transported for considerable distances downwind. Virtually all of the dust generated at the 15 facilities evaluated by U.S. EPA (1993g) in the *Cement Kiln Dust Report to Congress* may be suspended and transported in the wind (that is, the vast majority of particles are  $\leq 100$  micrometers), and over two-thirds of all CKD particles generated may be transported over long distances. Additionally, a significant percentage of the total dust generated (from 22 to 95 percent, depending on kiln type) comprises particles that are  $\leq 10$  micrometers.

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Physical data, including particle size distribution and density
- Chemical data, including organic and inorganic analytical tests similar to those used for sampling combustion gases
- Plant net CKD generation rate (how much CKD per year that is available for disposal)
- Ambient air monitoring data
- CKD management, transportation, storage, and disposal methods
- Containment procedures, including fugitive dust prevention measures and the area of exposed CKD
- Meteorological data, including wind speed and precipitation

#### 2.2.8.2 Estimation of CKD Fugitive Emissions

In general, this guidance does not address CKD risks in a quantitative fashion. However, risk assessments conducted for cement manufacturing facilities should, at a minimum, evaluate the fugitive emissions due to CKD on a qualitative basis. Readers are referred to the *Technical Background Document for the Report to Congress* (U.S. EPA 1993g), for methods to estimate the magnitude of fugitive emissions from the handling, storage, and disposal of CKD. In addition, an analysis of a specific facility's compliance with other environmental statutes and regulations may be an appropriate method to qualitatively evaluate risks associated the handling, storage, and disposal of CKD.

### 2.3 IDENTIFYING COMPOUNDS OF POTENTIAL CONCERN

Compounds of potential concern (COPCs) are those compounds evaluated throughout the risk assessment. The purposes of identifying COPCs are to focus the risk assessment on those compounds that are likely to pose the most risk to ecological receptors exposed to hazardous waste combustion emissions. The COPC identification process is conservative by design to avoid not including compounds that might pose an ecological risk.

There is no one definition of a COPC, because a compound that is a COPC at one hazardous waste combustion unit may not be a COPC at another combustion unit. COPCs in the emissions from hazardous waste combustion units vary widely, depending on (1) the type of combustion unit, (2) the type of hazardous waste feed being burned, and (3) the type of APCS used. Also considered as COPCs are products of incomplete combustion (PICs); which are any organic compounds emitted from a stack, such as (1) compounds initially present in the hazardous waste feed stream and not completely destroyed in the combustion process, and (2) compounds that are formed during the combustion process. Because PICs may be formed by trace toxic organic compounds in the waste feed stream, these compounds should be evaluated as PIC precursors, in addition to those compounds that constitute most of the hazardous waste feed.

PICs should not be confused with principal organic hazardous constituents (POHC), which are compounds in the waste feed stream used to measure DRE of the combustion unit during a trial burn test. Unburned POHCs and partially destroyed or reacted POHCs are PICs, but PICs are not necessarily related to POHCs.

Table A-1 (Appendix A) presents a comprehensive list of compounds typically identified (1) in hazardous waste, and (2) in hazardous waste combustion stack gas emissions. For each compound, Table A-1 identifies the Chemical Abstracts Service (CAS) number and also indicates whether a compound has been identified as a potential COPC by (1) U.S. EPA and state risk assessment reference documents, (2) emission test results that have identified the compound in the emissions from hazardous waste combustion facilities, or (3) other literature that suggests that the compound may be significant from a risk perspective. Table A-1 has been provided in this guidance in order to help risk assessors ensure that the trial burn considers the full range of compounds potentially emitted from a combustion unit and the

appropriate analytical method. Once the trial burn stack tests are completed, the COPC selection process is initiated based on the universe of stack test data, not Table A-1. The purpose of a risk assessment is not to arbitrarily evaluate every potential compound listed in Table A-1.

Based on U.S. EPA OSW review, COPCs previously identified in ecological risk assessments at combustion facilities are as follows:

- Polychlorinated dibenzo(p)dioxins (PCDD) and polychlorinated dibenzofurans (PCDF)
- Polynuclear aromatic hydrocarbons (PAH)
- Polychlorinated biphenyls (PCB)
- Pesticides
- Nitroaromatics
- Phthalates
- Other organics
- Metals

This list was compiled based on professional experience and is not meant to be either limiting or inclusive. The list enabled U.S. EPA OSW to focus on (1) developing receptor-specific and compound-specific bioconcentration factors as provided in Appendices C and D, (2) developing compound- and receptor-specific *TRVs* as provided in Appendix E, and (3) developing receptor exposure parameters and exposure equations discussed in Chapter 5 and provided in Appendix F. These focused compound-specific parameters and information are included to facilitate the performance of ecological risk assessments, and are not meant to be either limiting or inclusive for hazardous waste combustion facilities. Experience has shown that developing compound-specific and receptor-specific parameters for risk assessments can be one of the most labor- and time-intensive parts of completing the risk assessment, and U.S. EPA OSW intends that the information included in the Appendices of this guidance facilitates the risk process.

COPCs are identified from the trial burn data based on their potential to pose an increased risk. This identification process should focus on compounds that (1) are likely to be emitted, based on the potential presence of the compound or its precursors in the waste feed, (2) are potentially toxic to ecological

receptors, and/or (3) have a definite propensity for bioconcentrating in ecological receptors and bioaccumulating in food chains. Appendix E presents toxicity reference values of specific compounds to specific receptors. The toxicity information provided in this guidance is for informational purposes to help permitting authorities explain the basis for identifying compounds as COPCs and facilitate completing the risk assessment. Since toxicity information may change as additional research is conducted, permitting authorities should review the most current available information before completing a risk assessment to ensure that the toxicity data used in the risk assessment is based upon the most current Agency consensus.

As illustrated in Figure 2-3, the following steps should be used to identify the COPCs that will be evaluated for each facility (U.S. EPA 1993h; 1994d).

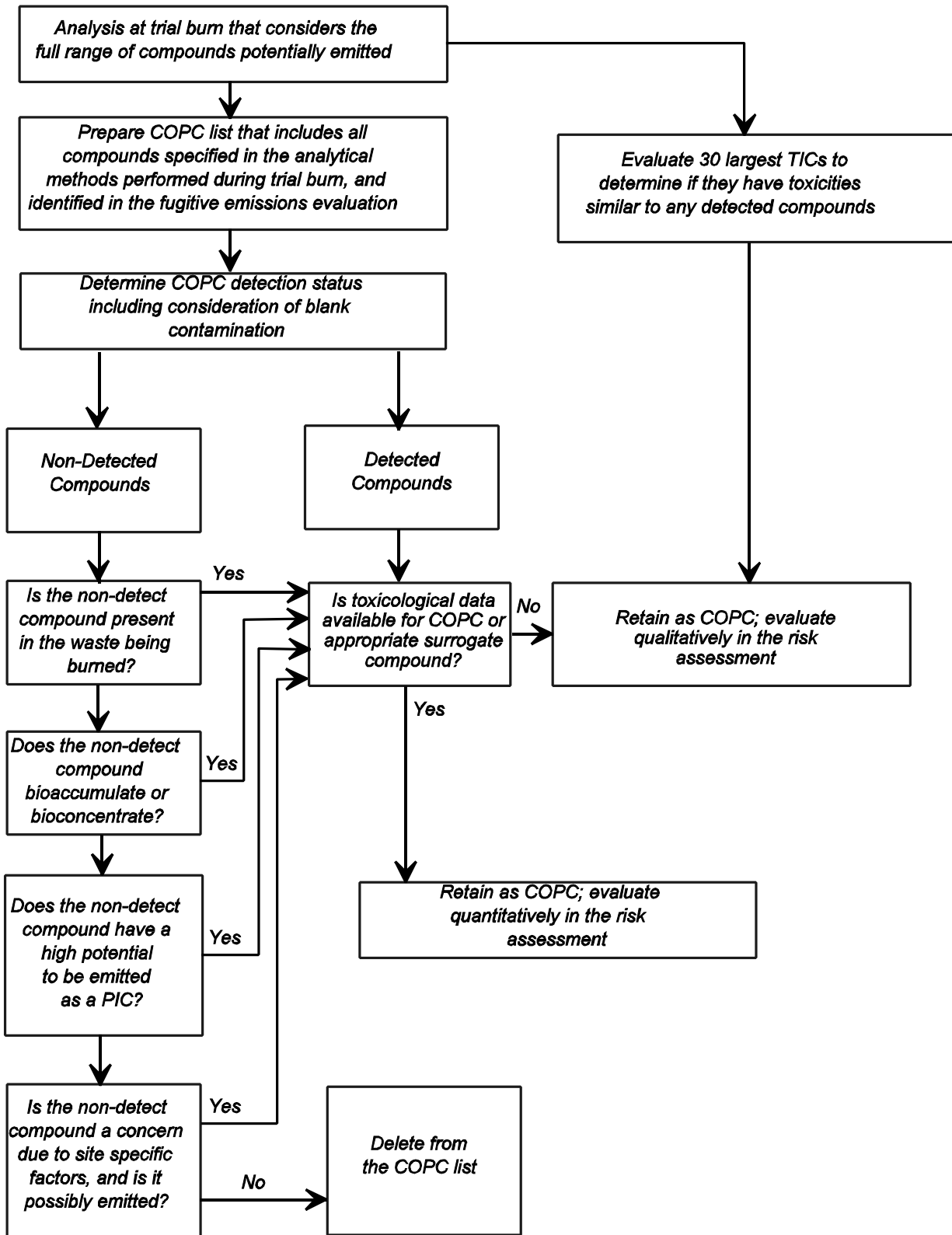
**Step 1:** Evaluate analytical data from the stack tests performed during the trial burn and compounds associated with fugitive emissions (see Section 2.2.5). Prepare a list which includes all the compounds specified in the analytical methods performed in the trial burn, and fugitive emission evaluation. Describe whether the compound was detected or not detected.

A detection in any one of the sample components (e.g., front half rinse, XAD resin, condensate, Tenax tube) in any run constitutes a detection for that specific compound. Evaluation of blank contamination results, included in the quality assurance (QA) data section of the trial burn report, should be considered when determining the non-detect status of the compounds (see Section 2.5).

**Step 2:** Evaluate the type of hazardous waste burned in the combustion unit—including all wastes that the unit will be permitted to burn—to determine whether any of the non-detect compounds should be retained for evaluation as COPCs because they are potentially present in the waste.

For example, if a facility is permitted to burn explosives which characteristically include nitroaromatic compounds, yet the stack test showed non-detect status for all nitroaromatic compounds, nitroaromatic compounds should still be evaluated in the risk assessment. This evaluation should also consider other materials fed to the combustion unit (e.g., raw materials or coal in a cement kiln). Regardless of the type of hazardous waste being burned in the combustion unit, every risk assessment should include PCDD/PCDFs and PAHs (the rationale for including these compounds is discussed in greater detail in Sections 2.3.1 and 2.3.2).

# COPC IDENTIFICATION



**Step 3:** Include as COPCs those compounds that are non-detect, but have a high potential to be emitted as PICs.

Although some compounds (nitroaromatics, phthalates, hexachlorobenzene, and petachlorophenol) have traditionally been automatically identified as PICs in previous U.S. EPA guidance, inclusion of these compounds should be based on consideration of potential to be emitted and waste feed composition (e.g., nitrogenated wastes, plastics, or highly chlorinated organic waste streams) (see Sections 2.3.4 through 2.3.6).

**Step 4:** Include as COPCs those compounds that are non-detect, but have a tendency to bioaccumulate or bioconcentrate. This includes organic chemicals with  $\log K_{ow}$  values equal to or greater than 4.0 (Connolly and Pederson 1987), and inorganic compounds with a whole-body  $BCF$  equal to or greater than 100.

U.S. EPA OSW understands that this step would not retain some nondetected compounds (such as VOCs with  $\log K_{ow}$  values less than 4.0) for further evaluation in the risk assessment and appears to provide the opportunity for detection limits for these compounds to be increased intentionally by the facility to escape the risk assessment process. However, U.S. EPA OSW anticipates that stack test data used in conducting the risk assessment will also be subject to evaluation in the human health risk assessment process, which would subsequently determine increased risk due to nondetected compounds with high detection limits. Therefore, the lowest achievable detection limits possible with standard U.S. EPA methods for all compounds are recommended, ensuring that the risk assessment process will result in the risk manager obtaining the information necessary to conclude that the facility has not potentially overlooked a serious risk.

**Step 5:** Evaluate the 30 largest tentatively identified compound (TIC) peaks obtained during gas chromatography (GC) analysis, to determine whether any of the TICs have toxicities similar to the detected compounds. If they do, consider surrogate toxicity data, as recommended for detected COPCs without toxicity information.

**Step 6:** Evaluate any compound that may be of concern due to other site-specific factors (e.g., community and regulatory concern, high background concentrations). Include as COPCs those compounds that (1) are a concern due to site-specific factors, and (2) may be emitted by the combustion unit.

If the compound in question does not have a reasonable potential of being present in the stack emissions, the risk assessment report should justify this assertion. This information will provide the risk manager with

the information necessary to evaluate potential for risk. By following Steps 1 through 6, the risk assessor will be able to identify COPCs from the typically exhaustive list of compounds tested in during the trial burn. To complete Step 4, log  $K_{ow}$  and  $BCF$  values for compounds typically identified in risk assessments as COPCs and listed at the beginning of this section are located in Appendices A and C, respectively.

The following subsections also focus on compounds that can drive risk assessments as indicated by past experience. These compounds include polychlorinated dibenzo(p)dioxins and dibenzofurans, polynuclear aromatic hydrocarbons, polychlorinated biphenyls, nitroaromatics, phthalates, hexachlorobenzene and pentachlorophenol, and metals. Volatile organic compounds are also discussed. Specific issues that affect the COPC identification process and evaluation of these compounds in the risk assessment are discussed. Because U.S. EPA's boiler and industrial furnace (BIF) regulations also regulate emission rates of PM and hydrochloric acid and chlorine gas, the risks associated with these compounds are also discussed. There is also a discussion of the emerging issues surrounding the class of compounds called "endocrine disruptors."

U.S. EPA OSW recognizes that, for many compounds, only limited information is available regarding potential effects. In addition, for some compounds for which effects have been identified, the relationship between dose and response may be poorly understood. U.S. EPA OSW advocates that the risk assessment use the sum of the available toxicological information and evaluate the uncertainty associated with these issues. As stated previously, toxicity benchmarks and information may change as additional research is conducted, permitting authorities should consult with the most current information before completing a risk assessment. Toxicity profiles for many of the compounds typically evaluated in ecological risk assessments are presented in Appendix H. U.S. EPA OSW prepared these profiles to promote consistency in risk assessments and to assist the uncertainty analysis.



### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Complete evaluation of hazardous wastes to be burned in the combustion unit
- Complete evaluation of any raw materials or primary fuels burned in the combustion unit
- Waste analysis procedures used to monitor the composition of hazardous waste feed streams
- Analytical data and calculations used to complete the COPC identification process

#### 2.3.1 Polychlorinated Dibenzo(p)dioxins and Dibenzofurans

Based on their combustion properties and toxicity, U.S. EPA OSW recommends that PCDDs and PCDFs should be included in every risk assessment. The general combustion properties and guidance for addressing toxicity of PCDDs and PCDFs are discussed in the following paragraphs and subsections, respectively.

One mode in which PCDDs and PCDFs form in dry APCSS is fly ash catalyzed reactions between halogens and undestroyed organic material from the furnace. PCDDs and PCDFs were first discovered as thermal decomposition products of polychlorinated compounds, including (1) the herbicide 2,4,5-T, (2) hexachlorophene, (3) PCBs, (4) pentachlorophenol, and (5) intermediate chemicals used to manufacture these compounds. In recent years, as chemical analytical methods have become more sensitive, additional sources of PCDDs and PCDFs have been identified, including (1) effluent from paper mills that use chlorine bleaches, and (2) combustion sources, including forest fires, municipal waste and medical incinerators, and hazardous waste combustion units. Duarte-Davidson et al. (1997) noted that the combustion of chlorine-containing materials in municipal solid waste is responsible for about two-thirds of the total annual emissions of newly formed TCDDs and TCDFs in the United Kingdom. In the United States, U.S. EPA (1998a) estimated that emissions of dioxin TEQs from municipal solid waste incinerators accounted for 37 percent of all emissions of dioxins into the environment in 1995.

PCDDs and PCDFs are formed at these combustion sources from the reaction of chlorine-containing chemicals and organic matter. Predicting the production of PCDDs and PCDFs in a specific situation is

difficult, because dechlorination, which produces PAHs from PCDDs and PCDFs, occurs under similar conditions. Recent studies (Addink et al. 1996; Environment Canada 1987; Fröese and Hutzinger 1996a, 1996b; Gullett et al. 1994; Kilgroe et al. 1991; Luijk et al. 1994; Robert 1994) have explored some of these complexities, including (1) the formation of PCDDs and PCDFs from simple organics (such as ethane) and complex organics (such as dibenzofuran), and (2) the catalysis of these organic compound reactions by various common metals, such as copper. Wikström et al. (1996) found that the form of chlorine—whether organic, as with chlorinated solvents, or inorganic, as with bleach and salts—has little effect on the quantity of PCDDs and PCDFs formed. However, their study found that the total concentration of chlorine is important. In particular, if the waste being burned exceeds 1 percent chlorine, the PCDD and PCDF formation rate increases significantly. The formation rate of PCDDs and PCDFs may also depend on the physical characteristics of the waste feed stream. Solid waste streams or high-ash-content liquid waste feed streams may increase particulate levels in the combustion system between the combustion unit and the APCs. The increased particulate levels provide additional surfaces for catalysis reactions to occur.

A review of currently available dioxin data for combustion units reveals that total PCDD/PCDF emission rates vary by more than 28-fold between different facilities, even though they use similar combustion units and APCs (U.S. EPA 1996h). Site-specific emission data are needed to enable completion of a more refined risk assessment at each combustion unit.

In evaluating fate-and-transport pathways, it is important to consider the chemical and physical properties of dioxins. In soil, sediment, and the water column, PCDDs and PCDFs are primarily associated with particulate and organic matter because of their high lipophilicity and low water solubility of the PCDDs and PCDFs. Evaluation of ambient air monitoring studies, in which researchers evaluated the partitioning of dioxin-like compounds between the vapor and particle phases, suggests that the higher chlorinated congeners (the hexa through hepta congeners) were principally sorbed to airborne particulates, whereas the tetra and penta congeners were significantly, if not predominantly, partitioned to the vapor phase (U.S. EPA 1994e). This finding is consistent with vapor/particle partitioning as theoretically modeled in Bidleman (1988). Dioxin-like compounds exhibit little potential for significant leaching or volatilization after they have been sorbed to particulate matter (U.S. EPA 1994e).

The guidance in Chapter 5 for modeling exposure to a COPC also applies generally to exposure assessment for PCDDs and PCDFs. However, procedures specific for these compounds should be followed because

congener-specific toxicity and bioaccumulation information is limited. As discussed below, exposure of receptors to PCDDs and PCDFs should be assessed using 2,3,7,8-TCDD toxicity equivalency factors (*TEF*) and 2,3,7,8-TCDD bioaccumulation equivalency factors (*BEF*) to convert the exposure media concentration of individual congeners to a 2,3,7,8-TCDD Toxicity Equivalent (TEQ).

U.S. EPA OSW is also aware of growing concern regarding the risks resulting from (1) fluorine- and bromine-substituted dioxins and furans, and (2) sulfur analogs of PCDDs and PCDFs. U.S. EPA guidance on considering these compounds as potential COPCs is discussed in Section 2.3.1.5.

### 2.3.1.1 Toxicity Equivalency Factors for PCDDs and PCDFs

There are 210 individual compounds or “congeners” of PCDDs and PCDFs. Evidence indicates that low levels of PCDD and PCDF congeners adversely affect ecological receptors, especially the 2,3,7,8-substituted congeners (U.S. EPA 1993p; Hodson et al. 1992; Walker and Peterson 1992). The 17 congeners containing chlorine substituents in at least the 2-, 3-, 7-, and 8-ring positions have been found to display dioxin-like toxicity (U.S. EPA 1993g; 1994h). Therefore, U.S. EPA OSW and other U.S. EPA guidance (1998; 1993h) recommend that all risk assessments include all PCDDs and PCDFs with chlorine molecules substituted in the 2, 3, 7, and 8 positions. In Appendix A, the 17 PCDD and PCDF congeners that should be evaluated in every risk assessment for potential risk are listed. Any other PCDD and PCDF congener identified as a COPC should be treated as an uncertainty (see Chapter 6).

As noted above, the toxicity of PCDDs and PCDFs is related to their structure and chlorine substitution pattern. The 17 listed congeners are known to share a common mechanism of toxicity involving binding to the Ah-receptor. Planar PCDDs and PCDFs are characteristic for high Ah-receptor affinity. Toxicity is also related to the chlorine substitution pattern, especially for chlorine atoms in the 2,3,7,8-positions. By extension, it is assumed that an additivity model may be used to characterize the toxicity of mixtures of these PCDDs and PCDFs. While these congeners share a similar toxicity mechanism, available information indicates that the toxicity of these PCDDs and PCDFs is congener-specific, resulting in a wide range of toxicities (U.S. EPA 1993p, World Health Organization [WHO] 1997). This has resulted in the development of TEFs for these 17 congeners to convert the exposure media concentration of individual congeners to a 2,3,7,8-TCDD TEQ; which are widely used to assess the risk of dioxin and dioxin-like compounds (U.S. EPA 1993p; WHO 1997).

The procedure used to assess risk on the basis of the relative toxicity of 2,3,7,8-TCDD, which is assumed the most toxic dioxin (U.S. EPA 1994f), assigns a TEF value to each congener relative to its toxicity in relation to 2,3,7,8-TCDD. For example, 2,3,7,8-TCDD has a TEF of 1.0, and the other PCDDs and PCDFs have TEF values between 0.0 and 1.0. To estimate the exposure media concentration, U.S. EPA OSW recommends that a risk assessment for PCDDs and PCDFs be completed using the congener-specific emission rates from the stack and fate and transport properties in the media concentration equations (see Chapter 3 and Appendix B) and food web equations (see Chapter 5 and Appendix F). For quantifying risk, the exposure media (e.g., may be sediment for evaluating risk to sediment community measurement receptors, or it may be the dose of one or more prey species for evaluating risk to class-specific guild measurement receptors) concentrations of the individual congeners should be converted to a 2,3,7,8-TCDD TEQ by multiplying by the congener-specific TEFs corresponding to the respective measurement receptor being evaluated. Use of the TEFs allows for the combined risk resulting from exposure to a mixture of the 17 dioxin-like congeners to be computed assuming that the risks are additive.

WHO (1997) recently convened a conference to discuss the derivation of TEFs for humans and wildlife. WHO (1997) discussed the compilation and review of relevant scientific information on the PCDD and PCDF toxicity to wildlife, and utilized this information to assist in identifying TEFs. The following table (see Table 2-3) lists congener-specific TEFs reported for fish, mammals, and birds (WHO 1997). U.S. EPA OSW believes that these conference proceedings reflect the best available information for screening the ecological risk of PCDDs and PCDFs. However, it should be noted that TEFs based on long term in-vivo studies should be used when available.

TABLE 2-3

POLYCHLORINATED DIBENZO-P-DIOXIN AND POLYCHLORINATED DIBENZOFURAN CONGENER  
 TOXICITY EQUIVALENCY FACTORS (TEFs) FOR FISH, MAMMALS, AND BIRDS

Congener	Receptor		
	Fish TEF	Mammal TEF	Bird TEF
2,3,7,8-TCDD	1.0	1.0	1.0
1,2,3,7,8-PeCDD	1.0	1.0	1.0
1,2,3,4,7,8-HxCDD	0.5	0.1	0.05
1,2,3,6,7,8-HxCDD	0.01	0.1	0.01
1,2,3,7,8,9-HxCDD	0.01	0.1	0.1
1,2,3,4,6,7,8-HpCDD	0.001	0.01	<0.001 <sup>a</sup>
OCDD	Not available	0.0001	Not available
2,3,7,8-TCDF	0.05	0.1	1.0
1,2,3,7,8-PeCDF	0.05	0.05	0.1
2,3,4,7,8-PeCDF	0.5	0.5	1.0
1,2,3,4,7,8-HxCDF	0.1	0.1	0.1
1,2,3,6,7,8-HxCDF	0.1	0.1	0.1
2,3,4,6,7,8-HxCDF	0.1	0.1	0.1
1,2,3,7,8,9-HxCDF	0.1	0.1	0.1
1,2,3,4,6,7,8-HpCDF	0.01	0.01	0.01
1,2,3,4,7,8,9-HpCDF	0.01	0.01	0.01
OCDF	0.0001	0.0001	0.0001

Notes:

<sup>a</sup> For exposure assessment, a value of 0.001, which estimates upper range of true value, should be used.

**Toxicity Equivalency Factors for Fish**

WHO (1997) reported the review of three scientific studies on the relative overt toxicity of PCDDs and PCDFs to fish from which TEFs could be determined. These included evaluation of rainbow trout sac fry mortality after egg injection (Walker and Peterson 1991; Zabel et al. 1995) and evaluation of rainbow trout sac fry mortality following waterborne exposure (Bol et al. 1989). WHO (1997) concluded that TEFs from the egg injection studies were more appropriate than the waterborne exposure study. WHO (1997)

also noted that since these TEFs were determined from the toxicity of each congener in relation to concentration in eggs, site-specific differences in exposure and bioavailability, and species-specific differences in toxicokinetic factors (deposition and metabolism) are accommodated. TEFs for PCDD and PCDF congeners in fish are presented in Table 2-3.

### Toxicity Equivalency Factors for Mammals

Current TEFs for mammals (for evaluating human health risk to PCDDs and PCDFs) are largely based on studies in rodents. To supplement existing rodent-based TEFs, WHO (1997) discussed a mink reproductive study (Tillitt et al. 1996) and a study which analyzed available data from mink reproductive toxicity tests (Leonard et al. 1994). WHO (1997) reported that the relative potencies of PCDD and PCDF congeners toward mink reproductive toxicity were similar to the rodent models. WHO (1997) also discussed recent information on *in vivo* tumor promotion and *in vivo* ethoxyresorufin-o-deethylase (EROD) induction potency. However, specific studies reporting this information were not cited. Based on their review, WHO (1997) reported updated TEFs for mammals, including new values for 1,2,3,7,8-PeCDD, OCDD, and OCDF. TEFs for PCDD and PCDF congeners in mammals are presented in Table 2-3.

### Toxicity Equivalency Factors for Birds

The experimental design of studies on the overt toxicity of PCDDs and PCDFs to birds precluded determination of the relative potency of these congeners. Other types of studies evaluated included embryo mortality following egg injection, *in vivo* biochemical effects following egg injection, biochemical effects in *in vitro* systems (Kennedy et al. 1996), and quantitative-structure activity relationship (QSAR) studies (Tysklind et al. 1995). The reviewed information indicated no significant differences between the *TEF* ranges for EROD induction and embryo mortality. Based on these results, WHO (1997) reported *TEFs* determined from EROD induction and QSAR studies. *TEFs* for PCDD and PCDF congeners in birds are presented in Table 2-3.

#### 2.3.1.2 Exposure Assessment for Community Measurement Receptors

To evaluate exposure of water, sediment, and soil communities to PCDDs and PCDFs, congener-specific concentrations in the respective media to which the community is exposed should be converted to a

2,3,7,8-TCDD *TEQ*; which allows for direct comparison to 2,3,7,8-TCDD toxicity benchmarks. A media-specific 2,3,7,8-TCDD *TEQ* is calculated and used in the exposure assessment because limited congener-specific toxicity information is available for community receptors (WHO 1997). The congener-specific concentrations in the media to which the community being evaluated is exposed, should be calculated consistent with the guidance presented in Chapters 4 and 5, and Appendix F, for assessing exposure of community measurement receptors to other COPCs. The concentration of each PCDD and PCDF congener in the media of exposure should then be multiplied by the congener-specific *TEF* for fish (see Table 2-3), and summed, to obtain the 2,3,7,8-TCDD *TEQ* (see Equation 2-3).

$$TEQ = \sum (C_{Mi} \cdot TEF_i) \quad \text{Equation 2-3}$$

where

<i>TEQ</i>	=	2,3,7,8-TCDD toxicity equivalence concentration ( $\mu\text{g/l}$ [water] or $\mu\text{g/kg}$ [soil or sediment])
$C_{Mi}$	=	Concentration of <i>i</i> th congener in abiotic media ( $\mu\text{g/L}$ [water] or $\mu\text{g/kg}$ [soil or sediment])
$TEF_i$	=	Toxicity equivalency factor (fish) for <i>i</i> th congener (unitless)

U.S. EPA OSW assumes that *TEFs* for fish accurately reflect the relative toxicity of PCDD and PCDF congeners to community receptors. This assumption is based on the requirement for congener-specific *TEFs* for this analysis, as an alternative to the overly conservative assumption that all congener concentrations in the media be evaluated directly as 2,3,7,8-TCDD. Evaluation of all congeners directly as 2,3,7,8-TCDD is assumed overly conservative based on the limited evidence of the Ah receptor or TCDD-like toxicity in invertebrates, and that invertebrates appear to be less sensitive to the toxic effects of dioxin-like compounds (WHO 1997). For the same reasons, *TEF* values specific to invertebrate have not been developed; requiring use of the surrogate *TEF* values for fish. The reported findings in WHO (1997) support the use of *TEFs*, in combination with chemical residue data, for the calculation of *TEQ* concentrations in various media, including animal tissues, soil, sediment, and water. However, in relation to the use of *TEFs* for abiotic media, it should be noted that the biological meaning of these values is obscure due to the fact that the assumed biological or toxicological effect is influenced by many physico-chemical factors before uptake occurs (WHO 1997). Nevertheless, *TEF* values can be used as relative measurements of concentrations within media.

Use of the *TEFs* allows for the combined risk resulting from exposure to a mixture of the 17 dioxin-like congeners to be computed assuming that the risks are additive. As discussed in Chapters 5 and 6, risk to the water, sediment, or soil community being evaluated is then subsequently estimated by comparing the media-specific 2,3,7,8-TCDD *TEQ* to the corresponding media-specific toxicity benchmark for 2,3,7,8-TCDD.

### 2.3.1.3 Exposure Assessment for Class-Specific Guild Measurement Receptors

To evaluate the exposure of class-specific guilds to PCDDs and PCDFs, congener-specific daily doses of all food items (i.e., media, plants, and animals) ingested by a measurement receptor should be converted to a 2,3,7,8-TCDD *TEQ* daily dose ( $DD_{TEQ}$ ); which allows for direct comparison to 2,3,7,8-TCDD toxicity benchmarks. The congener-specific daily doses of food items ingested by a measurement receptor should be calculated consistent with the guidance presented in Chapters 4 and 5, and Appendix F, for assessing exposure of class-specific guild measurement receptors to other COPCs. This includes the use of congener-specific media concentrations, congener-specific bioconcentration factors (*BCF*), and congener-specific food chain multipliers (*FCM*). The daily dose of each PCDD and PCDF congener ingested by a measurement receptor should then be multiplied by the congener-specific *TEFs* (see Table 2-3) that correspond to the respective measurement receptor, and summed, to obtain the  $DD_{TEQ}$ . Use of the *TEFs* allows for the combined risk resulting from exposure to a mixture of the 17 dioxin-like congeners to be computed assuming that the risks are additive. Following the general guidance provided in Chapters 5 and 6, risk to the class-specific guild being evaluated is then subsequently estimated by comparing the dose ingested term (represented by  $DD_{TEQ}$ ) of the measurement receptor to the receptor specific toxicity benchmark for 2,3,7,8-TCDD.

The  $DD_{TEQ}$  for each measurement receptor should be determined as indicated in the following equation:

$$DD_{TEQ} = \sum DD_i \cdot TEF_{(MeasurementReceptor)} \quad \text{Equation 2-4}$$

where

$$DD_{TEQ} = \text{Daily dose of 2,3,7,8-TCDD } TEQ \text{ } (\mu\text{g/kg BW/d})$$



$DD_i$	=	Daily dose of <i>i</i> th congener ( $\mu\text{g}/\text{kg BW}/\text{d}$ )
$TEF$	=	Toxicity equivalency factor (specific to measurement receptor) (unitless)

As noted above, the congener-specific daily doses ingested by the measurement receptor should be determined following guidance in Chapter 5 and using equations in Appendix F. These equations include the use of congener-specific *BCF* and *FCM* values. As discussed in Section 2.3.1.4, the limited availability of congener-specific *BCFs* requires that media to receptor *BCF* values for 2,3,7,8-TCDD be utilized in conjunction with congener-specific *BEF* values to obtain estimated congener-specific *BCF* values. The estimation of congener-specific *BCFs* and their resulting numeric values are further discussed in Appendices C and D. Calculation of a congener-specific daily dose also requires the use of congener-specific *FCMs*. Guidance on the appropriate use of *FCMs* in modeling exposure and congener-specific values are provided in Chapter 5 and Appendix A-2, respectively.

**2.3.1.4 Bioaccumulation Equivalency Factors**

As discussed in Section 2.3.1.3, modeling the exposure of PCDD and PCDF congeners through the food web requires the quantification of bioaccumulation potential. However, similar to the limited availability of congener-specific toxicity information, measured bioaccumulation data specific to each congener is also limited. Therefore, for use with *TEFs* in the development of wildlife water quality criteria for the Great Lakes, U.S. EPA (1995j) developed bioaccumulation equivalency factors (*BEFs*) as a measure of a congeners bioaccumulation potential relative to 2,3,7,8-TCDD. As indicated in Equation 2-5, *BEFs* are estimated as a ratio between each PCDD and PCDF congener-specific *BASF* to that of 2,3,7,8-TCDD (Lodge et al. 1994; U.S. EPA 1995j).

$$BEF_i = \frac{BSAF_i}{BSAF_{TCDD}} \quad \text{Equation 2-5}$$

where

$BEF_i$	=	Bioaccumulation equivalency factor for <i>i</i> th congener (unitless)
$BSAF_i$	=	Biota-sediment accumulation factor for <i>i</i> th congener (unitless)
$BSAF_{TCDD}$	=	Biota-sediment accumulation factor for 2,3,7,8-TCDD

*BEF* values reported by U.S. EPA (1995k) for the 17 PCDD and PCDF congeners are provided in Table 2-4. Although developed based on concentration data of PCDDs and PCDFs in sediment and surface water for application of *TEFs* in fish, U.S. EPA OSW assumes that these *BEFs* are applicable to other pathways and receptors. The estimation of PCDD and PCDF congener-specific *BCF* values using *BEFs* is indicated in Equation 2-5. Further discussion and resulting numeric values for congener-specific *BCFs* are provided in Appendices C and D.

$$BCF_i = BCF_{TCDD} \cdot BEF_i \quad \text{Equation 2-6}$$

where

- $BCF_i$  = Media-to-animal or media-to-plant bioconcentration factor for *i*th congener (L/kg [water], unitless [soil and sediment])
- $BCF_{TCDD}$  = Media-to-receptor BCF for 2,3,7,8-TCDD (L/kg [aquatic receptor], unitless [soil and sediment receptor])
- $BEF_i$  = Bioaccumulation equivalency factor for *i*th congener (unitless)

TABLE 2-4

PCDD AND PCDF BIOACCUMULATION EQUIVALENCY FACTORS (BEFs)

PCDD Congener	Bioaccumulation Equivalency Factor (unitless)	PCDF Congener	Bioaccumulation Equivalency Factor (unitless)
2,3,7,8-TCDD	1.0	2,3,7,8-TCDF	0.80
1,2,3,7,8-PeCDD	0.92	1,2,3,7,8-PeCDF	0.22
1,2,3,4,7,8-HxCDD	0.31	2,3,4,7,8-PeCDF	1.6
1,2,3,6,7,8-HxCDD	0.12	1,2,3,4,7,8-HxCDF	0.076
1,2,3,7,8,9-HxCDD	0.14	1,2,3,6,7,8-HxCDF	0.19
1,2,3,4,6,7,8-HpCDD	0.051	2,3,4,6,7,8-HxCDF	0.67
OCDD	0.012	1,2,3,7,8,9-HxCDF	0.63
		1,2,3,4,6,7,8-HpCDF	0.011
		1,2,3,4,7,8,9-HpCDF	0.39
		OCDF	0.016

Source: U.S. EPA 1995k

### 2.3.1.5 Fluorine, Bromine, and Sulfur PCDD/PCDF Analogs

U.S. EPA (U.S. EPA 1996l; 1996m) is currently evaluating the potential for the formation of (1) fluorine- and bromine-substituted dioxins and furans, and (2) sulfur analogs of PCDDs and PCDFs. Available information indicates that fluorinated dioxins and furans are not likely to be formed as PICs; however, the presence of free fluorine in the combustion gases may increase the formation of chlorinated dioxins (U.S. EPA 1996l). U.S. EPA OSW is not aware of any studies conducted to evaluate this relationship. Available information indicates the potential for the formation of brominated or chlorobrominated dioxins (U.S. EPA 1996d).

Although chlorinated dibenzothiophenes (the sulfur analogs of dibenzofurans) have been reported to form, no information is available to indicate the formation of chlorinated dioxin thioethers (the sulfur analogs of dibenzop[dioxins) (U.S. EPA 1996l). This may be because the carbon-oxygen bond is stronger than the carbon-sulfur bond, and the compound furan (which is part of the dibenzofuran structure) is more stable than thiophene (which is part of the dibenzothiophene structure) (U.S. EPA 1996n). Another possible

reason that chlorinated dioxin thioethers have not been observed is the potential instability of these compounds, which contain two carbon-sulfur bonds in the central ring of the structure (U.S. EPA 1996l). The likelihood of the formation or associated toxicity of these compounds is not currently well understood. Therefore, a quantitative toxicity assessment of fluorine, bromine, and sulfur analogs is not required for inclusion in the risk assessment report. Instead, the uncertainty section of the risk assessment report should discuss the potential for the formation of these analogs. It should be noted that there is currently no U.S. EPA approved method for the sampling or analysis of these dioxin analogs. The use of the method for total organics (see Section 2.2.1.3) is currently recommended to account for the potential presence of these compounds.

*TEF* values for brominated dioxins or furans have not been developed (U.S. EPA 1994e; WHO 1997). However, the toxicity of bromo- and chlorobromo-substituted dioxin analogs is comparable to that of chlorinated dioxins in short-term toxicity assays (U.S. EPA 1996m).

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Description of any combustion unit-specific operating conditions that may contribute to the formation of dioxins
- Any facility specific sampling information regarding PCDD and PCDF concentrations in air, soil, sediment, water, or biota
- Information regarding the concentration of sulfur, fluorine, and bromine in the combustion unit feed materials

### 2.3.2 Polynuclear Aromatic Hydrocarbons

Based on their combustion properties and toxicity, U.S. EPA OSW recommends that PAHs be included in every risk assessment. The following are commonly detected PAHs: benzo(a)pyrene (BaP); benzo(a)anthracene; benzo(b)fluoranthene; benzo(k)fluoranthene; chrysene; dibenz(a,h)anthracene; and indeno(1,2,3-cd)pyrene. The general combustion properties and guidance for addressing toxicity of PAHs are discussed in the following paragraph and subsection, respectively.

PAHs are readily formed in combustion units by either (1) dechlorination of other PAHs present in the waste feed or emissions stream (such as dioxins), or (2) the reaction of simple aromatic compounds (benzene or toluene) present in the waste feed or emissions stream. PAHs are well-known as the principal organic components of emissions from all combustion sources, including coal fires (soot), wood fires, tobacco smoke ("tar"), diesel exhaust, and refuse burning (Sandmeyer 1981). They are generally the only chemicals of concern in particulate matter (Manahan 1991), although the presence of metals and other inorganics in the waste feed can add other contaminants of concern. Therefore, based on the toxicity and combustion chemistry of PAHs, the absence of these compounds from stack emissions should always be confirmed via stack gas testing.

### **2.3.2.1 Exposure Assessment for PAHs**

U.S. EPA OSW recommends that individual PAH compounds be modeled from the emission source to media (i.e., soil, surface water, soil) and plants, using compound-specific emission rates and fate and transport properties, as required in the media concentration equations (see Chapter 3 and Appendix B). Evaluation of exposure of community and class-specific guild measurement receptors to individual PAHs, should be conducted consistent with guidance provided in Chapters 4 and 5, and utilizing equations in Appendix F.

### **2.3.3 Polychlorinated Biphenyls**

The use and distribution of polychlorinated biphenyls (PCBs) were severely restricted in the United States in the late 1970s—with additional bans and restrictions taking effect over the next decade (ATSDR 1995d). PCBs were produced commercially by the reaction of the aromatic hydrocarbon biphenyl with chlorine gas in the presence of a suitable catalyst, generally ferric chloride or another Lewis acid (ATSDR 1995d). The degree of chlorination was controlled by manipulation of the reaction conditions, including temperature, pressure, and the ratio of the reactants (Erickson 1992; Grayson 1985).

The most commercially useful property of PCBs is that they are chemically stable in relatively adverse conditions, such as a temperature of several hundred degrees in an oxygen-containing atmosphere; the more chlorinated congeners are more resistant to reaction. Therefore, destruction of PCBs by combustion

generally requires conditions of high temperatures (at least 1,200 °C) and an extended contact time (more than 2 seconds) in that temperature with adequate oxygen (Erickson 1992).

Limited data and studies, including laboratory and field, show that PCBs may be formed from the combustion of hazardous waste. Stack tests performed in U.S. EPA Region 10 on a boiler and an incinerator burning waste with 0.07 and 1.4 percent chlorine, respectively, confirmed the presence of PCBs in the stack gases (Kalama Chemical, Inc. 1996; Idaho National Engineering Laboratory 1997). The concentration of detected coplanar PCBs (see definition in Section 2.3.3.1) found in the boiler stack gas was 0.55 ng/dscm @ 7% O<sub>2</sub> at low temperature conditions (1,357° F) and 1.12 ng/dscm @ 7% O<sub>2</sub> at high temperature conditions (1,908° F). The concentration of total PCBs detected in the incinerator stack gas was 211 ng/dscm @ 7% O<sub>2</sub> at low temperature conditions (1,750° F) and 205 ng/dscm @ 7% O<sub>2</sub> at high temperature conditions (2,075° F). PCBs with more than four chlorines comprised 51 percent of the total PCBs in the low temperature test and 59 percent of the total PCBs in the high temperature test.

Other laboratory studies suggest the possible formation of PCBs as PICs from the combustion of hazardous waste with a high chlorine content. Bergman et al. (1984) heated samples of two chlorinated paraffins (CP) in conditions similar to incinerator conditions. A CP containing 70 percent chlorine did produce PCB (up to 0.3 percent of the amount of CP), as well as chlorinated benzenes (up to 0.5 percent), chlorinated toluenes (up to 0.6 percent), and chlorinated naphthalenes (up to 0.2 percent). Similar treatment of a CP containing 59 percent chlorine produced only chlorinated benzenes (up to 0.1 percent of the amount of CP, based on a detection limit of 0.0005 percent for each individual compound) and almost all of those (about 90 percent) were monochlorobenzene (Bergman et al. 1984). This study indicates that the combustion of highly chlorinated (60 percent or greater chlorine) wastes can produce PCBs.

PCBs should automatically be included as COPCs for combustion units that burn PCB-contaminated wastes or waste oils, highly variable waste streams such as municipal and commercial wastes for which PCB contamination is reasonable, and highly chlorinated waste streams.

Due to the toxicity and uncertainties associated with combustion chemistries the permitting authority may choose to confirm that the absence of these compounds from stack emissions via stack gas testing for units burning hazardous wastes.

### 2.3.3.1 Exposure Assessment for PCBs

Previous U.S. EPA combustion risk assessment guidance (1994b; 1994d; 1994c; 1994l) has recommended that all PCB congeners (209 different chemicals) be treated in a risk assessment as a mixture having a single toxicity. This recommendation was based on the U.S. EPA drinking water criteria for PCBs (U.S. EPA 1988).

However, since the compilation of U.S. EPA (1988), additional research on PCBs has been reported. The most important result of this research is the demonstration that some of the moderately chlorinated PCB congeners can have dioxin-like effects (U.S. EPA 1992f; U.S. EPA 1994i; ATSDR 1995d; WHO 1997).

WHO (1997) recently convened a conference to discuss the derivation of *TEFs* for humans and wildlife. Conference participants discussed the compilation and review of relevant scientific information on the PCB toxicity to wildlife, and utilized this information to assist in identifying *TEFs* for congeners that can have dioxin-like effects. U.S. EPA OSW believes that these conference proceedings reflect the best available information for screening the ecological risk of PCBs. The following table (see Table 2-5) lists PCB *TEFs* reported for fish, mammals, and birds (WHO 1997).

TABLE 2-5

PCB CONGENER TOXICITY EQUIVALENCY FACTORS (TEFs) FOR FISH, MAMMALS, AND BIRDS

PCB Congener	Receptor		
	Fish TEF	Mammals TEF	Birds TEF
3,4,4',5-TCB	0.0005	0.0001	0.1
3,3',4,4'-TCB	0.0001	0.0001	0.05
3,3',4,4',5-PeCB	0.005	0.1	0.1
3,3',4,4',5,5'-HxCB	0.00005	0.01	0.001
2,3,3',4,4'-PeCB	<0.000005	0.0001	0.0001
2,3,4,4',5-PeCB	<0.000005	0.0005	0.0001
2,3',4,4',5-PeCB	<0.000005	0.0001	0.00001
2',3,4,4',5-PeCB	<0.000005	0.0001	0.00001
2,3,3',4,4',5-HxCB	<0.000005	0.0005	0.0001
2,3,3',4,4',5-HxCB	<0.000005	0.0005	0.0001
2,3',4,4',5,5'-HxCB	<0.000005	0.00001	0.00001
2,3,3',4,4',5,5'-HpCB	<0.000005	0.0001	0.00001
2,2',3,3',4,4',5'-HpCB	Not Available	Not Available	Not Available
2,2',3,4,4',5,5'-HpCB	Not Available	Not Available	Not Available

Source: WHO (1997)

The listed congeners have four or more chlorine atoms with few substitutions in the ortho positions (positions designated 2, 2', 6, or 6'). They are sometimes referred to as coplanar PCBs, because the rings can rotate into the same plane if not blocked from rotation by ortho-substituted chlorine atoms. In this configuration, the shape of the PCB molecule is very similar to that of a PCDF molecule. Studies have shown that these dioxin-like congeners can then react with the aryl hydrocarbon receptor; this same reaction is believed to initiate the adverse effects of PCDDs and PCDFs. Additional congeners are suspected of producing similar reactions, but there is not yet enough data to derive *TEF* values for them.



High resolution gas chromatograph test methods (e.g., draft Method 1668), available at most commercial laboratories with dioxin/furan analytical capabilities, should be used to identify the specific concentration of individual coplanar PCBs in stack gas. U.S. EPA OSW recommends that permitting authorities estimate risks to community and class-specific guild measurement receptors from coplanar PCBs by computing a *TEQ* for PCBs, and then comparing to the appropriate toxicity benchmark for 2,3,7,8-TCDD.

The specific guidance, provided in Sections 2.3.1.2 and 2.3.1.2 for evaluating exposure to PCDDs and PCDFs, should be followed in evaluating exposure to dioxin-like PCBs. However, TEF values listed in Table 2-5 should be utilized in the *TEQ* calculations. Also, since congener-specific fate and transport and bioaccumulation data are not available for each of the PCBs listed in Table 2-5, U.S. EPA OSW recommends that the fate and transport properties for Aroclor 1254 be used in the modeling. This approach is reasonable because approximately 77 percent of Aroclor 1254 is composed of PCB congeners with more than 4 chlorines (Hutzinger et al. 1974).

In addition to the coplanar (dioxin-like) PCB congeners, the remaining PCBs should also be evaluated in the risk assessment consistent with the guidance provided in Chapters 4 and 5. When evaluating PCB mixtures containing isomers with more than 4 chlorines in quantities greater than 0.5 percent of the total PCBs, U.S. EPA OSW recommends that the fate and transport properties for Aroclor 1254 be used in the modeling. As discussed above for evaluating coplanar PCBs, this approach is reasonable because approximately 77 percent of Aroclor 1254 is composed of PCB congeners with more than 4 chlorines (Hutzinger et al. 1974). When assessing risks from PCB mixtures which contain less than 0.5 percent of PCB congeners with more than 4 chlorines, U.S. EPA OSW recommends that the fate and transport properties of Aroclor 1016 be used in the modeling. This approach is reasonable because approximately 99 percent of Aroclor 1016 is comprised of PCB congeners with 4 or less chlorines (Hutzinger et al. 1974).

#### 2.3.4 Nitroaromatics

Careful consideration should be made before the automatic inclusion of nitroaromatic organic compounds, including 1,3-dinitrobenzene; 2,4-dinitrotoluene; 2,6-dinitrotoluene; nitrobenzene; and pentachloronitrobenzene, in risk assessments for combustion units. These compounds or close relatives (such as toluenediamine [TDA] and toluene diisocyanate [TDI]—derivatives of dinitrotoluene) are typically associated with explosives and other highly nitrogenated hazardous wastes. Dinitrotoluene is used to make

two products: trinitrotoluene and TDA. TDA is, in turn, used to make TDI, which readily reacts with water and is, therefore, very unstable at ambient conditions; TDI is typically reacted with a polyol to form polyurethane (PU) plastics.

Combustion properties of these nitroaromatic compounds indicate that they will not be formed as PICs if they are not present in the waste feed stream, mainly because of the thermodynamic and chemical difficulty of adding a nitro group to an aromatic. The process requires that (1) nitronium ions be generated, and (2) an aromatic ring be reacted with the nitronium ion, resulting in the attachment of the nitronium ion to the ring. This reaction process is not likely to occur in a hazardous waste combustion unit because (1) the reaction is typically carried out by using a “nitrating acid” solution consisting of three parts concentrated nitric acid to one part sulfuric acid, and (2) nitronium ions are not usually formed in a combustion unit environment (if they are, a further thermodynamically favorable reaction will occur, thereby eliminating the nitronium ion) (Hoggett et al. 1971; Schofield 1980; March 1985).

Nitroaromatics should be included as COPCs if the hazardous waste feed streams include nitroaromatic compounds or close relatives (TDA and TDI). Also, combustion of feed streams containing unusually high amounts of fuel-bound nitrogen (greater than 5 percent) may lead to increased levels of nitrogenated PICs (U.S. EPA 1994c). Examples of waste feeds identified include heavy distillation fractions and bottoms streams from the production of coal tars and petroleum distillation. Combustion conditions most likely to result in nitrogenated PICs are associated with premature quenching of the primary flame—resulting from low temperature or excess air in the primary combustion chamber of the unit (U.S. EPA 1994c). Sampling for hydrogen cyanide is also recommended (U.S. EPA 1994c).

### 2.3.5 Phthalates

Careful consideration should be made before the automatic inclusion of phthalates, including bis(2-ethylhexyl)phthalate (BEHP) and di(n)octyl phthalate (DNOP), in risk assessments for combustion units. Among all phthalate plasticizers, BEHP—also referred to as di(2-ethylhexyl)phthalate or dioctyl phthalate—is produced in the largest volume; it is used in the manufacturing of polyvinyl chloride, which is the most widely produced plastic. DNOP is a plasticizer that is produced in large volumes and is used in the manufacture of plastics and rubber materials. Because plastics have become so widely used in society, phthalate plasticizers such as BEHP and DNOP have become widely distributed in food, water, and the

atmosphere (Howard 1990). Phthalate plasticizers are commonly found in the environment and are practically impossible to avoid, especially at the trace concentrations that modern analyses can detect.

Phthalates are synthesized by reacting alcohol with phthalic anhydride in the presence of an acidic catalyst in a nonaqueous solvent (ATSDR 1993; ATSDR 1995b). Phthalates and their predecessors are readily combusted compounds, as indicated by their flash points of 150 to 225 °C (NIOSH 1994). There is no apparent mechanism for phthalate PICs to be formed by the combustion of other chemical compounds. Therefore, phthalates are very unlikely to be emissions from a combustion unit, although some degradation products, such as PAHs, are likely to be emitted when phthalates are included in the waste feed. However, facilities that burn plastics or materials with phthalate plasticizers should carefully consider the potential for phthalate plasticizers to exist in the stack gas emissions due to incomplete combustion.

The evaluation of phthalate plasticizers in risk assessments should not be automatically discounted due to the toxicity and bioaccumulative potential of these compounds. Moreover, the uncertainties associated with combustion chemistry suggest that the absence of these compounds from stack emissions should always be confirmed via stack gas testing rather than process knowledge or waste feed characterization data. U.S. EPA OSW recommends that careful consideration should be given to including phthalates as COPCs based on the information presented above.

### **2.3.6 Hexachlorobenzene and Pentachlorophenol**

Careful consideration should be made before the automatic inclusion of hexachlorobenzene and pentachlorophenol in risk assessments for combustion units. Hexachlorobenzene and pentachlorophenol, like all chlorinated aromatics, are synthesized by the reaction of elemental chlorine with the parent aromatic (Deichmann and Keplinger 1981; Grayson 1985). The addition of the first chlorine atom to the benzene or phenol molecule is rapid, but further chlorination becomes progressively more difficult, requiring ferric chloride or another Lewis acid catalyst to complete the reaction (March 1985); therefore, these chlorinated compounds are difficult to make under controlled conditions. Hexachlorobenzene, but not pentachlorophenol, has been reported in emissions from the combustion of municipal solid waste and from other processes (such as the chlorination of wood pulp) that also produce PCDDs and PCDFs (ATSDR 1994a; ATSDR 1994b). Hexachlorobenzene is an impurity in pentachlorophenol while pentachlorophenol is formed from hexachlorobenzene in some factories (ATSDR 1994a; ATSDR 1994b). The combustion

properties of these chlorinated compounds indicate that they are not likely to be formed as PICs if they are not present in the waste feed stream.

Hexachlorobenzene and pentachlorophenol should be included as COPCs for units that burn waste feeds containing hexachlorobenzene and pentachlorophenol, wood preservatives, pesticides, and highly variable waste streams such as municipal solid waste. However, precluding these compounds from analytical testing during the trial burn based on process knowledge and waste feed characterization is not recommended. Because PCDDs and PCDFs can be formed from fly ash-catalyzed reactions between halogens and undestroyed organic material from the furnace, U.S. EPA guidance (U.S. EPA 1993h; 1994d) has recommended that potential precursor compounds be included in the risk assessment and trial burn (see Section 2.3). These precursor compounds may include chlorinated phenols (such as pentachlorophenol) and chlorinated aromatics (such as hexachlorobenzene). Furthermore, the toxicity and uncertainties associated with combustion chemistry suggest that the absence of these compounds from stack emissions should always be confirmed via stack gas testing. U.S. EPA OSW recommends that careful consideration should be given to including hexachlorobenzene and pentachlorophenol as COPCs based on the information presented above.

### **2.3.7 Metals**

U.S. EPA OSW recommends that the following inorganic substances be considered for evaluation in the risk assessment: aluminum, antimony, arsenic, barium, beryllium, cadmium, hexavalent chromium, copper, lead, mercury (elemental and divalent), nickel, selenium, silver, thallium, and zinc. All of these substances, except aluminum, copper, nickel, selenium, and zinc, are regulated by 40 CFR Part 266, Subpart H (the BIF regulations). In the case of metals not regulated by the BIF regulations, U.S. EPA has recommended that these metals be evaluated, to determine whether additional terms and conditions should be incorporated into the permit, by using U.S. EPA's omnibus authority provided under 40 CFR Part 270.32(b)(2) (U.S. EPA 1992c). Facilities may also apply the BIF regulation Tier I assumptions, that assume all metals in the waste feed pass through the combustion unit and APCS and are passed through to the emission stream (U.S. EPA 1992e).

It should be noted, that the presence of metals in the combustion unit's feed stream is not required for inclusion in the risk assessment. Although metals cannot be formed as PICs, U.S. EPA OSW is aware of combustion units with metal emissions resulting from waste feed leaching of stainless steel feed piping.

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Waste feed, raw material, and secondary fuel stream analytical data
- Metal emission rate sampling data or assumptions based on waste feed data
- Explanations for excluding specific metals from evaluation in the risk assessment

The following subsections provide additional information regarding U.S. EPA-recommended procedures for evaluating metals—chromium, mercury, and nickel—that may be specifically altered during the combustion process or require specific considerations in the risk assessment.

##### 2.3.7.1 Chromium

The oxidation state of chromium is a crucial issue in evaluating the toxicity of this metal and the risks associated with exposure. Hexavalent chromium ( $\text{Cr}^{+6}$ ) is the most toxic valence state of chromium. Trivalent chromium ( $\text{Cr}^{+3}$ ), a commonly found less oxidized and toxic form of chromium, is more commonly found in the environment. U.S. EPA (1990c; 1990d) has indicated that chromium emitted from a combustion unit is not likely to be in the hexavalent form; however, there is not sufficient evidence to reliably estimate the partitioning of chromium emissions into these two valence states. Also, media-specific chromium speciation information is often difficult to obtain within the scope of a screening risk assessment. However, U.S. EPA OSW recognizes that chromium may exist partially or in some cases entirely as trivalent chromium in various media. Therefore, unless site-sampling or process-specific information is provided to support a less conservative approach, the worst-case assumption—that 100 percent of the facility chromium emissions are in the hexavalent form—should be used as the initial assumption that all exposure is to hexavalent chromium.

The assumption that receptors are exposed to hexavalent chromium should be maintained in the absence of site specific data. However, permitting authorities may prepare supplemental calculations (that is, in addition to the site-specific data described above) considering chromium speciation at the points of potential exposure.

### **2.3.7.2 Mercury**

Consistent with previous U.S. EPA combustion risk assessment guidance (U.S. EPA 1993h, 1994d, 1994c, 1994l), U.S. EPA OSW recommends that mercury be evaluated as COPCs in the risk assessment. Air emissions of mercury contribute to local, regional, and global deposition. The U.S. Congress explicitly found this to be the case and required U.S. EPA to prioritize maximum achievable control technology (MACT) controls for mercury (U.S. Congress 1989).

Anthropogenic mercury releases are thought to be dominated on the national scale by industrial processes and combustion sources that release mercury into the atmosphere (U.S. EPA 1997b). Stack emissions containing mercury include both vapor and particulate forms. Vapor mercury emissions are thought to include both elemental ( $\text{Hg}^0$ ) and oxidized (e.g.,  $\text{Hg}^{+2}$ ) chemical species, while particulate mercury emissions are thought to be composed primarily of oxidized compounds due to the relatively high vapor pressure of elemental mercury (U.S. EPA 1997b). While coal combustion is responsible for more than half of all emissions of mercury in the U.S. anthropogenic sources, the fraction of coal combustion emissions in oxidized form is thought to be less than from waste incineration and combustion (U.S. EPA 1997b).

The analytical methods for mercury speciation of exit vapors and emission plumes are being refined, and there is still controversy in this field. Chemical reactions occurring in the emission plume are also possible. The speciation of mercury emissions is thought to depend on the fuel used, flue gas cleaning, and operating temperatures. The exit stream is thought to range from almost all divalent mercury to nearly all elemental mercury; with true speciation of mercury emissions from the various source types still uncertain and thought to vary, not only among source types, but also for individual plants as feed stock and operating conditions change (U.S. EPA 1997b). Most of the total mercury emitted at the stack outlet is found in the vapor phase; although exit streams containing soot or particulate can bind up some fraction of the mercury (U.S. EPA 1997b). Total mercury exiting the stack is assumed to consist of elemental and divalent species,

with no emissions of methylmercury assumed. The divalent fraction is split between vapor and particle-bound phases (Lindqvist et al. 1991). Much of the divalent mercury is thought to be mercuric chloride ( $\text{HgCl}_2$ ) (U.S. EPA 1997b); this is particularly the case for the combustion of wastes containing chlorine.

It should be noted that data on mercury speciation in emissions exiting the stack is very limited, as well as, the behavior of mercury emissions close to the point of release has not been extensively studied. This results in a significant degree of uncertainty implicit in modeling of mercury emissions. Additional examples of uncertainties include the precision of measurement techniques, estimates of pollution control efficiency, limited data specific to source class and activity level. Discussions of uncertainty and sensitivity analyses of several of the assumptions used in the modeling of mercury emissions are presented in the *Mercury Study Report to Congress* (U.S. EPA 1997b).

### Phase Allocation and Speciation of Mercury Exiting the Stack

As discussed above, stack emissions are thought to include both vapor and particle-bound forms; and speciated as both divalent and elemental mercury. Based on review of mercury emissions data presented for combustion sources in U.S. EPA (1997b) and published literature (Peterson et al. 1995), estimates for the percentage of vapor and particle-bound mercury emissions range widely from 20 to 80 percent. Therefore, at this time U.S. EPA OSW recommends a conservative approach that assumes phase allocation of mercury emissions from hazardous waste combustion of 80 percent of the total mercury in the vapor phase and 20 percent of total mercury in the particle-bound phase. This allocation is:

- Consistent with mercury emissions speciation data for hazardous waste combustion sources reported in literature (Peterson et al. 1995); and
- Believed to be reasonably conservative, since it results in the highest percentage of total mercury being deposited in proximity to the source, and therefore, indicative of the maximum exposure.

As indicated in the global cycle mass percentages in Figure 2-4, mercury exits the stack in both the elemental and divalent vapor forms. Based on U.S. EPA (1997b), a vast majority of mercury exiting the stack does not readily deposit and is transported outside of the U.S. or vertically diffused to the free atmosphere to become part of the global cycle (see Figure 2-4). The divalent form emitted, either in the

vapor phase or particle-bound, are thought to be subject to much faster atmospheric removal than elemental mercury (Lindberg et al. 1992; Peterson et al. 1995; and Shannon and Voldner 1994). In addition, vapor phase divalent mercury is thought to be more rapidly and effectively removed by both dry and wet deposition than particle-bound divalent mercury, as a result of the reactivity and water solubility of vapor divalent mercury (Lindberg et al. 1992; Peterson et al. 1995; and Shannon and Voldner 1994).

### **Vapor Phase Mercury**

As illustrated in Figure 2-4, of the 80 percent total mercury in the vapor phase, 20 percent of the total mercury is in the elemental vapor form and 60 percent of the total mercury is in the divalent vapor form (Peterson et al. 1995). A vast majority (assumed to be 99 percent) of the 20 percent vapor phase elemental mercury does not readily deposit and is transported outside of the U.S. or is vertically diffused to the free atmosphere to become part of the global cycle (U.S. EPA 1997b). Only a small fraction (assumed to be one percent) of vapor-phase elemental mercury either is adsorbed to particulates in the air and is deposited or converted to the divalent form to be deposited (assumed to be deposited as elemental mercury, see Figure 2-4). Of the 60 percent vapor phase divalent mercury, about 68 percent is deposited and about 32 percent is transported outside of the U.S. or is vertically diffused to the free atmosphere to become part of the global cycle (U.S. EPA 1997b).

### **Particle-bound Mercury**

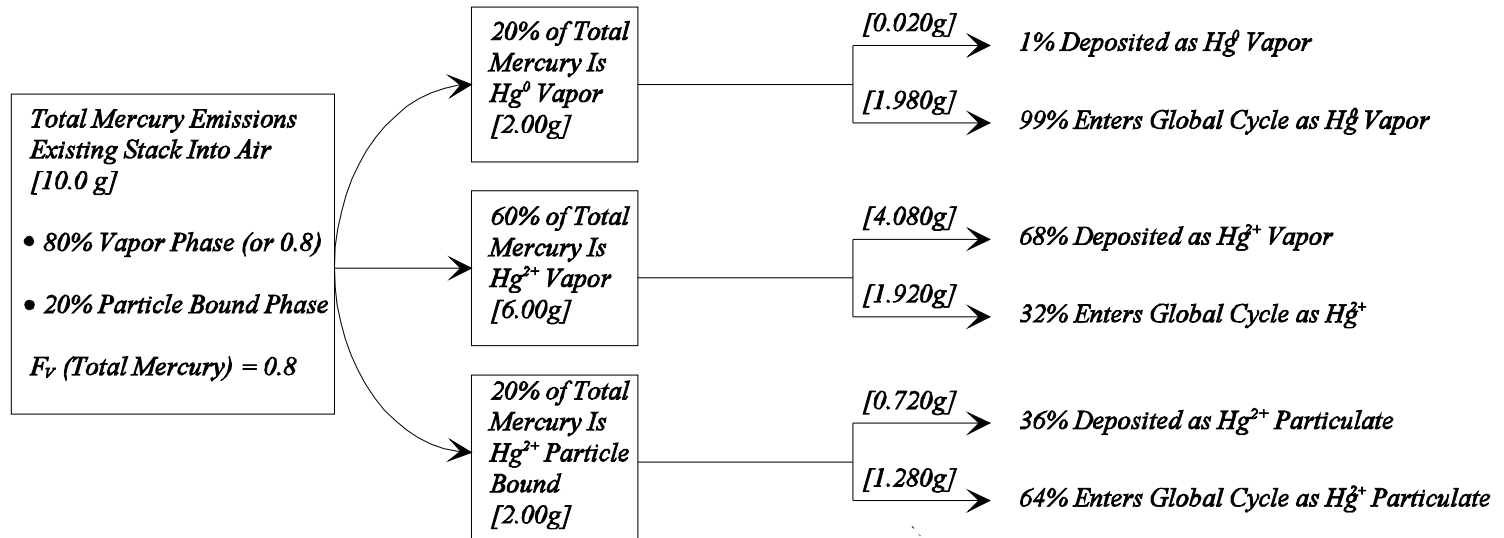
Of the 20 percent of the total mercury that is particle-bound, 99 percent (assumed to be 100 percent in Figure 2-4) is in the divalent form. U.S. EPA (1997b) indicates that only 36 percent of the particle-bound divalent mercury is deposited, and the rest is either transported outside of the U.S. or is vertically diffused to the free atmosphere to become part of the global cycle.

### **Deposition and Modeling of Mercury**

Consistent with U.S. EPA (1997b) and as shown in Figure 2-4, it is assumed that deposition to the various environmental media is entirely divalent mercury in either the vapor or particle-bound form. Without consideration of the global cycle, mercury speciations will result in 80 percent of the total mercury emitted being deposited as divalent mercury and the remaining 20 percent being deposited as elemental mercury.



**FIGURE 2-4**  
**PHASE ALLOCATION AND SPECIATION**  
**OF MERCURY IN AIR**



**LEGEND**

$Hg^0$  - Elemental Mercury  
 $Hg^{2+}$  - Divalent Mercury  
 [ ] - Example Mass Allocation

Without Consideration of Global Cycle

• 80% of Total Mercury Emitted is Deposited as  $Hg^{2+}$  [(6g + 2g) / 10g]

• 20% of Total Mercury Emitted is Deposited as  $Hg^0$  [2g / 10g]

Calculated  $F_V$

•  $F_V (Hg^{2+}) = [6g / (6g + 2g)] = 0.75$

•  $F_V (Hg^0) = [2g / 2g] = 1.0$

With Consideration of Global Cycle

• 48% of Total Mercury Emitted is Deposited as  $Hg^{2+}$  [(4.08g + 0.72g) / 10g]

• 0.2% of Total Mercury Emitted is Deposited as  $Hg^0$  [0.02g / 10g]

Calculated  $F_V$

•  $F_V (Hg^{2+}) = [4.08g / (4.08g + 0.72g)] = 0.85$

•  $F_V (Hg^0) = [0.02g / (0.02g + 0g)] = 1.0$

Compound Specific Emission Rate  $Q$

• Actual  $Q (Hg^{2+}) = 48% * Q$  (Total Mercury)

• Actual  $Q (Hg^0) = 0.2% * Q$  (Total Mercury)

U.S. EPA OSW recommends utilizing the percentages provided in U.S. EPA (1997b) to account for the global cycle, the percentage of total mercury deposited is reduced to a total of 48.2 percent (40.8 percent as divalent vapor, 7.2 percent as divalent particle-bound, and 0.2 percent as elemental vapor). As discussed in Appendix A-2, these speciation splits result in fraction in vapor phase ( $F_v$ ) values of 0.85 (40.8/48.2) for divalent mercury, and 1.0 (0.2/0.2) for elemental mercury. Also, to account for the remaining 51.8 percent of the total mercury mass that is not deposited, the deposition and media concentration equations (presented in Appendix B), multiply the compound-specific emission rate ( $Q$ ) for elemental mercury by a default value of 0.002; and divalent mercury by a default value of 0.48.

Consistent with U.S. EPA (1997b) and as shown in Figure 2-4, it is assumed that deposition to the various environmental media is entirely divalent mercury in either the vapor or particle-bound form. Deposited divalent mercury is also considered as a source of methyl mercury, which is assumed as a media-specific percentage of the total mercury deposited.

Also, only a small fraction (assumed to be one percent) of elemental mercury is in the vapor phase and is assumed to be deposited in its original form. Therefore, any resulting exposure to elemental mercury is considered to be much less significant, and will not be considered in the pathways of the ecological risk assessment.

Appendix A-2 provides the parameter values specific to the various forms of mercury, and Appendix B provides media concentration equations for modeling mercury through the exposure pathways assuming steady-state conditions.

### **Methylation of Mercury**

The net mercury methylation rate (the net result of methylation and demethylation) for most soils appears to be quite low; with much of the measured methyl mercury in soils potentially resulting from wet deposition (U.S. EPA 1997b). Consistent with U.S. EPA (1997b), a fraction of the divalent mercury that is deposited is assumed to speciate to organic mercury (methyl mercury) in soil. In soil, 98 percent of total mercury is assumed to be divalent mercury and the remaining mass as methyl mercury (U.S. EPA 1997b). A significant and important exception to mercury methylation rate being low in soils appears to be wetland soils. Wetlands appear to convert a small but significant fraction of the deposited mercury into methyl mercury; which can be

exported to nearby water bodies and potentially bioaccumulated in the aquatic food chain (U.S. EPA 1997b). Therefore, the assumed percentage of methyl mercury in wetland soils may be higher than the 2 percent assumed for non-wetland soils, and may closer approximate the 15 percent assumed for sediments.

Both watershed erosion and direct atmospheric deposition can be important sources of mercury to a water body (U.S. EPA 1997b). There appears to be a great deal of variability in the processing of mercury among water bodies. This variability is primarily a result of the characteristically wide range of chemical and physical properties of water bodies that influence the levels of methylated mercury. Some of the mercury entering the water body is methylated predominately through biotic processes (U.S. EPA 1997b). In the absence of modeling site-specific water body properties and biotic conditions, consistent with U.S. EPA (1997b), U.S. EPA OSW recommends 85 percent of total mercury in surface water is assumed to be divalent mercury and the remaining mass as methyl mercury.

For most environmental systems, the literature suggests that various physical and chemical conditions may influence the methylation of mercury. Consideration of these conditions, and the magnitude of their potential impact, may be required in some cases to assess the potential for over or under predicting mercury methylation in media and subsequent biotransfer up the food chain. Due to the extreme variance between environmental systems modeled, and at times disagreement, identified in literature reviewed regarding the quantitative influence of specific conditions on methylation, U.S. EPA OSW recommends that extensive research of literature, specific to the conditions prevalent at the site, be conducted before application and deviation from the conservative assumptions recommended above. The following table summarizes the qualitative effect some of the physical and chemical conditions, as reported in literature, may have on methylating:

Physical or Chemical Condition	Qualitative Influence on Methylation	Referenced Literature
Low dissolved oxygen	Enhanced methylation	Rudd et al. 1983; Parks et al. 1989
Decreased pH	Enhanced methylation in water column	Xun 1987; Gilmour and Henry 1991; Miskimmin et al. 1992
Decreased pH	Decreased methylation in sediment	Ramlal et al. 1985; Steffan et al. 1988
Increased dissolved organic carbon (DOC)	Enhanced methylation in sediment	Chois and Bartha 1994
Increased dissolved organic carbon (DOC)	Decreased methylation in water column	Miskimmin et al. 1992
Increased salinity	Decreased methylation	Blum and Bartha 1980
Increased nutrient concentrations	Enhanced methylation	Wright and Hamilton 1982; Jackson 1986; Regnell 1994; Beckvar et al. 1996
Increased selenium concentrations	Decreased methylation	Beckvar et al. 1996
Increased temperature	Enhanced methylation	Wright and Hamilton 1982; Parks et al. 1989
Increased sulfate concentrations	Enhanced methylation	Gilmour and Henry 1991; Gilmour et al. 1992
Increased sulfide concentrations	Enhanced methylation	Beckvar et al. 1996

To account for methylation of mercury in the media and its subsequent biotransfer assuming steady-state conditions, the deposition and media concentration equations (presented in Appendix B) have been modified specifically for modeling methyl mercury. Appendix A-2 provides the parameter values specific for methylmercury, and additional discussion and reference on their origin.

As noted above, methylation can be highly variable between environmental systems. This results in a significant degree of uncertainty implicit in modeling of mercury methylation. To expand on the qualitative information presented in the above table, and better understand conditions that may influence mercury methylation specific to a site, U.S. EPA OSW recommends review of information on this subject presented in the *Mercury Study Report to Congress* (U.S. EPA 1997b).

### Exposure Assessment for Mercury

For assessing exposure of community and class-specific guild measurement receptors to mercury, guidance provided in Chapters 4 and 5 should generally be followed. However, special consideration is required in evaluating the various forms of mercury modeled to the point of exposure.

To evaluate exposure of water, sediment, and soil communities to mercury, species-specific concentrations of divalent mercury and methyl mercury, in the respective media to which the community is exposed, should be directly compared to toxicity benchmarks specific to those compounds. The species-specific media concentrations should be calculated using equations and guidance presented in Chapter 3 and Appendix B. Media-specific toxicity benchmarks for divalent and methyl mercury are provided in Appendix E.

To evaluate the exposure of class-specific guilds to mercury, the media-specific concentrations of both divalent and methyl mercury should be modeled as independent COPCs through the food web, assuming no methylation of divalent mercury to the methyl mercury form within organisms. Therefore, the daily doses of all food items (i.e., media, plants, and animals) ingested by a measurement receptor should be considered for both divalent and methyl mercury, and compared to the respective toxicity benchmarks that are representative of the measurement receptor (see Appendix E). The daily doses of food items ingested by a measurement receptor should be calculated consistent with the guidance presented in Chapters 4 and 5, and Appendix F, for assessing exposure of class-specific guild measurement receptors to other COPCs. This includes the use of species-specific media concentrations, and methyl mercury bioconcentration factors (*BCF*) and food chain multipliers (*FCM*).

### Conclusion

In the event risks associated with mercury exceed target levels based on modeling with equations and initial conservative assumptions presented in this guidance, the permitting authority may approve use of more complex models that utilize more extensive site-specific data to predict transformation of chemical forms and biotransfer of mercury for evaluation at points of potential exposure. For example, the draft version of the ISCST3 dry gas algorithm for estimating dry gas deposition may be utilized. This draft model can be found

on the SCRAM bulletin (see Chapter 3); and specific default parameter values for mercury are presented in U.S. EPA (1997b). While this guidance does not address what models should be used or how data to support such models should be collected, the decision to use site-specific mercury models in a risk assessment is not precluded just because it is different; nor does this guidance automatically approve the use of such models. A permitting authority that chooses to use complex mercury models should carefully identify and evaluate their associated limitations, and clearly document these limitations in the uncertainty section of the risk assessment report.

U.S. EPA OSW encourages all facilities to implement a combination of waste minimization and control technology options to reduce mercury emission rates on an ongoing basis. Realistic expectations for mercury emission reduction efforts may be established by considering various technology-based mercury emission limits that apply to waste combustors (for example, standards for European combustors, the proposed MACT standards for hazardous waste combustors, or the MACT standards for municipal waste combustors). U.S. EPA OSW acknowledges that site-specific risk assessments as currently conducted may not identify the entire potential risk from mercury emissions. Mercury that does not deposit locally will ultimately enter the global mercury cycle for potential deposition elsewhere.

### **2.3.8 Particulate Matter**

PM is all condensed material suspended in air that has a mean aerodynamic diameter of 10 micrometers or less (PM<sub>10</sub>). PM can be classified as aerosols, dusts, fogs, fumes, mists, smogs, or smokes, depending on its physical state and origin. Anecdotal evidence suggests that uncontrolled particulate emissions from coal-burning industries has adversely affected local populations of wildlife (U.S. Fish and Wildlife Service [U.S. FWS] 1980). For wildlife, PM can adsorb to external surfaces or membranes, for example causing corneal damage. Wildlife exposure can also occur through ingestion of contaminated food, water, and hair (through grooming) (U.S. FWS 1980). However, PM dose-response information to evaluate risk of particulate matter to ecological receptors is limited. For this reason, U.S. EPA OSW does not recommend that PM be evaluated as a separate COPC in a risk assessment. However, PM is useful as an indicator parameter for other contaminants because it can be measured in real time and is sensitive to changes in combustion conditions.

### 2.3.9 Hydrogen Chloride/Chlorine Gas

Hydrogen chloride (which becomes hydrochloric acid when dissolved in water) and chlorine are two of the major products of the chemical industry, with uses too numerous to list. When chlorine gas dissolves in water (whether during drinking water treatment or when someone inhales chlorine), it hydrolyzes to form equal amounts of hydrochloric acid and hypochlorous acid.

Hydrogen chloride, as all other strong acids and bases, is an irritant on contact; adverse effects are seen only in the upper respiratory tract (including the nose, mouth, and throat). High concentrations can become corrosive and destroy tissues, producing chemical burns. Unless it is highly concentrated, ingested hydrochloric acid has only minimal adverse effects.

Because of the high concentrations of these compounds needed to produce observable effects, they are not expected to pose an ecological risk. Therefore, U.S. EPA OSW does not recommend that hydrogen chloride and chlorine gas be included as separate COPCs in the risk assessment.

### 2.3.10 Endocrine Disruptors

Endocrine disruptors are chemical compounds that interfere with the endocrine system's normal function and homeostasis in cells, tissues, and organisms. It has been hypothesized by U.S. EPA OSW that endocrine disruptors adversely affect the reproductive system by interfering with production, release, transport, receptor binding action, or elimination of natural blood-borne hormones and ligands.

Several studies have been conducted and serve as the basis for further experimentation to determine whether the hypothesis is correct. These studies include (1) wildlife reproduction (feminization of birds, alligators, and certain terrestrial mammals), (2) wildlife population ecology (population decline), (3) human reproductive physiology (decreased sperm count in males in industrialized nations), (4) molecular biology (data on receptor-mediated mode of action), and (5) endocrinology (increased understanding of mechanisms of hormone regulation and impacts of perturbations).

Some have attempted to classify chemical compounds as endocrine disruptors; however, several problems have been encountered. Only limited empirical data are available to support the designation of specific

chemicals as endocrine disruptors, and some of the data are conflicting. An absence of a clear structure-activity relationship is evident among the diverse groups of chemicals considered as endocrine disruptors. There is a lack of unifying dose-response relationship among the diverse group of chemicals. Also, multiple modes of action for chemicals are currently considered as endocrine disruptors.

Because the information currently available on endocrine disruptors is inconsistent and limited, U.S. EPA has not yet developed a methodology for quantitative assessments of risk resulting from potential endocrine disruptors (U.S. EPA 1996d). Currently, no quantitative U.S. EPA methods exist to specifically address the effects of endocrine disruptors in a risk assessment. Because the methods for addressing endocrine disruptors are developing at a rapid pace, permits writers and risk assessors should contact the Economics, Methods and Risk Analysis Division (EMRAD) of the Office of Solid Waste for the latest policy on how to deal with endocrine disruptors in site specific risk assessments. Additional information can also be obtained from review of available publications (e.g., EPA Special Report on Endocrine Disruption) at the web site “[www.epa.gov/ORD/WebPubs/endocrine/](http://www.epa.gov/ORD/WebPubs/endocrine/)”.

### **2.3.11 Radionuclides**

Radionuclides exist in (1) naturally occurring radioactive materials such as coal and other rocks, as (2) radioactive by-products of industrial processes. This risk assessment guidance does not consider the naturally occurring radioactive materials such as uranium and thorium (and their decay elements) based on U.S. EPA doctrine and technical limitations for measuring such low levels. However, radioactive wastes and materials, as defined by the U.S. Nuclear Regulatory Commission (NRC) and the U.S. Department of Energy (DOE), are subject to evaluation through interagency agreements on this subject. The U.S. NRC considers “radioactive waste” as waste that is, or contains, by-product material, source material, or special nuclear material (as defined in 10 CFR Part 20.1003). The U.S. NRC considers “mixed waste” as waste that is radioactive waste and hazardous waste defined by U.S. EPA. Radioactive and mixed waste must be handled in accordance with all relevant regulations, including U.S. EPA and U.S. NRC (10 CFR Part 20.2007) regulations. In particular, U.S. NRC licensees must comply with 10 CFR Part 20.2004—“Treatment or Disposal by Incineration”—and applicable U.S. EPA regulations.

U.S. EPA OSW recommends that the combustion of mixed waste and radioactive material should be evaluated in the risk assessment. Direct radiation (e.g., radiation from sealed sources such as instruments



that are not released to the environment) does not need to be evaluated in the risk assessment. Risk from both radiological and non-radiological contaminants should be presented along side each other in a risk summary table. Results should include a discussion of additivity and the uncertainties of additivity when combining risks from radiological and non-radiological contaminants. A radionuclide should be included as a COPC if it is in the combustion unit's waste feed.

U.S. EPA OSW recommends using the ISCST3 air dispersion model, utilizing the exponential decay option to calculate air concentrations and ground deposition rates. Intake should then be calculated with appropriate exposure scenario equations and parameters. ISCST3 is a good choice for facilities with multiple sources, complex terrain, building downwash and wet/dry deposition requirements.

A special consideration in integrating radioactive materials into risk calculations is related to decay and ingrowth of radionuclides, especially the few decay processes that involve a change of state. Decay should always be considered, both over the air transport time and the surface exposure duration. Ingrowth may be important, and special care must be taken in the use of radionuclide slope factors that include contributions from daughters ('+D' slope factors). Ingrowth involving change of physical states is another situation that will require special handling in the fate and transport modeling. For instance, solid radium-226 decays to gaseous radon-222, which then decays through solid polonium-218 to further decay elements.

Equations for fate and transport of radionuclides in soil and water should be consistent with those presented for non-radionuclides factoring in decay (and ingrowth if applicable). Food chain biotransfer parameters necessary to determine food concentrations are available in the *Handbook of Parameter Values for the Prediction of Radionuclide Transfer in Temperate Environments; IAEA Technical Report Series No. 364* (International Atomic Energy 1994).

Because the information currently available on ecological fate and effects for radionuclides is very limited, U.S. EPA OSW has not yet developed a methodology for quantitative assessments of ecological risk resulting from exposure. Ecological screening levels currently being used in some regions include 1 rad/day for aquatic receptors, based on population effects, (National Council on Radiation Protection and Measurements 1991), and 0.1 rad/day for terrestrial receptors (with the exception of pine trees and mammalian embryos) (International Atomic Energy Agency 1992). Additional references on evaluating ecological exposures to radiation include Barnthouse (1995) and Blaylock et al. (1993).

**USER NOTE**

*Prescriptive methodology for calculating risk from combustion facilities burning mixed waste is beyond the scope of the current document. The above information is provided to outline the methodology recommended by U.S. EPA OSW.*

**2.4 ESTIMATES OF COPC CONCENTRATIONS FOR NON-DETECTS**

The lowest level of an analyte that can be detected using an analytical method is generally termed the “detection limit.” One particularly difficult issue is the treatment of data in the risk assessment that are reported as below the “detection limit.” The following subsections (1) define commonly reported “detection limits,” (2) describe use in the risk assessment of data reported as non-detect, (3) describe statistical distribution techniques applied to address this issue, (4) summarize U.S. EPA OSW recommendations regarding quantification of non-detect issues in preparation of a risk assessment, and (5) clarify data flagged as estimated maximum possible concentration (EMPC) in the risk assessment.

**2.4.1 Definitions of Commonly Reported Detection Limits**

U.S. EPA’s commonly-used definition for the detection limit for non-isotope dilution methods has been the method detection limit (MDL), as promulgated in 40 CFR Part 136, Appendix B (U.S. EPA 1995i). A level above the MDL is the level at which reliable quantitative measurements can be made; generically termed the “quantitation limit” or “quantitation level.” In practice, numerous terms have been created to describe detection and quantitation levels. The significance and applicability of the more widely reported of these detection and quantitation levels by analytical laboratories are summarized below. These levels—listed generally from the lowest limit to the highest limit—include the following:

- Instrument Detection Limit (IDL) is the smallest signal above background that an instrument can reliably detect, but not quantify. Also, commonly described as a function of the signal-to-noise (S/N) ratio.
- Method Detection Limit (MDL) is the minimum concentration of a substance that can be measured (via non-isotope dilution methods) and reported with 99 percent confidence that the analyte concentration is greater than zero, and is determined from analysis of a sample in a specific matrix type containing the analyte. The MDL is considered the lowest level at which a compound can be reliably detected. The MDL is based on statistical analyses of laboratory data. In practice, the MDLs are determined on analytical reagents (e.g., water)

and not on the matrix of concern. MDLs for a given method, are laboratory and compound specific.

To determine the MDL as specified in 40 CFR Part 136, Appendix A, for example, at least seven replicate samples with a concentration of the compound of interest near the estimated MDL are analyzed. The standard deviation among these analyses is calculated and multiplied by 3.14. The result of the calculation becomes the MDL. The factor of 3.14 is based on a t-test with six degrees of freedom and provides a 99 percent confidence that the analyte can be detected at this concentration (U.S. EPA 1995i).

It should be noted that 40 CFR Part 136 is specific to the Clean Water Act, and therefore, it identifies the use of water as the matrix for the MDL determination. The MDL was promulgated in 1984, and is incorporated in more than 130 U.S. EPA analytical methods for the determination of several hundred analytes.

- Reliable Detection Level (RDL) is a detection level recommended by the National Environmental Research Laboratory in Cincinnati. It is defined as 2.623 times the MDL (U.S. EPA 1995i). The RDL is a total of 8 standard deviations above the MDL developmental test data (3.14 times 2.623).
- Estimated Detection Limit (EDL) is a quantitation level defined in SW-846 that has been applied to isotope dilution test methods (e.g., SW-846 Method 8290). A variation of the SW-846 defined EDL is also commonly reported by commercial laboratories, however, with the addition of a multiplication factor that generally elevates the EDL value by 3.5 to 5 times that of the SW-846 definition. Commercial laboratories sometimes report EDLs for non-isotope dilution methods such as SW-846 Method 8270, even though an EDL is not defined by the method.

**As defined in SW-846:** The EDL is defined in SW-846 (presented in various methods, e.g., Method 8280A) as the estimate made by the laboratory of the concentration of a given analyte required to produce a signal with a peak height of at least 2.5 times the background signal level. The estimate is specific to a particular analysis of the sample and will be affected by sample size, dilution, etc. The presented equation defining EDL is as follows:

$$EDL = \frac{2.5 \cdot Q_{is} \cdot (H_n^1 + H_n^2) \cdot D}{V \cdot (H_{is}^1 + H_{is}^2) \cdot RF_n} \quad \text{Equation 2-7}$$

where

<i>EDL</i>	=	Estimated detection limit (ng/L)
2.5	=	Peak height multiplier (unitless)
<i>Q<sub>is</sub></i>	=	Nanograms of the appropriate internal standard added to the sample prior to extraction (ng)

$H_n^1$ and $H_n^2$	=	The peak heights of the noise for both of the quantitation ions of the isomer of interest
$H_{is}^1$ and $H_{is}^2$	=	The peak heights of both the quantitation ions of the appropriate internal standards
$D$	=	Dilution factor - the total volume of the sample aliquot in clean solvent divided by the volume of the sample aliquot that was diluted (unitless)
$V$	=	Volume of sample extracted (L)
$RF_n$	=	Calculated relative response factor from calibration verification (unitless)

**Common commercial laboratory practice:** The EDL, generally reported by commercial laboratories, is defined as the detection limit reported for a target analyte that is not detected or presents an analyte response that is less than 2.5 times the background level. The area of the compound is evaluated against the noise level measured in a region of the chromatogram clear of genuine GC signals times an empirically derived factor. This empirical factor approximates the area to height ratio for a GC signal. This factor is variable between laboratories and analyses performed, and commonly ranges from 3.5 to 5. The equation is as follows:

$$EDL = \frac{2.5 \cdot Q_{\beta} \cdot (F \cdot H) \cdot D}{W \cdot A_{\beta} \cdot RRF_{\sigma}} \quad \text{Equation 2-8}$$

where

$EDL$	=	Estimated detection limit
2.5	=	Minimum response required for a GC signal
$Q_{\beta}$	=	The amount of internal standard added to the sample before extraction
$F$	=	An empirical factor that approximates the area to height ratio for a GC signal
$H$	=	The height of the noise
$D$	=	Dilution factor
$W$	=	The sample weight or volume
$RRF_{\sigma}$	=	The mean analyte relative response factor from the initial calibration

- Practical Quantitation Limit (PQL) is a quantitation level that is defined in 50 FR 46908 and 52 FR 25699 as the lowest level that can be reliably achieved with specified limits of precision and accuracy during routine laboratory operating conditions (U.S. EPA 1992g; 1995i). The PQL is constructed by multiplying the MDL, as derived above, by a factor (subjective and variable between laboratories and analyses performed) usually in the range of 5 to 10. However, PQLs with multipliers as high as 50 have been reported (U.S. EPA 1995i).

The PQL has been criticized because of the ambiguous nature of the multiplier and because the resulting levels have been perceived as too high for regulatory compliance purposes (U.S. EPA 1995i).

- Target Detection Limit (TDL) is a quantitation level constructed similar to the PQL.
- Reporting Limit (RL) is a quantitation level constructed similar to the PQL.
- Estimated Quantitation Limit (EQL) is a quantitation level constructed similar to the PQL.
- Sample Quantitation Limit (SQL) is a quantitation level that is sample-specific and highly matrix-dependent because it accounts for sample volume or weight, aliquot size, moisture content, and dilution. SQLs for the same compound generally vary between samples as moisture content, analyte concentration, and concentrations of interfering compounds vary. The SQL is generally 5 to 10 times the MDL, however, it is often reported at much higher levels due to matrix interferences.
- Contract Required Quantitation Limit (CRQL)/Contract Required Detection Limit (CRDL) is a quantitation pre-set by contract, which may incorporate U.S. EPA (1986b) SW-846 methods, Office of Water methods, or other methods deemed necessary to meet study objectives. These limits are typically administrative limits and may actually be one or two orders of magnitude above the MDL.

#### 2.4.2 Use In the Risk Assessment of Data Reported As Non-Detect

In collecting data for use in risk assessments or in setting regulatory compliance levels, the permitting authority is often faced with data quality objectives that require analyses near or below analytical detection or quantitation levels. In such situations, permittees often argue that the detection levels should be set with a large factor of certainty in order to be confident that measurements are reliable. Environmental groups frequently argue that a level of zero or a level at which a single researcher can demonstrate that the compound can be detected should be used as the set level. Because measurements made below analytical detection and quantitation levels are associated with increased measurement uncertainty, an understanding of these levels is important to the comprehension of the impact they may have when they are applied.

As a result of the quantitative differences between the various types of detection levels, “non-detected” compounds pose two questions: (1) Is the compound really present?, and (2) If so, at what concentration? The first question is generally hard to answer, and is dependent mainly on the analytical resources available. For the second question, the answer is “somewhere between true zero and the quantitation level applied.” For samples obtained during the trial burn that report compounds at below the detection limit, earlier U.S. EPA

(1994i) guidance has recommended that emission rates for non-detects be developed using one-half of the “detection limit” and applied in conducting the risk assessment. However, which detection limit should be used has not been explicitly defined or presented in quantitative terms.

To increase consistency and reproducibility in dealing with non-detects, U.S. EPA OSW recommends application of the MDL-derived RDL to quantify non-detects for COPCs analyzed with non-isotope dilution methods, and application of the method-defined EDL to quantify non-detects for COPCs analyzed with isotope dilution methods. Procedures for these applications are as follows:

***Non-isotope Dilution Methods:*** Non-detects for COPCs analyzed with non-isotope dilution methods should be quantified for use in the risk assessment using an MDL-derived RDL. Commonly used non-isotope dilution methods include SW-846 Method 8260 (volatiles), SW-846 Method 8270 (semivolatiles),

1. Require the laboratory to report the actual MDL for every non-detect compound analyzed, in addition to the commonly used reporting limit, such as an EDL, EQL, or PQL. The MDL should be derived in a manner consistent with 40 CFR Part 136 Appendix B. This would also apply for analysis of each individual component of multiple component samples (e.g., front half rinse, XAD resin, condensate, Tenax tube).

**Note:** Laboratories typically produce MDLs specific to each non-isotope dilution method performed by the laboratory on an annual basis.

2. Calculate an MDL-derived RDL for each COPC non-detect for quantitative application in the risk assessment. This would be obtained by multiplying the MDL, as reported by the laboratory, times 2.623 (interim factor) (U.S. EPA 1995i).
3. Adjust the RDL, as appropriate, to account for sample-specific volumetric treatments (e.g., splits and dilutions) that differ from those utilized in the Part 136 MDL determinations.

***Isotope Dilution Methods (SW-846 Methods 8290, 1624, 1625; and CARB 429, etc.):*** Non-detects for COPCs analyzed with isotope dilution methods should be quantified for use in the risk assessment using the EDL as defined by the analytical method without the use of empirical factors or other mathematical manipulations specific to the laboratory (e.g., EDL as defined in SW-846). Commonly used isotope dilution methods include SW-846 Methods 8290, 1624, and 1625.

It should be noted that the MDL definition used in 40 CFR Part 136 (see Section 2.4.1) addresses errors of the first type, false negatives. The 99 percent confidence limit stating that the MDL has only a 1 percent chance the detects will be misidentified as negative, when the compound of concern was present. Errors of the second type, false positives are not addressed. By not addressing false positives, or errors of the second type, the statistically defined default value become 50 percent. In other words, where 40 CFR did not

address false positives, the system required that 50 percent of the detects at the MDL would be false positives. This is a very conservative approach, and biased toward not missing any compounds of potential concern that may be present. The use of the MDL-derived RDL, and to a lesser extent the EDL, somewhat indirectly addresses the false positive issue. As described in defining the RDL (see Section 2.4.1), by the time the standard deviation has been multiplied by 8, the possibility of false positives is usually less than 1 percent.

### **2.4.3 Statistical Distribution Techniques**

Many statistical distribution techniques are available for calculating a range of standard deviations to quantify non-detect concentrations of COPCs. These include random replacement scenarios, such as: (1) the uniform fill-in (UFI) method, in which each LOD value is replaced with a randomly generated data point by using a uniform distribution; (2) the log fill-in LFI method which is the same as UFI, except for using a logarithmic distribution; (3) the normal fill-in (NFI) method which is the same as UFI, except for using a log-normal distribution; and (4) the maximum likelihood estimation (MLE) techniques (Cohen and Ryan 1989; Rao et al. 1991). If determined to be applicable by the permitting authority, a Monte Carlo simulation may also be used to determine a “statistical” value for each non-detect concentration.

### **2.4.4 U.S. EPA OSW-Recommendations on Quantifying Non-Detects**

Use of non-detects in risk assessments is dependent on the analytical method used to produce the data. In most cases, U.S. EPA will estimate emission rates for undetected COPCs (see Section 2.3) by assuming that COPCs are present at a concentration equivalent to the MDL-derived RDL for non-isotope dilution methods, or the method-defined EDL for isotope dilution methods. U.S. EPA OSW believes that these methods are reasonable and conservative, and that they represent a scientifically sound approach that allows maximum protection of the environment while recognizing the uncertainty associated with analytical measurements at very low concentrations in a real world sample matrix. It is also recognized that there are subjective components and limitations to each of the non-detect methodologies presented in this and previous guidance, including the recommended methods.

Some state permitting authorities have expressed the desire to obtain and use non-routine data (e.g., uncensored data) of defensible quality in the risk assessment as a way to deal with non-detect issues.

While this guidance does not address what forms or how such data may be used, the decision to use non-routine data in a risk assessment is not precluded just because it is different; nor does this guidance automatically approve the use of non-routine data. A permitting authority that chooses to use non-routine data should carefully identify and evaluate the limitations associated with non-routine data and clearly document this discussion in the uncertainty section of the risk assessment report.

For collection of data to be used in a risk assessment, U.S. EPA OSW recommends comprehensive sampling using typical sampling and analytical methods for VOCs, SVOCs, metals, PCDDs, PCDFs, total organics, and other appropriate constituents as necessary based on the type of waste that will be burned by the unit. A pretrial burn risk assessment can help to ensure that the desired quantitation limit (and, therefore, DREs and COPC stack gas emission rates) will be achieved during the trial burn test.

#### **2.4.5 Estimated Maximum Possible Concentration (EMPC)**

The EMPC, as defined in SW-846 Methods 8280A and 8290, is in most cases only used with the isotope dilution methods as stated. An EMPC is calculated for dioxin isomers that are characterized by a response with a signal to noise ratio of at least 2.5 for both the quantitation ions, and meet all the relevant identification criteria specified in the method, except the ion abundance ratio. Ion abundance ratios are affected by co-eluting interferences that contribute to the quantitative ion signals. As a result, one or both of the quantitative ions signals may possess positive biases.

An EMPC is a worst case estimate of the concentration. An EMPC is not a detection limit and should not be treated as a detection limit in the risk assessment. U.S. EPA OSW recommends that EMPC values be used as detections without any further manipulation (e.g., dividing by 2). However, because EMPCs are worst case estimates of stack gas concentrations, permitting authorities and facilities should consider techniques to minimize EMPCs when reporting trial and risk burn results, especially when the EMPC values result in risk estimates above regulatory levels of concern. Some techniques that may be applied to minimize EMPCs include performing additional cleanup procedures (as defined by the analytical method) on the sample or archived extract, and/or reanalyzing the sample under different chromatographic conditions.



### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Actual MDLs for all non-detect results
- Description of the method applied to quantify the concentration of non-detects

## 2.5 CONCENTRATIONS DETECTED IN BLANKS

Blank samples are intended to provide a measure of any contamination that may have been introduced into a sample either in the field while the samples were being collected, in transport to the laboratory, or in the laboratory during sample preparation or analysis. Blank samples are analyzed in the same manner as the site samples from the trail burn. In order to prevent the inclusion of non-site related compounds in the risk assessment, the concentrations of compounds detected in blanks should be compared to concentrations detected in site samples collected during the trial burn. Four types of blanks are defined in the *Risk Assessment Guidance for Superfund* (U.S. EPA 1989e): trip blanks, field blanks, laboratory calibration blanks, and laboratory reagent of method blanks. Detailed definitions of each are provided below.

**Trip Blank** - A trip blank is used to indicate potential contamination due to migration of volatile organic compounds from the air on the site or in sample shipping containers, through the septum or around the lid of sampling vials, and into the sample. The blank accompanies the empty sample bottles to the field as well as with the site samples returning to the laboratory for analysis. The blank sample is not opened until it is analyzed in the lab with the site samples, thus making the laboratory “blind” to the identity of the blanks.

**Field Blank** - A field blank is used to determine if field sampling or cleaning procedures (e.g., insufficient cleaning of sample equipment) result in cross-contamination of site samples. Like the trip blank, the field blank is transported to the field with empty sample bottles and is analyzed in the laboratory along with the site samples. Unlike the trip blank, however, the field blank sample is opened in the field and recovered in the same manner as the collected samples. As with trip blanks, the field blanks’ containers and labels should be the same as for site samples and blind to the laboratory.

**Instrument Blank** - An instrument blank is distilled, deionized water injected directly into an instrument without having been treated with reagents appropriate to the analytical method used to analyze actual site samples. This type of blank is used to indicate contamination in the instrument itself.

**Laboratory Reagent of Method Blank** - A laboratory reagent of method blank results from the treatment of distilled, deionized water with all of the reagents and manipulations (e.g., digestions or extractions) to which site samples will be subjected. Positive results in the reagent blank may indicate either contamination of the chemical reagents or the glassware and implements used to store or prepare the sample and resulting solutions. Although a laboratory following good laboratory practices will have its analytical processed under control, in some instances method blank contaminants cannot be entirely eliminated.

**Water Used for Blanks** - For all the blanks described above, results are reliable only if the water comprising the blank was clean. For example, if the laboratory water comprising the trip blank was contaminated with VOCs prior to being taken to the field, then the source of VOC contamination in the trip blank cannot be isolated.

Blank data should be compared with the results with which the blanks are associated. However, if the association between blanks and data can not be made, blank data should be compared to the results from the entire sample data set.

U.S. EPA (1989e) makes a division in comparison between blanks containing common laboratory contaminants and blanks containing contaminants not commonly used in laboratories. Compounds considered to be common laboratory contaminants are acetone, 2-butanone (methyl ethyl ketone), methylene chloride, toluene, and the phthalate esters. If compounds considered to be common laboratory contaminants are detected in the blanks, then sample results are not considered to be detected unless the concentrations in the sample are equal to or exceed ten times the maximum amount detected in the applicable blanks. If the concentration of a common laboratory contaminant in a sample is less than ten times the blank concentration, then the compound is treated as a non-detect in that particular sample.

In some limited cases, it may be appropriate to consider blanks which contain compounds that are not considered by U.S. EPA to be common laboratory contaminants as identified above. In these limited cases, sample results are not considered to be detected unless the concentrations in the sample exceed five times the maximum amount detected in the applicable blanks. If the concentration in a sample is less than five times the blank concentration, then the compound is treated as a non-detect in that particular sample.

Permitting authorities should carefully consider the evaluation of blank data in the overall context of the risk assessment and permitting process. U.S. EPA OSW expects that issues related to non-laboratory contaminant blanks to be minimal because data collection and analysis efforts in support of trial and risk burns are expected to be of high quality in strict conformance to QA/QC plans and SOPs. The trial and risk

burn data should be carefully evaluated to ensure that the level of contamination present in the blanks does not compromise the integrity of the data for purposes of risk assessment, or result in retesting in order to properly address data quality issues.

When considering blank contamination in the COPC selection process, permitting authorities should ensure that:

- (1) The facility or data gatherer has made every reasonable attempt to ensure good data quality and has rigorously implemented the QA/QC Plan and good industry sampling and testing practices.
- (2) Trial and risk burn data has not been submitted to the permitting authority as “blank corrected.” Rather, the permitting authority has the full opportunity to review the data absent additional manipulation by the data gatherer.
- (3) The effect of the blank correction on the overall risk estimates, if such an effect is considered, is clearly described in the uncertainty section of the risk assessment report.
- (4) The risk assessment reports emissions rates both as measured, and as blank corrected, in situations where there is a significant difference between the two values.

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# Chapter 3

## Air Dispersion and Deposition Modeling

### What's Covered in Chapter 3:

- ◆ U.S. EPA-Recommended Air Dispersion and Deposition Model
  - ◆ Air Model Development
  - ◆ Site-Specific Characteristics Required for Air Modeling
  - ◆ Use of Unit Emission Rate
  - ◆ Partitioning of Emissions
  - ◆ Meteorological Data Required for Air Modeling
  - ◆ Meteorological Preprocessors and Interface Programs
  - ◆ ISCST3 Model Input Files
  - ◆ ISCST3 Model Execution
  - ◆ Use of Modeled Output
  - ◆ Modeling Fugitive Emissions
  - ◆ Estimating Media Concentrations
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Combustion of materials produces residual amounts of pollution that may be released to the environment. Estimation of potential ecological risks associated with these releases requires knowledge of atmospheric pollutant concentrations and annual deposition rates in the areas around the combustion facility at habitat-specific scenario locations. Air concentrations and deposition rates are usually estimated by using air dispersion models. Air dispersion models are mathematical constructs that approximate the physical processes occurring in the atmosphere that directly influence the dispersion of gaseous and particulate emissions from the stack of a combustion unit. These mathematical constructs are coded into computer programs to facilitate the computational process.

This chapter provides guidance on the development and use of the standard U.S. EPA air dispersion model that U.S. EPA expects to be used in most situations—the Industrial Source Complex Short-Term

Model (ISCST3). ISCST3 requires the use of the following information for input into the model, and consideration of output file development:

- Site-specific characteristics required for air modeling (Section 3.2)
  - Surrounding terrain (Section 3.2.1)
  - Surrounding land use (Section 3.2.2)
  - Facility building characteristics (Section 3.2.3)
- Unit emission rate (Section 3.3)
- Partitioning of emissions (Section 3.4)
- Meteorological data (Section 3.5)
- Source Characteristics (Section 3.7)

ISCST3 also requires the use of several preprocessing computer programs that prepare and organize data for use in the model. Section 3.6 describes these programs. Section 3.7 describes the structure and format of the input files. Section 3.8 describes limitations to be considered in executing ISCST3. Section 3.9 describes use of the air modeling output in the risk assessment computations. Section 3.10 discusses air modeling of fugitive emissions. Section 3.11 describes how to estimate the media concentrations of COPCs in media.

If applicable, readers are encouraged to consult the air dispersion modeling chapter (Chapter 3) of the U.S. EPA OSW guidance document *Human Health Risk Assessment Protocol* (HHRAP) (U.S. EPA 1998c) before beginning the air modeling process to ensure the consideration of specific issues related to human health risk assessment. Additionally, the *Guideline on Air Quality Models* (GAQM) (U.S. EPA 1996c) is a primary reference for all US EPA and state agencies on the use of air models for regulatory purposes. The GAQM is incorporated in 40 CFR Part 51 as Appendix W. The Office of Air Quality Planning and Support (OAQPS) provides the GAQM and extensive information on air dispersion models, meteorological data, data preprocessors, user's guides, and model applicability on the Support Center for Regulatory Air Models (SCRAM) web site at address "<http://www.epa.gov/scram001/index.htm>". General questions regarding air modeling or information on the web site should be addressed to "[atkinson.dennis@epamail.epa.gov](mailto:atkinson.dennis@epamail.epa.gov)". Specific questions on the use of this guidance should be addressed to the appropriate permitting authority.

### 3.1 DEVELOPMENT OF AIR MODELS

This section (1) briefly describes the history of air model development, (2) introduces some data preprocessing programs developed to aid in preparing air model input files (these preprocessing programs are described in more detail in Sections 3.2.4 and 3.6, and (3) introduces ExInter Version 1.0, a preprocessor to ISCST3.

#### 3.1.1 History of Risk Assessment Air Dispersion Models

Before 1990, several air dispersion models were used by U.S. EPA and the regulated community. These models were inadequate for use in risk assessments because they considered only concentration, and not the deposition of contaminants to land. The original U.S. EPA guidance (1990a) on completing risk assessments identified two models that were explicitly formulated to account for the effects of deposition.

- COMPLEX terrain model, version 1 (COMPLEX I), from which a new model—COMPLEX terrain model with DEPosition (COMPDEP)—resulted
- Rough Terrain Diffusion Model (RTDM), from which a new model—RTDMDEP—resulted

COMPDEP was updated to include building wake effects from a version of the ISCST model in use at the time. Subsequent U.S. EPA guidance (1993h; 1994b) recommended the use of COMPDEP for air deposition modeling. U.S. EPA (1993h) specified COMPDEP Version 93252, and U.S. EPA (1994b) specified COMPDEP Version 93340. When these recommendations were made, a combined ISC-COMPDEP model (a merger of the ISCST2 and COMPLEX I model) was still under development. The merged model became known as ISCSTDFT. U.S. EPA guidance (1994i) recommended the use of the ISCSTDFT model. After reviews and adjustments, this model was released as ISCST3. The ISCST3 model contains algorithms for dispersion in simple, intermediate, and complex terrain; dry deposition; wet deposition; and plume depletion.

The use of the COMPDEP, RTDMDEP, and ISCST models is described in more detail in the following user's manuals; however, all models except the current version of ISCST3 are obsolete:

- Environmental Research and Technology (ERT). 1987. *User's Guide to the Rough Terrain Diffusion Model Revision 3.20*. ERT Document P-D535-585. Concord, Massachusetts.
- Turner, D.B. 1986. *Fortran Computer Code/User's Guide for COMPLEX I Version 86064: An Air Quality Dispersion Model in Section 4. Additional Models for Regulatory Use*. Source File 31 Contained in UNAMAP (Version 6). National Technical Information Service (NTIS) PB86-222361/AS.
- U.S. EPA. 1979. *Industrial Source Complex Dispersion Model User's Guide, Volume I*. Prepared by the H.E. Cramer Company. Salt Lake City, Utah. Prepared for the Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina. EPA 450/4-79/030. NTIS PB80-133044.
- U.S. EPA. 1980b. *User's Guide for MPTER: A Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment*. Environmental Sciences Research Laboratory. Research Triangle Park, North Carolina. EPA 600/8-80/016. NTIS PB80-197361.
- U.S. EPA. 1982a. *MPTER-DS: The MPTER Model Including Deposition and Sedimentation*. Prepared by the Atmospheric Turbulence and Diffusion Laboratory. National Oceanic and Atmospheric Administration (NOAA). Oak Ridge, Tennessee. Prepared for the Environmental Sciences Research Laboratory. Research Triangle Park, North Carolina. EPA 600/8-82/024. NTIS PB83-114207.
- U.S. EPA. 1987b. *On-Site Meteorological Program Guidance for Regulatory Modeling Applications*. Office of Air Quality Planning and Standards. Research Triangle Park, North Carolina.
- U.S. EPA. 1995c. *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volumes I and II*. Office of Air Quality Planning and Standards. Emissions, Monitoring, and Analysis Division. Research Triangle Park, North Carolina. EPA 454/B-95/003a. September.

Users of this document are advised that a draft version of ISCST3 that includes algorithms for estimating the dry gas deposition (currently referred to as the "Draft Dry Gas Deposition Model: GDISCDFT, Version 96248") is available on the SCRAM web site. Use of this version to support site specific air modeling applications is not required, because many of the parameters needed to execute the model are not available in guidance or the technical literature. Therefore, until the draft version is reviewed and approved, and the data is provided by U.S. EPA or in the technical literature, U.S. EPA OSW recommends that the current version of ISCST3, in conjunction with the procedure presented in this guidance (Appendix B) for estimating dry gas deposition using deposition velocity and gas concentration, should be used for risk assessments.

### 3.1.2 Preprocessing Programs

ISCST3 requires the use of additional computer programs, referred to as “preprocessing” programs. These programs manipulate available information regarding surrounding buildings and meteorological data into a format that can be used by ISCST3. Currently, these programs include the following:

- PCRAMMET (Personal Computer Version of the Meteorological Preprocessor for the old RAM program) prepares meteorological data for use in ISCST3. The program organizes data—such as precipitation, wind speed, and wind direction—into rows and columns of information that are read by ISCST3. The PCRAMMET User’s Guide contains detailed information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1995b).
- Building Profile Input Program (BPIP) calculates the maximum crosswind widths of buildings, which ISCST3 then uses to estimate the effects on air dispersion. This effect on dispersion by surrounding buildings is typically known as building downwash or wake effects. The BPIP User’s Guide contains detailed information for preparing the required building dimensions (length, height, and width) and locations for the ISCST3 model (U.S. EPA 1995d).
- Meteorological Processor for Regulatory Models (MPRM) prepares meteorological data for use in the ISCST3 by using on-site meteorological data rather than data from government sources (National Weather Service [NWS] or the Solar And Meteorological Surface Observational Network [SAMSON]). MPRM merges on-site measurements of precipitation, wind speed, and wind direction with off-site data from government sources into rows and columns of information that are read by ISCST3. The MPRM User’s Guide contains information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1996e).

Most air dispersion modeling performed to support risk assessments will use PCRAMMET and BPIP. MPRM will generally not be used unless on-site meteorological information is available. However, only MPRM is currently scheduled to be updated to include the meteorological parameters (solar radiation and leaf area index) required to execute the dry deposition of vapor algorithms included in the new version of ISCST3. The draft version of MPRM is available for review and comment on the SCRAM web site as GDMPRDFT (dated 96248).



### 3.1.3 Expert Interface (ExInter Version 1.0)

ExInter is an expert interface system enhanced by U.S. EPA Region 6 for the ISCST3 model. By enhancing ExInter, the goal of U.S. EPA Region 6 was to support the in-house performance of air dispersion modeling by regional U.S. EPA and state agency personnel at hazardous waste combustion units necessary to support risk assessments conducted at these facilities. ExInter enables the user to build input files and run ISCST3 and its preprocessor programs in a Windows-based environment. Specific procedures for developing input files are stored in an available knowledge database. The underlying premise of the ExInter system is that the knowledge of an “expert” modeler is available to “nonexpert” modeling personnel at all times. However, some air modeling experience is required to use ExInter and its components as recommended in this guidance. The ExInter program has been written in Microsoft Visual C++ in a Microsoft Windows environment.

ExInter allows for a generic source category that comprises point, area, and volume sources. For each source type, the program queries the relevant variables for the user. In addition to asking about the inputs regarding the source types, ExInter also asks about control options, receptors, meteorology, and output formats. ExInter then creates an input file, as required by the ISCST3 dispersion model. ExInter also allows the user to run the ISCST3 model and browse the results file.

Version 1.0 of ExInter provides for input parameters to model dry gas deposition included in a draft version of ISCST3. However, the data required for dry gas deposition requires a literature search and prior regulatory approval. The procedure presented in this guidance (Appendix B) for estimating dry gas deposition using deposition velocity and gas concentration is appropriate without prior approval. More detailed information on how to use ExInter can be found in the following:

- U.S. EPA. 1996i. *User's Guide for ExInter 1.0. Draft Version*. U.S. EPA Region 6 Multimedia Planning and Permitting Division. Center for Combustion Science and Engineering. Dallas, Texas. EPA/R6-096-0004. October.

ExInter is available on the SCRAM web site at “<http://www.epa.gov/scram001/index.htm>” under the Modeling Support section “Topics for Review”. Six self-extracting compressed files contain all components for installation and use. The user’s guide is accessed interactively using the help command. Individual user’s guides to ISCST3, BPIP, PCRAMMET, and MPRM also provide good references for

using ExInter components. ExInter requires a minimum of 15 megabytes of free hard disk space, Windows 3.1, 8 megabytes of system memory, and a 486 processor.

### **3.2 SITE-SPECIFIC INFORMATION REQUIRED TO SUPPORT AIR MODELING**

Site-specific information for the facility and surrounding area required to support air dispersion modeling includes (1) the elevation of the surrounding land surface or terrain, (2) surrounding land uses, and (3) characteristics of on-site buildings that may affect the dispersion of COPCs into the surrounding environment.

Often, site-specific information required to support air dispersion modeling can be obtained from review of available maps and other graphical data on the area surrounding the facility. The first step in the air modeling process is a review of available maps and other graphical data on the surrounding area. U.S. Geological Survey (USGS) 7.5-minute topographic maps (1:24,000) extending to 10 kilometers from the facility, and USGS 1:250,000 maps extending out to 50 kilometers, should be obtained to identify site location, nearby terrain features, waterbodies and watersheds, ecosystems, special ecological habitats, and land use. Aerial photographs are frequently available for supplemental depiction of the area. An accurate facility plot plan—showing buildings, stacks, property and fence lines—is also needed. Facility information including stack and fugitive source locations, building corners, plant property, and fence lines should be provided in Universal Transverse Mercator (UTM) grid coordinates in meters east and north in both USGS reference systems.

Most USGS paper 7.5-minute topographic maps are published in the North American Datum system established in 1927 (NAD 27). However, most digital elevation data (e.g., USGS Digital Elevation Mapping) is in the 1983 revised system (NAD 83). Special consideration should be given not to mix source data obtained from USGS maps based on NAD 27 with digital terrain elevation data based on NAD 83. Emission source information should be obtained in the original units from the facility data, and converted to metric units for air modeling, if necessary. Digital terrain data can be acquired from USGS or another documented source.

The specific information that must be collected is described in the following subsections. Entry of this information into the ISCST3 input files is described in Section 3.7.

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**RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT**

- All site-specific maps, photographs, or figures used in developing the air modeling approach
  - Mapped identification of facility information including stack and fugitive source locations, locations of facility buildings surrounding the emission sources, and property boundaries of the facility
- 

### 3.2.1 Surrounding Terrain Information

Terrain is important to air modeling because air concentrations and deposition rates are greatly influenced by the height of the plume above local ground level. Terrain is characterized by elevation relative to stack height. For air modeling purposes, terrain is referred to as “complex” if the elevation of the surrounding land within the assessment area—typically defined as anywhere within 50 kilometers from the stack—is above the top of the stack evaluated in the air modeling analysis. Terrain at or below stack top is referred to as “simple.” ISCST3 implements U.S. EPA guidance on the proper application of air modeling methods in all terrain if the modeler includes terrain elevation for each receptor grid node and specifies the appropriate control parameters in the input file.

Even small terrain features may have a large impact on the air dispersion and deposition modeling results and, ultimately, on the risk estimates. U.S. EPA OSW recommends that most air modeling include terrain elevations for every receptor grid node. Some exceptions may be those sites characterized by very flat terrain where the permitting authority has sufficient experience to comfortably defer the use of terrain data because its historical effect on air modeling results has been shown to be minimal.

In addition to maps which are used to orient and facilitate air modeling decisions, the digital terrain data used to extract receptor grid node elevations should be provided in electronic form. One method of obtaining receptor grid node elevations is using digital terrain data available from the USGS on the Internet at web site “<http://www.usgs.gov>”. An acceptable degree of accuracy is provided by the USGS “One Degree” (e.g., 90 meter data) data available as “DEM 250” 1:250,000 scale for the entire United States free of charge. USGS 30-meter data is available for a fee. Either 90-meter or 30-meter data is sufficient for most risk assessments which utilize 100 meter or greater grid spacing. Digital terrain data may also be purchased from a variety of commercial vendors which may require vendor-provided programs to extract

the data. The elevations may also be extracted manually at each receptor grid node from USGS topographic maps.

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Description of the terrain data used for air dispersion modeling
- Summary of any assumptions made regarding terrain data
- Description of the source of any terrain data used, including any procedures used to manipulate terrain data for use in air dispersion modeling

### 3.2.2 Surrounding Land Use Information

Land use information in the risk assessment is used for purposes of air dispersion modeling and the identification or selection of exposure scenario locations (see Chapter 4) in the risk assessment. Land use analysis for purposes of selecting exposure scenario locations usually occurs out to a radius of 50 kilometers from the centroid of the stacks to ensure identification of all receptors that may be impacted. However, in most cases, air modeling performed out to a radius of 10 kilometers allows adequate characterization for the evaluation of exposure scenario locations. If a facility with multiple stacks or emission sources is being evaluated, the radius should be extended from the centroid of a polygon drawn from the various stack coordinates.

Land use information is also important to air dispersion modeling, but at a radius closer (3 kilometers) to the emission source(s). Certain land uses, as defined by air modeling guidance, effect the selection of air dispersion modeling variables. These variables are known as dispersion coefficients and surface roughness. USGS 7.5-minute topographic maps, aerial photographs, or visual surveys of the area typically are used to define the air dispersion modeling land uses ([www.usgs.gov](http://www.usgs.gov)).

#### 3.2.2.1 Land Use for Dispersion Coefficients

The Auer method specified in the Guideline on Air Quality Models (40 CFR Part 51, Appendix W) is used to define land use for purposes of specifying the appropriate dispersion coefficients built into ISCST3.

Land use categories of “rural” or “urban” are taken from the methods of Auer (Auer 1978). Areas typically defined as rural include residences with grass lawns and trees, large estates, metropolitan parks and golf courses, agricultural areas, undeveloped land, and water surfaces. Auer typically defines an area as “urban” if it has less than 35 percent vegetation coverage or the area falls into one of the following use types:

Urban Land Use		
Type	Use and Structures	Vegetation
I1	Heavy industrial	Less than 5 percent
I2	Light/moderate industrial	Less than 5 percent
C1	Commercial	Less than 15 percent
R2	Dense single/multi-family	Less than 30 percent
R3	Multi-family, two-story	Less than 35 percent

In general, the Auer method is described as follows:

- Step 1** Draw a radius of 3 kilometers from the center of the stack(s) on the site map.
- Step 2** Inspect the maps, and define in broad terms whether the area within the radius is rural or urban, according to Auer’s definition.
- Step 3** Classify smaller areas within the radius as either rural or urban, based on Auer’s definition. (It may be prudent to overlay a grid [for example, 100 by 100 meters] and identify each square as primarily rural or urban)
- Step 4** Count the total of rural squares; if more than 50 percent of the total squares are rural, the area is rural; otherwise, the area is urban.

Alternatively, digital land use databases may be used in a computer-aided drafting system to perform this analysis.

**RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT**

- Description of the methods used to determine land use surrounding the facility
- Copies of any maps, photographs, or figures used to determine land use
- Description of the source of any computer-based maps used to determine land use

**3.2.2.2 Land Use for Surface Roughness Height (Length)**

Surface roughness height—also referred to as (aerodynamic) surface roughness length—is the height above the ground at which the wind speed goes to zero. Surface roughness affects the height above local ground level that a particle moves from the ambient air flow above the ground (for example in the plume) into a “captured” deposition region near the ground. That is, ISCST3 causes particles to be “thrown” to the ground at some point above the actual land surface, based on surface roughness height. Surface roughness height is defined by individual elements on the landscape, such as trees and buildings.

U.S. EPA (1995b) recommended that land use within 5 kilometers of the stack be used to define the average surface roughness height. For consistency with the method for determining land use for dispersion coefficients (Section 3.2.2.1), the land use within 3 kilometers generally is acceptable for determination of surface roughness. Surface roughness height values for various land use types are as follows:

Surface Roughness Heights for Land Use Types and Seasons (meters)				
Land Use Type	Spring	Summer	Autumn	Winter
Water surface	0.0001	0.0001	0.0001	0.0001
Deciduous forest	1.00	1.30	0.80	0.50
Coniferous forest	1.30	1.30	1.30	1.30
Swamp	0.20	0.20	0.20	0.05
Cultivated land	0.03	0.20	0.05	0.01
Grassland	0.05	0.10	0.01	0.001
Urban	1.00	1.00	1.00	1.00
Desert shrubland	0.30	0.30	0.30	0.15

Source: Sheih, Wesley, and Hicks (1979)

If a significant number of buildings are located in the area, higher surface roughness heights (such as those for trees) may be appropriate (U.S. EPA 1995b). A specific methodology for determining average surface roughness height has not been proposed in prior guidance documents. For facilities using National Weather Service surface meteorological data, the surface roughness height for the measurement site may be set to 0.10 meters (grassland, summer) without prior approval. If a different value is proposed for the measurement site, the value should be determined applying the following procedure to land use at the measurement site. For the application site, the following method should be used to determine surface roughness height:

- Step 1* Draw a radius of 3 kilometers from the center of the stack(s) on the site map.
- Step 2* Inspect the maps, and use professional judgment to classify the areas within the radius according to the PCRAMMET categories (for example water, grassland, cultivated land, and forest); a site visit may be necessary to verify some classifications.
- Step 3* Calculate the wind rose directions from the 5 years of meteorological data to be used for the study (see Section 3.4.1.1); a wind rose can be prepared and plotted by using the U.S. EPA WRPLOT program from the U.S. EPA's Support Center for Regulatory Air Models bulletin board system (SCRAM BBS).
- Step 4* Divide the circular area into 16 sectors of 22.5 degrees, corresponding to the wind rose directions (for example, north, north-northeast, northeast, and east-northeast) to be used for the study.
- Step 5* Identify a representative surface roughness height for each sector, based on an area-weighted average of the land use within the sector, by using the land use categories identified above.
- Step 6* Calculate the site surface roughness height by computing an average surface roughness height weighted with the frequency of wind direction occurrence for each sector.

Alternative methods of determining surface roughness height may be proposed for agency approval prior to use in an air modeling analysis.

### **3.2.3 Information on Facility Building Characteristics**

Building wake effects have a significant impact on the concentration and deposition of COPCs near the stack. Building wake effects are flow lines that cause plumes to be forced down to the ground much sooner than they would if the building was not there. Therefore, the ISCST3 model contains algorithms for

evaluating this phenomenon, which is also referred to as “building downwash.” The downwash analysis should consider all nearby structures with heights at least 40 percent of the height of the shortest stack to be modeled. The 40 percent value is based on Good Engineering Practice (GEP) stack height of 2.5 times the height of nearby structures or buildings (stack height divided by 2.5 is equal to 0.40 multiplied by the stack height [40 CFR Part 51 Appendix W]). Building dimensions and locations are used with stack heights and locations in BPIP to identify the potential for building downwash. BPIP and the BPIP user’s guide can be downloaded from the SCRAM web site and should be referred to when addressing specific questions. The BPIP output file is in a format that can be copied and pasted into the source (SO) pathway of the ISCST3 input file. The following procedure should be used to identify buildings for input to BPIP:

- Step 1** Lay out facility plot plan, with buildings and stack locations clearly identified (building heights must be identified for each building); for buildings with more than one height or roof line, identify each height (BPIP refers to each height as a tier).
- Step 2** Identify the buildings required to be included in the BPIP analysis by comparing building heights to stack heights. The building height test requires that only buildings at least 40 percent of the height of a potentially affected stack be included in the BPIP input file. For example, if a combustion unit stack is 50 feet high, only buildings at least 20 feet (0.40 multiplied by 50 feet) tall will affect air flow at stack top. Any buildings shorter than 20 feet should not be included in the BPIP analysis. The building height test is performed for each stack and each building.
- Step 3** Use the building distance test to check each building required to be included in BPIP from the building height test. For the building distance test, only buildings “nearby” the stack will affect air flow at stack top. “Nearby” is defined as “five times the lesser of building height or crosswind width” (U.S. EPA 1995d). A simplified distance test may be used by considering only the building height rather than the crosswind width. While some buildings with more height than width will be included unnecessarily using this simplification, BPIP will identify correctly only the building dimensions required for ISCST3.

As an example, if a plot plan identifies a 25-foot tall building that is 115 feet from the 50-foot tall combustion unit stack center to the closest building corner. The building distance test, for this building only, is five times the building height, or 125 feet (five multiplied by the building height, 25 feet). This building would be included in the BPIP analysis, because it passes the building height test and building distance test.

- Step 4** Repeat steps 2 and 3 for each building and each stack, identifying all buildings to be included in the BPIP. If the number of buildings exceeds the BPIP limit of eight buildings, consider combining buildings, modifying BPIP code for more buildings, or using third-party commercial software which implements BPIP. If two buildings are closer than the height of the taller building, the two buildings may be combined. For example, two buildings are 40 feet apart at their closest points. One building is 25 feet high, and the



other building is 50 feet high. The buildings could be combined into one building for input to BPIP. For input to BPIP, the corners of the combined building are the outer corners of the two buildings. For unusually shaped buildings with more than the eight corners allowed by BPIP, approximate the building by using the eight corners that best represent the extreme corners of the building. The BPIP User's Guide contains additional description and illustrations on combining buildings, and BPIP model limitations (U.S. EPA 1995d).

**Step 5** Mark off the facility plot plan with UTM grid lines. Extract the UTM coordinates of each building corner and each stack center to be included in BPIP input file. Although BPIP allows the use of "plant coordinates," U.S. EPA OSW requires that all inputs to the air modeling be prepared using UTM coordinates (meters) for consistency. UTM coordinates are rectilinear, oriented to true north, and in metric units required for ISCST3 modeling. Almost all air modeling will require the use of USGS topographic data (digital and maps) for receptor elevations, terrain grid files, location of plant property, and identification of surrounding site features. Therefore, using an absolute coordinate system will enable the modeler to check inputs at each step of the analysis. Also, the meteorological data are oriented to true north. Significant errors will result from ISCST3 if incorrect stack or building locations are used, plant north is incorrectly rotated to true north, or incorrect base elevations are used. With computer run times of multiple years of meteorological data requiring many hours (up to 40 hours for one deposition run with depletion), verification of locations at each step of preparing model inputs will prevent the need to remodel.

Several precautions and guidelines should be observed in preparing input files for BPIP:

- Before BPIP is run, the correct locations should be graphically confirmed. One method is to plot the buildings and stack locations by using a graphics program. Several commercial programs incorporating BPIP provide graphic displays of BPIP inputs.
- U.S. EPA OSW recommends, in addition to using UTM coordinates for stack locations and building corners, using meters as the units for height.
- Carefully include the stack base elevation and building base elevations by using the BPIP User's Guide instructions.
- Note that the BPIP User's Guide (revised February 8, 1995) has an error on page 3-5, Table 3-1, under the "TIER(i,j)" description, which incorrectly identifies tier height as base elevation.
- BPIP mixes the use of "real" and "integer" values in the input file. To prevent possible errors in the input file, note that integers are used where a count is requested (for example, the number of buildings, number of tiers, number of corners, or number of stacks).
- The stack identifications (up to eight characters) in BPIP must be identical to those used in the ISCST3 input file, or ISCST3 will report errors.

For most sites, BPIP executes in less than 1 minute. The array of 36 building heights and 36 building widths (one for each of 36 10-degree direction sectors) are input into the ISCST3 input file by cutting and pasting from the BPIP output file. The five blank spaces preceding "SO" in the BPIP output file must be deleted so that the "SO" begins in the first column of the ISCST3 input file.

One use of BPIP is to design stack heights for new facilities or determine stack height increases required to avoid the building influence on air flow, which may cause high concentrations and deposition near the facility. The output for BPIP provides the GEP heights for stacks. Significant decreases in concentrations and deposition rates will begin at stack heights at least 1.2 times the building height, and further decreases occur at 1.5 times building height, with continual decreases of up to 2.5 times building height (GEP stack height) where the building no longer influences stack gas.

### **3.3 USE OF UNIT EMISSION RATE**

The ISCST3 model is usually run with a unit emission rate of 1.0 g/s in order to preclude having to run the model for each specific COPC. The unitized concentration and deposition output from ISCST3, using a unit emission rate, are adjusted to the COPC-specific air concentrations and deposition rates in the estimating media concentration equations (see Section 3-11) by using COPC-specific emission rates obtained during the trial burn (see Chapter 2). Concentration and deposition are directly proportional to a unit emission rate used in the ISCST3 modeling.

For facilities with multiple stacks or emission sources, each source must be modeled separately. The key to not allowing more than one stack in a single run is the inability to estimate stack-specific risks, which limits the ability of a permitting agency to evaluate which stack is responsible for the resulting risks. Such ambiguity would make it impossible for the agency to specify protective, combustion unit-specific permit limits. If a facility has two or more stacks with identical characteristics (emissions, stack parameters, and nearby locations), agency approval may be requested to represent the stacks with a single set of model runs.

### **3.4 PARTITIONING OF EMISSIONS**

COPC emissions to the environment occur in either vapor or particle phase. In general, most metals and organic COPCs with very low volatility (refer to fraction of COPC in vapor phase  $[F_v]$  less than 0.05, as

presented in Appendix A-2) are assumed to occur only in the particle phase. Organic COPCs occur as either only vapor phase (refer to  $F_v$  of 1.0, as presented in Appendix A-2) or with a portion of the vapor condensed onto the surface of particulates (e.g., particle-bound). COPCs released only as particulates are modeled with different mass fractions allocated to each particle size than the mass fractions for the organics released in both the vapor and particle-bound phases. Due to the limitations of the ISCST3 model, estimates of vapor phase COPCs, particle phase COPCs, and particle-bound COPCs cannot be provided in a single pass (run) of the model. Multiple runs are required. An example of this requirement is the risk assessment for the WTI incinerator located in East Liverpool, Ohio. The study used three runs; a vapor phase run for organic COPCs, a particle run with mass weighting of the particle phase metals and organic COPCs with very low volatility, and a particle run with surface area weighting of the particle-bound organic COPCs.

### **3.4.1 Vapor Phase Modeling**

ISCST3 output for vapor phase air modeling runs are vapor phase ambient air concentration and wet vapor deposition at receptor grid nodes based on the unit emission rate. Vapor phase runs do not require a particle size distribution in the ISCST3 input file. One vapor phase run is required for each receptor grid that is modeled (see Section 3.7).

### **3.4.2 Particle Phase Modeling (Mass Weighting)**

ISCST3 uses algorithms to compute the rate at which dry and wet removal processes deposit particulate-phase COPCs emitted from a combustion unit stack to the Earth's surface. Particle size is the main determinant of the fate of particles in air flow, whether dry or wet. The key to dry particle deposition rate is the terminal, or falling, velocity of a particle. Particle terminal velocity is calculated mainly from the particle size and particle density. Large particles fall more rapidly than small particles and are deposited closer to the stack. Small particles have low terminal velocities, with very small particles remaining suspended in the air flow. Wet particle deposition also depends on particle size as larger particles are more easily removed, or scavenged, by falling liquid (rain) or frozen (snow or sleet) precipitation. An ISCST3 modeling analysis of particle phase emissions for deposition rate requires an initial estimate of the particle size distribution, distinguished on the basis of particle diameter.

The diameters of small particulates contained in stack emissions are usually measured in micrometers. The distribution of particulate by particle diameter will differ from one combustion process to another, and is greatly dependent on (1) the type of furnace, (2) the design of the combustion chamber, (3) the composition of the feed fuel, (4) the particulate removal efficiency, (5) the design of the APCS, (6) the amount of air, in excess of stoichiometric amounts, that is used to sustain combustion, and (7) the temperature of combustion. However, based on these variables, the particle size distribution cannot be calculated, but only directly measured or inferred from prior data. Unfortunately, few studies have been performed to directly measure particle size distributions from a variety of stationary combustion sources (U.S. EPA 1986a).

U.S. EPA OSW recommends that existing facilities perform stack tests to identify particle size distribution. These data should represent actual operating conditions for the combustion unit and air pollution control device (APCD) that remove particulate from the stack gas. A table of particle size distribution data should be prepared using stack test data in the format in Table 3-1.

U.S. EPA OSW expects that stack test data will be different from the values presented in Table 3-1 because of the use of particle “cut size” for the different cascade impactor filters (or Coulter counter-based distributions) used during actual stack sampling. The test method will drive the range of particle sizes that are presented in the results of the stack test. However, because ISCST3 requires mean particle diameter for each particle size distribution, and the stack test data identifies only the mass (“weight”) of particles in a range bounded by two specific diameters, stack test data must be converted into a mean particle diameter which approximates the diameter of all the particles within a defined range. Consistent with U.S. EPA 1993h, the mean particle diameter is calculated by using the following equation:

$$D_{mean} = [0.25 \cdot (D_1^3 + D_1^2 D_2 + D_1 D_2^2 + D_2^3)]^{0.33} \quad \text{Equation 3-1}$$

where

- $D_{mean}$  = Mean particle diameter for the particle size category ( $\mu\text{m}$ )
- $D_1$  = Lower bound cut of the particle size category ( $\mu\text{m}$ )
- $D_2$  = Upper bound cut of the particle size category ( $\mu\text{m}$ )

For example, the mean particle diameter of 5.5  $\mu\text{m}$  in Table 3-1 is calculated from a lower bound cut size (assuming a cascade impactor is used to collect the sample) of 5.0  $\mu\text{m}$  to an upper bound cut size of 6.15  $\mu\text{m}$ . In this example, the mean particle diameter is calculated as:

$$D_{mean} = [0.25 (5.0^3 + (5.0)^2(6.15) + (5.0)(6.15)^2 + 6.15^3)]^{0.33} = 5.5 \mu\text{m}$$

TABLE 3-1

**GENERALIZED PARTICLE SIZE DISTRIBUTION, AND PROPORTION OF AVAILABLE SURFACE AREA, TO BE USED AS A DEFAULT IN DEPOSITION MODELING IF SITE-SPECIFIC DATA ARE UNAVAILABLE**

1	2	3	4	5	6
Mean Particle Diameter <sup>a</sup> ( $\mu\text{m}$ )	Particle Radius ( $\mu\text{m}$ )	Surface Area/ Volume ( $\mu\text{m}^{-1}$ )	Fraction of Total Mass <sup>b</sup>	Proportion Available Surface Area	Fraction of Total Surface Area
> 15.0	7.50	0.400	0.128	0.0512	0.0149
12.5	6.25	0.480	0.105	0.0504	0.0146
8.1	4.05	0.741	0.104	0.0771	0.0224
5.5	2.75	1.091	0.073	0.0796	0.0231
3.6	1.80	1.667	0.103	0.1717	0.0499
2.0	1.00	3.000	0.105	0.3150	0.0915
1.1	0.55	5.455	0.082	0.4473	0.1290
0.7	0.40	7.500	0.076	0.5700	0.1656
< 0.7	0.40	7.500	0.224	1.6800	0.4880

Notes:

- a Geometric mean diameter in a distribution from U.S. EPA (1980a), as presented in U.S. EPA (1993h)
- b The terms mass and weight are used interchangeably when using stack test data

From Table 3-1, the mean particle diameter is 5.5  $\mu\text{m}$ . The mass of particulate from the 5.0  $\mu\text{m}$  stack test data is then assigned to the 5.5  $\mu\text{m}$  mean particle diameter for the purpose of computing the “fraction of total mass.”

Typically, eight to ten mean particle diameters are available from stack test results. As determined from a sensitivity analysis conducted by The Air Group-Dallas under contract to U.S. EPA Region 6 ([www.epa.gov/region06](http://www.epa.gov/region06)), a minimum of three particle size categories (> 10 microns, 2-10 microns, and < 2 microns) detected during stack testing are generally the most sensitive to air modeling with ISCST-3 (U.S. EPA 1997). For facilities with stack test results which indicate mass amounts lower than the detectable limit (or the filter weight is less after sampling than before), a single mean particle size diameter of 1.0 microns should be used to represent all mass (e.g., particle diameter of 1.0 microns or a particle mass fraction of 1.0) in the particle and particle-bound model runs. Because rudimentary methods for stack testing may not detect the very small size or amounts of COPCs in the particle phase, the use of a 1.0 micron particle size will allow these small particles to be included properly as particles in the risk assessment exposure pathways while dispersing and depositing in the air model similar in behavior to a vapor.

After calculating the mean particle diameter (Column 1), the fraction of total mass (Column 4) per mean particle size diameter must be computed from the stack test results. For each mean particle diameter, the stack test data provides an associated mass of particulate. The fraction of total mass for each mean particle diameter is calculated by dividing the associated mass of particulate for that diameter by the total mass of particulate in the sample. In many cases, the fractions of total mass will not sum to 1.0 due to rounding errors. In these instances, U.S. EPA OSW advocates that the remaining mass fraction be added into the largest mean particle diameter mass fraction to force the total mass to 1.0.

Direct measurements of particle-size distributions at a proposed new facility may be unavailable, so it will be necessary to provide assumed particle distributions for use in ISCST3. In such instances, a representative distribution may be used. The unit on which the representative distribution is based should be as similar as practicable to the proposed unit. For example, the default distribution provided in Table 3-1 is not appropriate for a hazardous waste burning boiler with no APCD or a wet scrubber, because it is based on data from different type of unit. However, the generalized particle size (diameter) distribution in Table 3-1 may be used as a default for some combustion facilities equipped with either ESPs

or fabric filters, because the distribution is relatively typical of particle size arrays that have been measured at the outlet to advanced equipment designs (Buonicore and Davis 1992; U.S. EPA 1986a; U.S. EPA 1987a).

After developing the particulate size distribution based on mass, this distribution is used in ISCST3 to apportion the mass of particle phase COPCs (metals and organics with  $F_v$  values less than 0.05) based on particle size. Column 4 of Table 3-1 (as developed from actual stack test data) is used in the ISCST3 input file to perform a particulate run with the particle phase COPCs apportioned based on mass weighting.

### 3.4.3 Particle-Bound Modeling (Surface Area Weighting)

A surface area weighting, instead of mass weighting, of the particles is used in separate particle runs of ISCST3. Surface area weighting approximates the situation where a semivolatile organic contaminant that has been volatilized in the high temperature environment of a combustion system and then condensed to the surface of particles entrained in the combustion gas after it cools in the stack. Thus, the apportionment of emissions by particle diameter becomes a function of the surface area of the particle that is available for chemical adsorption (U.S. EPA 1993h).

The first step in apportioning COPC emissions by surface area is to calculate the proportion of available surface area of the particles. If particle density is held constant (such as  $1 \text{ g/m}^3$ ), the proportion of available surface area of aerodynamic spherical particles is the ratio of surface area ( $S$ ) to volume ( $V$ ), as follows:

- Assume aerodynamic spherical particles.
- Specific surface area of a spherical particle with a radius,  $r$ — $S = 4 \pi r^2$
- Volume of a spherical particle with a radius,  $r$ — $V = 4/3 \pi r^3$
- Ratio of  $S$  to  $V$ — $S/V = 4 \pi r^2 / (4/3 \pi r^3) = 3/r$

The following uses the particle size distribution in Table 3-1 as an example of apportioning the emission rate of the particle-bound portion of the COPC based on surface area. This procedure can be followed for apportioning actual emissions to the actual particle size distribution measured at the stack. In Table 3-1, a



spherical particle having a diameter of 15  $\mu\text{m}$  (Column 1) has a radius of 7.5  $\mu\text{m}$  (Column 2). The proportion of available surface area (assuming particle density is constant) is 0.400 ( $S/V = 3/7.5$ ), which is the value in Column 3. Column 4 shows that particles with a mean diameter of 15  $\mu\text{m}$ , constitute 12.8 percent of the total mass. Multiplication of Column 3 by Column 4 yields a value in Column 5 of 0.0512. This value is an approximation of the relative proportion of total surface area, based on the percent of particles that are 15  $\mu\text{m}$  in diameter. The sum of Column 5 yields the total surface area of all particles in the particle size distribution. In this example, the sum is 3.4423. Column 6 is the fraction of total surface area represented by the specific particle diameter in the distribution, and is calculated by dividing the relative proportion of surface area (Column 5) for a specific diameter by the total relative proportion of surface area (3.4423 square micrometers [ $\mu\text{m}^2$ ]). In the example of the 15  $\mu\text{m}$ -diameter particle, the fraction of total surface area available for adsorption is 0.0149 ( $0.0512/3.4423$ ). This procedure is then repeated for all particle sizes in the array.

After developing the particulate size distribution based on surface area, this distribution is used in ISCST3 to apportion mass of particle-bound COPCs (most organics) based on particle size. Column 6 of Table 3-1 (as developed from actual stack test data) is used in the ISCST3 input file to perform a particulate run for the particle-bound COPCs apportioned based on surface area weighting.

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Copies of all stack test data used to determine particle size distribution
- Copies of all calculations made to determine particle size distribution, fraction of total mass, and fraction of total surface area

### 3.5 METEOROLOGICAL DATA

To model air concentration and deposition, the ISCST3 model requires a variety of meteorological information:

1. Air concentration
  - a. Hourly values

- (1) Wind direction (degrees from true north)
  - (2) Wind speed (m/s)
  - (3) Dry bulb (ambient air) temperature (K)
  - (4) Opaque cloud cover (tenths)
  - (5) Cloud ceiling height (m)
- b. Daily values
- (1) Morning mixing height (m)
  - (2) Afternoon mixing height (m)
2. Deposition
- a. Dry particle deposition—hourly values for surface pressure (millibars)
  - b. Wet particle deposition—hourly values
    - (1) Precipitation amount (inches)
    - (2) Precipitation type (liquid or frozen)
  - c. Dry vapor deposition (when available)—hourly values for solar radiation (watts/m<sup>2</sup>)

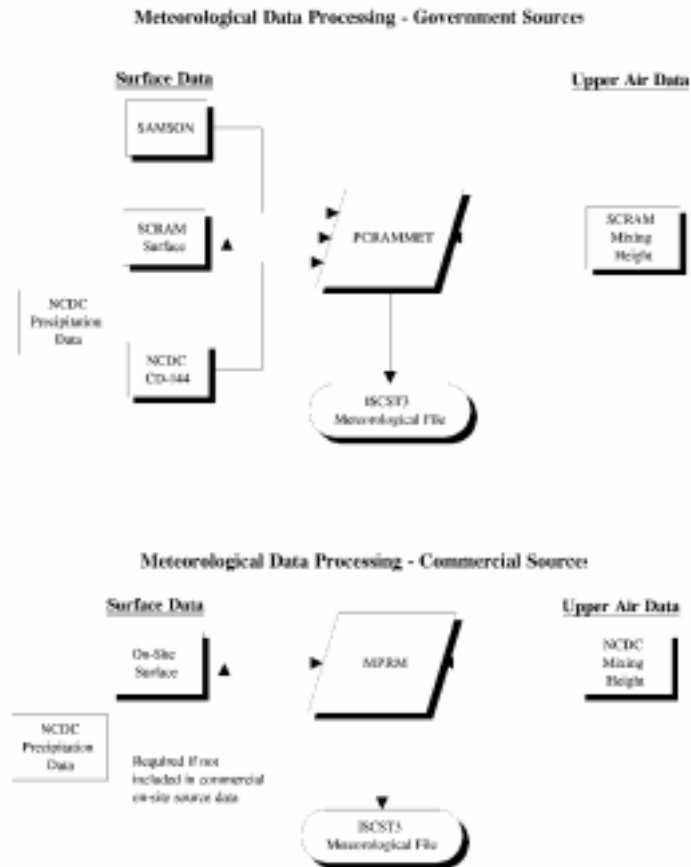
As shown in Figure 3-1, these data are available from several different sources. For most air modeling, five years of data from a representative National Weather Service station is recommended. However, in some instances where the closest NWS data is clearly not representative of site specific meteorological conditions, and there is insufficient time to collect 5 years of onsite data, 1 year of onsite meteorological data (consistent with GAQM) may be used to complete the risk assessment. The permitting authority should approve the representative meteorological data prior to performing air modeling.

The following subsections describe how to select the surface and upper air data that will be used in conjunction with the ISCST3 model. Section 3.7 describes the computer programs used to process the meteorological data for input to the ISCST3 model.

#### **RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT**

- Identification of all sources of meteorological data

FIGURE 3-1  
SOURCES OF METEOROLOGICAL DATA



### 3.5.1 Surface Data

Surface data can be obtained from SAMSON in CD-ROM format. SAMSON data are available for 239 airports across the U.S. for the period of 1961 through 1990. The National Climate Data Center (NCDC) recently released the update to SAMSON through 1995 surface data. However, since the upper air (mixing height) data available from the U.S. EPA SCRAM web site has not been updated to cover this recent data period, it is acceptable to select the representative 5 years of meteorological data from the period up through 1990. SAMSON data contain all of the required input parameters for concentration, dry and wet particle deposition, and wet vapor deposition. SAMSON also includes the total solar radiation data required for dry vapor deposition, which may be added to ISCST3 in the future. Alternatively, some meteorological files necessary for running ISCST3 are also available on the SCRAM BBS for NWS stations located throughout the country (SCRAM BBS is part of the Office of Air Quality and Planning and Standards Technology Transfer Network [OAQPS TTN]). The meteorological data, preprocessors, and user's guides are also located on the SCRAM web site at "<http://www.epa.gov/scram001/index.htm>". However, these files do not contain surface pressure, types of precipitation (present weather), or precipitation amount. Although the ISCST3 model is not very sensitive to surface pressure variations, and a default value may be used, precipitation types and amounts are necessary for air modeling wet deposition. Precipitation data are available from the National Climatic Data Center (NCDC), and are processed by PCRAMMET to supplement the SCRAM BBS surface data. NCDC also has surface data in CD-144 format, which contains all of the surface data, including precipitation.

The SAMSON CD-ROM for the eastern, central, or western (Volumes I, II, and III) United States may be purchased from NCDC in Asheville, North Carolina.

<b>National Climatic Data Center                  Federal Building                  37 Battery Park Avenue                  Asheville, NC 28801-2733</b>	
<b>Customer Service: (704) 271-4871</b>	
File type:	File name:
Hourly precipitation amounts	NCDC TC-3240
Hourly surface observations with precipitation type	NCDC TD-3280
Hourly surface observations with precipitation type	NCDC SAMSON CD-ROM (Vol. I, II, and/or III)
Twice daily mixing heights from nearest station	NCDC TD-9689 (also available on SCRAM web site for 1984 through 1991)

PCRAMMET and MPRM are the U.S. EPA meteorological preprocessor programs for preparing the surface and upper air data into a meteorological file of hourly parameters for input into the ISCST3 model. Most air modeling analyses will use PCRAMMET to process the National Weather Service data. However, both preprocessors require the modeler to replace any missing data. Before running PCRAMMET or MPRM, the air modeler must fill in missing data to complete 1 full year of values. A procedure recommended by U.S. EPA for filling missing surface and mixing height data is documented on the SCRAM BBS under the meteorological data section. If long periods of data are missing, and these data are not addressed by the U.S. EPA procedures on the SCRAM BBS, then a method must be developed for filling in missing data. One option is to fill the time periods with “surrogate place holder” data in the correct format with correct sequential times to complete preparation of the meteorological file. Place holder data are typically considered the last valid hourly data of record. Then, when ISCST3 is running, the MSGPRO keyword in the Control pathway can be used to specify that data are missing. Note that the DEFAULT keyword must not be used with MSGPRO. Since the missing data keyword is not approved generally for regulatory air modeling, the appropriate agency must provide approval prior to use. All processing of meteorological data should be completely documented to include sources of data, decision criteria for selection, consideration for precipitation amounts, preprocessor options selected, and filled missing data.

The most recently available 5 years of complete meteorological data contained on SAMSON, or more recent sources, should be used for the air modeling. It is desirable, but not mandatory, that the 5 years are

consecutive. The use of less than five years of meteorological data should be approved by appropriate authorities. The following subsections describe important characteristics of the surface data.

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**RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT**

- Electronic copy of the ISCST3 input code used to enter meteorological information
  - Description of the selection criteria and process used to identify representative years used for meteorological data
  - Identification of the 5 years of meteorological selected
  - Summary of the procedures used to compensate for any missing data
- 

### **3.5.1.1 Wind Speed and Wind Direction**

Wind speed and direction are two of the most critical parameters in ISCST3. The wind direction promotes higher concentration and deposition if it persists from one direction for long periods during a year. A predominantly south wind, such as on the Gulf Coast, will contribute to high concentrations and depositions north of the facility. Wind speed is inversely proportional to concentration in the ISCST3 algorithms. The higher the wind speed, the lower will be the concentration. If wind speed doubles, the concentration and deposition will be reduced by one-half. ISCST3 needs wind speed and wind direction at the stack top. Most air modeling is performed using government sources of surface data. Wind data are typically measured at 10 meters height at NWS stations. However, since some stations have wind speed recorded at a different height, the anemometer height must always be verified so that the correct value can be input into the PCRAMMET meteorological data preprocessing program. ISCST3 assumes that wind direction at stack height is the same as measured at the NWS station height. ISCST3 uses a wind speed profile to calculate wind speed at stack top. This calculation exponentially increases the measured wind speed from the measured height to a calculated wind speed at stack height (U.S. EPA 1995d).

### **3.5.1.2 Dry Bulb Temperature**

Dry bulb temperature, or ambient air temperature, is the same temperature reported on the television and radio stations across the country each day. It is measured at 2 meters above ground level. Air temperature

is used in ISCST3 in the buoyant plume rise equations developed by Briggs (U.S. EPA 1995c). The model results are not very sensitive to air temperature, except at extremes. However, buoyant plume rise is very sensitive to the stack gas temperature. Buoyant plume rise is mainly a result of the difference between stack gas temperature and ambient air temperature. Conceptually, it is similar to a hot air balloon. The higher the stack gas temperature, the higher will be the plume rise. High plume heights result in low concentrations and depositions as the COPCs travel further and are diluted in a larger volume of ambient air before reaching the surface. The temperature is measured in K, so a stack gas temperature of 450°F is equal to 505 K. Ambient temperature of 90°F is equal to 305 K, and 32°F is 273 K. A large variation in ambient temperature will affect buoyant plume rise, but not as much as variations in stack gas temperature.

### **3.5.1.3 Opaque Cloud Cover**

PCRAMMET uses opaque cloud cover to calculate the stability of the atmosphere. Stability determines the dispersion, or dilution, rate of the COPCs. Rapid dilution occurs in unstable air because of surface heating that overturns the air. With clear skies during the day, the sun heats the Earth's surface, thereby causing unstable air and dilution of the stack gas emission stream. Stable air results in very little mixing, or dilution, of the emitted COPCs. A cool surface occurs at night because of radiative loss of heat on clear nights. With a cloud cover, surface heating during the day and heat loss at night are reduced, resulting in moderate mixing rates, or neutral stability. Opaque cloud cover is a measure of the transparency of the clouds. For example, a completely overcast sky with 10/10ths cloud cover may have only 1/10th opaque cloud cover if the clouds are high, translucent clouds that do not prevent sunlight from reaching the Earth's surface. The opaque cloud cover is observed at NWS stations each hour.

### **3.5.1.4 Cloud Ceiling Height**

Cloud height is required in PCRAMMET to calculate stability. Specifically, the height of the cloud cover affects the heat balance at the Earth's surface. Cloud ceiling height is measured or observed at all NWS stations provided on the SAMSON CD-Roms and the U.S. EPA SCRAM web site.

### 3.5.1.5 Surface Pressure

Surface pressure is required by ISCST3 for calculating dry particle deposition. However, ISCST3 is not very sensitive to surface pressure. SAMSON and NCDC CD-144 data include surface pressure. SCRAM BBS surface data do not include surface pressure. U.S. EPA believes that, if SCRAM BBS surface data are used, a default value of 1,000 millibars can be assumed, with little impact on modeled results.

### 3.5.1.6 Precipitation Amount and Type

The importance of precipitation to ISCST3 results was discussed in the selection of the meteorological data period (see Section 3.5.1). Precipitation is measured at 3 feet (1 meter) above ground level. Precipitation amount and type are required to be processed by PCRAMMET or MPRM into the ISCST3 meteorological file to calculate wet deposition of vapor and particles. The amount of precipitation, or precipitation rate, will directly influence the amount of wet deposition at a specific location. Particles and vapor are both captured by falling precipitation, known as precipitation scavenging. Scavenging coefficients are required as inputs to ISCST3 for vapors with a rate specified for liquid and frozen precipitation. The precipitation type in a weather report in SAMSON or CD-144 data file will identify to ISCST3 which event is occurring for appropriate use of the scavenging coefficients entered (see Section 3.7.2.6). SCRAM BBS surface data do not include precipitation data. Supplemental precipitation files from NCDC may be read into PCRAMMET for integration into the ISCST3 meteorological file.

### 3.5.1.7 Solar Radiation (Future Use for Dry Vapor Deposition)

The current version of ISCST3 does not use solar radiation. Several U.S. EPA models, including the Acid Deposition and Oxidant Model (ADOM), incorporate algorithms for dry vapor deposition. At such time as U.S. EPA approves the draft version of ISCST3 which includes dry gas deposition, the hourly total solar radiation will be required. Solar radiation affects the respiratory activity of leaf surfaces, which affects the rate of vapor deposition. With a leaf area index identified in the ISCST3 input file in the future, the model will be able to calculate dry vapor deposition.



### 3.5.2 Upper Air Data

Upper air data, also referred to as mixing height data, are required to run the ISCST3 model. ISCST3 requires estimates of morning and afternoon (twice daily) mixing heights. PCRAMMET and MPRM use these estimates to calculate an hourly mixing height by using interpolation methods (U.S. EPA 1996e). The mixing height files are typically available for the years 1984 through 1991 on the U.S. EPA SCRAM web site. U.S. EPA OSW recommends that only years with complete mixing height data be used as input for air modeling. In some instances, data may need to be obtained from more than one station to complete five years of data. The selection of representative data should be discussed with appropriate authorities prior to performing air modeling.

Mixing height data for years prior to 1983, in addition to current mixing height data, may be purchased from NCDC as described in Section 3.5.1. The years selected for upper air data must match the years selected for surface data. If matching years of mixing height data are not available from a single upper air station, another upper air station should be used for completing the five years.

## 3.6 METEOROLOGICAL PREPROCESSORS AND INTERFACE PROGRAMS

After the appropriate surface and upper air data is selected following the procedures outlined in Section 3.5, additional data manipulation is necessary before the data is used with the ISCST3 model. The following subsections describe the meteorological preprocessors and interface programs used for these manipulation tasks. To eliminate any need to repeat air modeling activities, U.S. EPA OSW recommends that the selection of representative mixing height and surface data be approved by the appropriate regulatory agency before preprocessing or air modeling is conducted. Permitting authority approval also is recommended in the selection of site-specific parameter values required as input to the meteorological data preprocessors.

### 3.6.1 PCRAMMET

U.S. EPA OSW recommends preparing a meteorological file for ISCST3 that can be used to calculate any concentration or deposition. By preparing a file that PCRAMMET terms a "WET DEPOSITION" file, all required parameters will be available to ISCST3 for any subsequent concentration or deposition modeling.

For example, if only the concentration option is selected in ISCST3 for a specific run, ISCST3 will ignore the precipitation values in the meteorological file. For subsequent air deposition modeling, ISCST3 will access the precipitation data from the same preprocessed meteorological file.

PCRAMMET may use SAMSON, SCRAM web site, and NCDC CD-144 surface data files. U.S. EPA OSW recommends using the SAMSON option in PCRAMMET to process the SAMSON surface data and U.S. EPA SCRAM web site mixing height data. The PCRAMMET User's Guide in the table "Wet Deposition, SAMSON Data" (U.S. EPA 1995b) identifies the PCRAMMET input requirements for creating an ASCII meteorological file for running ISCST3 to calculate air concentration, and wet and dry deposition. The meteorological file created for ISCST3 will contain all of the parameters needed for air modeling of concentration and deposition.

PCRAMMET requires the following input parameters representative of the measurement site:

- Monin-Obukhov length
- Anemometer height
- Surface roughness height (at measurement site)
- Surface roughness height (at application site)
- Noon-time albedo
- Bowen ratio
- Anthropogenic heat flux
- Fraction of net radiation absorbed at surface

The PCRAMMET User's Guide contains detailed information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1995b). The parameters listed are briefly described in the following subsections. These data are not included in the surface or mixing height data files obtained from the U.S. EPA or NCDC. Representative values specific to the site to be modeled should be carefully selected using the tables in the PCRAMMET User's Guide or reference literature. The selected values should be approved prior to processing the meteorological data.

### 3.6.1.1 Monin-Obukhov Length

The Monin-Obukhov length ( $L$ ) is a measure of atmospheric stability. It is negative during the day, when surface heating causes unstable air. It is positive at night, when the surface is cooled with a stable atmosphere. In urban areas during stable conditions, the estimated value of  $L$  may not adequately reflect the less stable atmosphere associated with the mechanical mixing generated by buildings or structures. However, PCRAMMET requires an input for minimum urban Monin-Obukhov length, even if the area to be analyzed by ISCST3 is rural. A nonzero value for  $L$  must be entered to prevent PCRAMMET from generating an error message. A value of 2.0 meter for  $L$  should be used when the land use surrounding the site is rural (see Section 3.2.2.1). For urban areas, Hanna and Chang (1991) suggest that a minimum value of  $L$  be set for stable hours to simulate building-induced instability. The following are general examples of  $L$  values for various land use classifications:

Land Use Classification	Minimum $L$
Agricultural (open)	2 meters
Residential	25 meters
Compact residential/industrial	50 meters
Commercial (19 to 40-story buildings)	100 meters
Commercial (>40-story buildings)	150 meters

PCRAMMET will use the minimum  $L$  value for calculating urban stability parameters. These urban values will be ignored by ISCST3 during the air modeling analyses for rural sites.

### 3.6.1.2 Anemometer Height

The height of the wind speed measurements is required by ISCST3 to calculate wind speed at stack top. The wind sensor (anemometer) height is identified in the station history section of the Local Climatological Data Summary available from NCDC for every National Weather Service station. Since 1980, most National Weather Service stations measure wind speed at the height of 10 meters. However, some stations operate at other heights or have valid representative data during years of operation at more than one height. The modeler must verify the correct measurement height for each year of data prior to processing with

PCRAMMET and running the ISCST3 model. ISCST3 modeled results are very sensitive to small variations in wind speed.

### 3.6.1.3 Surface Roughness Height at Measurement Site

Surface roughness height is a measure of the height of obstacles to wind flow. It is important in ISCST3 because it determines how close a particle must be above the ground before it is “captured” for deposition on the ground. Dramatic differences in ISCST3 calculations may result from slight variations in surface roughness. For surface meteorological data from a National Weather Station, a value of 0.10 meters for the “measurement site” typically may be used without prior approval. Surface roughness is proportional, but not equal, to the physical height of the obstacles. The table in Section 3.2.2.2 lists the roughness heights that can be used as input values. These values are based on the general land use in the vicinity of the measurement site. These values should be considered in discussions with the appropriate agency modeler prior to air modeling.

### 3.6.1.4 Surface Roughness Height at Application Site

Determination of surface roughness height is also required at the facility (application site) for performing PCRAMMET processing to prepare an ISCST3 meteorological file. ISCST3 model results are very sensitive to the value used in PCRAMMET for this parameter. The table in Section 3.2.2.2 is applicable to the application site. A site-specific computation of a single surface roughness value representative of the site is required using the method described in Section 3.2.2.2. The computed value of surface roughness height for the application site, along with maps or photographs illustrating land use, must be approved by the appropriate agency prior to use.

### 3.6.1.5 Noon-Time Albedo

“Noon-time albedo” is the fraction of the incoming solar radiation that is reflected from the ground when the sun is directly overhead. Albedo is used in calculating the hourly net heat balance at the surface for calculating hourly values of Monin-Obukhov length. PCRAMMET automatically adjusts for the variation in albedo with solar elevation angle. Experience suggests that ISCST3 modeling results are not sensitive to the value selected for this parameter. Typical albedo values are presented in Table 3-2. As shown in Table

3-2, albedo values vary from 0.10 to 0.20 on water surfaces from summer to winter. The most variability is for cultivated farmland, which varies from 0.14 during spring when land is tilled to expose dark earth, to 0.60 in winter when areas are snow-covered.

Based on the information in Table 3-2, albedos are estimated to vary in rural areas from 0.14 to 0.20 for cultivated land, and from 0.18 to 0.20 for grassland. For urban areas, the variation without snow is from 0.14 to 0.18. For practical purposes, the selection of a single value for noon-time albedo to process a complete year of meteorological data is desirable. For example, the single value of 0.18 may be appropriate to process all meteorological data for an urban site. For rural sites, a single albedo value of 0.18 representative of grassland and cultivated land may be appropriate for areas without significant snow cover during winter months. For desert shrubland, a single value of 0.28 may be appropriate. A single value of 0.12 could be representative of forested areas. The permitting authority should review proposed values used in the processing of the meteorological data.

TABLE 3-2

ALBEDO OF NATURAL GROUND COVERS FOR LAND USE TYPES AND SEASONS

Land Use Type	Season <sup>a</sup>			
	Spring	Summer	Autumn	Winter
Water surface	0.12	0.10	0.14	0.20
Deciduous forest	0.12	0.12	0.12	0.50
Coniferous forest	0.12	0.12	0.12	0.35
Swamp	0.12	0.14	0.16	0.30
Cultivated land	0.14	0.20	0.18	0.60
Grassland	0.18	0.18	0.20	0.60
Urban	0.14	0.16	0.18	0.35
Desert shrubland	0.30	0.28	0.28	0.45

Notes:

Source—Iqbal (1983)

<sup>a</sup> The various seasons are defined by Iqbal (1983) as follows:

- Spring: Periods when vegetation is emerging or partially green; this is a transitional situation that applies for 1 to 2 months after the last killing frost in spring.
- Summer: Periods when vegetation is lush and healthy; this is typical of mid-summer, but also of other seasons in which frost is less common.
- Autumn: Periods when freezing conditions are common, deciduous trees are leafless, crops are not yet planted or are already harvested (bare soil exposed), grass surfaces are brown, and no snow is present.
- Winter: Periods when surfaces are covered by snow and temperatures are below freezing. Winter albedo depends on whether a snow cover is present continuously, intermittently, or seldom. Albedo ranges from about 0.30 for bare snow cover to about 0.65 for continuous cover.

### 3.6.1.6 Bowen Ratio

The Bowen ratio is a measure of the amount of moisture at the surface. The presence of moisture affects the heat balance resulting from evaporative cooling, which, in turn, affects the hourly Monin-Obukhov length calculated by PCRAMMET. Surface moisture is highly variable. Daytime Bowen ratios are presented in Table 3-3.

Bowen ratio values vary throughout the country. For example, in urban areas where annual rainfall is less than 20 inches, a single Bowen ratio value of 4.0 may be representative. For rural areas, a Bowen ratio value of 2.0 may be appropriate for grassland and cultivated land. For areas where annual rainfall is greater than 20 inches, U.S. EPA OSW recommends a single Bowen ratio value of 2.0 for urban areas; and 0.7 for rural forests, grasslands, and cultivated lands. The applicable permitting authority should review proposed values used in the processing of the meteorological data.

### 3.6.1.7 Anthropogenic Heat Flux

Anthropogenic heat is the surface heating caused by human activity, including automobiles and heating systems. It is used to calculate hourly  $L$  values (Monin-Obukhov lengths). Table 3-4 presents anthropogenic heat flux ( $Q_f$ ) values that have been calculated for several urban areas around the world. In rural areas, U.S. EPA OSW recommends that a value of 0.0 Watts/m<sup>2</sup> be used for the  $Q_f$ . A value of 20.0 Watts/m<sup>2</sup> is appropriate for large urban areas based on the annual value from Table 3-4 for Los Angeles.

### 3.6.1.8 Fraction of Net Radiation Absorbed at the Ground

Also used for calculating hourly values of Monin-Obukhov length, fraction of net radiation absorbed at the ground is the last component of radiative heat balance. Based on the net radiation ( $Q_*$ ) values presented in Table 3-4, and recommendations presented in the PCRAMMET User's Manual based on Oke (1982), U.S. EPA OSW recommends values of 0.15 for rural areas and 0.27 for urban areas (U.S. EPA 1995b).

**TABLE 3-3**  
**DAYTIME BOWEN RATIOS BY LAND USE, SEASON,**  
**AND PRECIPITATION CONDITIONS**

Land Use	Season <sup>a</sup>			
	Spring	Summer	Autumn	Winter
<b>Dry Conditions</b>				
Water (fresh and salt)	0.1	0.1	0.1	2.0
Deciduous forest	1.5	0.6	2.0	2.0
Coniferous forest	1.5	0.6	1.5	2.0
Swamp	0.2	0.2	0.2	2.0
Cultivated land	1.0	1.5	2.0	2.0
Grassland	1.0	2.0	2.0	2.0
Urban	2.0	4.0	4.0	2.0
Desert shrubland	5.0	6.0	10.0	2.0
<b>Average Conditions</b>				
Water (fresh and salt)	0.1	0.1	0.1	1.5
Deciduous forest	0.7	0.3	1.0	1.5
Coniferous forest	0.7	0.3	0.8	1.5
Swamp	0.1	0.1	0.1	1.5
Cultivated land	0.3	0.5	0.7	1.5
Grassland	0.4	0.8	1.0	1.5
Urban	1.0	2.0	2.0	1.5
Desert shrubland	3.0	4.0	6.0	6.0



**TABLE 3-3**  
**DAYTIME BOWEN RATIO BY LAND USE, SEASON,**  
**AND PRECIPITATION CONDITIONS**  
**(Continued)**

Land Use	Season <sup>a</sup>			
	Spring	Summer	Autumn	Winter
<b>Wet Conditions</b>				
Water (fresh and salt)	0.1	0.1	0.1	0.3
Deciduous forest	0.3	0.2	0.4	0.5
Coniferous forest	0.3	0.2	0.3	0.3
Swamp	0.1	0.1	0.1	0.5
Cultivated land	0.2	0.3	0.4	0.5
Grassland	0.3	0.4	0.5	0.5
Urban	0.5	1.0	1.0	0.5
Desert shrubland	1.0	5.0	2.0	2.0

Note:

Source—Paine (1987)

<sup>a</sup> The various seasons are defined by Iqbal (1983) as follows:

- Spring: Periods when vegetation is emerging or partially green; this is a transitional situation that applies for 1 to 2 months after the last killing frost in spring.
- Summer: Periods when vegetation is lush and healthy; this is typical of mid-summer, but also of other seasons in which frost is less common.
- Autumn: Periods when freezing conditions are common, deciduous trees are leafless, crops are not yet planted or are already harvested (bare soil exposed), grass surfaces are brown, and no snow is present
- Winter: Periods when surfaces are covered by snow and temperatures are below freezing.

**TABLE 3-4**  
**ANTHROPOGENIC HEAT FLUX ( $Q_f$ ) AND NET RADIATION ( $Q_*$ )**  
**FOR SEVERAL URBAN AREAS**

Urban Area (Latitude)	Population (Millions)	Population Density (Persons/km <sup>2</sup> )	Per Capita Energy Use (MJ x 10 <sup>3</sup> /year)	$Q_f$ (Watts/m <sup>2</sup> ) (Season)	$Q_*$ (Watts/m <sup>2</sup> )
Manhattan (40° North)	1.7	28,810	128	117 (Annual) 40 (Summer) 198 (Winter)	93 (Annual)
Montreal (45° North)	1.1	14,102	221	99 (Annual) 57 (Summer) 153 (Winter)	52 (Annual) 92 (Summer) 13 (Winter)
Budapest (47° North)	1.3	11,500	118	43 (Annual) 32 (Summer) 51 (Winter)	46 (Annual) 100 (Summer) -8 (Winter)
Sheffield (53° North)	0.5	10,420	58	19 (Annual)	56 (Annual)
West Berlin (52° North)	2.3	9,830	67	21 (Annual)	57 (Annual)
Vancouver (49° North)	0.6	5,360	112	19 (Annual) 15 (Summer) 23 (Winter)	57 (Annual) 107 (Summer) 6 (Winter)
Hong Kong (22° North)	3.9	3,730	34	4 (Annual)	110 (Annual)
Singapore (1° North)	2.1	3,700	25	3 (Annual)	110 (Annual)
Los Angeles (34° North)	7.0	2,000	331	21 (Annual)	108 (Annual)
Fairbanks (64° North)	0.03	810	740	19 (Annual)	18 (Annual)

Note:

Source—Oke (1978)

### **3.6.2 MPRM**

For on-site data, a new version of MPRM is used to mesh on-site data with NWS data in the preparation of the meteorological input file. MPRM performs the same meteorological file preparation as PCRAMMET, except the source of the surface data in MPRM consists of on-site measurements (U.S. EPA 1996e).

MPRM includes extensive QA/QC for values that are out of range. MPRM also checks for missing data and summarizes values that require editing to fill missing data. After a complete surface file passes the quality checks, it is processed with NCDC mixing height data. NCDC data are purchased to correspond to the collection period of the on-site surface data. Mixing height data available on SCRAM's web site ends in 1991. A delay of about 3 months can occur for obtaining mixing height data from NCDC to process with recent on-site surface data.

Inputs to MPRM for preparing an ISCST3 meteorological file for concentration and deposition are the same as for PCRAMMET. Section 3.6.1 provides methods for determining values for these parameters.

Draft versions of ISCST3 and MPRM are available for review which implement dry vapor deposition. These versions are GDISCDFT (dated 96248) and GDMPRDFT (dated 96248), respectively. They may be found on the U.S. EPA SCRAM web site under "Topics for Review". These draft models are not the current regulatory versions and should not be used without approval from the appropriate permitting authority.

### **3.7 ISCST3 MODEL INPUT FILES**

A thorough instruction of how to prepare the input files for ISCST3 is presented in the ISC3 User's Guide, Volume I (U.S. EPA 1995c), which is available for downloading from the SCRAM BBS. The example ISCST3 input file is provided in Figure 3-2 from the air dispersion modeling chapter (Chapter 3) of the U.S. EPA HHRAP (U.S. EPA 1998). This example illustrates a single year run (1984), for particle phase COPC emissions from a single stack, to compute acute (1-hour average) and chronic (annual average) and provide single year results in one hour and annual average plot files for post-processing. For ecological risk assessments, only the annual average air parameters are required, not the 1-hour values. However, by modeling both the 1-hour and annual averages in a single set of runs, the ISCST3 air dispersion model will

provide the necessary air parameters for use in both the human health and ecological risk assessments. The specification of a terrain grid file in the TG pathway is optional. Each air modeling analysis has unique issues and concerns that should be addressed in the risk assessment report. U.S. EPA OSW recommends that the air modeling methodology be consistent in data collection, model set-up, and model output. This consistency will assist both the modeler and U.S. EPA in communicating and interpreting model results. The risk assessment report should document each section of the ISCST3 input file to identify consistent methods.

Three sets of ISCST3 runs are required for each COPC emission source. As discussed in Section 3.4, separate ISCST3 runs are required to model vapor phase COPCs, particle phase COPCs, and particle-bound phase COPCs for each source (stack or fugitive) of COPCs. The ISCST3 “Control Secondary Keywords” used for these three runs are:

Vapor Phase:	CONC	WDEP		
Particle Phase:	CONC	DDEP	WDEP	DEPOS
Particle-Bound Phase:	CONC	DDEP	WDEP	DEPOS

For ISCST3 modeling to provide air parameters for ecological risk assessments, only the total deposition (DEPOS) of the particle and particle-bound phases are required. The control secondary keywords for concentration in the air (CONC) and the components of deposition to the ground, dry deposition (DDEP) and wet deposition (WDEP), are not required to be output separately by ISCST3. However, by specifying these control secondary keywords as illustrated, the ISCST3 model will compute the needed air parameters for both human health and ecological risk assessments. ISCST3 requires site-specific inputs for source parameters, receptor locations, meteorological data, and terrain features. The model is prepared for

execution by creating an input file. The input file is structured in five (or six if a terrain grid file is used) sections, or pathways, designated by two-letter abbreviations:

ISCST3 INPUT FILE SECTIONS	
Section	Abbreviation
Control	CO
Source	SO
Receptor	RE
Meteorology	ME
<i>Terrain Grid (Optional)</i>	<i>TG</i>
Output	OU

The following subsections describe how to specify the parameters for each pathway in the ISCST3 input file.

### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Electronic and hard copies of ISCST3 input file for all air modeling runs

#### 3.7.1 Control Pathway

Model options (MODELOPT) are specified in the COntrol pathway to direct ISCST3 in the types of computations to perform. U.S. EPA OSW recommends that air modeling specify the DFAULT parameter to use the following regulatory default options:

- Use stack-tip downwash (except for Schulman-Scire downwash).
- Use buoyancy-induced dispersion (except for Schulman-Scire downwash).
- Do not use final plume rise (except for building downwash).
- Use the calms processing routines.

- Use upper-bound concentration estimates for sources influenced by building downwash from super-squat buildings.
- Use default wind speed profile exponents.
- Use default vertical potential temperature gradients.

The CONC parameter specifies calculation of air concentrations for vapor and particles. The DDEP and WDEP parameters specify dry and wet deposition. The DEPOS specifies computation of total (wet and dry) deposition flux. Since ISCST3 currently does not include an algorithm for the dry deposition of vapor phase COPCs, only wet deposition is specified for vapor phase runs. Note that dry deposition of vapor phase is addressed in the pathway equations during the risk assessment using the concentration of the vapor phase and a deposition velocity. DRYDPLT and WETDPLT are used for plume depletion resulting from dry and wet removal. U.S. EPA OSW recommends the following command lines for each of the three runs (these are for rural areas; substitute URBAN for urban areas):

Vapor: CO MODELOPT DFAULT CONC WDEP WETDPLT RURAL

Particle Phase: CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL

Particle-Bound: CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL

Note that only the total deposition (DEPOS) air parameter values are required for the ecological risk assessment pathways. The modeler may elect not to include CONC, DDEP and WDEP as separate output components from ISCST3 if the air modeling results will not be used for a human health risk assessment. However, the control secondary keywords must always be specified for plume depletion through the dry deposition (DRYDPLT) and wet deposition (WETDPLT) processes.

FIGURE 3-2

EXAMPLE INPUT FILE FOR "PARTICLE PHASE"

```
CO STARTING
CO TITLEONE Example input file, particle phase run
CO TITLETWO 1984 met data, Baton Rouge Surface, Boothville Upper Air
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL
CO AVERTIME 1 ANNUAL
CO POLLUTID UNITY
CO TERRHGTS ELEV
CO RUNORNOT RUN
CO SAVEFILE 84SAVE1 5 84SAVE2
** Restart incomplete runs with INITFILE, changing '**' to 'CO'
** INITFILE 84SAVE1
CO FINISHED

SO STARTING
SO LOCATION STACK1 POINT 637524. 567789. 347.
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29
SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
SO PARTDENS STACK1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5 4E-5 9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
SO SRCGROUP ALL
SO FINISHED

RE STARTING
RE ELEVUNIT METERS
RE DISCCART 630000. 565000. 352.
RE DISCCART 630500. 565000. 365.
RE DISCCART 631000. 565000. 402.
...
      (ARRAY OF DISCRETE RECEPTORS)
...
RE DISCCART 635000. 570000. 387.
RE FINISHED

ME STARTING
ME INPUTFIL 84BTR.WET
ME ANEMHGHT 10.0
ME SURFDATA 13970 1984 BATON_ROUGE
ME UAIRDATA 12884 1984 BOOTHVILLE
ME FINISHED

TG STARTING
TG INPUTFIL TERRAIN.TER
TG LOCATION 0.0 0.0
TG ELEVUNIT METERS
TG FINISHED

OU STARTING
OU RECTABLE ALLAVE FIRST
OU PLOTFILE 1 ALL FIRST BTR841.PLT
OU PLOTFILE ANNUAL ALL BTR84A.PLT
OU FINISHED
```

For each of the three runs for each emission source, 5 years of off-site (e.g., National Weather Service from SAMSON) meteorological data are completed. For sites with meteorological data collected on-site, the appropriate permitting authority should be notified for the data period required for a risk assessment. The averaging times (AVERTIME) should be specified as 'ANNUAL' to compute long-term (annual average) ecological risk. Optionally, the '1' may be specified for convenience in modeling for the maximum 1-hour averages used in computing acute human health risks. Each phase run may be repeated five times (one for each year, or a total of 15 ISCST3 runs) to complete a set of 15 runs for the full five years of meteorological data.

Alternatively, the modeler may combine the 5 years of meteorological data into a single meteorological data file and complete only 3 runs for each emission source (one run for each phase). Section 3.5.1.1 of the ISC3 User's Guide (U.S. EPA 1995c), includes a complete discussion of combining multiple years of meteorological data into a single file prior to running ISCST3. The modeler should select the 'ANNUAL' averaging time for all risk assessment runs, regardless of the number of years in the meteorological data file. The incorrect selection of 'PERIOD' will not compute the correct deposition rates required by the risk assessment equations (refer to Section 3.2.3 of the ISC3 User Guide, Volume I). No additional ISCST3 model execution time is required to obtain 1-year or 5-year air modeling values.

In addition, ISCST3 allows the specification of COPC half-life and decay coefficients. Unless approved by the permitting authority with documentation of COPC-specific data, these keywords should not be used when conducting air modeling to support risk assessments. The TERRHGTS keyword with the ELEV parameter typically should be used to model terrain elevations at receptor grid nodes. The FLAGPOLE keyword specifies receptor grid nodes above local ground level and is not typically used for most air modeling to perform impacts at ground level.

U.S. EPA OSW also recommends that SAVEFIL be used to restart ISCST3 in the event of a computer or power failure during long runs. SAVEFIL is best used by specifying two save files, each with a different name. The save interval should be no longer than 5 days for large runs. If two save files are used, and a



failure occurs during writing to the savefile, no more than 10 days will be lost. The INITFILE command should be used to restart the runs after the failure, as shown in the following example:

```
CO SAVEFILE SAVE1 5 SAVE2
** INITFILE SAVE1
```

ISCST3 will save the results alternately to SAVE1 and SAVE2 every 5 days. If the run fails after successfully writing to SAVE1, the ISCST3 run can be restarted by replacing the two asterisks (\*) in the INITFILE line with CO and running ISCST3 again. The run will begin after the last day in SAVE1. The modeler should change the names of the save files (e.g., SAVE3 and SAVE4) in the 'CO SAVEFILE' command line prior to restarting ISCST3 to avoid overwriting the SAVE1 and SAVE2 files containing valid data from the interrupted run. Note that the MULTYEAR keyword is not used for computing long-term averages and should not be specified.

The following is an example of the COntrol pathway computer code for a single-year ISCST3 particle run:

```
CO STARTING
CO TITLEONE Example input file, particle pahse run, 1 year
CO TITLETWO 1984 met data, Baton Rouge Surface, Boothville Upper Air
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL
CO AVERTIME 1 ANNUAL
CO POLLUTID UNITY
CO TERRHGTS ELEV
CO RUNORRUN RUN
CO SAVEFILE 84SAVE1 5 84SAVE2
** Restart incomplete runs with INITFILE, changing `**` to `CO`
** INITFILE SAVE1
CO FINISHED
```

Additional runs for the other 4 years are set up with the same COntrol pathway, except for the title description and SAVEFILE filenames.

### **3.7.2 Source Pathway**

As discussed in Section 3.3, ISCST3 normally uses a unit emission rate of 1.0 g/s. Additional source characteristics required by the model (typically obtained from the Part B permit application and trial burn report) include the following:

- Source type (point source for stack emissions; area or volume for fugitive emissions)
- Source location (UTM coordinates, m)
- Source base elevation
- Emission rate (1.0 g/s)
- Stack height (m)
- Stack gas temperature (K)
- Stack gas exit velocity (m/s)
- Stack inside diameter (m)
- Building heights and widths (m)
- Particle size distribution (percent)
- Particle density (g/cm<sup>3</sup>)
- Particle and gas scavenging coefficients (unitless)

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Input values with supporting documentation for each parameter identified in Section 3.7.2

##### 3.7.2.1 Source Location

The location keyword of the SOurce pathway (SO LOCATION) identifies source type, location, and base elevation. The source type for any stack is referred to as a point source in ISCST3. Fugitive source emissions are discussed in section 3.10. The source location must be entered into ISCST3. Locations should be entered in UTM coordinates. The easterly coordinate is entered to the nearest meter; for example, 637524 meters UTM-E (no commas are used). The northerly coordinate is entered to the nearest meter; for example, a northerly coordinate of 4,567,789 meters UTM-N is entered as 4567789. The base

elevation of each stack must be entered in meters. Base elevation may be obtained from a USGS topographic map, facility plot plans or USGS digital data base.

An example input for the location keyword on the SOurce pathway includes source type, location, and base elevation in the following format:

```
SO LOCATION STACK1 POINT 637524. 4567789. 347.
```

### 3.7.2.2 Source Parameters

The source parameters keyword of the SOurce pathway (`SO SRCPARAM`) identifies the emission rate, stack height, stack temperature, stack velocity, and stack diameter. The unit emission rate is entered as 1.0 g/s. Stack height is the height above plant base elevation on the `SO LOCATION` keyword. Stack exit temperature is the most critical stack parameter for influencing concentration and deposition. High stack temperatures result in high buoyant plume rise, which, in turn, lowers concentration and deposition rates. Stack temperatures should be based on stack sampling tests for existing stacks. For new or undefined stacks, manufacturer's data for similar equipment should be used. Stack exit velocity should be calculated from actual stack gas flow rates and stack diameter. Actual stack gas flow rates should be determined for existing stacks during stack sampling. Representative values for new or undefined sources should be obtained from manufacturer's data on similar equipment. Stack diameter is the inside diameter of the stack at exit.

Following is an example of the source parameter input in the SOurce pathway for emission rate (grams per second), stack height (meters), stack temperature (K), stack velocity (meters per second), and stack diameter (meters):

```
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
```

### 3.7.2.3 Building Parameters

The building height and width keywords of the SOurce pathway (`SO BUILDHGT`; `SO BUILDWID`) identify the building dimensions that most influence the air flow for each of the 36 10-degree directions

surrounding a stack. The dimensions are calculated by using the U.S. EPA program BPIP, as described in Section 3.2.4.

The BPIP output file is input as follows:

```
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29

SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
```

### 3.7.2.4 Particle Size Distribution

ISCST3 requires particle size distribution for determining deposition velocities. U.S. EPA OSW recommends site-specific stack test data for existing sources. New or undefined sources may use the particle size distribution presented in Table 3-1.

The following example is the ISCST3 input for particle phase run. From Table 3-1, the distribution for 9 mean diameter sizes includes the data required for the keywords of the SOURCE pathway

(SO PARTDIAM; SO MASSFRAX). The PARTDIAM is taken from Column 1 (Mean Particle Diameter).

The MASSFRAX is taken from Column 4 (Fraction of Total Mass).

```
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
```

The example for the ISCST3 input for the particle-bound run is described below. From Table 3-1, the PARTDIAM is the same. The MASSFRAX is taken from Column 6 (Fraction of Total Surface Area).

```
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.49 0.17 0.13 0.09 0.05 0.02 0.02 0.01 0.02
```

### 3.7.2.5 Particle Density

Particle density is also required for modeling the air concentration and deposition rates of particles. Site-specific measured data on particle density should be determined for all existing sources when possible. For new or undefined sources requiring air modeling, a default value for particle density of 1.0 g/cm<sup>3</sup> may be used. Particles from combustion sources, however, may have densities that are less than 1.0 g/cm<sup>3</sup> (U.S. EPA 1994a), which would reduce the modeled deposition flux.

Following is an example of the particle density input in the SOurce pathway (SO PARTDENS) for the 9 mean particle size diameters of the previous example:

```
SO PARTDENS STACK1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
```

### 3.7.2.6 Scavenging Coefficients

Wet deposition flux is calculated within ISCST3 by multiplying a scavenging ratio by the vertically integrated concentration. The scavenging ratio is the product of a scavenging coefficient and a precipitation rate. Studies have shown that best fit values for the scavenging coefficients vary with particle size. For vapors, wet scavenging depends on the properties of the COPCs involved. However, not enough data are now available to adequately develop COPC-specific scavenging coefficients. Therefore, vapors are assumed to be scavenged at the rate of the smallest particles with behavior in the atmosphere that is assumed to be influenced more by the molecular processes that affect vapors than by the physical processes that may dominate the behavior of larger particles (U.S. EPA 1995c).

To use the wet deposition option in ISCST3, users must input scavenging coefficients for each particle size and a file that has hourly precipitation data. For wet deposition of vapors, a scavenging coefficient for a 0.1- $\mu$ m particle may be input to simulate wet scavenging of very small (molecular) particles. Alternatively, site-specific measured washout data or a calculation based on Henry's Law constant may be approved by the appropriate permitting authority prior to analysis. Wet deposition results only during precipitation. Scavenging coefficients should be determined for each particle size from the best fit curve based on the work of Jindal and Heinhold (1991) presented in the ISC3 User's Guide (U.S. EPA 1995c). The curves are

limited to a maximum particle size of 10- $\mu$ m, so all scavenging coefficients for particle sizes greater than or equal to 10- $\mu$ m are assumed to be equal. This assumption follows research on wet scavenging of particles (Jindal and Heinhold 1991).

The ISCST3 model input also differentiates between frozen and liquid scavenging coefficients. As a conservative estimate, the frozen scavenging coefficients are assumed to be equal to the liquid scavenging coefficients (PEI and Cramer 1986). If desired, the user may input separate scavenging coefficients for frozen precipitation. Research on sulfate and nitrate data has shown that frozen precipitation scavenging coefficients are about one-third of the values of liquid precipitation (Scire, Strimaitis, and Yamartino 1990; Witby 1978).

Following is an example of the particle liquid (rain) and frozen (sleet or snow) scavenging coefficients input in the SOurce pathway for 9 mean particle size diameters assuming particles are scavenged by frozen precipitation at 1/3 the rate of liquid precipitation:

```
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5 4E-5 9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
```

The complete SOurce pathway for the example particle phase input file is as follows:

```
SO STARTING
SO LOCATION STACK1 POINT 637524. 4567789. 347.
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29
SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
SO PARTDENS STACK1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5 4E-5 9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
SO SRCGROUP ALL
SO FINISHED
```

When modeling air vapors using ISCST3, the following is an example of the SOURCE pathway input for wet vapor scavenging coefficients that replaces the PARTDIAM, MASSFRAX, PARTDENS, PARTSLIQ and PARTSICE lines in the above example:

```
SO GAS-SCAV STACK1 LIQ 1.7E-4  
SO GAS-SCAV STACK1 ICE 0.6E-4
```

### 3.7.3 REceptor Pathway

The REceptor pathway identifies sets or arrays of receptor grid nodes identified by UTM coordinates for which ISCST3 generates estimates of air parameters including air concentration, dry and wet deposition, and total deposition. Previous U.S. EPA guidance (U.S. EPA 1994a) recommended using a polar receptor grid to identify maximum values, because polar grids provide coverage over large areas with a reduced number of receptor grid nodes, thereby reducing computer run times. However, U.S. EPA Region 6 experience indicates that, although the use of polar grids may reduce computer run times, air modelers typically choose a different option, because the benefit of reduced run time is offset by difficulties in identifying polar grid locations in absolute UTM coordinates for (1) extracting terrain values from digital terrain files, and (2) selecting receptor grid node locations for evaluation of ecosystems and special ecological habitats (see Chapter 4).

Receptor grid node arrays may be generated by using ISCST3 grid generation. However, assigning terrain elevations for each receptor grid node in an array associated with the generated grid can result in errors. One method of obtaining a Cartesian grid with terrain elevations is to open the USGS DEM file in a graphics program (e.g., SURFER<sup>®</sup>). Selection of the grid option samples the DEM file, at the user-specified spacing, over a range of east (x) and north (y) values. The specified x and y locations extract terrain elevation (z) from the DEM file at the desired receptor grid node for air modeling with the appropriate terrain elevations at each receptor grid node. These x, y, and z values are saved as a text file with one receptor grid node per line. A text editor is used to prefix each line with "RE DISCCART" to specify a discrete receptor grid node in ISCST3 format. Commercial receptor grid generators are also available. One commercial program (Lakes Environmental Software) generates the recommended receptor grid node array and extracts terrain elevations from the USGS DEM downloaded files, or any terrain file in x-y-z format.

The following is an example of the REceptor pathway for discrete receptor grid nodes at 500-meter spacing and including terrain elevations (in meters):

```
RE STARTING
RE ELEVUNIT METERS
RE DISCCART 630000. 565000. 352.
RE DISCCART 630500. 565000. 365.
RE DISCCART 631000. 565000. 402.
      ↓
RE DISCCART 635000. 570000. 387.
RE FINISHED
```

U.S. EPA OSW recommends that air modeling for each risk assessment include, at a minimum, an array of receptor grid nodes covering the area within 10 kilometers of the facility with the origin at the centroid of a polygon formed by the locations of the stack emission sources. This receptor grid node array should consist of a Cartesian grid with grid nodes spaced 100 meters apart extending from the centroid of the emission sources out to 3 kilometers from the centroid. For the distances from 3 kilometers out to 10 kilometers, the receptor grid node spacing can be increased to 500 meters. The single grid node array contains both grid node spacings. This same receptor grid node array is included in the REceptor pathway for all ISCST3 runs for all years of meteorological data and for all emission sources.

Terrain elevations should be specified for all receptor grid nodes. Several methods are available for assigning terrain elevations to grid nodes using digital terrain data. The 1:250,000 scale DEM digital data are available for download at the USGS Internet site:

Worldwide Web: <http://edcwww.cr.usgs.gov/pub/data/dem/250>

FTP (two options): <ftp://edcwww.cr.usgs.gov/pub/data/dem/250>  
<ftp://edcftp.cr.usgs.gov/pub/data/dem/250>

This data has horizontal spacing between digital terrain values of approximately 90 meters which provides sufficient accuracy for air modeling.

In addition to the receptor grid node array evaluated for each facility out to 10 kilometers, other grid node arrays may be considered for evaluation of water bodies and their watersheds, ecosystems and special ecological habitats located beyond 10 kilometers. Grid node spacing of 500 meters between nodes is



recommended for grid node arrays positioned at distances greater than 10 kilometers from the emission source. An equally spaced grid node array facilitates subsequent computation of area averages for deposition rates.

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Summary of all information regarding the coordinates and placement of the receptor grid node array used in air modeling
- Copies of any maps, figures, or aerial photographs used to develop the receptor grid node array
- Map presenting UTM locations of receptor grid nodes, along with other facility information.

#### 3.7.4 MEteorological Pathway

The file containing meteorological data is specified in the MEteorological pathway. PCRAMMET creates individual files for each of 5 years, as ASCII files, to be read into ISCST3 for computing hourly concentrations and deposition rates. The modeler may specify a single year of meteorological data in each ISCST3 run, or combine the total period of meteorological data into a single meteorological file for processing by ISCST3 in a single 5-year run. When combining meteorological files, the modeler is cautioned to consider the following:

- Preprocess each year separately using PCRAMMET or MPRM into an ASCII format
- Combine the years into a single file (using a text editor or DOS COPY command)
- The first line (header) of the combined file is read by ISCST3 for comparison to the Surface and Upper Air Station ID numbers specified in the input file ME pathway
- The header for subsequent years is read by ISCST3 only if not deleted in the combined file. If subsequent year headers are included in the combined file, ISCST3 will compare the station IDs to the input file station ID. For air modeling analysis which use meteorological data from more than one surface station or upper air station (e.g., the upper air station is moved after the third year of the period and assigned a new station ID by the National Weather Service), the modeler should delete the headers for subsequent years in the combined file.

- For sites where the anemometer height is changed during the 5 year period (e.g., for the period 1984-1988, the anemometer was relocated from 20 feet to 10 meters on December 15, 1985), the modeler should run each year separately to specify the correct anemometer height in the ISCST3 input file ME pathway which corresponds to the correct height for that year of meteorological data.

Details of specifying the meteorological data file are in the ISC3 User's Guide (Section 3.5.1.1). Each year within the file must be complete with a full year of data (365 days, or 366 days for leap years). The anemometer height must be verified for the surface station from Local Climate Data Summary records, or other sources, such as the state climatologist office. U.S. EPA OSW recommends that the anemometer height ANEMHGHT for the wind speed measurements at the surface station be correctly identified before air modeling.

The following is an example input section for the MEteorological pathway, using the 1984 Baton Rouge file, with an anemometer height of 10 meters and station identification numbers:

```
ME STARTING
ME INPUTFIL 84BR.WET
ME ANEMHGHT 10.0
ME SURFDATA 13970 1984 BATON_ROUGE
ME UAIRDATA 12884 1984 BOOTHVILLE
ME FINISHED
```

### 3.7.5 Terrain Grid (TG) Pathway

The computation of dry plume depletion is sensitive to terrain elevation. In the absence of a terrain grid file, ISCST3 automatically assumes that the terrain slope between the stack base and the receptor grid node elevation is linear. In concept, this assumption may underestimate plume deposition. However, based on experience, the magnitude of the differences in computed concentrations and deposition rates is nominal. Since the inclusion of a terrain grid file in the TG pathway significantly increases model execution time, U.S. EPA OSW recommends that a terrain grid file is not necessary for all sites. If a terrain grid file is desired for a specific site based on highly variable terrain over short distances, the format of the TG file is described in the ISC3 User's Guide.

The location keyword of the TG pathway (TG LOCATION) identifies the x and y values to be added to the source and receptor grid to align with the terrain file coordinates. If the source and receptor grid nodes are in relative units such that the source is at location 0,0, the location keywords in the TG pathway would be the UTM coordinates of the source. U.S. EPA OSW requires that all emission sources and receptor grid nodes be specified in UTM coordinates (NAD27 or NAD83 format), and that the TG file, if used, be in UTM coordinates. Therefore, the location of the origin of the TG file relative to the source location will be 0,0. Also, U.S. EPA OSW recommends that the terrain elevations in the TG file be presented in meters.

Following is an example of the TG pathway:

```
TG STARTING
TG INPUTFIL TERRAIN.TER
TG LOCATION 0.0 0.0
TG ELEVUNIT METERS
TG FINISHED
```

### **3.7.6 Output Pathway**

ISCST3 provides numerous output file options in addition to the results in the output summary file specified in receptor tables (RECTABLE). The plot file is most useful for facilitating post-processing of the air parameter values in the model output. The plot file lists the x and y coordinates and the concentration or deposition rate values for each averaging period in a format that can be easily pulled into a post-processing program (or spreadsheet). Note that the ISCST3 generated 'plot' file is not the same format as the ISCST3 generated 'post' file. U.S. EPA OSW recommends using the plot file, not the post file.

Following is an example Output file specification for single-year run of 1-hour and annual average plot files:

```
OU STARTING
OU RECTABLE ALLAVE FIRST
OU PLOTFILE 1 ALL FIRST BTR841.PLT
OU PLOTFILE ANNUAL ALL BTR84A.PLT
OU FINISHED
```

For ecological risk assessments, the 1-hour average plot file is not needed. If the modeler has directed in the ISCST3 control pathway for 1-hour averages to be computed for use in a human health acute risk

assessment, then the 1-hour average plot file also should be specified (U.S. EPA 1998). The second line in the example directs ISCST3 to create a table of values for each receptor grid node for all averaging periods in the model run (annual and optionally 1-hour). The third line directs ISCST3 to create a separate plot file of the 1-hour average results, if desired by the modeler. The fourth line directs ISCST3 to create another separate plot file of the annual average results for all sources in the run for each receptor grid node.

### **3.8 ISCST3 MODEL EXECUTION**

Model execution time should be considered for each analysis. A complete air modeling run—including air concentration, wet and dry deposition, and plume depletion—may require 10 times the run time for the same source and receptor grid nodes for air concentration only. Even if only the total deposition is specified, ISCST3 must compute air concentration and the dry and wet deposition components in order to compute the total deposition air parameter values required for the ecological risk assessment. For example, an ISCST3 particle run of one source with 800 receptor grid nodes, on 1 year of meteorological data, with the options for air concentration, wet and dry deposition, and plume depletion required about 40 hours on a personal computer with a 486 processor running at 66 megahertz (486/66). The same run can be completed in about 10 hours on a 586/120 personal computer. Five years of meteorological data and an additional 1,600 receptor grid nodes result in total run times of 120 hours for 1 year, and 600 hours for a 5-year analysis on a 486/66 personal computer. Run time on a 586/120 personal computer is estimated at about 150 hours. A significant loss of modeling effort and analysis time can be prevented by verifying input parameters and conducting test runs prior to executing the ISCST3 runs.

Long run times result mainly from two algorithms—plume depletion and terrain grid file. ISCST3 run times are increased as much as tenfold for runs applying plume depletion. U.S. EPA OSW believes that constituent mass must be conserved between suspended concentration and deposition rate by allowing for depletion of deposited mass from the plume concentration in ISCST3. The overestimate of plume concentration, and the subsequent overestimate of deposition, which results when plume depletion is not allowed, is too conservative. However, the nominal benefits of including a terrain grid file do not justify the added run times. Therefore, plume depletion should always be included, but terrain grid files are not recommended.

### 3.9 USE OF MODELED OUTPUT

The ISCST3 modeled output (air concentrations and deposition rates) are provided on a unit emission rate (1.0 g/s) basis from the combustion unit or emission source, and are not COPC-specific. The estimating media equations presented in Section 3.11 and Appendix B require the model output (air parameters, see Table 3-5) directly without converting the unit based output to COPC-specific output. However, there may be some instances where the risk assessor will need to convert modeled output to COPC-specific output for the risk assessment. For example, the risk assessor may want to compare modeled COPC concentrations in ambient media to concentrations actually measured in the field.

#### 3.9.1 Unit Rate Output vs. COPC-Specific Output

The relationship between the unit emission rate and the unit air parameter values (air concentrations and deposition rates) is linear. Similarly, the relationship between the COPC-specific emission rate ( $Q$ ) and the COPC-specific air parameter values (air concentrations and deposition rates) would also be linear if the COPC-specific emission rate was used in the air model. Section 3.3 discussed the use of the unit emission rate and advanced the theory that a unit emission rate should be used instead of the COPC-specific emission rate in order to preclude having to run the ISCST3 model separately for each individual COPC. The use of a unit emission rate in the air modeling is advocated because a common ratio relationship can be developed between the unit emission rate and the COPC-specific emission rate based on the fact that in the air model, both individual relationships are linear. This ratio relationship can be expressed by the following equation:

**TABLE 3-5**  
**AIR PARAMETERS FROM ISCST3 MODELED OUTPUT**

<b>Air Parameter</b>	<b>Description</b>	<b>Units</b>
<i>Cyv</i>	Unitized yearly average air concentration from vapor phase	$\mu\text{g-s/g-m}^3$
<i>Cyp</i>	Unitized yearly average air concentration from particle phase	$\mu\text{g-s/g-m}^3$
<i>Dyvv</i>	Unitized yearly average wet deposition from vapor phase	$\text{s/m}^2\text{-yr}$
<i>Dydp</i>	Unitized yearly average dry deposition from particle phase	$\text{s/m}^2\text{-yr}$
<i>Dywp</i>	Unitized yearly average wet deposition from particle phase	$\text{s/m}^2\text{-yr}$
<i>Cyww</i>	Unitized yearly (water body or watershed) average air concentration from vapor phase	$\mu\text{g-s/g-m}^3$
<i>Dywww</i>	Unitized yearly (water body or watershed) average wet deposition from vapor phase	$\text{s/m}^2\text{-yr}$
<i>Dytwp</i>	Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase	$\text{s/m}^2\text{-yr}$

$$\frac{\text{COPC-Specific Air Concentration}}{\text{COPC-Specific Emission Rate}} = \frac{\text{Modeled Output Air Concentration}}{\text{Unit Emission Rate}} \quad \text{Equation 3-2}$$

Use of this equation requires that three of the variables be known. The modeled output air concentration (or deposition rate) is provided by the air model, the unit emission is 1.0 g/s, and the COPC-specific emission rate; which is obtained directly from stack or source test data.

### 3.9.1.1 Determination of the COPC-Specific Emission Rate ( $Q$ )

The COPC-specific emission rate can usually be determined with information obtained directly from the trial burn report. The COPC-specific emission rate from the stack is a function of the stack gas flow rate and the stack gas concentration of each COPC; which can be calculated from the following equation:

$$Q = SGF \cdot \frac{SGC \cdot CFO_2}{1 \times 10^6} \quad \text{Equation 3-4}$$

where

$Q$	=	COPC-specific emission rate (g/s)
$SGF$	=	Stack gas flow rate at dry standard conditions (dscm/s)
$SGC$	=	COPC stack gas concentration at 7 percent O <sub>2</sub> as measured in the trial burn (μg/dscm)
$CFO_2$	=	Correction factor for conversion to actual stack gas concentration O <sub>2</sub> (unitless)
$1 \times 10^6$	=	Unit conversion factor (μg/g)

Guidance for determining COPC-specific emission rates for fugitive emission sources can be found in Chapter 2. Also, it is sometimes necessary to derive the COPC-specific emission rate from surrogate data, such as for a new facility that has not yet been constructed and trial burned (see Chapter 2).

### 3.9.1.2 Converting Unit Output to COPC-Specific Output

Once the three of the four variables in Equation 3-1 are known, the COPC-specific air concentrations and deposition rates can be obtained directly by multiplication, as follows:

$$\text{COPC-Specific Air Concentration} = \frac{\text{Modeled Output Air Concentration} \cdot \text{COPC-Specific Emission Rate}}{\text{Unit Emission Rate}} \quad \text{Equation 3-3}$$

For example, if COPC A is emitted at a rate of 0.25 g/s, and the ISCST3 modeled concentration at a specific receptor grid node is 0.2 μg/m<sup>3</sup> per the 1.0 g/s unit emission rate, the concentration of COPC A at that receptor grid node is 0.05 μg/m<sup>3</sup> (0.25 multiplied by 0.2). Deposition is calculated similarly, proportional to the emission rate of each COPC. Readers are reminded once again that this process of

converting modeled unitized output into COPC-specific output is taken directly into account in the estimating media concentration equations in Section 3.11 and Appendix B.

### 3.9.2 Output from the ISCST3 Model

The ISCST3 output is structured and the risk assessor must understand how to read the output in order to ensure accurate use of modeled output in the risk assessment. The output from each ISCST3 model run is written to two separate file formats. The 'output file' is specified by name at run time in the execution command. Typical command line nomenclature is:

```
ISCST3 inputfile.INP outputfile.OUT
```

where

ISCST3:	specifies execution of the ISCST3 model
inputfile.INP:	is the input file name selected by the modeler
outputfile.OUT:	is the output file name selected by the modeler, typically the same as the input file name

For example, the following ISCST3 input line would run the input file (PART84.INP) created by the modeler for particulate emissions using 1984 meteorological data. The output file (PART84.OUT) from the run will automatically be written by ISCST3 during model execution.

```
ISCST3 PART84.INP PART84.OUT
```

The output 'plot file' is specified by the modeler in the ISCST3 input file OUTPUT pathway and created by ISCST3 during the run (see Section 3.7.6). Figure 3-3 is an example of the first few lines in the particle phase plot file with single-year annual average concentration, total deposition, dry deposition and wet deposition values for each receptor grid node. The total deposition is the sum of the dry and wet components of deposition. The single-year values at each receptor grid node being evaluated must be averaged to a 5-year value. The 5-year averaged values at the receptor grid nodes selected for evaluation in the risk assessment (see Section 3.9.3), are used in the estimating media concentration equations. This file is usually imported into a post-processing program (or spreadsheet) before entry into the risk assessment computations.



Similar plot files are produced for the particle-bound and vapor phase runs. The output for the vapor phase runs will be average concentration and wet deposition. The output for the particle and particle-bound phase runs will be average concentration, dry deposition, wet deposition and total deposition. Again, the 1-year values at each receptor grid node must be averaged to a 5-year value at each node unless a single five-year ISCST3 run using a combined meteorological file is used. If the 5-year combined file is used, the results from the ISCST3 plot file may be used directly in the risk assessment without averaging over the five years.

All values are defined as used in the estimating media concentration equations (see Section 3.11).

### **3.9.3 Use of Model Output in Estimating Media Equations**

Section 3.4 discussed how consideration of partitioning of the COPCs effects the development of ISCST3 modeling runs. The selection of which air modeled air parameter values (air concentrations and deposition rates) to use in the estimating media concentration equations is based on this same partitioning theory.

#### **3.9.3.1 Vapor Phase COPCs**

ISCST3 output generated from vapor phase air modeling runs are vapor phase air concentrations (unitized  $C_{yv}$  and unitized  $C_{yww}$ ) and wet vapor depositions (unitized  $D_{ywv}$  and unitized  $D_{ywwv}$ ) for organic COPCs at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC organics except the polycyclic aromatic hydrocarbons dibenzo(a,h)anthracene and indeno(1,2,3-cd)pyrene, which have vapor phase fractions,  $F_v$ , less than five percent. The air concentration (unitized  $C_{yv}$ ) and wet vapor deposition (unitized  $D_{ywv}$ ) from the vapor phase run is also used in the estimating media concentration equations for mercury. Values for these COPCs are selected from the vapor phase run because the mass of the COPC emitted by the combustion unit is assumed to have either all or a portion of its mass in the vapor phase (see Appendix A-2).

### 3.9.3.2 Particle Phase COPCs

ISCST3 output generated from particle phase air modeling runs are air concentration (unitized  $C_{yp}$ ), dry deposition (unitized  $D_{ydp}$ ), wet deposition (unitized  $D_{ywp}$ ), and combined deposition (unitized  $D_{ytwp}$ ) for inorganics and relatively non-volatile organic COPCs at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC inorganics (except mercury, see Chapter 2 and Appendix A-2) and polycyclic aromatic hydrocarbons with fraction of vapor phase,  $F_v$ , less than 0.05 (e.g., dibenzo(a,h)anthracene and indeno(1,2,3-cd)pyrene). Values for inorganic and relatively non-volatile COPCs are selected from the particle phase run because the mass of the COPC emitted by the combustion unit is assumed to have all of its mass in the particulate phase (see Appendix A-2), apportioned across the particle size distribution based on mass weighting.

### 3.9.3.3 Particle-Bound COPCs

ISCST3 output generated from particle-bound air modeling runs are air concentration (unitized  $C_{yp}$ ), dry deposition (unitized  $D_{ydp}$ ), wet deposition (unitized  $D_{ywp}$ ), and combined deposition (unitized  $D_{ytwp}$ ) for organic COPCs and mercury (see Chapter 2 and Appendix A-2) at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC organics and mercury to account for a portion of the vapor condensed onto the surface of particulates. Values for these COPCs are selected from the particle-bound run because the mass of the COPC emitted by the combustion unit is assumed to have a portion of its mass condensed on particulates (see Appendix A-2), apportioned across the particle size distribution based on surface area weighting.

## 3.10 MODELING OF FUGITIVE EMISSIONS

Fugitive source emissions, as defined in Chapter 2, should be modeled using the procedures presented throughout this chapter for stack source emissions. However, the fugitive emissions should be represented in the ISCST3 input file SSource pathway as either “area” or “volume” source types. Fugitive emissions of volatile organics are modeled only in the vapor phase. Fugitive emissions of ash are modeled only in the particle and particle-bound phases, not vapor phase.

As discussed in Chapter 2, fugitive emissions of volatile organic vapors are associated with combustion units that include storage vessels, pipes, valves, seals and flanges. The horizontal area of the fugitive source (which can be obtained from the facility plot plan) is entered into the ISCST3 input file following the instructions presented in the ISC3 User's Guide, Volume I (U.S. EPA 1995c). The height of the fugitive source is defined as the top of the vertical extent of the equipment. If the vertical extent of the fugitive source is not known, a default height of ground level (release height of zero) may be input, providing a conservative estimate of potential impacts. The ISCST3 model run time is faster for volume source types than for area source types, and should be considered for most applications. The methods in the ISCST3 User's Guide should be followed in defining the input parameters to represent the fugitive source.

FIGURE 3-3  
 EXAMPLE PLOT FILE

```

*ISCST3 (96113): Example Particle Phase Run, Single Year 1990
*MODELING OPTIONS USED:
* CONC   DEPOS   DDEP   WDEP   RURAL  ELEV           DFAULT           DRYDPL WETDPL

*          PLOT FILE OF ANNUAL VALUES FOR SOURCE GROUP: ALL
*          FOR A TOTAL OF      21 RECEPTORS.
*          FORMAT: (6(1X,F13.5),1X,F8.2,2X,A6,2X,A8,2X,I8,2X,A8)
*          X          Y          AVERAGE CONC  TOTAL DEPO  DRY DEPO  WET DEPO  ZELEV  AVE  GRP  NUM HRS  NET
*          _____  _____  _____  _____  _____  _____  _____  _____  _____  _____  _____
691600.00000 3342050.00000    0.29900    0.28658    0.20024    0.08634    4.00    ANNUAL  ALL    8760    NA
691700.00000 3342050.00000    0.30203    0.35416    0.23884    0.11532    5.00    ANNUAL  ALL    8760    NA

691800.00000 3342050.00000    0.25174    0.42461    0.25976    0.16485    5.00    ANNUAL  ALL    8760    NA
691900.00000 3342050.00000    0.13256    0.50524    0.23852    0.26672    5.00    ANNUAL  ALL    8760    NA
692000.00000 3342050.00000    0.00322    0.61790    0.05850    0.55940    5.00    ANNUAL  ALL    8760    NA
692100.00000 3342050.00000    0.00000    6.32022    0.00000    6.32022    6.00    ANNUAL  ALL    8760    NA
692200.00000 3342050.00000    0.00319    0.32218    0.06577    0.25641    6.00    ANNUAL  ALL    8760    NA
692300.00000 3342050.00000    0.13768    0.39938    0.21734    0.18204    6.00    ANNUAL  ALL    8760    NA
692400.00000 3342050.00000    0.23546    0.33855    0.20975    0.12880    6.00    ANNUAL  ALL    8760    NA
692500.00000 3342050.00000    0.25673    0.27475    0.17903    0.09572    6.00    ANNUAL  ALL    8760    NA
692600.00000 3342050.00000    0.24706    0.22195    0.14812    0.07384    6.00    ANNUAL  ALL    8760    NA
691600.00000 3342150.00000    0.37348    0.40644    0.25958    0.14685    5.00    ANNUAL  ALL    8760    NA
691700.00000 3342150.00000    0.37166    0.51388    0.31119    0.20269    5.00    ANNUAL  ALL    8760    NA
    
```

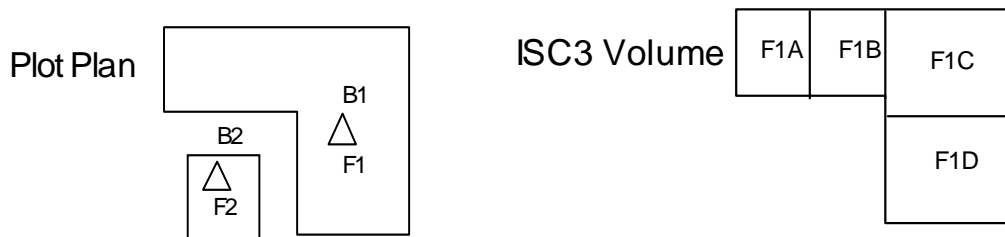
**Protocol for Screening Level Human Health Risk Assessment**  
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**February 28, 1997**

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691800.00000	3342150.00000	0.34332	0.68794	0.39582	0.29212	5.00	ANNUAL	ALL	8760	NA
691900.00000	3342150.00000	0.22930	0.98039	0.54883	0.43156	5.00	ANNUAL	ALL	8760	NA
692000.00000	3342150.00000	0.03473	0.90823	0.37421	0.53402	6.00	ANNUAL	ALL	8760	NA
692100.00000	3342150.00000	0.00098	0.62882	0.15736	0.47146	6.00	ANNUAL	ALL	8760	NA
692200.00000	3342150.00000	0.02605	0.48160	0.15582	0.32578	7.00	ANNUAL	ALL	8760	NA
692300.00000	3342150.00000	0.17300	0.49313	0.22998	0.26315	7.00	ANNUAL	ALL	8760	NA
692400.00000	3342150.00000	0.24520	0.29443	0.19715	0.09729	7.00	ANNUAL	ALL	8760	NA
692500.00000	3342150.00000	0.25561	0.23482	0.16744	0.06738	7.00	ANNUAL	ALL	8760	NA

The following example is for organic fugitive emissions modeled as a volume source type. For a facility which may have two stack emission sources (B1, B2) and two fugitive emission sources (areas F1, F2); a total of four runs for each year (or 5-year combined file) of meteorological data is required. One run is required for each of the two stacks as point sources. One run is required for each of the two fugitive areas as volume sources (Note: modeler may alternatively model as an area source). Since the emissions are fugitive volatile organics, only the vapor phase is modeled. The vertical extent of the pipes, valves, tanks and flanges associated with each fugitive emission area is 15 feet (about 5 meters) above plant elevation. To define the sources for input to ISCST3, the release height is specified as 2.5 meters (½ of vertical extent of fugitive emissions). The initial vertical dimension is specified as 1.16 meters (vertical extent of 5 meters divided by 4.3 as described in the ISC3 User’s Guide).



The initial horizontal dimension is the side length of the square fugitive area (footprint) divided by 4.3. If fugitive area F2 has a measured side of 30 meters, the initial horizontal dimension is 6.98 (30 meters divided by 4.3). For fugitive area F1, the area on the plot plan must be subdivided (ISC3 Volume) to create square areas for input to ISCST3. The four areas depicted represent subdivision into square areas. The resulting four square areas are input into a single ISCST3 run for Fugitive source F1 as four separate volume sources (F1A, F1B, F1C, F1D). The initial horizontal dimension for each volume source is the side of the square divided by 4.3. It is very important to allocate proportionately the unit emission rate (1.0 gram per second) among the subdivided areas. For example, if the areas of the subdivided squares in the ISC3 Volume figure results in F1A equal to F1B each with 1/8th the total area, the proportion of the unit emissions allocated to each of these volume sources is 0.125 grams per second. The remaining two areas are each 3/8ths of the total area of fugitive F1, so that 0.375 grams per second is specified for the emission rate from each source. The total emissions for the four volume sources sum to the unit emission rate for the F1 fugitive source ( $0.125 + 0.125 + 0.375 + 0.375 = 1.0$  g/s). By specifying all sources to be included in the model results from ISCST3 (SO SRCGROUP ALL), the ISCST3 model will appropriately

combine all four volume source subdivisions of fugitive source F1 into combined impact results for fugitive source F1. The resulting air parameter values in the plot files may be used directly in the risk assessment equations, the same as if a stack emission were modeled as a single point source. The initial vertical dimension is defined the same as F2, using the vertical extent of 5 meters divided by 4.3 and a release height of 2.5 meters ( $\frac{1}{2}$  vertical extent). For volume sources, the location is specified by the x and y coordinates of the center of each square area.

The CONTROL parameters should follow the recommendations for setting up a vapor phase computation.

CO CONC WDEP

Fugitive emissions of ash particles are from the storage piles associated with combustion units. The horizontal area of the storage pile is entered into the ISCST3 input file following the ISCST3 User's Guide, Volume I (U.S. EPA 1995c). The height of emissions is input as the top of the pile. If the vertical extent is not known, the height may be input as ground level (or zero height). Fugitive ash will typically be modeled as area source type. However, volume source type may be considered by the appropriate regulatory agency prior to air modeling. The methods in the ISCST3 User's Guide should be followed in defining the input parameters to represent the ash release as an area source.

The CONTROL parameters should follow the recommendations for setting up a particulate phase computation.

CO CONC DDEP WDEP DEPOS

The emissions characterization and source type must be documented.

### 3.11 ESTIMATION OF COPC CONCENTRATIONS IN MEDIA

As discussed in Section 3.9 (see also Table 3-5), the ISCST3 modeled output of unitized air parameters (air concentrations and deposition rates) are provided on a unit emission (1.0 g/s) basis from the combustion unit, and are not COPC-specific. The estimating media concentration equations, presented in this section, accept these unitized output values directly to calculate COPC-specific media concentrations

for use in characterizing ecological risk. Selection of the appropriate ISCST3 modeled output for use in the equations is discussed in Section 3.9.

This section presents the estimating media concentration equations used for calculating, from the appropriate ISCST3 unitized model output and COPC-specific emission rates, COPC-specific media concentrations in soil, surface water, and sediment. Determining COPC media concentrations is relevant to estimating risks to potentially impacted ecosystems through exposure of ecological receptors to COPCs in air (plant only), soil, surface water, and sediment. This section also includes equations for calculating COPC-specific concentrations in terrestrial plants resulting from foliar and root uptake.

Section 3.11.1 describes the equations for calculating COPC-specific concentration in soils. Section 3.11.2 describes the equations for calculating COPC-specific concentrations in surface water and sediment. Section 3.11.3 describes the equations for calculating COPC-specific plant concentrations from foliar and root uptake. In addition, Appendix B also provides in more detail the media concentration equations and default input variables recommended by U.S. EPA OSW.

### **3.11.1 CALCULATION OF COPC CONCENTRATIONS IN SOIL**

As depicted in Figure 3-4, COPC concentrations in soil are calculated by summing the particle and vapor phase deposition of COPCs to the soil. Wet and dry deposition of particles and vapors are considered, with dry deposition of vapors calculated from the vapor air concentration and the dry deposition velocity. Soil concentrations may require many years to reach steady state. As a result, the equations used to calculate the soil concentration over the period of deposition were derived by integrating the instantaneous soil concentration equation over the period of deposition. U.S. EPA OSW recommends that the highest 1-year annual average COPC concentration in soil be used as the soil concentration for estimating ecological risk, which would typically occur at the end of the time period of combustion (see Section 3.11.1).



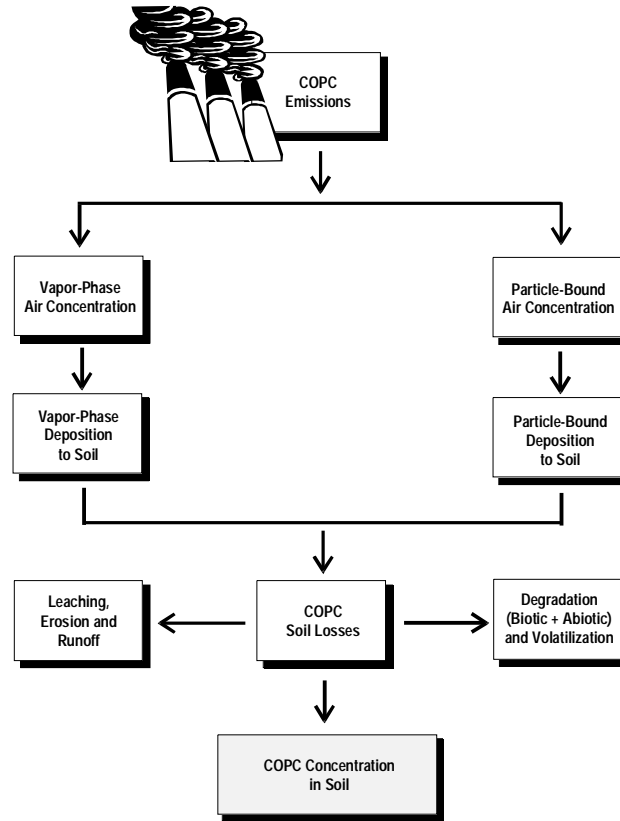


Figure 3-4 - COPC Concentration in Soil

Following deposition, the calculation of soil concentration also considers losses of COPCs by several mechanisms, including leaching, erosion, runoff, degradation (biotic and abiotic), and volatilization. All of these loss mechanisms may lower the soil concentration if included in the soil concentration calculation (see Section 3.11.1.2). Soil conditions—such as pH, structure, organic matter content, and moisture content—can also affect the distribution and mobility of COPCs in soil. Loss of COPCs from the soil is modeled using a combination of default and site-specific values to account for the physical and chemical characteristics of the soil.

COPCs may also be physically incorporated into the upper layers of soil through tilling. The concentration in the top 20 centimeters of soil should be computed for estimating a COPC concentration in soils that are

physically disturbed or tilled. The COPC concentration in the top 1 centimeter of soil should be computed for estimating a COPC concentration in soils that are not tilled (see Section 3.11.1.4).

### 3.11.1.1 Calculating Highest Annual Average COPC Concentration in Soil

U.S. EPA OSW recommends the following equation for calculating the highest average annual COPC soil concentration.

---

**Recommended Equations for Calculating:  
Highest Annual Average COPC Concentration in Soil ( $C_s$ )**

---

$$C_s = \frac{D_s \cdot [1 - \exp(-k_s \cdot tD)]}{k_s} \qquad \text{Equation 3-7}$$

where

$C_s$	=	COPC concentration in soil (mg COPC/kg soil)
$D_s$	=	Deposition term (mg/kg-yr)
$k_s$	=	COPC soil loss constant due to all processes ( $\text{yr}^{-1}$ )
$tD$	=	Total time period over which deposition occurs (time period of combustion) (yr)

This equation calculates the highest annual average soil concentration, which is typically expected to occur at the end of the time period of deposition (U.S. EPA 1994i; 1998c). Derivation of the equation is presented in U.S. EPA (1998c). Appendix B, Table B-1-1 also describes the equation, definitions of its terms, and default values for the variables.

### 3.11.1.2 Calculating the COPC Soil Loss Constant ( $k_s$ )

COPCs may be lost from the soil by several processes that may or may not occur simultaneously. In Equation 3-8, the soil loss constant,  $k_s$ , expresses the rate at which a COPC is lost from soil (U.S. EPA 1993h; 1998c). The constant  $k_s$  is determined by using the soil's physical, chemical, and biological characteristics to consider the losses resulting from:

- (1) biotic and abiotic degradation,

- (2) erosion,
- (3) surface runoff,
- (4) leaching, and
- (5) volatilization.

Consistent with earlier U.S. EPA guidance (U.S. EPA 1993h; 1994i; 1998c), U.S. EPA OSW recommends using Equation 3-8 to compute the soil loss constant.

---

**Recommended Equation for Calculating:  
COPC Soil Loss Constant ( $k_s$ )**

---

$$k_s = k_{sg} + k_{se} + k_{sr} + k_{sl} + k_{sv} \quad \text{Equation 3-8}$$

where

$k_s$	=	COPC soil loss constant due to all processes ( $\text{yr}^{-1}$ )
$k_{sg}$	=	COPC loss constant due to degradation ( $\text{yr}^{-1}$ )
$k_{se}$	=	COPC loss constant due to erosion ( $\text{yr}^{-1}$ )
$k_{sr}$	=	COPC loss constant due to runoff ( $\text{yr}^{-1}$ )
$k_{sl}$	=	COPC loss constant due to leaching ( $\text{yr}^{-1}$ )
$k_{sv}$	=	COPC loss constant due to volatilization ( $\text{yr}^{-1}$ )

The use of Equation 3-8 assumes that COPC loss can be defined by using first-order reaction kinetics. First-order reaction rates depend on the concentration of one reactant (Bohn, McNeal, and O'Connor 1985). The loss of a COPC by a first-order process depends only on the concentration of the COPC in the soil, and a constant fraction of the COPC is removed from the soil over time. Those processes that apparently exhibit first-order reaction kinetics without implying a mechanistic dependence on a first-order loss rate are termed “apparent first-order” loss rates (Sparks 1989). The assumption that COPC loss follows first-order reaction kinetics may be an oversimplification because—at various concentrations or under various environmental conditions—the loss rates from soil systems will resemble different kinetic expressions. However, at low concentrations, a first-order loss constant may be adequate to describe the loss of the COPC from soil (U.S. EPA 1990a).

COPC loss in soil can also follow zero or second-order reaction kinetics. Zero-order reaction kinetics are independent of reactant concentrations (Bohn, McNeal, and O'Connor 1985). Zero-order loss rates describe processes in which the reactants are present at very high concentrations. Under zero-order kinetics, a constant amount of a COPC is lost from the soil over time, independent of its concentration. Processes that follow second-order reaction kinetics depend on the concentrations of two reactants or the concentration of one reactant squared (Bohn, McNeal, and O'Connor 1985). The loss constant of a COPC following a second-order process can be contingent on its own concentration, or on both its concentration and the concentration of another reactant, such as an enzyme or catalyst.

Because COPC loss from soil depends on many complex factors, it may be difficult to model the overall rate of loss. In addition, because the physical phenomena that cause COPC loss can occur simultaneously, the use of Equation 3-8 may also overestimate loss rates for each process (Valentine 1986). When possible, the common occurrence of all loss processes should be taken into account.

The following subsections discuss issues associated with the calculation of the  $k_{sl}$ ,  $k_{se}$ ,  $k_{sr}$ ,  $k_{sg}$ , and  $k_{sv}$  variables. Appendix B, Tables B-1-2 through B-1-6 present the equations for computing the overall and individual soil loss constant, except for loss due to degradation, which is discussed below.

#### **COPC Loss Constant Due to Biotic and Abiotic Degradation ( $k_{sg}$ )**

Soil losses resulting from biotic and abiotic degradation ( $k_{sg}$ ) are determined empirically from field studies and should be addressed in the literature (U.S. EPA 1990a). Lyman et al. (1982) states that degradation rates can be assumed to follow first order kinetics in a homogenous media. Therefore, the half-life of a compound can be related to the degradation rate constant. Ideally,  $k_{sg}$  is the sum of all biotic and abiotic rate constants in the soil media. Therefore, if the half-life of a compound (for all of the mechanisms of transformation) is known, the degradation rate can be calculated. However, literature sources do not provide sufficient data for all such mechanisms, especially for soil. Therefore, Appendix A-2 presents U.S. EPA OSW recommended values for this COPC specific variable.

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**Recommended Values for:  
COPC Loss Constant Due to Biotic and Abiotic Degradation (*k<sub>sg</sub>*)**

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See Appendix A-2

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The rate of biological degradation in soils depends on the concentration and activity of the microbial populations in the soil, the soil conditions, and the COPC concentration (Jury and Valentine 1986). First-order loss rates often fail to account for the high variability of these variables in a single soil system. However, the use of simple rate expressions may be appropriate at low chemical concentrations (e.g., nanogram per kilogram soil) at which a first-order dependence on chemical concentration may be reasonable. The rate of biological degradation is COPC-specific, depending on the complexity of the COPC and the usefulness of the COPC to the microorganisms. Some substrates, rather than being used by the organisms as a nutrient or energy source, are simply degraded with other similar COPCs, which can be further utilized. Environmental and COPC-specific factors that may limit the biodegradation of COPCs in the soil environment (Valentine and Schnoor 1986) include:

- (1) availability of the COPC,
- (2) nutrient limitations,
- (3) toxicity of the COPC, and
- (4) inactivation or nonexistence of enzymes capable of degrading the COPC.

Chemical degradation of organic compounds can be a significant mechanism for removal of COPCs in soil (U.S. EPA 1990a). Hydrolysis and oxidation-reduction reactions are the primary chemical transformation processes occurring in the upper layers of soils (Valentine 1986). General rate expressions describing the transformation of some COPCs by all non-biological processes are available, and these expressions are helpful when division into component reactions is not possible.

Hydrolysis in aqueous systems is characterized by three processes: acid-catalyzed, base-catalyzed, and neutral reactions. The overall rate of hydrolysis is the sum of the first-order rates of these processes (Valentine 1986). In soil systems, sorption of the COPC can increase, decrease, or not affect the rate of hydrolysis, as numerous studies cited in Valentine (1986) have shown. The total rate of hydrolysis in soil can be predicted by adding the rates in the soil and water phases, which are assumed to be first-order

reactions at a fixed pH (Valentine 1986). Methods for estimating these hydrolysis constants are described by Lyman et al. (1982).

Organic and inorganic compounds also undergo oxidation-reduction (redox) reactions in the soil (Valentine 1986). Organic redox reactions involve the exchange of oxygen and hydrogen atoms by the reacting molecules. Inorganic redox reactions may involve the exchange of atoms or electrons by the reactants. In soil systems where the identities of oxidant and reductant species are not specified, a first-order rate constant can be obtained for describing loss by redox reactions (Valentine 1986). Redox reactions involving metals may promote losses from surface soils by making metals more mobile (e.g., leaching to subsurface soils).

### COPC Loss Constant Due to Soil Erosion ( $k_{se}$ )

U.S. EPA (1993h) recommended the use of Equation 3-8A to calculate the constant for soil loss resulting from erosion ( $k_{se}$ ).

$$k_{se} = \frac{0.1 \cdot X_e \cdot SD \cdot ER}{BD \cdot Z_s} \cdot \frac{Kd_s \cdot BD}{\theta_{sw} + (Kd_s \cdot BD)} \quad \text{Equation 3-8A}$$

where:

$k_{se}$	=	COPC soil loss constant due to soil erosion
0.1	=	Units conversion factor (1,000 g/kg/10,000 cm <sup>2</sup> -m <sup>2</sup> )
$X_e$	=	Unit soil loss (kg/m <sup>2</sup> -yr)
$SD$	=	Sediment delivery ratio (unitless)
$ER$	=	Soil enrichment ratio (unitless)
$Kd_s$	=	Soil-water partition coefficient (mL/g)
$BD$	=	Soil bulk density (g/cm <sup>3</sup> soil)
$Z_s$	=	Soil mixing zone depth (cm)
$\theta_{sw}$	=	Soil volumetric water content (mL/cm <sup>3</sup> soil)

Unit soil loss ( $X_e$ ) is calculated by using the Universal Soil Loss Equation (USLE), as described in Section 3.11.2. Variables associated with Equation 3-8A are further discussed in Appendix B, Table B-1-3.

U.S. EPA guidance (1994b and 1994l) have stated that all *kse* values are equal to zero. U.S. EPA (1994l) stated that *kse* is equal to zero because of contaminated soil eroding onto and off of the site.

Consistent with earlier U.S. EPA guidance (1994b and 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that the constant for the loss of soil resulting from erosion (*kse*) should be set equal to zero.

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**Recommended Value for:  
COPC Loss Constant Due to Erosion (*kse*)**

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0

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For additional information on addressing *kse*, U.S. EPA OSW recommends consulting the methodologies described in U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press). The use of *kse* values is also further described in Appendix B, Table B-1-3.

**COPC Loss Constant Due to Runoff (*ksr*)**

Consistent with earlier U.S. EPA guidance (1993h; 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that Equation 3-8B be used to calculate the constant for the loss of soil resulting from surface runoff (*ksr*). The use of this equation is further described in Appendix B, Table B-1-4.

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**Recommended Equation for Calculating:  
COPC Loss Constant Due to Runoff (*ksr*)**

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$$ksr = \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \left( \frac{1}{1 + (Kd_s \cdot BD / \theta_{sw})} \right) \quad \text{Equation 3-8B}$$

where

<i>ksr</i>	=	COPC loss constant due to runoff (yr <sup>-1</sup> )
<i>RO</i>	=	Average annual surface runoff from pervious areas (cm/yr)
$\theta_{sw}$	=	Soil volumetric water content (mL/cm <sup>3</sup> soil)

$Z_s$	=	Soil mixing zone depth (cm)
$Kd_s$	=	Soil-water partition coefficient (mL/g)
$BD$	=	Soil bulk density (g/cm <sup>3</sup> soil)

**COPC Loss Constant Due to Leaching (*ksl*)**

Consistent with earlier U.S. EPA guidance (1993h and 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that Equation 3-8C be used to calculate the COPC loss constant due to leaching (*ksl*). The use of this equation is further described in Appendix B, Table B-1-5.

**Recommended Equation for Calculating:  
 COPC Loss Constant Due to Leaching (*ksl*)**

$$ksl = \frac{P + I - RO - E_v}{\theta_{sw} \cdot Z_s \cdot [1.0 + (BD \cdot Kd_s / \theta_{sw})]} \quad \text{Equation 3-8C}$$

where

$ksl$	=	COPC loss constant due to leaching (yr <sup>-1</sup> )
$P$	=	Average annual precipitation (cm/yr)
$I$	=	Average annual irrigation (cm/yr)
$RO$	=	Average annual surface runoff from pervious areas (cm/yr)
$E_v$	=	Average annual evapotranspiration (cm/yr)
$\theta_{sw}$	=	Soil volumetric water content (mL/cm <sup>3</sup> soil)
$Z_s$	=	Soil mixing zone depth (cm)
$Kd_s$	=	Soil-water partition coefficient (mL/g)
$BD$	=	Soil bulk density (g/cm <sup>3</sup> soil)

Appendix B, Table B-1-5 further describes the variables associated with Equation 3-8C. The average annual volume of water ( $P + I - RO - E_v$ ) available to generate leachate is the mass balance of all water inputs and outputs from the area under consideration.



**COPC Loss Constant Due to Volatilization ( $k_{sv}$ )**

Semi-volatile and volatile COPCs emitted in high concentrations may become adsorbed to soil particles and exhibit volatilization losses from soil. The loss of a COPC from the soil by volatilization depends on the rate of movement of the COPC to the soil surface, the chemical vapor concentration at the soil surface, and the rate at which vapor is carried away by the atmosphere (Jury 1986).

Consistent with U.S. EPA (In Press), U.S. EPA OSW recommends that Equation 3-8D be used to calculate the constant for the loss of soil resulting from volatilization ( $k_{sv}$ ). The soil loss constant due to volatilization ( $k_{sv}$ ) is based on gas equilibrium coefficients and gas phase mass transfer. The first order decay constant,  $k_{sv}$ , is obtained by adapting the Hwang and Falco equation for soil vapor phase diffusion (Hwang and Falco 1986). The use of this equation is further described in Appendix B, Table B-1-6.

**Recommended Equation for Calculating:  
 COPC Loss Constant Due to Volatilization ( $k_{sv}$ )**

$$k_{sv} = \left( \frac{3.1536 \times 10^7 \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \left( \frac{D_a}{Z_s} \right) \cdot \left[ 1 - \left( \frac{BD}{\rho_s} \right) - \Theta_{sw} \right] \quad \text{Equation 3-8D}$$

where

$k_{sv}$	=	COPC loss constant due to volatilization ( $\text{yr}^{-1}$ )
$3.1536 \times 10^7$	=	Units conversion factor (s/yr)
$H$	=	Henry's Law constant ( $\text{atm} \cdot \text{m}^3/\text{mol}$ )
$Z_s$	=	Soil mixing zone depth (cm)
$Kd_s$	=	Soil-water partition coefficient (mL/g)
$R$	=	Universal gas constant ( $\text{atm} \cdot \text{m}^3/\text{mol} \cdot \text{K}$ )
$T_a$	=	Ambient air temperature (K) = 298.1 K
$BD$	=	Soil bulk density ( $\text{g}/\text{cm}^3$ soil)
$D_a$	=	Diffusivity of COPC in air ( $\text{cm}^2/\text{s}$ )
$\Theta_{sw}$	=	Soil volumetric water content ( $\text{mL}/\text{cm}^3$ soil)
$\rho_s$	=	Solids particle density ( $\text{g}/\text{cm}^3$ )

Appendix B, Table B-1-5 further describes the variables associated with Equation 3-8C. In cases where high concentrations of volatile organic compounds are expected to be present in the soil, U.S. EPA OSW

recommends consulting the methodologies described in U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press). The use of *k<sub>sv</sub>* values is also further described in Appendix B, Table B-1-6.

**3.11.1.3 Deposition Term (*D<sub>s</sub>*)**

U.S. EPA OSW recommends that Equation 3-9 be used to calculate the deposition term (*D<sub>s</sub>*). This equation is further described in Appendix B, Table B-1-1. The use of Equation 3-11 to calculate the deposition term is consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), which both incorporate a deposition term (*D<sub>s</sub>*) into Equation 3-7 for the calculation of the COPC concentration in soil (*C<sub>s</sub>*) (see also Section 3.11.1.1).

**Recommended Equation for Calculating:  
 Deposition Term (*D<sub>s</sub>*)**

$$D_s = \left[ \frac{100 \cdot Q}{Z_s \cdot BD} \right] \cdot [F_v(0.31536 \cdot V_{dv} \cdot C_{yv} + D_{y_{wv}}) + (D_{y_{wp}} + D_{y_{dp}}) \cdot (1 - F_v)] \quad \text{Equation 3-9}$$

where

- D<sub>s</sub>* = Deposition term (mg COPC/kg soil-yr)
- 100 = Units conversion factor (m<sup>2</sup>-mg/cm<sup>2</sup>-kg)
- Q* = COPC-specific emission rate (g/s)
- Z<sub>s</sub>* = Soil mixing zone depth (cm)
- BD* = Soil bulk density (g/cm<sup>3</sup> soil)
- F<sub>v</sub>* = Fraction of COPC air concentration in vapor phase (unitless)
- 0.31536 = Units conversion factor (m-g-s/cm-μg-yr)
- V<sub>dv</sub>* = Dry deposition velocity (cm/s)
- C<sub>yv</sub>* = Unitized yearly average air concentration from vapor phase (μg-s/g-m<sup>3</sup>)
- D<sub>y<sub>wv</sub></sub>*
- D<sub>y<sub>dp</sub></sub>*
- D<sub>y<sub>wp</sub></sub>*

Section 3.9 further describes the ISCST3 unitized air parameters (*C<sub>yv</sub>*, *D<sub>y<sub>wv</sub></sub>*, *D<sub>y<sub>dp</sub></sub>*, and *D<sub>y<sub>wp</sub></sub>*) obtained as output from the air dispersion modeling. Appendix B describes the determination of other variables

associated with Equation 3-9. The proper use of this equation is also further described in Appendix B, Table B-1-1.

#### 3.11.1.4 Site-Specific Parameters for Calculating Soil Concentration

As discussed in the previous sections, calculating the COPC concentration in soil ( $C_s$ ) requires some site-specific parameter values, which must be calculated or derived from available literature or site-specific data. These site-specific parameters include the following:

- Soil mixing zone depth ( $Z_s$ )
- Soil bulk density ( $BD$ )
- Available water ( $P + I - RO - E_v$ )
- Soil volumetric water content ( $\theta_{sw}$ )

Determination of values for these parameters is further described in the following subsections, and in Appendix B.

##### Soil Mixing Zone Depth ( $Z_s$ )

When exposures to COPCs in soils are modeled, the depth of contamination is important in calculating the appropriate soil concentration. Due to leaching and physical disturbance (e.g., tilling) COPCs may migrate deeper in the soil in for some areas. Therefore, the value for the depth of soil contamination, or soil mixing zone depth ( $Z_s$ ), used in modeling ecological risk should be considered specific to tilled (e.g., large plowed field) or untilled soil areas.

In general, previous U.S. EPA combustion risk assessment guidance (1990a) has estimated that if the area under consideration is tilled or mechanically disturbed, the soil mixing zone depth is about 10 to 20 centimeters depending on local conditions and the equipment used. If soil is not moved, COPCs are assumed to be retained in the shallower, upper soil layer. In this case, earlier U.S. EPA guidances (U.S. EPA 1990a; U.S. EPA 1993h) have typically recommended a value of 1 centimeter.

Consistent with earlier U.S. EPA guidance (1990a) and U.S. EPA (1998c), U.S. EPA OSW recommends the following values for the soil mixing zone depth ( $Z_s$ ).

---

<b>Recommended Values for: Soil Mixing Zone Depth (<math>Z_s</math>)</b>
1 cm - untilled 20 cm - tilled

---

### Soil Bulk Density ( $BD$ )

$BD$  is the ratio of the mass of soil to its total volume. This variable is affected by the soil structure, type, and moisture content (Hillel 1980). Consistent with U.S. EPA (1990a; 1994b) and information presented in Hoffman and Baes (1979), U.S. EPA OSW recommends the following value for the soil dry bulk density ( $BD$ ).

---

<b>Recommended Value for: Soil Dry Bulk Density (<math>BD</math>)</b>
1.50 g/cm <sup>3</sup> soil

---

For determination of actual field values specific to a specified location at a site, U.S. EPA (1994I) recommended that wet soil bulk density be determined by weighing a thin-walled, tube soil sample (e.g., a Shelby tube) of known volume and subtracting the tube weight (ASTM Method D2937). Moisture content can then be calculated (ASTM Method 2216) to convert wet soil bulk density to dry soil bulk density.

### Available Water ( $P + I - RO - E_v$ )

The average annual volume of water available ( $P + I - RO - E_v$ ) for generating leachate is the mass balance of all water inputs and outputs from the area under consideration. A wide range of values for these variables may apply in the various U.S. EPA regions.

The average annual precipitation ( $P$ ), irrigation ( $I$ ), runoff ( $RO$ ), and evapotranspiration ( $E_v$ ) rates and other climatological data may be obtained from either data recorded on site or from the Station Climatic Summary for a nearby airport.

Meteorological parameters—such as the evapotranspiration rate and the runoff rate—may also be found in resources such as Geraghty, Miller, van der Leeden, and Troise (1973). Surface runoff may also be estimated by using the curve number equation developed by the U.S. Soil Conservation Service (U.S. EPA 1990a). U.S. EPA (1985b) cites isopleths of mean annual cropland runoff corresponding to various curve numbers developed by Stewart, Woolhiser, Wischmeier, Caro, and Frere (1975). Curve numbers are assigned to an area on the basis of soil type, land use or cover, and the hydrologic condition of the soil (U.S. EPA 1990a).

Using these different references may introduce uncertainties and limitations. For example, Geraghty, van der Leeden, and Troise (1973) present isopleths for annual surface water contributions that include interflow and ground water recharge; these values should be adjusted downward to reflect surface runoff only. U.S. EPA (1994b) recommends that these values be reduced by 50 percent.

### Soil Volumetric Water Content ( $\theta_{sw}$ )

The soil volumetric water content  $\theta_{sw}$  depends on the available water and the soil structure. A wide range of values for these variables may apply in the various U.S. EPA regions. Consistent with earlier guidance documents (U.S. EPA 1994b), U.S. EPA OSW recommends the following value for  $\theta_{sw}$ .

---

**Recommended Value for:**  
**Soil Volumetric Water Content ( $\theta_{sw}$ )**

---

0.2 ml/cm<sup>3</sup> soil

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Additional information on soil water content is presented in Appendix B, specific to the equations in which it is used.

### 3.11.2 CALCULATION OF COPC CONCENTRATIONS IN SURFACE WATER AND SEDIMENTS

COPC concentrations in surface water and sediments are calculated for all water bodies selected for evaluation in the risk assessment. Mechanisms considered for determination of COPC loading of the water column are:

- (1) Direct deposition,
- (2) Runoff from impervious surfaces within the watershed,
- (3) Runoff from pervious surfaces within the watershed,
- (4) Soil erosion over the total watershed,
- (5) Direct diffusion of vapor phase COPCs into the surface water, and
- (6) Internal transformation of compounds chemically or biologically.

Other potential mechanisms may require consideration on a case-by-case basis (e.g., tidal influences), however, contributions from other potential mechanisms are assumed to be negligible in comparison with those being evaluated.

The USLE and a sediment delivery ratio are used to estimate the rate of soil erosion from the watershed. To evaluate the COPC loading to a water body from its associated watershed, the COPC concentration in watershed soils should be calculated. As described in Section 3.11.1, the equation for COPC concentration in soil includes a loss term that considers the loss of contaminants from the soil after deposition. These loss mechanisms may all lower the soil concentration associated with a specific deposition rate.

Surface water concentration algorithms include a sediment mass balance, in which the amount of sediment assumed to be buried and lost from the water body is equal to the difference between the amount of soil introduced to the water body by erosion and the amount of suspended solids lost in downstream flow. As a result, the assumptions are made that sediments do not accumulate in the water body over time, and an equilibrium is maintained between the surficial layer of sediments and the water column. The total water column COPC concentration is the sum of the COPC concentration dissolved in water and the COPC

concentration associated with suspended solids. Partitioning between water and sediment varies with the COPC. The total concentration of each COPC is partitioned between the sediment and the water column.

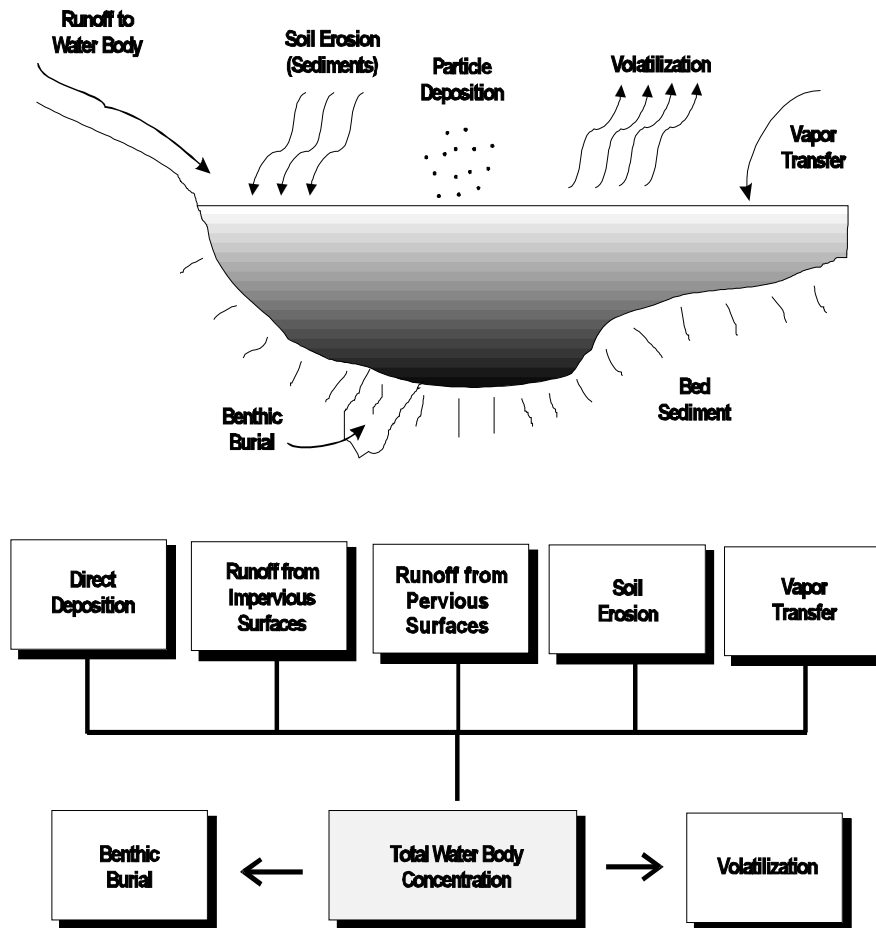


Figure 3-5 COPC Loading to the Water Body

Section 3.11.2.1 describes equations for computing COPC loading to a water body. Section 3.11.2.2 describes equations for computing total COPC concentration in a water body. Section 3.11.2.3 present the equations for computing COPC concentration in water column and in sediment. These equations are also presented and further defined in Appendix B.

3.11.2.1 Total COPC Loading to a Water Body ( $L_T$ )

Consistent with earlier U.S. EPA guidance (1994I) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-10 to calculate the total COPC load to a water body ( $L_T$ ). This equation is also further described in Appendix B, Table B-2-1.

---

**Recommended Equation for Calculating:  
Total COPC Load to the Water Body ( $L_T$ )**

---

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E + L_I \quad \text{Equation 3-10}$$

where

$L_T$	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
$L_{DEP}$	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
$L_{dif}$	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
$L_{RI}$	=	Runoff load from impervious surfaces (g/yr)
$L_R$	=	Runoff load from pervious surfaces (g/yr)
$L_E$	=	Soil erosion load (g/yr)
$L_I$	=	Internal transfer (g/yr)

Due to the limited data and uncertainty associated with the chemical or biological internal transfer,  $L_I$ , of compounds into daughter products, U.S. EPA OSW recommends a default value for this variable of zero. However, if a permitting authority determines that site-specific conditions indicate calculation of internal transfer should be considered, U.S. EPA OSW recommends following the methodologies described in U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S EPA In Press). Calculation of each of the remaining variables ( $L_{DEP}$ ,  $L_{dif}$ ,  $L_{RI}$ ,  $L_R$ , and  $L_E$ ) is discussed in the following subsections.



**Total (Wet and Dry) Particle Phase and Wet Vapor Phase Contaminant Direct Deposition Load to Water Body ( $L_{DEP}$ )**

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends Equation 3-11 to calculate the load to the water body from the direct deposition of wet and dry particles and wet vapors onto the surface of the water body ( $L_{DEP}$ ). The equation is also further described in Appendix B, Table B-2-2.

---

**Recommended Equation for Calculating:  
Total Particle Phase and Wet Vapor Phase Direct Deposition Load to Water Body ( $L_{DEP}$ )**

---

$$L_{DEP} = Q \cdot [ F_v \cdot Dy_{www} + (1 - F_v) \cdot Dy_{twp} ] \cdot A_w \quad \text{Equation 3-11}$$

where

$L_{DEP}$	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
$Q$	=	COPC emission rate (g/s)
$F_v$	=	Fraction of COPC air concentration in vapor phase (unitless)
$Dy_{www}$	=	Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m <sup>2</sup> -yr)
$Dy_{twp}$	=	Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m <sup>2</sup> -yr)
$A_w$	=	Water body surface area (m <sup>2</sup> )

Section 3.9 describes the unitized air parameters,  $Dy_{www}$  and  $Dy_{twp}$ , obtained as output from the ISCST3 air dispersion modeling. The determination of water body surface area,  $A_w$ , is described in Chapter 4.

Appendix A-2 describes determination of the compound-specific parameter,  $F_v$ .

**Diffusion Load to Water Body ( $L_{dif}$ )**

Consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-12 to calculate the dry vapor phase COPC diffusion load to the water body ( $L_{dif}$ ). The equation is described in detail in Appendix B, Table B-2-3.

**Recommended Equation for Calculating:  
 Vapor Phase COPC Diffusion (Dry Deposition) Load to Water Body ( $L_{Dif}$ )**

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot C_{yww} \cdot A_w \cdot 1 \times 10^{-6}}{R \cdot T_{wk}} \quad \text{Equation 3-12}$$

where

$L_{dif}$	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
$K_v$	=	Overall COPC transfer rate coefficient (m/yr)
$Q$	=	COPC emission rate (g/s)
$F_v$	=	Fraction of COPC air concentration in vapor phase (unitless)
$C_{yww}$	=	Unitized yearly (water body and watershed) average air concentration from vapor phase ( $\mu\text{g-s/g-m}^3$ )
$A_w$	=	Water body surface area ( $\text{m}^2$ )
$10^{-6}$	=	Units conversion factor ( $\text{g}/\mu\text{g}$ )
$H$	=	Henry's Law constant ( $\text{atm-m}^3/\text{mol}$ )
$R$	=	Universal gas constant ( $\text{atm-m}^3/\text{mol-K}$ )
$T_{wk}$	=	Water body temperature (K)

The overall COPC transfer rate coefficient ( $K_v$ ) is calculated by using the equation in Appendix B, Table B-2-13. Consistent with previous U.S. EPA guidance (1994l; 1993h) and U.S. EPA (1998c), U.S. EPA OSW recommends a water body temperature ( $T_{wk}$ ) of 298 K (or 25°C). Section 3.9 describes the determination of the modeled air parameter,  $C_{yww}$ . The determination of water body surface area,  $A_w$ , is described in Chapter 4. Appendix A-2 describes determination of compound-specific parameters,  $F_v$  and  $H$ .

### Runoff Load from Impervious Surfaces ( $L_{RI}$ )

In some watershed soils, a fraction of the wet and dry deposition in the watershed will be to impervious surfaces. Dry deposition may accumulate and be washed off during rain events. Consistent with U.S. EPA (1994) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-13 to calculate impervious runoff load to a water body ( $L_{RI}$ ). The equation is also presented in Appendix B, Table B-2-4.

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**Recommended Equation for Calculating:  
Runoff Load from Impervious Surfaces ( $L_{RI}$ )**

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$$L_{RI} = Q \cdot [ F_v \cdot Dy_{www} + (1.0 - F_v) \cdot Dy_{twp} ] \cdot A_I \quad \text{Equation 3-13}$$

where

$L_{RI}$	=	Runoff load from impervious surfaces (g/yr)
$Q$	=	COPC emission rate (g/s)
$F_v$	=	Fraction of COPC air concentration in vapor phase (unitless)
$Dy_{www}$	=	Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m <sup>2</sup> -yr)
$Dy_{twp}$	=	Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m <sup>2</sup> -yr)
$A_I$	=	Impervious watershed area receiving COPC deposition (m <sup>2</sup> )

Impervious watershed area receiving COPC deposition ( $A_I$ ) is the portion of the total effective watershed area that is impervious to rainfall (i.e., roofs, driveways, streets, and parking lots) and drains to the water body.

### Runoff Load from Pervious Surfaces ( $L_R$ )

Consistent with U.S. EPA (1994) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-14 to calculate the runoff dissolved COPC load to the water body from pervious soil surfaces in the watershed ( $L_R$ ). The equation is also presented in Appendix B, Table B-2-5.

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**Recommended Equation for Calculating:  
Runoff Load from Pervious Surfaces ( $L_R$ )**

---

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{C_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.01 \quad \text{Equation 3-14}$$

---

where

$L_R$	=	Runoff load from pervious surfaces (g/yr)
$RO$	=	Average annual surface runoff from pervious areas (cm/yr)
$A_L$	=	Total watershed area receiving COPC deposition (m <sup>2</sup> )
$A_I$	=	Impervious watershed area receiving COPC deposition (m <sup>2</sup> )
$C_s$	=	COPC concentration in soil (in watershed soils) (mg COPC/kg soil)
$BD$	=	Soil bulk density (g soil/cm <sup>3</sup> soil)
$\theta_{sw}$	=	Soil volumetric water content (mL water/cm <sup>3</sup> soil)
$Kd_s$	=	Soil-water partition coefficient (cm <sup>3</sup> water/g soil)
$0.01$	=	Units conversion factor (kg-cm <sup>2</sup> /mg-m <sup>2</sup> )

Appendix B describes the determination of site-specific parameters,  $RO$ ,  $A_L$ ,  $A_I$ ,  $BD$ , and  $\theta_{sw}$ . The calculation of the COPC concentration in soil ( $C_s$ ) is discussed in Section 3.11.1 and Appendix B. Soil bulk density ( $BD$ ) and soil water content ( $\theta_{sw}$ ) are described in Section 3.11.1.4.

### Soil Erosion Load ( $L_E$ )

Consistent with U.S. EPA (1994) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-15 to calculate soil erosion load ( $L_E$ ). The equation is also presented in Appendix B, Table B-2-6.

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**Recommended Equation for Calculating:  
Soil Erosion Load ( $L_E$ )**

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$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{C_s \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001 \quad \text{Equation 3-15}$$

where

$L_E$	=	Soil erosion load (g/yr)
$X_e$	=	Unit soil loss (kg/m <sup>2</sup> -yr)
$A_L$	=	Total watershed area (evaluated) receiving COPC deposition (m <sup>2</sup> )
$A_I$	=	Impervious watershed area receiving COPC deposition (m <sup>2</sup> )
$SD$	=	Sediment delivery ratio (watershed) (unitless)
$ER$	=	Soil enrichment ratio (unitless)
$C_s$	=	COPC concentration in soil (in watershed soils) (mg COPC/kg soil)
$BD$	=	Soil bulk density (g soil/cm <sup>3</sup> soil)
$\theta_{sw}$	=	Soil volumetric water content (mL water/cm <sup>3</sup> soil)
$Kd_s$	=	Soil-water partition coefficient (mL water/g soil)
0.001	=	Units conversion factor (k-cm <sup>2</sup> /mg-m <sup>2</sup> )

Unit soil loss ( $X_e$ ) and watershed sediment delivery ratio ( $SD$ ) are calculated as described in the following subsections and in Appendix B. COPC concentration in soil ( $C_s$ ) is described in Section 3.11.1 and Appendix B, Table B-1-1. Soil bulk density ( $BD$ ) and soil water content ( $\theta_{sw}$ ) are described in Section 3.11.1.4.

**Universal Soil Loss Equation - USLE**

U.S. EPA OSW recommends that the universal soil loss equation (USLE), Equation 3-16, be used to calculate the unit soil loss ( $X_e$ ) specific to each watershed. This equation is further described in Appendix B, Table B-2-7. Appendix B also describes determination of the site- and watershed-specific values for each of the variables associated with Equation 3-16. The use of Equation 3-16 is consistent with U.S. EPA (1994b; 1994l) and U.S. EPA (1998c).

**Recommended Equation for Calculating:  
 Unit Soil Loss ( $X_e$ )**

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047} \quad \text{Equation 3-16}$$

where

$X_e$	=	Unit soil loss (kg/m <sup>2</sup> -yr)
$RF$	=	USLE rainfall (or erosivity) factor (yr <sup>-1</sup> )
$K$	=	USLE erodibility factor (ton/acre)
$LS$	=	USLE length-slope factor (unitless)
$C$	=	USLE cover management factor (unitless)
$PF$	=	USLE supporting practice factor (unitless)
907.18	=	Units conversion factor (kg/ton)
4047	=	Units conversion factor (m <sup>2</sup> /acre)

The USLE  $RF$  variable, which represents the influence of precipitation on erosion, is derived from data on the frequency and intensity of storms. This value is typically derived on a storm-by-storm basis, but average annual values have been compiled (U.S. Department of Agriculture 1982). Information on determining site-specific values for variables used in calculating  $X_e$  is provided in U.S. Department of Agriculture (U.S. Department of Agriculture 1997) and U.S. EPA guidance (U.S. EPA 1985b). Refer to Appendix B, Table B-2-7 for additional discussion of the USLE.

**Sediment Delivery Ratio (*SD*)**

U.S. EPA OSW recommends the use of Equation 3-17 to calculate sediment delivery ratio (*SD*). The use of this equation is further described in Appendix B, Table B-2-8.

---

**Recommended Equation for Calculating:  
Sediment Delivery Ratio (*SD*)**

---

$$SD = a \cdot (A_L)^{-b} \qquad \text{Equation 3-17}$$

where

<i>SD</i>	=	Sediment delivery ratio (watershed) (unitless)
<i>a</i>	=	Empirical intercept coefficient (unitless)
<i>b</i>	=	Empirical slope coefficient (unitless)
<i>A<sub>L</sub></i>	=	Total watershed area (evaluated) receiving COPC deposition (m <sup>2</sup> )

The sediment delivery ratio (*SD*) for a large land area, a watershed or part of a watershed, can be calculated, on the basis of the area of the watershed, by using an approach proposed by Vanoni (1975). Accordingly, U.S. EPA (1993h) recommended the use of Equation 3-17 to calculate the sediment delivery ratio.

According to Vanoni (1975), sediment delivery ratios vary approximately with the -0.125 power of the drainage area. Therefore, the empirical slope coefficient is assumed to be equal to 0.125. An inspection of the data presented by Vanoni (1975) indicates that the empirical intercept coefficient varies with the size of the watershed, as illustrated in Appendix B, Table B-2-8.

*A<sub>L</sub>* is the total watershed surface area affected by deposition that drains to the body of water. A watershed includes all of the land area that contributes water to a water body. In assigning values to the watershed surface area affected by deposition, consideration should be given to (1) the distance from the stack, (2) the location of the area affected by deposition fallout with respect to the water body, and (3) in the absence of

any deposition considerations, watershed hydrology. Total sediment in a water body may have originated from watershed soils that are (or have the potential to be) both affected and unaffected by deposition of combustion emissions. If a combustor is depositing principally on a land area that feeds a tributary of a larger river system, consideration must be given to an “effective” area. An effective drainage area will almost always be less than the watershed.

**3.11.2.2 Total Water Body COPC Concentration ( $C_{wtot}$ )**

U.S. EPA OSW recommends the use of Equation 3-18 to calculate total water body COPC concentration ( $C_{wtot}$ ). The total water body concentration includes both the water column and the bed sediment. The equation is also presented in Appendix B, Table B-2-9.

**Recommended Equation for Calculating:  
 Total Water Body COPC Concentration ( $C_{wtot}$ )**

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} + k_{wt} \cdot A_W \cdot (d_{wc} + d_{bs})} \quad \text{Equation 3-18}$$

where

- $C_{wtot}$  = Total water body COPC concentration (including water column and bed sediment) (g COPC/m<sup>3</sup> water body)
- $L_T$  = Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
- $Vf_x$  = Average volumetric flow rate through water body (m<sup>3</sup>/yr)
- $f_{wc}$  = Fraction of total water body COPC concentration in the water column (unitless)
- $k_{wt}$  = Overall total water body COPC dissipation rate constant (yr<sup>-1</sup>)
- $A_W$  = Water body surface area (m<sup>2</sup>)
- $d_{wc}$  = Depth of water column (m)
- $d_{bs}$  = Depth of upper benthic sediment layer (m)

The total COPC load to the water body ( $L_T$ )—including deposition, runoff, and erosion—is described in Section 3.11.2.1 and Appendix B, Table B-2-1. The depth of the upper benthic layer ( $d_{bs}$ ), which represents the portion of the bed that is in equilibrium with the water column, cannot be precisely specified;



however, U.S. EPA (1993h) recommended values ranging from 0.01 to 0.05. Consistent with U.S. EPA (1994; 1998c), U.S. EPA OSW recommends a default value of 0.03, which represents the midpoint of the specified range. Issues related to the remaining parameters are summarized in the following subsections.

**Fraction of Total Water Body COPC Concentration in the Water Column ( $f_{wc}$ ) and Benthic Sediment ( $f_{bs}$ )**

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-19 to calculate fraction of total water body COPC concentration in the water column ( $f_{wc}$ ), and Equation 3-20 to calculate fraction of total water body contaminant concentration in benthic sediment ( $f_{bs}$ ). The equations are also presented in Appendix B, Table B-2-10.

**Recommended Equation for Calculating:  
 Fraction of Total Water Body COPC Concentration in  
 the Water Column ( $f_{wc}$ ) and Benthic Sediment ( $f_{bs}$ )**

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z + (\theta_{bs} + Kd_{bs} \cdot BS) \cdot d_{bs} / d_z} \quad \text{Equation 3-19}$$

$$f_{bs} = 1 - f_{wc} \quad \text{Equation 3-20}$$

where

- $f_{wc}$  = Fraction of total water body COPC concentration in the water column (unitless)
- $f_{bs}$  = Fraction of total water body COPC concentration in benthic sediment (unitless)
- $Kd_{sw}$  = Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
- $TSS$  = Total suspended solids concentration (mg/L)
- $1 \times 10^{-6}$  = Units conversion factor (kg/mg)
- $d_z$  = Total water body depth (m)
- $\theta_{bs}$  = Bed sediment porosity ( $L_{water} / L_{sediment}$ )

$Kd_{bs}$	=	Bed sediment/sediment pore water partition coefficient (L water/kg bottom sediment)
$BS$	=	Benthic solids concentration (g/cm <sup>3</sup> [equivalent to kg/L])
$d_{wc}$	=	Depth of water column (m)
$d_{bs}$	=	Depth of upper benthic sediment layer (m)

U.S. EPA (1993h) and NC DEHNR (1997) recommended the use of Equations 3-19 and 3-20 to calculate the fraction of total water body concentration occurring in the water column ( $f_{wc}$ ) and the bed sediments ( $f_{bs}$ ). The partition coefficient  $Kd_{sw}$  describes the partitioning of a contaminant between sorbing material, such as soil, surface water, suspended solids, and bed sediments (see Appendix A-2). NC DEHNR (1997) also recommended adding the depth of the water column to the depth of the upper benthic layer ( $d_{wc} + d_{bs}$ ) to calculate the total water body depth ( $d_z$ ).

NC DEHNR (1997) recommended a default total suspended solids (*TSS*) concentration of 10 mg/L, which was adapted from U.S. EPA (1993h). However, due to variability in water body specific values for this variable, U.S. EPA OSW recommends the use of water body-specific measured *TSS* values representative of long-term average annual values for the water body of concern. Average annual values for *TSS* are generally expected to be in the range of 2 to 300 mg/L; with additional information on anticipated *TSS* values available in the U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press).

If measured data is not available, or of unacceptable quality, a calculated *TSS* value can be obtained for non-flowing water bodies using Equation 3-21.

$$TSS = \frac{X_e \cdot (A_L - A_I) \cdot SD \cdot 1x10^3}{Vf_x + D_{ss} \cdot A_W} \quad \text{Equation 3-21}$$

where

$TSS$	=	Total suspended solids concentration (mg/L)
$X_e$	=	Unit soil loss (kg/m <sup>2</sup> -yr)
$A_L$	=	Total watershed area (evaluated) receiving COPC deposition (m <sup>2</sup> )
$A_I$	=	Impervious watershed area receiving COPC deposition (m <sup>2</sup> )

$SD$	=	Sediment delivery ratio (watershed) (unitless)
$Vf_x$	=	Average volumetric flow rate through water body (value should be 0 for quiescent lakes or ponds) ( $m^3/yr$ )
$D_{ss}$	=	Suspended solids deposition rate (a default value of 1,825 for quiescent lakes or ponds) ( $m/yr$ )
$A_w$	=	Water body surface area ( $m^2$ )

The default value of 1,825  $m/yr$  provided for  $D_{ss}$  is characteristic of Stoke's settling velocity for an intermediate (fine to medium) silt.

Also, to evaluate the appropriateness of watershed-specific values (specific for non-flowing water bodies) used in calculating the unit soil loss ( $X_e$ ), as described in Section 3.11.2.1 and Appendix B, the water-body specific measured  $TSS$  value should be compared to the calculated  $TSS$  value obtained using Equation 3-21. If the measured and calculated  $TSS$  values differ significantly, parameter values used in calculating  $X_e$  should be re-evaluated. This re-evaluation of  $TSS$  and  $X_e$  should also be conducted if the calculated  $TSS$  value is outside of the normal range expected for average annual measured values, as discussed above.

Bed sediment porosity ( $\theta_{bs}$ ) can be calculated from the benthic solids concentration by using the following equation (U.S. EPA 1993h):

$$\theta_{bs} = 1 - \frac{BS}{\rho_s}$$

where

$\theta_{bs}$	=	Bed sediment porosity ( $L_{water}/L_{sediment}$ )
$\rho_s$	=	Bed sediment density ( $kg/L$ )
$BS$	=	Benthic solids concentration ( $kg/L$ )

U.S. EPA OSW recommends the following default value for bed sediment porosity ( $\theta_{bs}$ ), which was adapted from U.S. EPA (1993h) and U.S. EPA (1998c):

**Recommended Value for:  
 Bed Sediment Porosity ( $\theta_{bs}$ )**

$$\theta_{bs} = 0.6 \frac{L_{\text{water}}}{L_{\text{sediment}}}$$

(assuming  $\rho_s = 2.65 \text{ kg/L}$  [bed sediment density] and  $BS = 1 \text{ kg/L}$  [benthic solids concentration])

Values for the benthic solids concentration ( $BS$ ) and depth of upper benthic sediment layer ( $d_{bs}$ ) range from 0.5 to 1.5 kg/L and 0.01 to 0.05 meters, respectively. However, consistent with earlier U.S. EPA guidance (1993h; 1994l) and U.S. EPA (1998c), 1 kg/L is a reasonable default for most applications of the benthic solids concentration ( $BS$ ), and 0.03 meter is the default depth of the upper benthic layer ( $d_{bs}$ ). The default depth of 0.03 meters is based on the midpoint of the range presented above. The use of this equation is further described in Appendix B, Table B-2-10.

**Overall Total Water Body COPC Dissipation Rate Constant ( $k_{wt}$ )**

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-22 to calculate the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial. The equation is also presented in Appendix B, Table B-2-11.

**Recommended Equation for Calculating:  
 Overall Total Water Body COPC Dissipation Rate Constant ( $k_{wt}$ )**

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b \quad \text{Equation 3-22}$$

where

- $k_{wt}$  = Overall total water body dissipation rate constant ( $\text{yr}^{-1}$ )
- $f_{wc}$  = Fraction of total water body COPC concentration in the water column (unitless)
- $k_v$  = Water column volatilization rate constant ( $\text{yr}^{-1}$ )
- $f_{bs}$  = Fraction of total water body COPC concentration in benthic sediment (unitless)
- $k_b$  = Benthic burial rate constant ( $\text{yr}^{-1}$ )

The variables  $f_{wc}$  and  $f_{bs}$  are discussed in the previous section, Equations 3-19 and 3-20, and calculated by using the equations presented in Appendix B, Table B-2-10.

**Water Column Volatilization Rate Constant ( $k_v$ )**

Consistent with U.S. EPA (1994I) and U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-23 to calculate water column volatilization rate constant. The equation is also presented in Appendix B, Table B-2-12.

**Recommended Equation for Calculating:  
 Water Column Volatilization Rate Constant ( $k_v$ )**

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})} \quad \text{Equation 3-23}$$

where

- $k_v$  = Water column volatilization rate constant (yr<sup>-1</sup>)
- $K_v$  = Overall COPC transfer rate coefficient (m/yr)
- $d_z$  = Total water body depth (m)
- $Kd_{sw}$  = Suspended sediments/surface water partition coefficient (L water/kg suspended sediments)
- $TSS$  = Total suspended solids concentration (mg/L)
- $1 \times 10^{-6}$  = Units conversion factor (kg/mg)

Total water body depth ( $d_z$ ), suspended sediment and surface water partition coefficient ( $Kd_{sw}$ ), and total suspended solids concentration ( $TSS$ ), are previously described in this section.  $Kd_{sw}$  is discussed in Appendix A-2. The overall transfer rate coefficient ( $K_v$ ) is described in the following subsection.

**Overall COPC Transfer Rate Coefficient ( $K_v$ )**

Volatile organic chemicals can move between the water column and the overlying air. The overall transfer rate  $K_v$ , or conductivity, is determined by a two-layer resistance model that assumes that two “stagnant

films” are bounded on either side by well-mixed compartments. Concentration differences serve as the driving force for the water layer diffusion. Pressure differences drive the diffusion for the air layer. From balance considerations, the same mass must pass through both films; the two resistances thereby combine in series, so that the conductivity is the reciprocal of the total resistance.

Consistent with U.S. EPA (1993h) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-24 to calculate the overall transfer rate coefficient ( $K_v$ ). The equation is also presented in Appendix B, Table B-2-13.

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**Recommended Equation for Calculating:  
 Overall COPC Transfer Rate Coefficient ( $K_v$ )**

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$$K_v = \left( K_L^{-1} + \left( K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right)^{-1} \cdot \theta^{T_{wk} - 293} \quad \text{Equation 3-24}$$

where

$K_v$	=	Overall COPC transfer rate coefficient (m/yr)
$K_L$	=	Liquid phase transfer coefficient (m/yr)
$K_G$	=	Gas phase transfer coefficient (m/yr)
$H$	=	Henry’s Law constant (atm·m <sup>3</sup> /mol)
$R$	=	Universal gas constant (atm·m <sup>3</sup> /mol·K)
$T_{wk}$	=	Water body temperature (K)
$\theta$	=	Temperature correction factor (unitless)

The value of the conductivity  $K_v$  depends on the intensity of turbulence in the water body and the overlying atmosphere. As Henry’s Law constant increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. Conversely, as Henry’s Law constant decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

The liquid and gas phase transfer coefficients,  $K_L$  and  $K_G$ , respectively, vary with the type of water body. The liquid phase transfer coefficient ( $K_L$ ) is calculated by using Equations 3-25 and 3-26. The gas phase transfer coefficient ( $K_G$ ) is calculated by using Equations 3-27 and 3-28.

Henry's Law constants generally increase with increasing vapor pressure of a COPC and generally decrease with increasing solubility of a COPC. Henry's Law constants are compound-specific and are presented in Appendix A-2. The universal ideal gas constant,  $R$ , is  $8.205 \times 10^{-5}$  atm-m<sup>3</sup>/mol-K, at 20°C. The temperature correction factor ( $\theta$ ), which is equal to 1.026, is used to adjust for the actual water temperature. Volatilization is assumed to occur much less readily in lakes and reservoirs than in moving water bodies.

### Liquid Phase Transfer Coefficient ( $K_L$ )

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends using Equations 3-25 and 3-26 to calculate liquid phase transfer coefficient. ( $K_L$ ). The use of these equations is further described in Appendix B, Table B-2-14.

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**Recommended Equation for Calculating:  
 Liquid Phase Transfer Coefficient ( $K_L$ )**

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**For flowing streams or rivers:**

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7 \quad \text{Equation 3-25}$$

**For quiescent lakes or ponds:**

$$K_L = (C_d^{0.5} \cdot W) \cdot \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_w}{\rho_w \cdot D_w}\right)^{-0.67} \cdot 3.1536 \times 10^7 \quad \text{Equation 3-26}$$

where

$K_L$	=	Liquid phase transfer coefficient (m/yr)
$D_w$	=	Diffusivity of COPC in water (cm <sup>2</sup> /s)
$u$	=	Current velocity (m/s)
$1 \times 10^{-4}$	=	Units conversion factor (m <sup>2</sup> /cm <sup>2</sup> )
$d_z$	=	Total water body depth (m)
$C_d$	=	Drag coefficient (unitless)
$W$	=	Average annual wind speed (m/s)

$\rho_a$	=	Density of air (g/cm <sup>3</sup> )
$\rho_w$	=	Density of water (g/cm <sup>3</sup> )
$k$	=	von Karman's constant (unitless)
$\lambda_z$	=	Dimensionless viscous sublayer thickness (unitless)
$\mu_w$	=	Viscosity of water corresponding to water temperature (g/cm-s)
$3.1536 \times 10^7$	=	Units conversion factor (s/yr)

For a flowing stream or river, the transfer coefficients are controlled by flow-induced turbulence. For these systems, the liquid phase transfer coefficient is calculated by using Equation 3-25, which is the O'Connor and Dobbins (1958) formula, as presented in U.S. EPA (1993h).

For a stagnant system (quiescent lake or pond), the transfer coefficient is controlled by wind-induced turbulence. For quiescent lakes or ponds, the liquid phase transfer coefficient can be calculated by using Equation 3-26 (O'Connor 1983; U.S. EPA 1993h).

The total water body depth ( $d_z$ ) for liquid phase transfer coefficients is discussed previously in this section.

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of the following default values. These values are further described in Appendix A-2:

- (1) a diffusivity of chemical in water ranging ( $D_w$ ) from  $1.0 \times 10^{-5}$  to  $8.5 \times 10^{-2}$  cm<sup>2</sup>/s,
- (2) a dimensionless viscous sublayer thickness ( $\lambda_z$ ) of 4,
- (3) a von Karman's constant ( $k$ ) of 0.4,
- (4) a drag coefficient ( $C_d$ ) of 0.0011 which was adapted from U.S. EPA (1993h),
- (5) a density of air ( $\rho_a$ ) of 0.0012 g/cm<sup>3</sup> at standard conditions (temperature = 20°C or 293 K, pressure = 1 atm or 760 millimeters of mercury) (Weast 1986),
- (6) a density of water ( $\rho_w$ ) of 1 g/cm<sup>3</sup> (Weast 1986),
- (7) a viscosity of water ( $\mu_w$ ) of a 0.0169 g/cm-s corresponding to water temperature (Weast 1986).



**Gas Phase Transfer Coefficient ( $K_G$ )**

U.S. EPA OSW recommends using Equations 3-27 and 3-28 to calculate gas phase transfer coefficient ( $K_G$ ). The equation is also discussed in Appendix B, Table B-2-15.

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**Recommended Equation for Calculating:  
 Gas Phase Transfer Coefficient ( $K_G$ )**

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**For flowing streams or rivers:**

$$K_G = 36500 \text{ m/yr} \qquad \text{Equation 3-27}$$

**For quiescent lakes or ponds:**

$$K_G = (C_d^{0.5} \cdot W) \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a}\right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 3-28}$$

where

$K_G$	=	Gas phase transfer coefficient (m/yr)
$C_d$	=	Drag coefficient (unitless)
$W$	=	Average annual wind speed (m/s)
$k$	=	von Karman's constant (unitless)
$\lambda_z$	=	Dimensionless viscous sublayer thickness (unitless)
$\mu_a$	=	Viscosity of air corresponding to air temperature (g/cm-s)
$\rho_a$	=	Density of air corresponding to water temperature (g/cm <sup>3</sup> )
$D_a$	=	Diffusivity of COPC in air (cm <sup>2</sup> /s)
$3.1536 \times 10^7$	=	Units conversion factor (s/yr)

U.S. EPA (1993h) indicated that the rate of transfer of a COPC from the gas phase for a flowing stream or river is assumed to be constant, in accordance with O'Connor and Dobbins (1958) (Equation 3-27).

For a stagnant system (quiescent lake or pond), the transfer coefficients are controlled by wind-induced turbulence. For quiescent lakes or ponds, U.S. EPA OSW recommends that the gas phase transfer coefficient be computed by using the equation presented in O'Connor (1983) (Equation 3-28).

Consistent with U.S. EPA (1994I) and U.S. EPA (1998c), U.S. EPA OSW recommends  $1.81 \times 10^{-4}$  g/cm-s for the viscosity of air corresponding to air temperature.

**Benthic Burial Rate Constant ( $k_b$ )**

U.S. EPA OSW recommends using Equation 3-29 to calculate benthic burial rate ( $k_b$ ). The equation is also discussed in Appendix B, Table B-2-16.

**Recommended Equation for Calculating:  
 Benthic Burial Rate Constant ( $k_b$ )**

$$k_b = \left( \frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^3 - Vf_x \cdot TSS}{A_w \cdot TSS} \right) \cdot \left( \frac{TSS \cdot 1 \times 10^{-6}}{BS \cdot d_{bs}} \right) \quad \text{Equation 3-29}$$

where

$k_b$	=	Benthic burial rate constant ( $\text{yr}^{-1}$ )
$X_e$	=	Unit soil loss ( $\text{kg}/\text{m}^2\text{-yr}$ )
$A_L$	=	Total watershed area (evaluated) receiving deposition ( $\text{m}^2$ )
$SD$	=	Sediment delivery ratio (watershed) (unitless)
$Vf_x$	=	Average volumetric flow rate through water body ( $\text{m}^3/\text{yr}$ )
$TSS$	=	Total suspended solids concentration ( $\text{mg}/\text{L}$ )
$A_w$	=	Water body surface area ( $\text{m}^2$ )
$BS$	=	Benthic solids concentration ( $\text{g}/\text{cm}^3$ )
$d_{bs}$	=	Depth of upper benthic sediment layer (m)
$1 \times 10^{-6}$	=	Units conversion factor ( $\text{kg}/\text{mg}$ )
$1 \times 10^3$	=	Units conversion factor ( $\text{g}/\text{kg}$ )

The benthic burial rate constant ( $k_b$ ), which is calculated in Equation 3-29, can also be expressed in terms of the rate of burial ( $Wb$ ):

$$Wb = k_b \cdot d_{bs} \quad \text{Equation 3-30}$$

where

$Wb$	=	Rate of burial (m/yr)
$k_b$	=	Benthic burial rate constant ( $\text{yr}^{-1}$ )
$d_{bs}$	=	Depth of upper benthic sediment layer (m)

According to U.S. EPA (1994i) and U.S. EPA (1998c), COPC loss from the water column resulting from burial in benthic sediment can be calculated by using Equation 3-29. These guidance documents also recommend a benthic solids concentration ( $BS$ ) value ranging from 0.5 to 1.5 kg/L, which was adapted from U.S. EPA (1993h). U.S. EPA OSW recommends the following default value for benthic solids concentration ( $BS$ ).

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**Recommended Default Value for:  
Benthic Solids Concentration ( $BS$ )**

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1.0 kg/L

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The calculated value for  $k_b$  should range from 0 to 1.0; with low  $k_b$  values expected for water bodies characteristic of no or limited sedimentation (rivers and fast flowing streams), and  $k_b$  values closer to 1.0 expected for water bodies characteristic of higher sedimentation (lakes). This range of values is based on the relation between the benthic burial rate and rate of burial expressed in Equation 3-30; with the depth of upper benthic sediment layer held constant. For  $k_b$  values calculated as a negative (water bodies with high average annual volumetric flow rates in comparison to watershed area evaluated), a  $k_b$  value of 0 should be assigned for use in calculating the total water body COPC concentration ( $C_{wtot}$ ) in Equation 3-18. If the calculated  $k_b$  value exceeds 1.0, re-evaluation of the parameter values used in calculating  $X_e$  should be conducted.

### 3.11.2.3 Total COPC Concentration in Water Column ( $C_{wtot}$ )

U.S. EPA OSW recommends using Equation 3-31 to calculate total COPC concentration in water column ( $C_{wtot}$ ). The equation is also discussed in Appendix B, Table B-2-17.

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**Recommended Equation for Calculating:  
Total COPC Concentration in Water Column ( $C_{wctot}$ )**

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$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}} \quad \text{Equation 3-31}$$

where

$C_{wctot}$	=	Total COPC concentration in water column (mg COPC/L water column)
$f_{wc}$	=	Fraction of total water body COPC concentration in the water column (unitless)
$C_{wtot}$	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
$d_{wc}$	=	Depth of water column (m)
$d_{bs}$	=	Depth of upper benthic sediment layer (m)

The use of Equation 3-31 to calculate total COPC concentration in water column is consistent with U.S. EPA (1994l; 1998c).

Total water body COPC concentration—including water column and bed sediment ( $C_{wtot}$ ) and fraction of total water body COPC concentration in the water column ( $f_{wc}$ )—should be calculated by using Equation 3-18 and Equation 3-19, respectively. Depth of upper benthic sediment layer ( $d_{bs}$ ) is discussed previously.

**Dissolved Phase Water Concentration ( $C_{dw}$ )**

U.S. EPA OSW recommends the use of Equation 3-32 to calculate the concentration of COPC dissolved in the water column ( $C_{dw}$ ). The equation is discussed in detail in Appendix B, Table B-2-18.

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**Recommended Equation for Calculating:  
Dissolved Phase Water Concentration ( $C_{dw}$ )**

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$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}} \quad \text{Equation 3-32}$$

where

$C_{dw}$	=	Dissolved phase water concentration (mg COPC/L water)
$C_{wctot}$	=	Total COPC concentration in water column (mg COPC/L water column)
$Kd_{sw}$	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
$TSS$	=	Total suspended solids concentration (mg/L)
$1 \times 10^{-6}$	=	Units conversion factor (kg/mg)

The use of Equation 3-32 to calculate the concentration of COPC dissolved in the water column is consistent with U.S. EPA (1994l; 1998c).

The total COPC concentration in water column ( $C_{wctot}$ ) is calculated by using the Equation 3-31 (see also Appendix B, Table B-2-17). The surface water partition coefficient ( $Kd_{sw}$ ) and total suspended solids concentration ( $TSS$ ) are discussed previously.

### **COPC Concentration in Bed Sediment ( $C_{sed}$ )**

U.S. EPA OSW recommends the use of Equation 3-33 to calculate COPC concentration in bed sediment ( $C_{sed}$ ). The equation is also presented in Appendix B, Table B-2-19.

**Recommended Equation for Calculating:  
 COPC Concentration in Bed Sediment ( $C_{sed}$ )**

$$C_{sed} = f_{bs} \cdot C_{wtot} \cdot \left( \frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot BS} \right) \cdot \left( \frac{d_{wc} + d_{bs}}{d_{bs}} \right) \quad \text{Equation 3-33}$$

where

$C_{sed}$	=	COPC concentration in bed sediment (mg COPC/kg sediment)
$f_{bs}$	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
$C_{wtot}$	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
$Kd_{bs}$	=	Bed sediment/sediment pore water partition coefficient (L COPC/kg water body)
$\theta_{bs}$	=	Bed sediment porosity ( $L_{\text{pore water}}/L_{\text{sediment}}$ )
$BS$	=	Benthic solids concentration ( $g/cm^3$ )
$d_{wc}$	=	Depth of water column (m)
$d_{bs}$	=	Depth of upper benthic sediment layer (m)

The use of Equation 3-33 to calculate the COPC concentration in bed sediment is consistent with U.S. EPA (1994l; 1998c).

The total water body COPC concentration—including water column and bed sediment ( $C_{wtot}$ ) and the fraction of total water body COPC concentration that occurs in the benthic sediment ( $f_{bs}$ )—is calculated by using Equations 3-18 and 3-20, respectively. The bed sediment and sediment pore water partition coefficient ( $Kd_{bs}$ ) is discussed in Appendix A-2. Bed sediment porosity ( $\theta_{bs}$ ), benthic solids concentration ( $BS$ ), depth of water column ( $d_{wc}$ ), and depth of upper benthic layer ( $d_{bs}$ ) are discussed previously.

### 3.11.3 CALCULATION OF COPC CONCENTRATIONS IN PLANTS

The concentration of COPCs in plants is assumed to occur by three possible mechanisms:

- **Direct deposition of particles**—wet and dry deposition of particle phase COPCs onto the exposed plant surfaces.
- **Vapor transfer**—uptake of vapor phase COPCs by plants through their foliage.

- **Root uptake**—root uptake of COPCs available from the soil and their transfer to the aboveground portions of the plant.

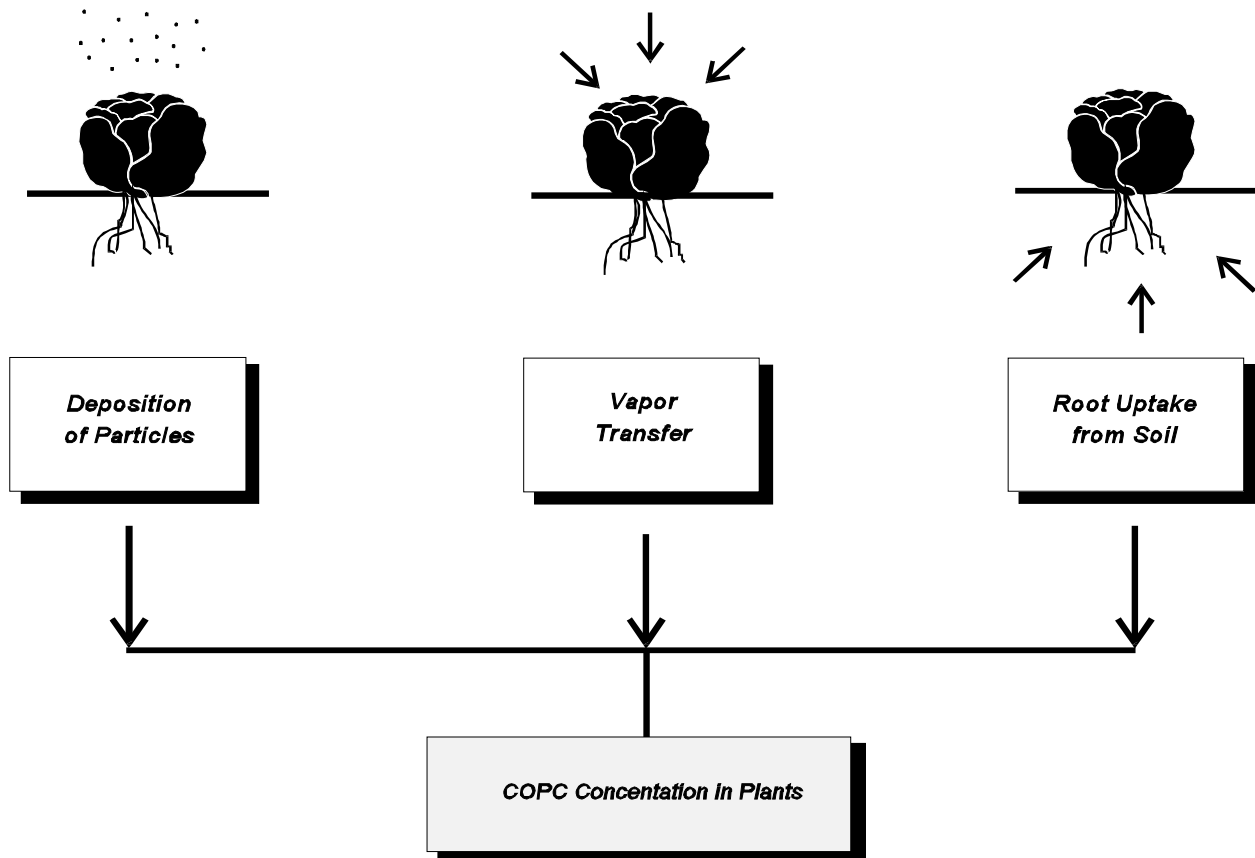


Figure 3-6 COPC Concentration in Plants

The total COPC concentration in terrestrial plants,  $C_{TP}$  is calculated as a sum of contamination occurring through all three of these mechanisms.

3.11.3.1 Calculating Plant Concentration Due to Direct Deposition ( $P_d$ )

Consistent with previous U.S. EPA guidance (1994I) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-34 to calculate COPC concentration in plants due to direct deposition. The use of this equation is further described in Appendix B, Table B-3-1.

**Recommended Equation for Calculating:  
 Plant Concentration Due to Direct Deposition ( $P_d$ )**

$$P_d = \frac{1,000 \cdot Q \cdot (1 - F_v) \cdot [Dydp + (F_w \cdot Dywp)] \cdot R_p \cdot [1.0 - \exp(-k_p \cdot T_p)] \cdot 0.12}{Y_p \cdot k_p} \quad \text{Equation 3-34}$$

where

$P_d$	=	Plant concentration due to direct (wet and dry) deposition (mg COPC/kg WW)
1,000	=	Units conversion factor (mg/g)
$Q$	=	COPC emission rate (g/s)
$F_v$	=	Fraction of COPC air concentration in vapor phase (unitless)
$Dydp$	=	Unitized yearly average dry deposition from particle phase (s/m <sup>2</sup> -yr)
$F_w$	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$Dywp$	=	Unitized yearly wet deposition from particle phase (s/m <sup>2</sup> -yr)
$R_p$	=	Interception fraction of the edible portion of plant (unitless)
$k_p$	=	Plant surface loss coefficient (yr <sup>-1</sup> )
$T_p$	=	Length of plant exposure to deposition per harvest of the edible portion of the <i>i</i> th plant group (yr)
0.12	=	Dry weight to wet weight conversion factor (unitless)
$Y_p$	=	Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m <sup>2</sup> )

Section 3.9 describes the use of the unitized air parameters,  $Dydp$  and  $Dywp$ , obtained as output from the air dispersion modeling. Appendix A-3 describes determination of  $F_v$ . Appendix B describes determination of  $F_w$ ,  $R_p$ ,  $k_p$ ,  $T_p$ , and  $Y_p$ . The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz et al. 1991).



### 3.11.3.2 Calculating Plant Concentration Due to Air-to-Plant Transfer ( $P_v$ )

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-35 to calculate the plant concentration due to air-to-plant transfer ( $P_v$ ). The use of this equation is further described in Appendix B, Table B-3-2.

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**Recommended Equation for Calculating:  
Plant Concentration Due to Air-to-Plant Transfer ( $P_v$ )**

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$$P_v = Q \cdot F_v \cdot 0.12 \cdot \frac{C_{yv} \cdot B_v}{\rho_a} \quad \text{Equation 3-35}$$

where

$P_v$	=	Plant concentration due to air-to-plant transfer (mg COPC/kg WW)
$Q$	=	COPC emission rate (g/s)
$F_v$	=	Fraction of COPC air concentration in vapor phase (unitless)
$C_{yv}$	=	Unitized yearly average air concentration from vapor phase ( $\mu\text{g-s/g-m}^3$ )
$B_v$	=	Air-to-plant biotransfer factor ([mg COPC/g DW plant]/[mg COPC/g air]) (unitless)
0.12	=	Dry weight to wet weight conversion factor (unitless)
$\rho_a$	=	Density of air ( $\text{g/m}^3$ )

Section 3.9 describes the use of the unitized air parameter,  $C_{yv}$ . Appendix A-3 describes determination of the COPC-specific parameters,  $F_v$  and  $B_v$ . The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz et al. 1991). Appendix B further describes use of Equation 3-35, including determination of  $F_w$  and  $\rho_a$ .

### 3.11.3.3 Calculating Plant Concentration Due to Root Uptake ( $P_r$ )

Consistent with previous U.S. EPA guidance (1994g; 1994i; 1995h) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-36 to calculate the plant concentration due to root uptake ( $P_r$ ). The use of this equation is further described in Appendix B, Table B-3-3.

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**Recommended Equation for Calculating:  
Plant Concentration Due to Root Uptake (*Pr*)**

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$$Pr = Cs \cdot BCF_r \cdot 0.12 \qquad \text{Equation 3-36}$$

where

<i>Pr</i>	=	Plant concentration due to root uptake (mg COPC/kg WW)
<i>BCF<sub>r</sub></i>	=	Plant-soil biotransfer factor (unitless)
<i>C<sub>s</sub></i>	=	COPC concentration in soil (mg COPC/kg soil)
0.12	=	Dry weight to wet weight conversion factor (unitless)

Equation 3-36 is based on the soil-to-aboveground plant transfer approach developed by Travis and Arms (1988). The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz et al. 1991). Appendix A-3 describes determination of the COPC-specific parameter *BCF<sub>r</sub>*. Section 3.11.1 and Appendix B describe calculation of *C<sub>s</sub>*.

### 3.12 REPLACING DEFAULT PARAMETER VALUES

As discussed in Chapter 1, default parameter values are provided in this guidance for numerous inputs to the fate and transport modeling. After completing a risk assessment based on the default parameter values recommended in this guidance, risk assessors may choose to investigate replacing default parameter values with measured or published values if a more representative estimate of site-specific risk can be obtained. Use of parameter values other than those specified in this guidance should always be clearly described in the risk assessment report and work plan, and approved by the permitting authority. U.S. EPA OSW recommends that requests to change default parameter values include the following information, as appropriate:

1. An explanation of why the use of a measured or published value other than the default value is warranted (e.g., the default parameter value is based on data or studies at sites in the northwestern U.S., but the facility is located in the southeast);
2. The supporting technical basis of the replacement parameter value, including readable copies (printed in English) of any relevant technical literature or studies;

3. The basis of the default parameter value, as understood by the requestor, including readable copies (printed in English) of the referenced literature or studies (if available);
4. A comparison of the weight-of-evidence between the competing studies (e.g., the proposed replacement parameter value is based on a study that is more representative of site conditions, a specific exposure setting being evaluated, or a more scientifically valid study than the default parameter value, the proposed replacement parameter is based on the analysis of 15 samples as opposed to 5 for the default parameter value, or the site-specific study used more stringent quality control/quality assurance procedures than the study upon which the default parameter value is based);
5. A description of other risk assessments or projects where the proposed replacement parameter value has been used, and how such risk assessments or projects are similar to the risk assessment in consideration.

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# Chapter 4

## Problem Formulation

### What's Covered in Chapter 4:

- ◆ Exposure Setting Characterization
  - ◆ Food Web Development
  - ◆ Selecting Assessment Endpoints
  - ◆ Identifying Measures of Effect
- 
- 

Problem formulation establishes the exposure setting used as the basis for exposure analysis and risk characterization. Problem formulation includes (1) characterization of the exposure setting for identification of potentially exposed habitats in the assessment area (Section 4.1); (2) development of food webs representative of the habitats to be evaluated (Section 4.2); (3) selection of assessment endpoints relevant to food web structure and function (Section 4.3); and (4) identification of measurement receptors (Section 4.4).

### 4.1 EXPOSURE SETTING CHARACTERIZATION

Exposure setting characterization is important in the identification of habitats consisting of ecological receptors in the assessment area that may be impacted as a result of exposure to compounds emitted from a facility. Ecological receptors within a potentially impacted habitat can be evaluated through consideration of the combination of exposure pathways to which ecological receptors representing a habitat-specific food web may be exposed to a compound. The habitats identified to be evaluated are selected based on existing habitats surrounding the facility (see Section 4.1.1); and also support which habitat-specific food webs are evaluated in risk characterization. Consideration of ecological receptors representative of the habitats also provides the basis for selecting measurement receptors, as well as, it supports demonstration of the presence or absence of federal and state species of special interest (see Section 4.1.1.3).

Exposure setting characterization is generally focused geographically to the assessment area that is defined as the area surrounding the facility that is impacted from facility emissions as predicted by ISCST3 air dispersion modeling; with additional consideration typically extending by a 50-km radius, taken from the centroid of a polygon (also used as the origin of ISCST3 receptor grid node array, see Chapter 3) identified by the UTM coordinates of the facility's emission sources. A 50-km radius is generally the recognized limit of the ISCST3 air dispersion model and its predecessors (U.S. EPA 1990a; 1995c). Resources for characterizing the exposure setting should focus on the areas impacted from emissions as predicted by air dispersion modeling. As discussed in Section 4.1.1, habitats (potentially including water bodies and their associated watersheds)—both within and outside the facility property boundary—should be considered for evaluation.

The following subsections provide information on selection of habitats, and identification of ecological receptors representative of those habitats, to be considered for evaluation in the risk assessment.

#### **4.1.1 Selection of Habitats**

Habitats to be considered in the risk assessment are selected by identifying similar habitats surrounding the facility that are potentially impacted by facility emissions, and when overlaid with the air dispersion modeling results, define which habitat-specific food webs should be evaluated in the risk assessment.

Habitats can be defined based on their biotic and abiotic characteristics, and are generally divided into two major groups (i.e., terrestrial and aquatic) that can be classified as follows:

- Terrestrial
  - Forest
  - Shortgrass prairie
  - Tallgrass prairie
  - Agricultural/Cropland
  - Scrub/Shrub
  - Desert
  
- Aquatic
  - Freshwater
  - Brackish/Intermediate
  - Marine

Habitat types can typically be identified by reviewing hard copy and/or electronic versions of land use land classification (LULC) maps, topographic maps, and aerial photographs. Sources and general information associated with each of these data types or maps are presented below. Also, as noted in Chapter 3, the UTM coordinate system format (NAD27 or NAD83) for all mapping information should be verified to ensure consistency and prevent erroneous georeferencing of locations and areas.

***Land Use Land Cover (LULC) Maps*** - LULC maps can be downloaded directly from the USGS web site (<http://mapping.usgs.gov/index.html>), at a scale of 1:250,000 in a file type GIRAS format. LULC maps can also be downloaded from the EPA web site (<ftp://ftp.epa.gov/pub>), at a scale of 1:250,000, in an Arc/Info export format. These maps provide detailed habitat information based upon the classification system and definitions of Level II Land Use and Land Cover information. Exact boundaries of polygon land use area coverages, in areas being considered for evaluation, should be verified using available topographic maps and aerial photographic coverages.

***Topographic Maps*** - Topographic maps are readily available in both hard copy and electronic format directly from USGS or numerous other vendors. These maps are commonly at a scale of 1:24,000, and in a file type of TIFF format with TIFF World File included for georeferencing.

***Aerial Photographs*** - Hard copy aerial photographs can be purchased directly from USGS in a variety of scales and coverages. Electronic format aerial photographs of Digital Ortho Quarter Quads (DOQQs) can also be purchased directly from USGS, or from an increasing number of commercial sources. Properly georeferenced DOQQs covering a 3-km or more radius of the assessment area, overlays of the LULC map coverage, and the ISCST3 modeled receptor grid node array provide an excellent reference for identifying land use areas and justifying selection of exposure locations.

While these data types or maps do not represent the universe of information available on habitats or land use, they are readily available from a number of governmental sources (typically accessible via the Internet), usually can be obtained free or for a low cost, and, when used together, provide sufficient information to reliably identify and define boundaries of habitats to be considered for evaluation in risk characterization. However, while the use of these or other data can be very accurate, verifying identified habitats by conducting a site visit is recommended. Also, these data sources may be dated, and may not reflect current habitat boundaries or land use (i.e., expanded cropland or urban developments, new lakes).

Additional information useful for habitat identification can be obtained from discussions with representatives of private and government organizations which routinely collect and evaluate ecosystem or habitat information including the following: (1) Soil Conservation Service, (2) U.S. Fish and Wildlife

Service (FWS), (3) U.S Department of Agriculture, (4) state natural resource, wildlife, and park agencies, and (5) local government agencies.

U.S. EPA OSW recommends that habitats identified during exposure setting characterization and selected for evaluation in the risk assessment be clearly mapped and include the following supporting information:

- Facility boundaries
- Facility emission source location(s)
- Habitat types and boundaries
- Water bodies and their associated watersheds
- Special ecological areas (see Section 4.1.1.2)

A facility location map, including land-use and land cover data, which allows for identification of habitats to support selection of habitat-specific food webs to be evaluated in the risk assessment. The map should also note the UTM coordinate system format (NAD27 or NAD83) for all information presented to ensure consistency and prevent erroneous georeferencing of locations and areas; including accurate identification of exposure scenario locations and water bodies within the habitat to be evaluated, as discussed in the following subsections.

#### **4.1.1.1 Selection of Exposure Scenario Locations Within Terrestrial Habitats**

Exposure scenario locations to be evaluated within the terrestrial habitats identified during the exposure setting characterization, are selected at specific receptor grid nodes based on evaluation of the magnitude of air parameter values estimated by ISCST3 (see Chapter 3). U.S. EPA OSW would like to note that the methodology and resulting selection of receptor grid nodes as exposure scenario locations is one of the most critical parts of the risk assessment process, ensuring standardization across all facilities evaluated and reproducibility of results. The estimates of risk can vary significantly in direct response to the receptor grid nodes that are selected as exposure scenario locations because the grid node-specific ISCST3 modeled air parameter values are used as inputs into the media equations.

U.S. EPA OSW recommends that, at a minimum, the procedures described below be used in the selection of receptor grid nodes as exposure scenario locations; and that the selected exposure scenario locations correspond to actual ISCST3 modeled receptor grid node locations defined by UTM coordinates. In addition to consistency and reproducibility, these procedures ensure that the exposure scenario location(s) selected for evaluation over a specified habitat do not overlook the most highly impacted locations.

Exposure scenario locations, at actual receptor grid nodes, should be selected as follows:

***Step 1: Define Terrestrial Habitats To Be Evaluated*** - All habitats, identified during exposure setting characterization for evaluation in the risk assessment, should be defined and habitat boundaries mapped in a format (NAD 27 or NAD 83 UTM) consistent with that used to define locations of facility emission sources and modeled ISCST3 receptor grid nodes.

***Step 2: Identify Receptor Grid Node(s) Within Each Habitat To Be Evaluated*** - For each habitat to be evaluated, identify the receptor grid nodes within that area or on the boundary of that area (defined in Step 1) that represent the locations of highest yearly average concentration for each ISCST3 modeled air parameter (i.e., air concentration, dry deposition, wet deposition) for each phase (i.e., vapor, particle, particle-bound). This determination should be performed for each emission source (i.e., stacks, fugitives) and all emissions sources at the facility combined. This results in the selection of one or more receptor grid nodes as exposure scenario locations, within a defined habitat area to be evaluated, and that meet one or more of the following criteria:

- Highest modeled unitized vapor phase air concentration
- Highest modeled unitized vapor phase wet deposition rate
- Highest modeled unitized particle phase air concentration
- Highest modeled unitized particle phase wet deposition rate
- Highest modeled unitized particle phase dry deposition rate
- Highest modeled unitized particle-bound phase air concentration
- Highest modeled unitized particle-bound phase wet deposition rate
- Highest modeled unitized particle-bound phase dry deposition rate

Only ISCST3 modeled air parameters corresponding to a single receptor grid node should be used per exposure scenario location as inputs into the media equations, without averaging or statistical manipulation. However, based generally on the number and location of facility emission sources, multiple exposure scenario locations may be selected to represent the highest potential impact area for a specific habitat being evaluated.



Modeling of the above air parameter criteria for habitats at actual sites being evaluated in U.S. EPA Region 6, using actual modeled air parameters, indicates that only 1 to 3 receptor nodes are typically selected per habitat. This is because, in most cases, the location of some of the highest air concentration and deposition rate, within a habitat for several of the modeled air parameters, occurs at the same receptor grid node. The number of receptor grid nodes with maximum air parameters depends on many factors, including number of and distance between emissions sources, habitat size and shape, distance and direction from facility, topographic features, and meteorological patterns. It should also be noted, that while these criteria minimize overlooking maximum risk within a habitat, they do not preclude the risk assessor from selecting additional exposure scenario locations within that same habitat based on site-specific risk considerations.

Also, a water body and associated watershed in close proximity to the exposure scenario location being evaluated should be identified to represent a drinking water source for applicable receptors (see Appendix F). Although the locations and type of sources (i.e., free water, consumption of water as part of food items) of water ingested by an animal through diet are expected to vary depending on the receptor and availability, COPC intake by the receptor through ingestion of water can be estimated by assuming only water intake from a defined water body for which a COPC concentration can be calculated. Therefore, a representative water body should be defined and evaluated following the guidance provided in Section 4.1.1.2, and a COPC concentration in the water column,  $C_{water}$ , calculated as described in Chapter 3 and Appendix B.

If a definable water body is not located within or in close proximity to the terrestrial habitat being evaluated, receptor drinking water intake terms in the exposure equations presented in Appendix F should be adjusted accordingly (i.e., ingestion of drinking water set equal to zero). However, for sites where the permitting authority or risk manager identifies that receptor exposure through ingestion of drinking water may be significant, an available option is to assume that a small water body exists at the same receptor grid node as the exposure scenario location being evaluated. If multiple exposure scenario locations within the habitat are being evaluated, a single assumed water body can be located at the closest receptor grid node located equal distance from each of the exposure scenario locations being evaluated, and utilized as a drinking water source for evaluation of each exposure scenario location within the habitat. Since the assumed water body represents a pool or other drinking source too small for identification on an aerial

photograph or map, it can be assumed to have a unit volume (i.e., surface area of 1 meter square, water column depth of 1 meter). The assumed water body should not have flow or an associated watershed.

#### 4.1.1.2 Selection of Habitat Exposure Scenario Locations Within Aquatic Habitats

Exposure scenario locations to be evaluated within the aquatic habitats identified during the exposure setting characterization may first require differentiating water bodies from land areas within aquatic habitats not typically covered by water (e.g., flood plains or wetland areas transitioning to terrestrial and upland habitats). Exposure scenario locations within land areas of aquatic habitats not characteristic of a standing water body are selected following the same steps as for terrestrial habitats (see Section 4.1.1.1). However, exposure scenario locations for defined water bodies within aquatic habitats should be selected following the guidance provided in this section. The associated watershed contributing COPC loading to the water body being evaluated should also be defined.

U.S. EPA OSW recommends that, at a minimum, the following procedures be used in the selection of exposure scenario locations within defined water body areas of aquatic habitats as follows:

***Step 1: Define Aquatic Habitats To Be Evaluated*** - All habitats, identified during exposure setting characterization for evaluation in the risk assessment, should be defined and habitat boundaries mapped in a format (NAD 27 or NAD 83 UTM) consistent with that used to define locations of facility emission sources and modeled ISCST3 receptor grid nodes. Water body boundaries should reflect annual average shoreline elevations. The area extent of watersheds associated with water bodies to be evaluated should also be defined.

***Step 2: Identify Receptor Grid Node(s) Within Each Habitat To Be Evaluated*** - For each water body and associated watershed to be evaluated, the receptor grid nodes within that area and on the boundary of that area (defined in Step 1) should be considered. For water bodies, the risk assessor can select the receptor grid node that represent the locations of highest yearly average concentration for each ISCST3 modeled air parameter (i.e., air concentration, dry deposition, wet deposition) for each phase (i.e., vapor, particle, particle-bound), or average the air parameter values for all receptor grid nodes within the area of the water body. This determination should be performed for each emission source (i.e., stacks, fugitives), and all emissions sources at the facility combined. For watersheds, the modeled air parameter values should be averaged for all receptor grid nodes within the area extent or effective area of the watershed (excluding the area of the water body).

For evaluating the COPC loading to the water body from its associated watershed, the area extent of the watershed should be defined and the ISCST3 modeled air parameter values at each receptor grid node

within the watershed area (excluding the water body) averaged. These averaged air parameter values are then used in the estimating media equations presented in Chapter 3 and Appendix B for calculating the COPC loading to the water body.

For water bodies identified as potentially impacted from emission sources and selected for evaluation, the area extent of the associated watershed that contributes water to the water body should also be identified and defined by UTM coordinates. The area extent of a watershed is generally defined by topographic highs that result in downslope drainage into the water body. The watershed can be important to determining the overall water body COPC loading, because pervious and impervious areas of the watershed, as well as the soil concentration of COPCs resulting from emissions from facility sources, are also used in the media concentration equations to calculate the water body COPC concentrations resulting from watershed runoff (see Chapter 3 and Appendix B). The total watershed area that contributes water to the water body can be very extensive relative to the area that is impacted from facility emissions. Therefore, it is important that the area extent of all watersheds to be evaluated should be approved by the permitting authority, to ensure that the watershed and its contribution to the water body is defined appropriately in consideration of the aquatic habitat being evaluated and subsequent estimated risk.

For example, if facility emissions impact principally a land area that feeds a specific tributary that drains to a large swamp system and immediately upstream of the ISCST3 receptor grid nodes identified as exposure scenario locations for the aquatic habitat defined by the swamp, the risk assessor should consider evaluating an “effective” watershed area rather than the entire watershed area of the large swamp system. For such a large swamp system, the watershed area can be on the order of thousands of square kilometers and can include numerous tributaries draining into the swamp at points that would have no net impact on the water body COPC concentration at the exposure point(s) of interest.

Similar to large watersheds, water bodies may also be extensive in size relative to the area that is impacted from facility emissions and exposure point(s) of interest. In such cases, the risk assessor should consider defining and evaluating an “effective” area of the water body that focuses the assessment specific to areas potentially impacted and of most concern when considering potential for exposure. Therefore, as with watersheds, it is important that the area extent of all water bodies to be evaluated should be approved by the permitting authority, to ensure that potential impacts and exposure are appropriately considered.

The recommended ISCST3 modeled receptor grid node array extends out about 10 km from facility emission sources (see Chapter 3). To address evaluation of habitat areas, water bodies, or watersheds located beyond the coverage provided by the recommended receptor grid node array (greater than 10 km from the facility), the ISCST3 modeling can be conducted with an additional receptor grid node array specified to provide coverage of the area of concern, or the steps above can be executed using the closest receptor grid nodes from the recommended array. However, using the closest receptor grid nodes from the recommended receptor grid node array will in most cases provide a conservative estimate of risk since the magnitude of air parameter values at these receptor grid nodes would most likely be higher than at receptor grid nodes located further from the facility sources and actually within the area of concern.

#### **RECOMMENDED INFORMATION FOR RISK ASSESSMENT**

- Identification and/or mapping of habitats, water bodies, and associated watersheds potentially impacted by facility emissions of COPCs, including surface area of the water body and area extent of the contributing watershed defined by UTM coordinates
- Rational for selection or exclusion from evaluation, habitats within the assessment area
- Description of rational and assumptions made to limit the watershed area to an “effective” area
- Copies of all maps, photographs, or figures used to define characteristics of habitats, water bodies, and watersheds

#### **4.1.1.3 Special Ecological Areas**

A special ecological area is a habitat that could require protection or special consideration on a site-specific basis because (1) unique and/or rare ecological receptors and natural resources are present, or (2) legislatively-conferred protection (e.g., a national monument) has been established. All potentially exposed special ecological areas in the assessment area should be identified for consideration. The following are examples of special ecological habitats (U.S. EPA 1997c):

- Marine Sanctuaries
- National river reaches
- Spawning areas critical for maintenance of fish/shellfish species

- Terrestrial areas utilized for breeding by large or dense aggregations of animals
- Migratory pathways and feeding areas critical for maintenance of anadromous fish species
- National Preserves
- Federal lands designated for protection of natural ecosystems
- National or State Wildlife Refuges
- Critical areas identified under the Clean Lakes Program
- Habitats known to be used by Federal or State designated or proposed endangered or threatened species
- Areas identified under the Coastal Zone Management Act
- Sensitive areas identified under the National Estuary Program or Near Coastal Waters Program
- Designated Federal Wilderness Areas
- State lands designated for wildlife or game management
- Federal- or State-designated Scenic or Wild Rivers, or Natural Areas
- Wetlands

#### RECOMMENDED INFORMATION FOR RISK ASSESSMENT

- Identification and mapping of habitats in the assessment area, information on which the identification is based, and information on any special ecological areas. Maps, photographs, or additional sources used to determine habitats and define boundaries should be referenced. Maps and figures should also note the UTM coordinate system format (NAD27 or NAD83) for all information presented to ensure consistency and prevent erroneous georeferencing of locations and areas.

#### 4.1.2 Identification of Ecological Receptors

Identification of ecological receptors during exposure setting characterization is used to define food webs specific to potentially impacted habitats to be evaluated in the risk assessment. Ecological receptors for each habitat potentially impacted should be identified to ensure (1) plant and animal communities representative of the habitat are represented by the habitat-specific food web, and (2) potentially complete exposure pathways are identified. Examples of sources and general information available for identification of site-specific ecological receptors are presented below:

**Government Organizations** - U.S. Fish and Wildlife Service (National Wetland Inventory Maps - <http://nwi.fws.gov>) and State Natural Heritage Programs (see Appendix H) provide maps or lists

of species based on geographic location, and are very helpful in identifying threatened or endangered species or areas of special concern.

**General Literature (field guides)** - Examples of information describing the flora and fauna of North America and useful in the development of habitat-specific food webs (see Section 4.2) include the following: Wharton 1982; Craig et al. 1987; Baker et al. 1991; Carr 1994; Ehrlich et al. 1988; National Geographic Society (1987, 1992); Whitaker 1995; Burt and Grossenheider 1980; Behler 1995; Smith and Brodie 1982; Tynning 1990; and Farrand Jr. 1989.

**Private or Local Organizations** - Additional private or professional organizations that are examples of sources of information include: National Audubon Society, National Geographic Society, Local Wildlife Clubs, State and National Parks Systems, and Universities.

Ecological receptor identification should include species both known and expected to be present in a specific habitat being evaluated, and include resident and migratory populations. Identification of flora should be based on major taxonomic groups represented in the assessment area. Natural history information may also be useful during food web development in assigning individual receptors to specific habitats and guilds based on feeding behavior (as discussed in Section 4.2.).

## 4.2 FOOD WEB DEVELOPMENT

Information obtained during exposure setting characterization should be used to develop one or more habitat-specific food web(s) that represent communities and guilds of receptors potentially exposed to emissions from facility sources. Food webs are interlocking patterns of food chains, which are the straight-line transfer of energy from a food source (e.g., plants) to a series of organisms feeding on the source or on other organisms feeding on the food source (Odum 1971). While energy and, therefore, transfer of a compound in a food chain, is not always linear, it is assumed in this guidance that energy and, thus, compounds, are always transferred to a higher trophic level. The importance of a food chain as an exposure pathway primarily depends on receptor dietary habits, the receptors in the food chain, and other factors including bioavailability and depuration of the compound evaluated.

Habitat-specific food webs are developed for use in the risk assessment to:

- Define direct and indirect exposure pathways
- Formulate assessment endpoints

- Develop mathematical relationships between guilds
- Perform quantitative exposure analysis for ecological receptors

Food webs can be developed using the “community approach” (Cohen 1978), which includes (1) identification of potential receptors in a given habitat (see Section 4.1.2) for grouping into feeding guilds by class and communities (see Section 4.2.1), (2) organizing food web structure by trophic level (e.g., primary producer, secondary consumer; see Section 4.2.2), and (3) defining dietary relationships between guilds and communities (see Section 4.2.3). The result is a complete food web for a defined habitat, which should be developed for each habitat in the assessment area to be evaluated in risk characterization. An example of food web development is presented in Section 4.2.4.

#### **4.2.1 Grouping Receptors into Feeding Guilds and Communities**

The first step in developing a habitat-specific food web is to identify, based on the dietary habits and feeding strategies of receptors compiled in Section 4.1.2, the major feeding guilds for birds, mammals, reptiles, amphibians, and fish. A guild is a group of species that occupies a particular trophic level and shares similar feeding strategies. Invertebrates and plants are not assigned to guilds, rather these receptors are grouped into their respective community by the environmental media they inhabit. The distinction for grouping upper-trophic-level receptors into class-specific guilds, and invertebrates and plants into communities, is made because the risk to these groups is characterized differently (see Chapter 5).

Once the major feeding guilds are identified (e.g., herbivore, omnivore, carnivore, insectivore), receptors should be grouped by class (e.g., mammals, birds, amphibians and reptiles, and fish). As noted, invertebrates and plants are grouped into their respective community by the media they inhabit (i.e, soil invertebrates, terrestrial vegetation, sediment fauna, water column invertebrates, phytoplankton, and rooted aquatic vegetation).

#### **4.2.2 Organizing Food Web Structure By Trophic Level**

The structure of a food web should be organized by trophic level. A trophic level is one of the successive levels of nourishment in a food web or food chain. The first trophic level (TL1) contains the primary producers or the green plants. Members of this trophic level produce their own food from nutrients,

sunlight, carbon dioxide, and water. These primary producers are also the source of food for members of the second trophic level (TL2). The second trophic level is often referred to as the primary consumers and is composed of animals that eat plants (herbivores) and animals that subsist on detritus (decaying organic matter) found in sediment and soil (detritivores). The third trophic level (TL3), contains both omnivores and carnivores. Omnivores are animals that eat both plant and animal matter, while carnivores eat primarily animal matter. The fourth trophic level (TL4), contains only carnivores and is sometimes referred to as the dominant carnivores. TL4 contains animals at the top of the food chain (e.g., raptorial birds).

Some species can occupy more than one trophic level at a time depending on life stage. For this reason, professional judgement should be used to categorize receptors without making the food web unduly complex.

#### **4.2.3 Defining Dietary Relationships Between Guilds and Communities**

After species have been grouped into the appropriate guilds and communities, and organized by trophic level, dietary relationships between guilds and communities should be defined. Guilds and communities should be linked together based on dietary relationships by evaluating the dietary composition of the receptors for each guild and community. Although most organisms have a complex diet, it should be assumed that the majority of their diet is composed of a limited number of prey items and, therefore, a limited number of feeding guild interactions occur. Therefore, U.S. EPA OSW recommends that generally only those interactions that contribute more than five percent of the total diet should be considered for development of a food web. This recommendation of five percent of the total diet as a general cutoff is based on the assumption that the food web can be simplified without underestimating exposure.

#### **RECOMMENDED INFORMATION FOR RISK ASSESSMENT**

- Habitat-specific food web(s) that include identification of (1) media (e.g., soil, sediment, water), (2) trophic levels that include at a minimum producers (TL 1), primary consumers (TL 2), secondary consumers (TL 3), and carnivores (TL 4), (3) guilds divided into classes (e.g., herbivorous mammals, omnivorous birds) and communities, and (4) major dietary interactions.

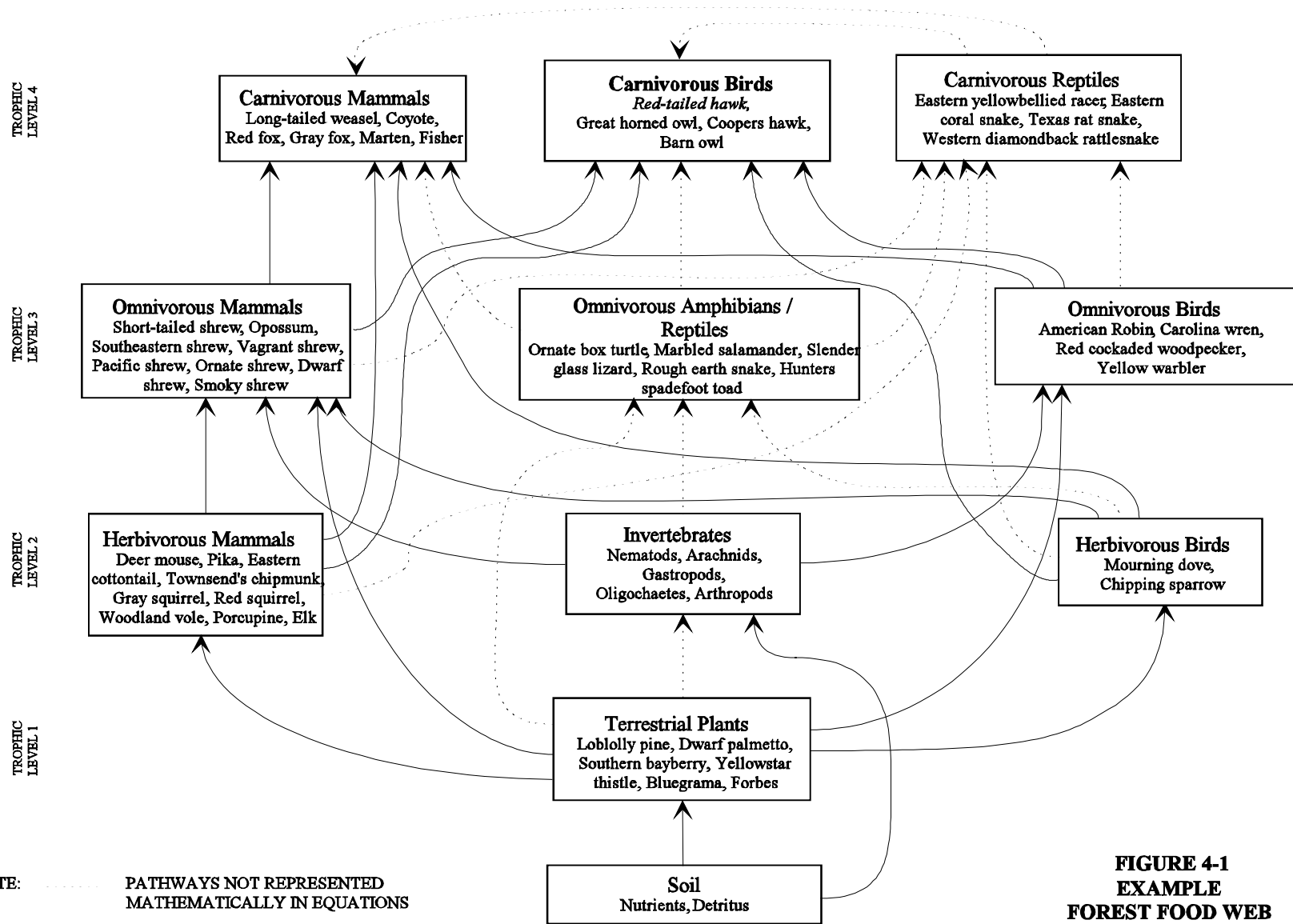


#### 4.2.4 Example Habitat-Specific Food Webs

To better illustrate food web development as discussed in the previous sections (see Sections 4.2.1 through 4.2.3), seven habitat-specific example food webs are presented as Figures 4-1 through 4-7. The habitats represented include:

- Forest
- Tallgrass prairie
- Shortgrass prairie
- Shrub/Scrub
- Freshwater/Wetland
- Salt marsh
- Brackish/Intermediate marsh

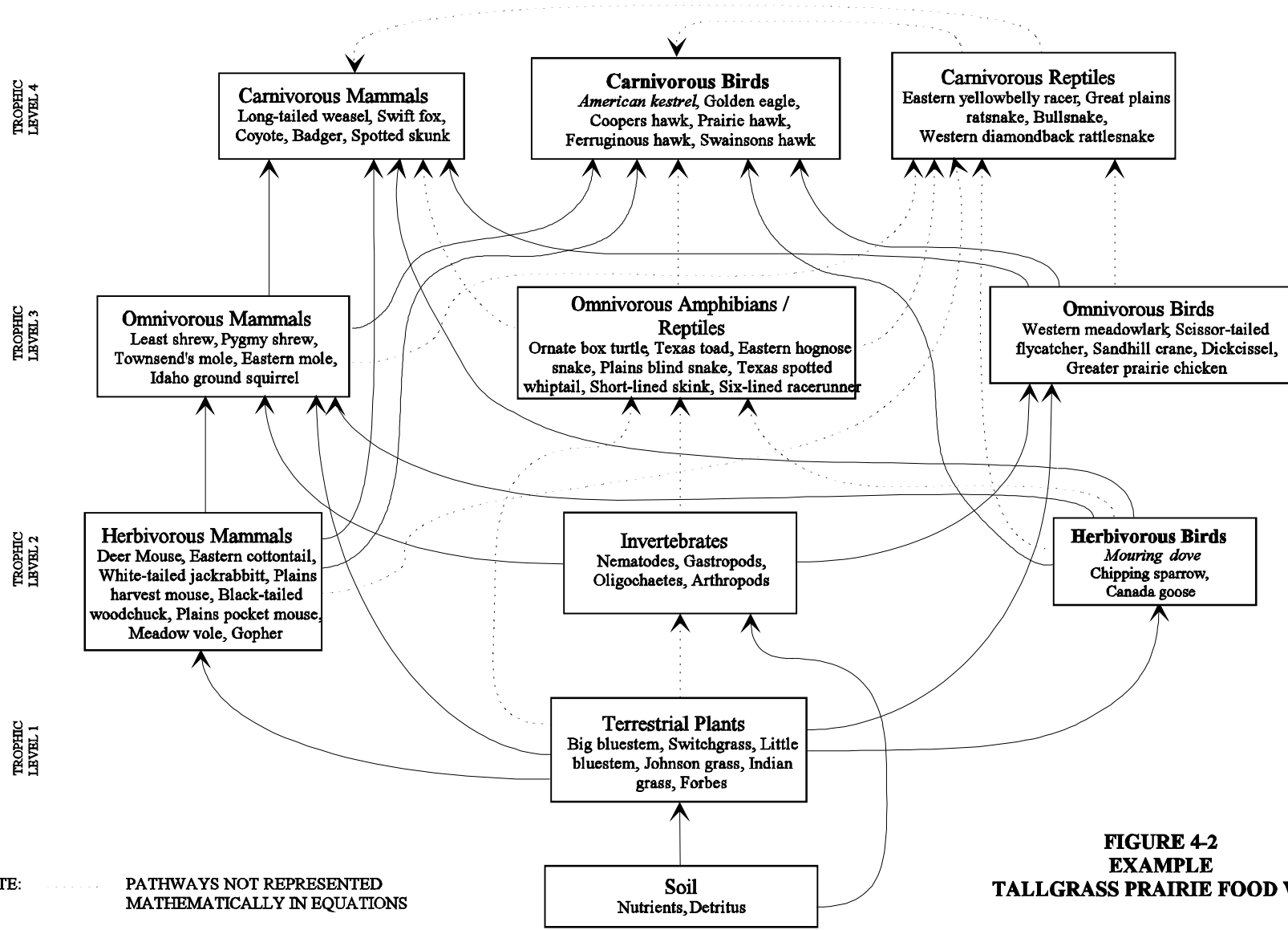
The terrestrial and aquatic example food webs are based on information describing the flora and fauna of North America (U.S. FWS 1979; Wharton 1982; Craig et al. 1987; Baker et al. 1991). Supplemental information was collected from field guides and U.S. EPA's *Wildlife Exposure Factors Handbook* (Carr 1994; Ehrlich et al. 1988; National Geographic Society 1987; U.S. EPA 1993o; Whitaker 1995; Burt and Grossenheider 1980; Behler 1995; Smith and Brodie 1982; Tynning 1990; National Geographic Society 1992; Farrand Jr. 1989).



**FIGURE 4-1  
 EXAMPLE  
 FOREST FOOD WEB**

NOTE: ..... PATHWAYS NOT REPRESENTED  
 MATHEMATICALLY IN EQUATIONS

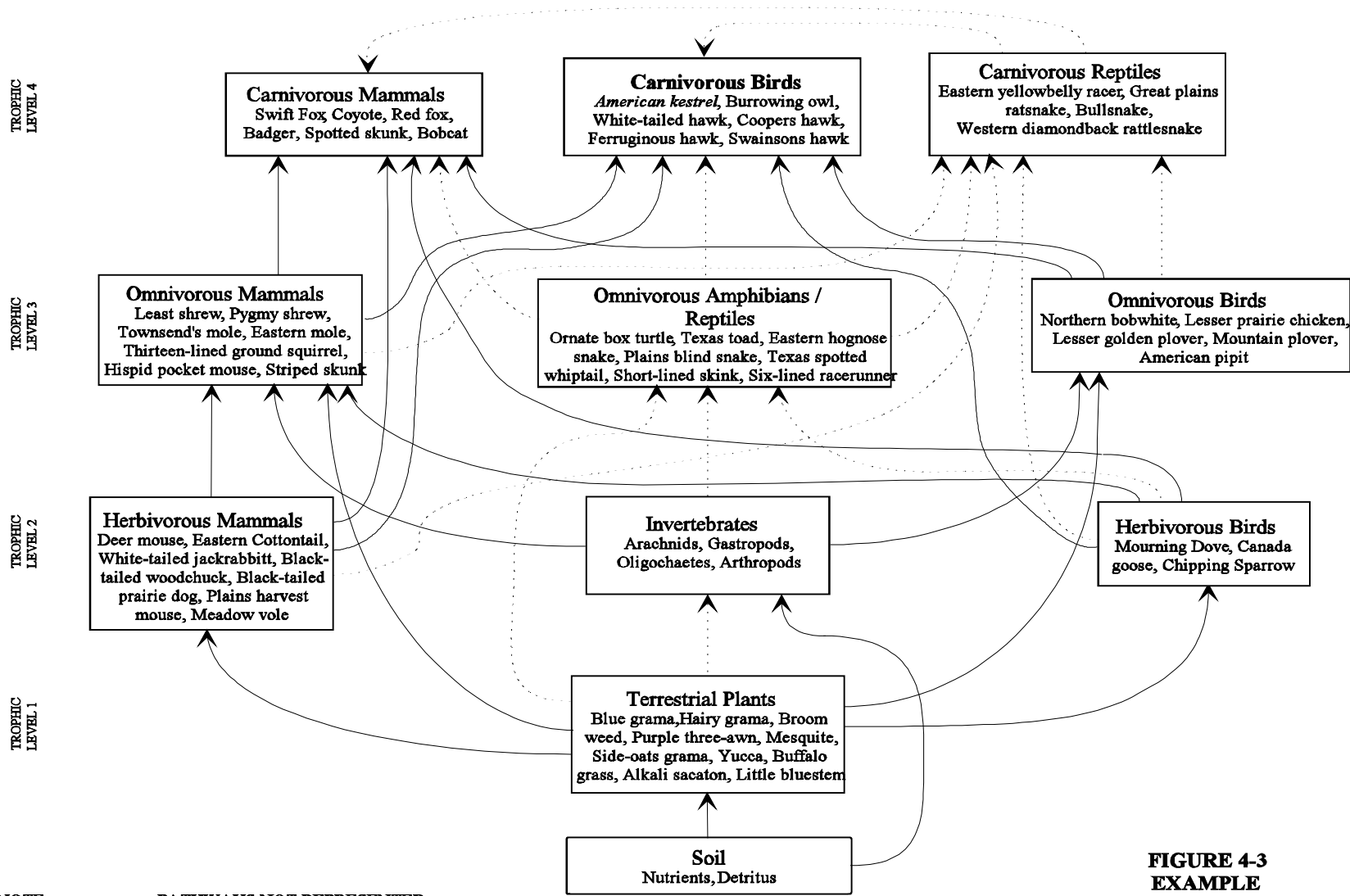
RECEPTORS LISTED IN ITALICS  
 ARE MEASUREMENT RECEPTORS



NOTE: ..... PATHWAYS NOT REPRESENTED  
 MATHEMATICALLY IN EQUATIONS

RECEPTORS LISTED IN ITALICS  
 ARE MEASUREMENT RECEPTORS

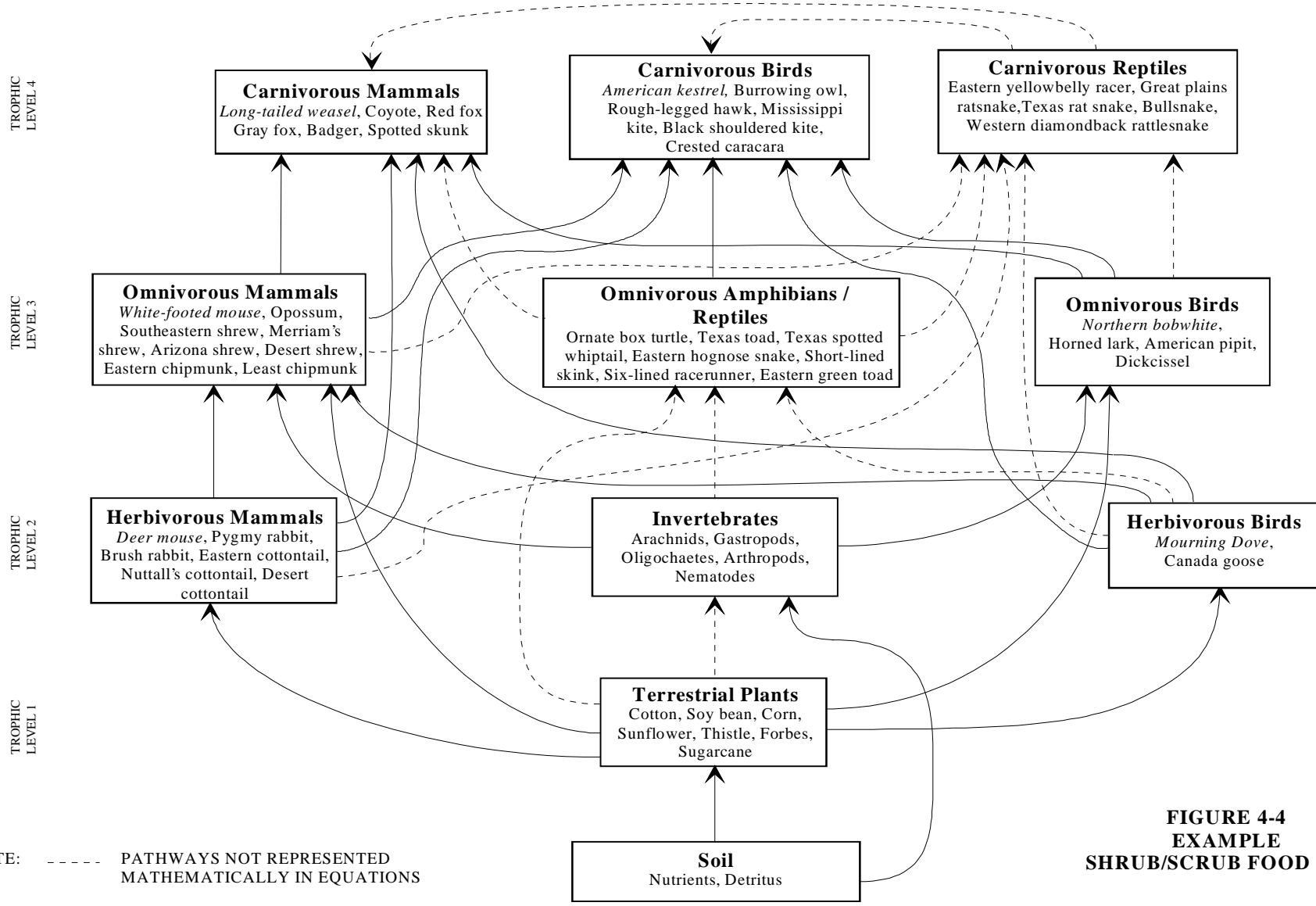
**FIGURE 4-2  
 EXAMPLE  
 TALLGRASS PRAIRIE FOOD WEB**



**FIGURE 4-3  
 EXAMPLE  
 SHORTGRASS PRAIRIE FOOD WEB**

NOTE: ..... PATHWAYS NOT REPRESENTED  
 MATHEMATICALLY IN EQUATIONS

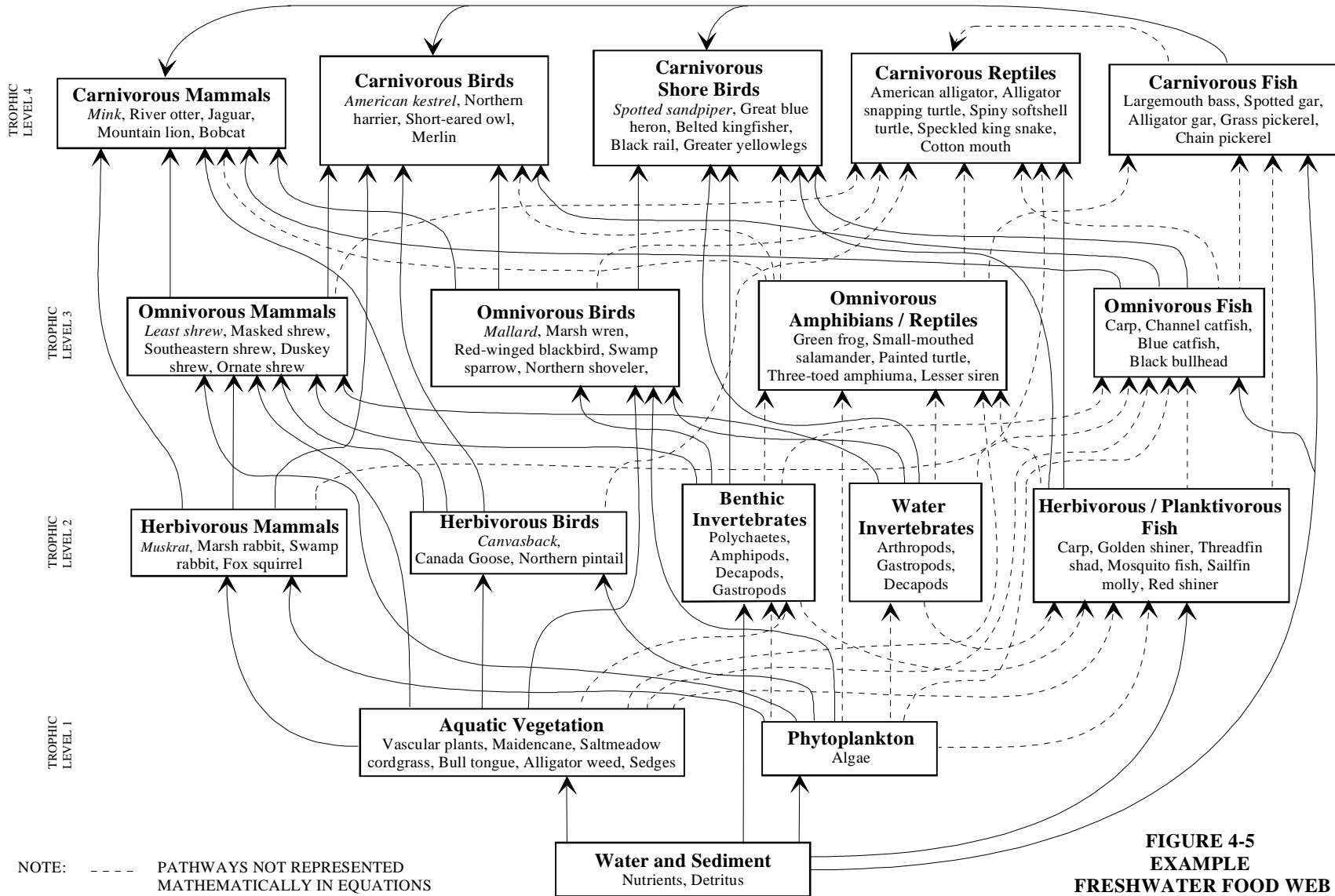
RECEPTORS LISTED IN ITALICS  
 ARE MEASUREMENT RECEPTORS



**FIGURE 4-4**  
**EXAMPLE**  
**SHRUB/SCRUB FOOD WEB**

NOTE: - - - - PATHWAYS NOT REPRESENTED  
 MATHEMATICALLY IN EQUATIONS

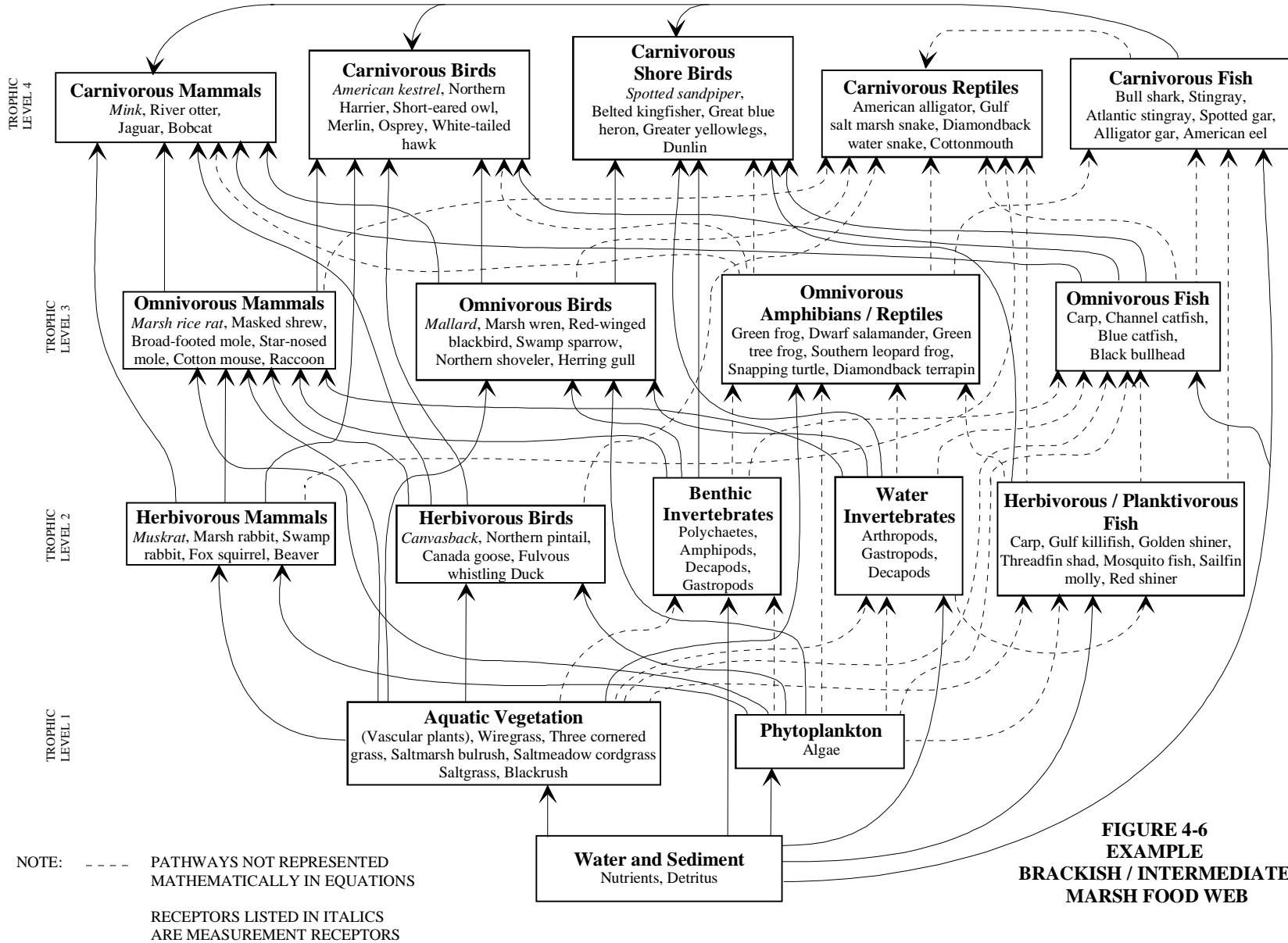
RECEPTORS LISTED IN ITALICS  
 ARE MEASUREMENT RECEPTORS



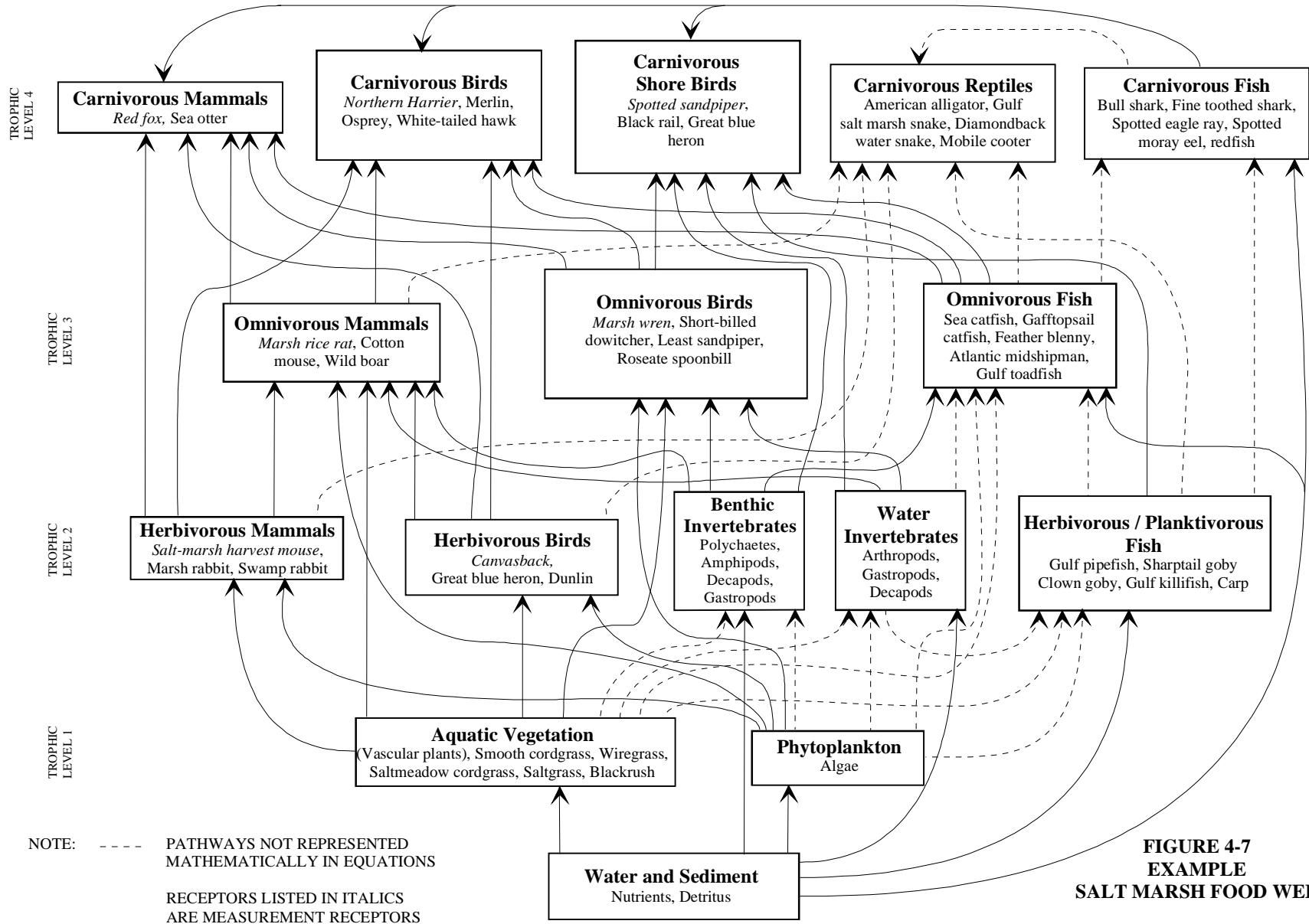
**FIGURE 4-5  
 EXAMPLE  
 FRESHWATER FOOD WEB**

NOTE: - - - PATHWAYS NOT REPRESENTED  
 MATHEMATICALLY IN EQUATIONS

RECEPTORS LISTED IN ITALICS  
 ARE MEASUREMENT RECEPTORS



**FIGURE 4-6  
 EXAMPLE  
 BRACKISH / INTERMEDIATE  
 MARSH FOOD WEB**



**FIGURE 4-7  
 EXAMPLE  
 SALT MARSH FOOD WEB**



### 4.3 SELECTING ASSESSMENT ENDPOINTS

An assessment endpoint is an expression of an ecological attribute that is to be protected (U.S. EPA 1997c). A critical ecological attribute of a guild or community is a characteristic that is relevant to ecosystem (food web) structure and function. Protection of the critical ecological attributes of each guild and community is assumed to also ensure the protectiveness of habitat-specific food web structure and function. Therefore, assessment endpoints should be identified specific to each class-specific guild and community within each trophic level of the habitat-specific food web.

Examples of assessment endpoints for guilds include:

- Seed disperser
- Major food source for predator
- Decomposer/detritivore
- Pollinator
- Regulate populations of prey (e.g., forage fish, small rodents)

Examples of assessment endpoints for communities include:

- Diversity or species richness
- Community composition
- Productivity
- Major food source for consumer
- Habitat for wildlife

Descriptions of ecological attributes to be protected (i.e., assessment endpoints) associated with several guilds and communities in a terrestrial ecosystem are provided as examples below.

- Herbaceous plant abundance, habitat, and productivity are attributes to be preserved in a terrestrial ecosystem. As food, herbaceous plants provide an important pathway for energy and nutrient transfer from soil to herbivorous (e.g., rabbit) and omnivorous (e.g., mouse) receptors. Herbaceous plants also provide critically important habitat for small animals.

- Woody plant habitat and productivity are critical attributes to be protected. As food, woody plants provide an important pathway for energy and nutrient transfer from soil to herbivorous and omnivorous vertebrates (e.g., white-tailed deer, yellow-bellied sapsucker). Woody plants also provide critically important habitat for terrestrial wildlife.
- Herbivore productivity is an attribute to be protected in the terrestrial ecosystem because herbivores incorporate energy and nutrients from plants and transfer it to higher trophic levels, such as first- and second-order carnivores (e.g., snakes and owls, respectively). Herbivores also are integral to the success of terrestrial plants, through such attributes as seed dispersal.
- Omnivore productivity is an attribute to be protected in the terrestrial ecosystem because omnivores incorporate energy and nutrients from lower trophic levels and transfer it to higher levels, such as first- and second-order carnivores.
- First-order carnivore productivity is an attribute to be protected in the terrestrial ecosystem because these carnivores provide food to other carnivores (both first- and second-order), omnivores, scavengers, and microbial decomposers. They also affect the abundance, reproduction, and recruitment of lower trophic level receptors, such as vertebrate herbivores and omnivores, through predation.
- Second-order carnivore productivity is an attribute to be protected in the terrestrial ecosystem because carnivores affect the abundance, reproduction, and recruitment of species in lower trophic levels in the food web.
- Soil invertebrate productivity and function as a decomposer are attributes to be preserved in a terrestrial ecosystem, because they provide a mechanism for the physical breakdown of detritus for microbial decomposition, which is a vital function. Soil invertebrates also function as a major food source for omnivorous birds.

Selection of assessment endpoints represents a scientific and management decision point. Since risk characterization, and subsequently final risk management decisions, are dependent on the selection of assessment endpoints, they should be developed with input from risk managers and other stakeholders.

Table 4-1 lists the assessment endpoints for guilds and communities in the three aquatic and four terrestrial example habitat-specific food webs.

**TABLE 4-1**  
**ASSESSMENT ENDPOINTS FOR GUILDS AND COMMUNITIES IN EXAMPLE FOOD WEBS**

Representative Receptors		Example Critical Ecological Attributes
<b>Aquatic Receptors</b>		
Aquatic Plants	Phytoplankton, Vascular plants	Primary producers convert light energy into biomass, and are the first link in aquatic food chains supporting higher trophic level aquatic consumers and wildlife. Rooted vegetation also provides habitat and bottom stability.
Water Invertebrates	Crustaceans, Rotifers, Amphipods	Aquatic invertebrates are an important food source for many higher trophic level consumers. Zooplankton regulate phytoplankton populations, and are a critical link in energy transfer to higher trophic levels in aquatic ecosystems.
Herbivorous / Planktivorous Fish	Carp, Gulf killifish, Threadfin shad, Molly, Golden Shiner, Goby, Mosquito Fish, Red Shiner	Herbivorous/Planktivorous Fish are an important prey species for higher trophic level predators in the aquatic and terrestrial ecosystems, and provide a critical link for energy transfer from primary producers to higher trophic level consumers. They generally comprise the majority of tissue biomass in aquatic ecosystems, and provide an important role to the ecosystem through regulating algae and plankton biomass.
Omnivorous Fish	Carp, Channel catfish, Gafftopsail fish, Atlantic midshipman, Feather blenny, Gulf toad fish, Bluecat, Bullhead	Omnivorous fish are an important prey item for higher trophic level predators. Through predation, they may also regulate population levels in lower trophic level fish and invertebrates.
Carnivorous Fish	Largemouth bass, Spotted gar, Bull shark, Redfish, Grass pickerel, Alligator gar, Chain pickerel, American eel, Atlantic stingray, Spotted moray eel, Fine toothed shark	Carnivorous fish provide an important function for the aquatic environment by regulating lower trophic populations through predation. They are also an important prey item for many top level mammal and bird carnivores.
<b>Sediment Receptors</b>		
Sediment Invertebrates	Oligochaetes, Pelecypods, Amphipods, Decapods, Polychaetes, Gastropods	Sediment invertebrates are an important food source for many higher trophic level predators. They also provide an important role as decomposers/detritivores in nutrient cycling.
<b>Soil Receptors</b>		
Terrestrial Plants	Vascular plants, Grasses, Forbs, Lichens	Primary producers provide a critical food source and are the first link in the terrestrial food chain for higher trophic level consumers. In addition, vegetation provides critical habitat for wildlife.

**TABLE 4-1 (Continued)**  
**ASSESSMENT ENDPOINTS FOR GUILDS AND COMMUNITIES IN EXAMPLE FOOD WEBS**

Representative Receptors		Example Critical Ecological Attributes
Soil Invertebrates	Nematodes, Gastropods, Oligochaetes, Arthropods	Soil invertebrates provide an important food source for many higher trophic level species. As decomposers/detritivores they play a critical role in nutrient cycling. They also aid in soil aeration and infiltration by increasing macro, and micro porosity.
<b>Upper Trophic Level Avian and Mammalian Wildlife</b>		
Herbivorous Mammals	Deer mouse, Nutria, Eastern cottontail, Prairie vole, Fox squirrel, Grey squirrel, Swamp rabbit, Eastern wood rat, White-tailed deer, Fulvous harvest mouse, Black-tailed jackrabbit, Hispid cotton rat, Hispid pocket mouse, Black-tailed prairie dog,	Herbivorous mammals are an important prey item for many higher trophic level predators. They provide an important link for energy transfer between primary producers and higher trophic level consumers. In addition, these organisms generally comprise the majority of the terrestrial tissue biomass, and are important in seed dispersal and pollination for many plant species.
Herbivorous Birds	Mourning dove, Canada goose, Chipping sparrow, Northern pintail	Herbivorous birds are an important prey item for many higher trophic level predators. They are important in seed dispersal for many plants in both terrestrial and aquatic ecosystems. Aquatic herbivorous birds may also play an important role in egg dispersion for fish and invertebrate species.
Omnivorous Mammals	Least shrew, Raccoon, Muskrat, Marsh rice rat, Wild boar, Cotton mouse, Eastern spotted skunk, Coyote, Nine-banded armadillo, Virginia opossum, Elliot's short-tailed shrew, Striped skunk, Golden mouse, Seminole bat.	Omnivorous mammals are an important prey item for higher trophic level predators, and influence lower trophic level populations through predation. They play an important role in seed dispersal for many types of terrestrial vegetation and aquatic plants.
Omnivorous Birds	American robin, Northern bobwhite, Marsh wren, Carolina wren, Swamp sparrow, Yellow warbler, Lesser prairie chicken, Roadrunner, Mallard, Least sandpiper, Red cockaded wood pecker, Roseate spoonbill, Greater prairie chicken, Scissor-tailed flycatcher, Sandhill crane, Dickcissel, Canada goose, Red-winged blackbird, Hooded merganser, Northern shovler.	Omnivorous birds are an important prey item for higher trophic level predators. They play an important role in seed dispersal and pollination for many types of terrestrial vegetation and aquatic plants. In addition, aquatic species provide egg dispersal for some fish and invertebrate species.
Omnivorous Amphibians and Reptiles	Ornate box turtle, Green frog, Texas toad, Eastern hognose snake, Plains blind snake, Small-mouthed salamander, Diamondback terrapin, Short-lined skink, Six-lined racerunner, Eastern green toad, Marbled salamander, Slender glass lizard,	Omnivorous amphibians and reptiles provide an important food source for predators. They also provide seed dispersal for many plants and regulate lower trophic level populations through predation.

**TABLE 4-1 (Continued)**  
**ASSESSMENT ENDPOINTS FOR GUILDS AND COMMUNITIES IN EXAMPLE FOOD WEBS**

Representative Receptors		Example Critical Ecological Attributes
Carnivorous Mammals	Grey fox, Swift fox, River otter, Bobcat, Mountain lion, Long-tailed weasel, American badger, Red fox, American mink, Red wolf	Carnivorous mammals provide an important functional role to the environment by regulating lower trophic level prey populations.
Carnivorous Birds	Red-tailed hawk, American kestrel, Marsh hawk, Great-horned owl, Barn owl, Burrowing owl, White-tailed hawk, Ferruginous hawk, Swansons hawk, Golden eagle, Mississippi kite, Prairie hawk, Merlin	Carnivorous Birds provide an important functional role to the environment by regulating lower trophic level prey populations.
Carnivorous Shore Birds	Great blue heron, Belted kingfisher, Spotted sandpiper, Black rail, Greater yellowlegs, Dunlin,	Carnivorous Shore Birds provide an important functional role to the environment by regulating lower trophic level prey populations, and influencing species composition in terrestrial and aquatic ecosystems. They also provide egg dispersal for some fish and aquatic invertebrates.
Carnivorous Reptiles	Eastern yellowbelly racer, Eastern coral snake, Texas rat snake, Western Diamondback rattlesnake, American alligator, Bullsnake, Alligator snapping turtle, Cotton mouth, Speckled king snake, Spiny softshell turtle, Gulf salt marsh snake,	Carnivorous Reptiles provide an important functional role to the environment by regulating lower trophic level prey and are an important prey item for other upper trophic level predators.

#### 4.4 IDENTIFYING MEASUREMENT RECEPTORS TO EVALUATE MEASURES OF EFFECT

Measures of effect are measures used to evaluate “the response of the assessment endpoint when exposed to a stressor (formerly measurement endpoints)” (U.S. EPA 1997c). Measures of exposure are measures of how exposure may be occurring, including how a stressor may co-occur with the assessment endpoint (U.S. EPA 1997c). Measures of effect, in conjunction with measures of exposure, are used to make inferences about potential changes in the assessment endpoint (U.S. EPA 1997c).

Measures of effect are selected as: (1) toxicity values developed and/or adopted by federal or state agencies (e.g., ambient water quality criteria [AWQC], NOAA effects range low [ERL] values) for protection of media-specific communities, or (2) receptor-specific chronic no-observed-adverse-effects-levels (NOAELs) or their equivalent for ecologically relevant endpoints (see Chapter 5) for this screening assessment. Measures of exposure are selected as the COPC concentrations in media or dose (e.g., ingestion of contaminated media and/or tissue) to which exposure occurs, and determined as discussed in Chapter 5.

The evaluation of the measure of effect to the assessment endpoint (see Chapters 5 and 6) requires identification of a measurement receptor representative of the assessment endpoint. The measurement receptor is selected based on consideration of factors such as (1) ecological relevance, (2) exposure potential, (3) sensitivity, (4) social or economic importance, and (5) availability of natural history information.

A measurement receptor, specific to each guild, may be selected as a species, population, community, or assemblage of communities. For communities (i.e., soil, surface water, sediment), the community or assemblage of communities is selected as the measurement receptor, and no specific species is selected. For guilds, individual species are selected as measurement receptors. Sections 4.4.1 and 4.4.2 discuss measurement receptors for communities and for mammals and birds, respectively. Section 4.4.3 discusses selection of measurement receptors for the example food webs (see Section 4.2).

#### 4.4.1 Measurement Receptors for Communities

For communities (i.e., soil, surface water, sediment), the community or assemblage of communities are selected as the measurement receptors, and no specific species are selected. Therefore, it is inferred that critical ecological attributes of these communities are not adversely affected if a COPC concentration in that respective media does not exceed the toxicity benchmark specific for that community (see Section 5.1). Representative measurement receptors for soil, surface water, sediment communities include:

- Soil—Soil invertebrate community and terrestrial plant community
- Surface Water—Phytoplankton community, water invertebrate community
- Sediment—Benthic invertebrate community

#### 4.4.2 Measurement Receptor for Guilds

A measurement receptor should be selected for each class-specific guild to model (1) COPC dose ingested, and (2) whole body COPC concentration in prey eaten by predators. The selected measurement receptor should be representative of other species in the guild, with respect to the guild's feeding niche in the ecosystem. The risk assessment should demonstrate that using the measurement receptor ensures that risk to other species in the guild is not underestimated. The following factors should be evaluated to identify a measurement receptor:

- **Ecological Relevance** - Highly relevant receptors provide an important functional or structural aspect in the ecosystem. Attributes of highly relevant receptors typically fall under the categories of food, habitat, production, seed dispersal, pollination, and decomposition. Critical attributes include those that affect or determine the function or survival of a population. For example, a sustainable population of forage fish might be critical to the sustainability of a population of carnivorous game fish.
- **Exposure Potential** - Receptors with high exposure potentials are those that, due to their metabolism, feeding habits, location, or reproductive strategy, tend to have higher potentials for exposure than other receptors. For example, the metabolic rates of small receptors are generally higher than those for large animals. This results in a higher ingestion per body weight (i.e., increased exposure potential).
- **Sensitivity** - Highly susceptible receptors include those with low tolerances to a COPC as well as receptors with enhanced COPC susceptibility due to other concomitant stressors that may not be related to a COPC, such as reduced habitat availability. For example,

raptorial birds are highly sensitive to the effects of chlorinated pesticides that bioaccumulate through the food chain.

- ***Social or Economic Importance*** - An assessment endpoint may also be based on socially or economically important receptors. These types of receptors include species valued for economic importance such as crayfish and game fish. For these receptors, critical attributes include those that affect survival, production, and fecundity characteristics. For example, swamp crayfish are highly sensitive to some heavy metals through adverse effects to behavioral characteristics.
- ***Availability of Natural History Information*** - Natural history information is essential to quantitatively evaluate risk to measurement receptors. If this information such as body weight, food, water, soil, and sediment ingestion rates is unavailable for the desired measurement receptor, a surrogate species should be selected. Uncertainty associated with using a surrogate species should be discussed.

It should be noted that more than one measurement receptor can be selected per assessment endpoint.

Also, although each of these factors should be evaluated when selecting the measurement receptor, at least one of the measurement receptors selected to represent a class-specific guild should have the highest exposure potential (i.e., ingestion rate on a body weight basis). This ensures that risk to other species in the guild is not underestimated.

U.S. EPA's *Wildlife Exposure Factors Handbook* (U.S. EPA 1993o) is an example of an excellent source of dietary and other natural history information. However, it is recommended that receptor information obtained from it or any source be verified and documented during measurement receptor identification.

#### 4.4.3 Measurement Receptors for Example Food Webs

Consistent with the discussions presented in Section 4.4, measurement receptors were selected for the example food webs presented in Section 4.2. Receptor information documented in *Wildlife Exposure Factors Handbook* (U.S. EPA 1993o) and available literature was evaluated to determine suitable measurement receptors for each class-specific guild represented in the example food webs.

Ecological relevance, exposure potential, sensitivity, social or economic importance and availability of natural history information (see Section 4.4.3) were evaluated to identify measurement receptors for the example food webs. It should be noted that since these measurement receptors have been provided as examples to facilitate understanding of the previously described selection process, not every assessment



endpoint has been represented (e.g., TL3 omnivorous fish, TL3 omnivorous amphibians and reptiles, and TL4 carnivorous fish) as may be expected for a complete ecological risk assessment at a site. Discussions on each of the example measurement receptors follow.

### **American Kestrel**

The American kestrel (*Falco sparverius*), or sparrow hawk, was selected as the measurement receptor for the carnivorous bird guild in the example shortgrass prairie, tallgrass prairie, shrub/scrub, freshwater wetland, and brackish/intermediate marsh food webs based on the following information:

- The kestrel is important in regulating small mammal populations through predation. Predators of the kestrel include larger raptors such as red-tailed hawks, golden eagles, and great horned owls.
- The kestrel's prey include a variety of invertebrates such as worms, spiders, scorpions, beetles, and other large insects, as well as an assortment of small to medium-sized birds and mammals. Winter home ranges vary from a few hectares to hundreds of hectares, depending on the amount of available prey in the area.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### **American Robin**

The American robin (*Turdus migratorius*) was selected as the measurement receptor for the omnivorous bird guild in the example forest food web based on the following information:

- The robin serves an important function in seed dispersion for many fruit species, making it a valuable component of the ecosystem.
- Habitats include forests, wetlands, swamps, and habitat edge where forested areas are broken with agricultural and range land. The robin forages on snails and other soil invertebrates, seeds, and fruit.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

## Canvasback

The Canvasback (*Aythya valisineria*) was selected as the measurement receptor for the herbivorous bird guild in all three example aquatic food webs based on the following information:

- The Canvasback provides a valuable functional role to aquatic habitats by dispersing seeds for aquatic vegetation.
- The Canvasback is the largest member of the Pochards (bay ducks) and is common throughout North America. They breed from Alaska to Nebraska, and in intermountain marshes of Washington, Oregon, and northern California. Their diet consists of aquatic vegetation, and small invertebrates, which they obtain by digging in sediments. Although the canvasback consumes aquatic invertebrates during certain times of the year, in winter when they are present along coastal regions, a large portion of their diet is aquatic vegetation and was therefore selected to represent the herbivorous bird guild.
- Since natural history information on the canvasback was scarce, the Lesser Scaup (*Aythya affinis*), for which natural history information is readily available, was selected as a surrogate receptor.

## Deer Mouse

The deer mouse (*Peromyscus maniculatus*) was selected as the measurement receptor for the herbivorous mammal guild in the example forest, shortgrass prairie, tallgrass prairie, shrub/scrub food webs based on the following information:

- The deer mouse is preyed upon by owls, snakes, and small carnivorous mammals, making it a very important prey item. This animal also plays an important ecological role in seed and fruit dispersion for many types of vegetation. In addition, their burrowing activities influence soil composition and aeration.
- The deer mouse is almost strictly nocturnal and feeds chiefly on seeds, fruits, bark, roots, and herbage. Due to its burrowing and dietary habits, there is a high potential for direct and indirect exposure. The home range for a deer mouse is rarely over 100 meters, and it spends most of its day in an underground burrow.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Least Shrew

The least shrew (*Cryptotis parva*) was selected as the measurement receptor for the omnivorous mammal guild in the example tallgrass prairie, shortgrass prairie, and freshwater wetland food webs based on the following information:

- Because of the shrews abundance and high population density, they make up a large portion of the diet of owls, hawks, and snakes.
- Shrews feed on snails, insects, sow bugs, and other small invertebrates. The home range size is on average 0.39 hectares. Their diet of invertebrates and their burrowing behavior result in a high potential of direct and indirect exposure to contaminants.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Long-tailed Weasel

The long-tailed weasel (*Mistily Renata*) was selected as the measurement receptor for the carnivorous mammal guild in the example forest, tallgrass prairie and shrub/scrub food webs based on the following information:

- The long-tailed weasel is important in regulating small mammal populations through predation. Predators of the weasel include cats, foxes, snakes, and large raptors such as hawks and owls.
- Habitats are varied and include forested, brushy, open areas including farm lands preferably near water, where they prey on rabbits, chipmunks, shrews, mice, rats and birds.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Mallard Duck

The mallard duck (*Anas platyrhynchos*) was chosen as the measurement receptor for the omnivorous bird guild for the freshwater wetland and brackish/intermediate marsh food webs based on the following information:

- The mallard serves as a valuable component in aquatic food webs providing dispersion of seeds for aquatic vegetation, and due to their role in the nutrient cycle of wetlands. In addition, the mallard is a major prey item for carnivorous mammals, birds, and snakes.
- The mallard is present in a diverse amount of aquatic habitats throughout the United States. Although their diet is considered omnivorous, 90 percent of their diet may be plant material at some times of the year. Mallards are surface feeders that will often filter through soft mud and sediment searching for food items.
- The mallard is very important game species, representing approximately one-third of all waterfowl harvested.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Marsh Rice Rat

The marsh rice rat (*Oryzomys palustris*) was selected as the measurement receptor for the omnivorous mammal guild in the example brackish/intermediate and salt marsh food web based on the following information:

- The marsh rice rat inhabits marsh and wetland areas where it feeds on crabs, insects, fruits, snails, and aquatic plants. The rice rat plays an important role in seed dispersal and is a major food item for many predators including raptors, cats, weasels and snakes.
- The marsh rice rat has a high potential for exposure due to their aquatic diet and direct contact with media.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Marsh Wren

The marsh wren (*Cistothorus palustris*) was selected as the measurement receptor for the omnivorous bird guild in the example salt marsh food web based on the following information:

- The marsh wren consumes large numbers of aquatic insects thus regulating their populations, which make it a valuable component of the ecosystem. Main predators are snakes and turtles which prey heavily upon the eggs.
- The marsh wren is common throughout the United States, inhabiting freshwater, brackish, and saltwater marshes. Its diet consists mainly of aquatic invertebrates, although snails

and spiders may be taken. In addition, its diet of aquatic invertebrates makes it susceptible to accumulation and toxicity of bioaccumulative chemicals

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Mink

The mink (*Mustela vison*) was selected as the measurement receptor for the carnivorous mammal guild in the example brackish/intermediate marsh and freshwater food webs based on the following information:

- As a high trophic level predator, the mink provides an important component to the ecosystem by influencing the population dynamics of their prey. Their main predators include fox, bobcats, and great-horned owls.
- The mink is one of the most abundant carnivorous mammals in North America, inhabiting rivers, creeks, lakes, and marshes. They are distributed throughout North America, except in extreme north Canada, Mexico, and areas of the southwestern United States. Mink are predominantly nocturnal hunters, although they are sometimes active during the day. They are opportunistic feeders and will consume whatever prey is most abundant including: small mammals, fish, birds, reptiles, amphibians, crustaceans, and insects.
- They have been shown to be sensitive to PCBs and similar chemicals, and have a high potential for exposure due to their aquatic diet and direct contact with the media.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Mourning Dove

The Mourning Dove (*Zenaida macroura*) was selected as the measurement receptor for the herbivorous bird guild in all four example terrestrial food webs based on the following information:

- The dove plays an important functional role in seed dispersion for many grasses and forbs. Doves provide an important prey item for many higher trophic level omnivores and carnivores. Predators of the mourning dove include falcons, hawks, fox, and snakes.
- The mourning dove inhabits open woodlands, forests, prairies, and croplands. It feeds mostly on seeds, which comprise 99 percent of its diet. It may ingest insignificant amounts of animal matter and green forage incidently.
- Mourning doves have a high potential for exposure through ingestion of inorganic contaminants.

- Mourning doves are an important game species, contributing significantly as a food and economic resource.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### **Muskrat**

The muskrat (*Ondrata zibethicus*) was selected as the measurement receptor for the herbivorous mammal guild in the example freshwater wetland and brackish/intermediate marsh food webs based on the following information:

- The muskrat is important to the overall structure of the aquatic ecosystem by regulating aquatic vegetation diversity and biomass, resulting in stream bank stability and increased habitat diversity for aquatic organisms including fish. It was also chosen as the measurement receptor based on its value to the ecosystem including its large population densities and importance as a prey species (e.g., prey for hawks, mink, otters, owls, red fox, snapping turtles, alligators, and water snakes).
- The muskrat spends a large part of its time in the water, and is common in fresh, brackish, and saltwater habitats. It has relatively high food and water ingestion rates, and a diet that consists mainly of aquatic vegetation, clams, crayfish, frogs, and small fish.
- Due to the large numbers, the muskrat plays an important economic role in the fur industry, and as a food item for some cultures.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### **Northern Bobwhite**

The northern bobwhite (*Colinus virginianus*) was selected as the measurement receptor for the omnivorous bird guild in the example shortgrass prairie and shrub/scrub food webs based on the following information:

- The bobwhite plays an important role in seed dispersion for many plant species, and is an important prey item for snakes, and other small mammals. If habitat conditions permit, their numbers will increase rapidly, providing an additional food source for many predators. They also are valuable in controlling insect populations during certain times of the year.
- The bobwhite's diet consists mainly of seeds and invertebrates, although in the winter green vegetation can dominate its diet. During breeding season, the bobwhite's home

range may encompass several hectares, including areas for foraging, cover, and a nest site. In non-breeding season, the bobwhite's home range can be as large as 16 hectares. It has a high potential for exposure through ingestion and dermal contact with soil during dust bathing.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Northern Harrier

The Northern harrier (*Circus cyaneus*), also called the Marsh hawk was selected as the measurement receptor for carnivorous bird guild in the example salt marsh food web based on the following information:

- The marsh hawk plays an important role in the ecosystem in regulating small mammal populations through predation.
- The marsh hawks diet consists of small mammals, birds, and occasionally snakes, frogs, and insects. Their habitat preferences include wetlands or marshes.
- In addition, the marsh hawk has demonstrated sensitivity to pesticides, which bioaccumulate through food chains.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Red Fox

The red fox (*Vulpes vulpes*) was selected as the measurement receptor for the carnivorous mammal guild in the example salt marsh food web based on the following information:

- Red fox have a high potential for exposure due to bioaccumulation through the food chain, and are a valuable component to ecosystem structure by regulating the abundance, reproduction, distribution, and recruitment of lower trophic level prey.
- Although omnivorous in dietary habits, the majority of the diet consists of cottontail rabbits, voles, mice, birds, and other small mammals. This animal was chosen because of its status as a top carnivore and its widespread distribution in the United States, inhabiting chaparral, wooded and brushy areas, coastal areas and rim rock country.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Red-tailed Hawk

The red-tailed hawk (*Buteo jamaicensis*) was selected as the measurement receptor in the carnivorous bird guild in the example forest food web based on the following information:

- The red-tailed hawks position as a high trophic level predator makes them a valuable component of terrestrial food webs through their regulation of populations of lower trophic level prey species.
- The red-tailed hawk is widely distributed in the United States among a diverse number of habitat types ranging from woodlands to pastures. Its diet includes small mammals (such as mice, shrews, voles, rabbits, and squirrels), birds, lizards, snakes, and large insects. It is an opportunistic feeder, preying on whatever species is most abundant. Red-tailed hawks are territorial throughout the year, and have home ranges that can be over 1,500 hectares.
- Red-tailed hawks have shown sensitivity to many chemicals which disrupt reproduction or egg development.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Salt Marsh Harvest Mouse

The salt marsh harvest mouse (*Reithrodontomys raviventris*) was selected as the measurement receptor for the herbivorous mammal guild in the example salt marsh food web based on the following information:

- The salt marsh harvest mouse plays an important functional role in aquatic habitats through seed dispersal for aquatic vegetation.
- Predators include owls, snakes, and many mammals including weasels, fox, and cats.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Short-tailed Shrew

The short-tailed shrew (*Blarina brevicauda*) was selected as the measurement receptor for the omnivorous mammal guild in the example forest food web based on the following information:

- The short-tailed shrews value as a prey species for many high level predators is very important to the health of an ecosystem. They also play an important role in soil recycling and aeration, through tunnel excavation.



- The short-tailed shrew is one of the most common mammals in the United States. It is a small insectivorous mammal that represents secondary consumers (insectivores) present in terrestrial ecosystems. Their diet of invertebrates such as earthworms and their burrowing behavior result in a high potential of direct and indirect exposure to contaminants. It has a very high metabolism rate which requires almost constant feeding. The most common habitats are wooded and wet areas in the drier parts of the range.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Spotted Sandpiper

The spotted sandpiper (*Actitis macularia*) was selected as the measurement receptor for the carnivorous shore bird guild in the example freshwater wetland, brackish/intermediate, and salt marsh food webs based on the following information:

- The spotted sandpiper inhabits a wide variety of habits usually associated with water or marsh.
- Spotted sandpipers have a high potential for exposure through ingestion of aquatic insects, worms, fish, crustaceans, mollusks, and carrion.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Swift Fox

The Swift Fox (*Vulpes velox*) was selected as the measurement receptor for the carnivorous mammal guild in the example shortgrass prairie food web based on the following information:

- The swift fox fills an important functional role by regulating the population dynamics of many prey species.
- The swift fox is mainly nocturnal and its diet consists of small mammals, insects, birds, lizards, and amphibians. It spends most of its days in a den, emerging at night to hunt. Their home range extends several kilometers.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### Western Meadow Lark

The western meadow lark (*Sturnella neglecta*) was selected as the measurement receptor for the omnivorous bird guild in the example tallgrass prairie food web based on the following information:

- The western meadow lark serves an important function in seed dispersion for many forb and grass species, making it a valuable component of the ecosystem.
- Habitats include grassland, savanna, pasture, and cultivated fields. The western meadow lark forages on spiders, sowbugs, snails, and grass and forb seeds.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

### White-footed Mouse

The white-footed mouse (*Peromyscus polionotus*) was selected as the measurement receptor for the omnivorous mammal guild in the example shrub/scrub food web based on the following information:

- The white-footed mouse plays an important role in seed dispersal and provide an important food source for raptors, snakes and other mammals including cats, weasels and fox.
- The white-footed mouse feeds on nuts, seeds, fruits, beetles, caterpillars, and other insects. Due to its burrowing and dietary habits, there is a high potential for direct and indirect exposure.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

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# Chapter 5

## Analysis

### What's Covered in Chapter 5:

- ◆ Exposure Assessment
  - ◆ Toxicity Assessment
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The analysis phase of a risk assessment consists of assessing (1) exposure of a measurement receptor to a compound of potential concern (COPC), and (2) toxicity of a COPC to a measurement receptor. The exposure assessment (Section 5.1), and the toxicity assessment (Section 5.4) are used to characterize ecological risk, as discussed in Chapter 6.

### 5.1 EXPOSURE ASSESSMENT

Exposure is the contact (e.g., ingestion) of a receptor with a COPC. Exposure of ecological receptors to COPCs emitted from facility sources are evaluated through consideration of exposure pathways. All exposure pathways that are potentially complete should be evaluated. The existence of a potentially complete exposure pathway indicates the potential for a receptor to contact a COPC; it does not require that a receptor be adversely affected. Exposure pathways considered in this guidance include all direct uptake pathways of a COPC from media (e.g., soil, sediment, and surface water) for lower trophic level receptors evaluated at the community level, and ingestion of a COPC contaminated organism (plant or animal food item) or media for higher trophic level receptors evaluated as class-specific guilds. It should be noted that exposure pathways currently not addressed in this guidance due to the limitation of data include (1) inhalation and dermal exposure pathways for upper trophic level organisms, (2) ingestion via grooming and preening, and (3) foliar uptake of dissolved COPCs by aquatic plants.

Exposure assessment consists of quantifying exposure of a measurement receptor to a COPC. As previously noted (see Chapter 4), exposure to community and class-specific guild measurement receptors is assessed using different approaches. This is because the available toxicity reference values (*TRVs*) used in

risk characterization (see Chapter 6) for lower trophic level communities are media specific; whereas *TRVs* for upper trophic level class-specific guilds are provided in terms of dose ingested.

For community measurement receptors (e.g., water, sediment, and soil communities), the exposure assessment consists of determining the COPC concentration in the media that the particular community inhabits. For example, the COPC concentration in soil is determined during the exposure assessment for comparison to the NOAEL for terrestrial plants and soil invertebrates during risk characterization. For class-specific guild measurement receptors, exposure is assessed by quantifying the daily dose ingested of contaminated media and/or organism (expressed as the mass of COPC ingested per kilogram body weight per day). The following sections provide guidance on assessing exposure to community and class-specific guild measurement receptors.

## 5.2 Assessing Exposure to Community Measurement Receptors

Since exposure to communities is assumed to be primarily through contact with COPCs within the media they inhabit, the assessment of exposure for community measurement receptors is simply the determination of the COPC concentration in the media that they inhabit. Exposure for water, sediment, and soil community measurement receptors should be determined as follows:

***Water Community*** - Exposure to the water community as a measurement receptor (e.g., water invertebrates or phytoplankton in the freshwater/wetland food web) is assessed by determining the COPC dissolved water concentration (*C<sub>dw</sub>*) (see Chapter 3 and Appendix B) at the specific location being evaluated (see Chapter 4).

***Sediment Community*** - Exposure to the sediment community as a measurement receptor (e.g., sediment invertebrates in the brackish/intermediate food web) is assessed by determining the COPC concentration in bed sediment (*C<sub>sed</sub>*) (see Chapter 3 and Appendix B) at the specific location being evaluated (see Chapter 4).

***Soil Community*** - Exposure to the soil community as a measurement receptor (e.g., soil invertebrates or terrestrial plants in the forest food web) is assessed by determining the COPC concentration in soil (*C<sub>s</sub>*) (see Chapter 3 and Appendix B) at the specific location being evaluated (see Chapter 4).

### 5.3 Assessing Exposure to Class-Specific Guild Measurement Receptors

Exposure to measurement receptors of class-specific guilds is assessed by quantifying the daily dose ingested of contaminated food items (i.e., plant and animal), and media. COPC daily dose ingested (expressed as the mass of COPC ingested per kilogram body weight per day) depends on the COPC concentration in plant and animal food items and media, the measurement receptor's trophic level (i.e., consumer), the trophic level of animal food items (i.e., prey), and the measurement receptor's ingestion rate of each food item and media. The complexity of the daily dose equation will depend on (1) the number of food items in a measurement receptor's diet, (2) the trophic level of each food item and of the measurement receptor. The daily dose of COPC ingested by a measurement receptor, considering all food items and media ingested, can be calculated from the following generic equation:

$$DD = \sum IR_F \cdot C_i \cdot P_i \cdot F_i + \sum IR_M \cdot C_M \cdot P_M \quad \text{Equation 5-1}$$

where

$DD$	=	Daily dose of COPC ingested (mg COPC/kg BW-day)
$IR_F$	=	Measurement receptor plant or animal food item ingestion rate (kg/kg BW-day)
$C_i$	=	COPC concentration in $i$ th plant or animal food item (mg COPC/kg)
$P_i$	=	Proportion of $i$ th food item that is contaminated (unitless)
$F_i$	=	Fraction of diet consisting of plant or animal food item $i$ (unitless)
$IR_M$	=	Measurement receptor media ingestion rate (kg/kg BW-day [soil or bed sediment] or L/kg BW-day [water])
$C_M$	=	COPC concentration in media (mg/kg [soil or bed sediment] or mg/L [water])
$P_M$	=	Proportion of ingested media that is contaminated (unitless)

Sections 5.3.1 through 5.3.2 (also see Appendix F) provide guidance for determining values for the above parameters; including (1) the determination of measurement receptor food item and media ingestion rates, and (2) the calculation of COPC concentrations in plant and animal food items. The use of *BCFs* and *FCMs* in calculating COPC concentrations in plant and animal food items is also discussed in the following sections. The daily dose should be computed using COPC media (i.e., soil, sediment, surface water, air) concentrations, at the location within the habitat supporting the food web being evaluated (see Chapter 4), for determination of (1) the COPC concentration in the plant or animal food item ingested, and (2) the

COPC concentration in the media ingested. Guidance on the calculation of COPC concentrations in media being ingested is provided in Chapter 3 and Appendix B.

The daily dose of COPC ingested by a measurement receptor should be determined by summing the contributions from each contaminated plant, animal, and media food item. Equation 5-1 and consumer specific equations in Appendix F, are derived to account for 100 percent of the measurement receptor's diet (total daily mass of food items ingested) which can potentially be contaminated. However, if a food item or media at an actual site location is not contaminated (i.e., the COPC concentration in the media or resulting food item is zero), then the daily mass of that food item or media ingested does not contribute to the daily dose of COPC ingested. Also, Equation 5-1 does not directly include a term for home range, as defined spatially. However, the term accounting for the proportion of plant or animal food item that is contaminated,  $P_i$ , numerically accounts for the fraction of a respective food item that may potentially be obtained from outside the geographical limits of the impacted habitat (i.e., outside the area of contamination) being evaluated.

For measurement receptors ingesting more than one plant or animal food item, U.S. EPA OSW recommends that exposure be separately quantified assuming that the measurement receptor ingests both "equal" and "exclusive" diets. Not only does this constitute the most complete evaluation of exposure potential for a measurement receptor; if warranted, it also identifies which pathways are driving risk specific to a COPC and measurement receptor, and allows risk management efforts to be prioritized. Guidance for calculating  $DD$  assuming "equal diet" and "exclusive diet" is provided below.

**Equal Diet** - To evaluate exposure to a measurement receptor based on an equal diet, the daily dose of COPC ingested is calculated assuming that the fraction of daily diet consumed by the measurement receptor is equal among food item groups. This is computed by setting the value for fraction of diet consisting of plant and/or animal food items,  $F_i$ , equal to 1.0 divided by the total number of plant and animal food item groups ingested. Therefore,  $F_i$  values within a specific  $DD$  equation would be the same numerically.

**Exclusive Diet** - To evaluate exposure to a measurement receptor based on exclusive diets, the daily dose of COPC ingested is calculated assuming that the fraction of daily diet consumed by the measurement receptor is exclusively (100 percent) one food item group. This is computed by setting the value for  $F_i$  equal to 1.0 for each food item group at a time, while the  $F_i$  values for the remaining food item groups are set equal to zero. The food item designated as exclusive is alternated to each respective food item represented in the  $DD$  equation to obtain a numeric range of exposure values based on exclusive diets. If the daily diet of a food item (i.e., prey) of a measurement receptor (i.e., consumer) also consists of more than one plant or animal food item,

then an equal diet should be assumed for the food item being consumed while evaluating exposure to the measurement receptor.

In addition to quantifying exposure based on equal and exclusive diets for measurement receptors, U.S. EPA OSW recommends that the following assumptions be applied in a screening level risk assessment.

- The COPC concentrations estimated to be in food items and media ingested are bioavailable.
- Only contributions of COPCs from the sources (e.g., combustion stacks, fugitives) included in the risk assessment are considered in estimating COPC concentrations in food items and media.
- The measurement receptor's most sensitive life stage is present in the assessment area being evaluated in the risk assessment.
- The body weights and food ingestion rates for measurement receptors are conservative.
- Each individual species in a community or class-specific guild is equally exposed.
- The proportion of ingested food items and ingested media that is contaminated is assumed to be 100 percent (i.e.,  $P_i$  is assigned a value of 1.0); which assumes that a measurement receptor feeds only in the assessment area.

Although conservative in nature, U.S. EPA OSW recommends use of these assumptions considering that the results of a screening level risk assessment are intended to support development of permits and focus risk management efforts. Site-specific exposure characterization that may warrant deviation from these screening level assumptions should be reviewed and approved by the appropriate permitting authority following recommendations provided in Section 3.12.

### 5.3.1 Ingestion Rates for Measurement Receptors

As indicated in Equation 5-1 above, species specific ingestion rates of food items and media, on a body weight basis, are required for calculating the daily dose of COPC ingested for each measurement receptor. As specified for use in the equations presented in Appendix F, it is important to ensure that food (i.e., plants and animals) and water ingestion rates are on a wet weight basis, and ingestion rates for soil and sediment are on a dry weight basis (see Appendix F). Table 5-1 provides values for ingestion rates for measurement receptors identified in the example food webs presented in Chapter 4. These values are primarily obtained from the allometric equations presented in the *Wildlife Exposure Factors Handbook*

(U.S. EPA 1993o). Soil ingestion rates were calculated using the percent soil in estimated diets of wildlife as described in Beyer et al. (1994).

Species specific ingestion rates including food and water have been measured for few wildlife species. Therefore, allometric equations presented in the *Wildlife Exposure Factors Handbook* were used to calculate species specific food and media ingestion rates. Allometry is defined as the study of the relationship between the growth and size of one body part to the growth and size of the whole organism, including ingestion rates, and can be used to estimate species specific values for ingestion (U.S. EPA 1993o). Allometric equations should only be used for those taxonomic groups used to develop the allometric relationship. For example, equations developed for carnivorous mammals should not be used to calculate food ingestion rates for herbivorous mammals. For a detailed discussion on the development and limitations of the allometric equations used to obtain ingestion rate values presented in Table 5-1, see U.S. EPA (1993o) and Nagy (1987).

The use of individual species body weights may result in some uncertainty, since individual species usually exhibit values somewhat different from those predicted by allometric modeling derived using multiple species. However, this uncertainty is expected to be minimal since measurement receptors were selected to maximize exposure for each class-specific guild, as discussed in Section 4.4.2.

If species specific values are not available in U.S. EPA (1993o), or can not be represented by the allometric equations presented, other sources to evaluate include:

- U.S. Fish and Wildlife Service (FWS) publications (e.g., U.S. FWS 1979)
- State wildlife resource management agencies
- Published scientific literature
- Publications by wildlife conservation organizations (such as The National Audubon Society)



TABLE 5-1

INGESTION RATES FOR EXAMPLE MEASUREMENT RECEPTORS

Measurement Receptor	Example Food Web <sup>a</sup>								
		Body Weight (kg)	Reference	Food IR <sup>e</sup> (kg WW/kg BW-day)	Reference	Water IR (L/kg BW-day)	Reference	Soil/Sed IR <sup>m</sup> (kg DW/kg BW-day)	Reference
American Kestrel	SG, TG, SS, FW, BR	1.00E-01	U.S. EPA 1993o	4.02E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	1.25E-01 <sup>k</sup>	U.S. EPA 1993o	1.39E-03 <sup>n</sup>	Pascoe et al. 1996
American Robin	F	8.00E-02	U.S. EPA 1993o	4.44E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	1.37E-01 <sup>k</sup>	U.S. EPA 1993o	1.43E-02 <sup>o</sup>	Beyer et al. 1994
Canvas Back	FW, BR, SW	7.70E-01 <sup>b</sup>	U.S. EPA 1993o	1.99E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	6.43E-02 <sup>k</sup>	U.S. EPA 1993o	1.82E-03 <sup>p</sup>	Beyer et al. 1994
Deer Mouse	TG, F, SG, SS	1.48E-02	U.S. EPA 1993o	5.99E-01 <sup>g</sup>	U.S. EPA 1993o; Nagy 1987	1.51E-01 <sup>l</sup>	U.S. EPA 1993o	1.44E-03 <sup>q</sup>	Beyer et al. 1994
Least Shrew	SG, FW, TG	4.00E-03	National Audubon Society 1995	6.20E-01 <sup>h</sup>	U.S. EPA 1993o	1.72E-01 <sup>l</sup>	U.S. EPA 1993o	1.36E-02 <sup>o</sup>	Beyer et al. 1994
Long Tailed Weasel	TG ,F, SS	8.50E-02	National Audubon Society 1995	3.33E-01 <sup>i</sup>	U.S. EPA 1993o; Nagy 1987	1.27E-01 <sup>l</sup>	U.S. EPA 1993o	2.98E-03 <sup>r</sup>	Beyer et al. 1994
Mallard Duck	BR, FW	1.04E+00	U.S. EPA 1993o	1.79E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	5.82E-02 <sup>k</sup>	U.S. EPA 1993o	3.18E-03	Beyer et al. 1994
Marsh Rice Rat	BR, SW	3.00E-02	National Audubon Society 1995	4.40E-01 <sup>g</sup>	U.S. EPA 1993o; Nagy 1987	1.41E-01 <sup>l</sup>	U.S. EPA 1993o	2.33E-03 <sup>s</sup>	Beyer et al. 1994
Marsh Wren	SW	1.00E-02	U.S. EPA 1993o	9.26E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	2.75E-01 <sup>k</sup>	U.S. EPA 1993o	1.96E-02 <sup>o</sup>	Beyer et al. 1994
Mink	FW, BR	9.74E-01	U.S. EPA 1993o	2.16E-01 <sup>i</sup>	U.S. EPA 1993o; Nagy 1987	9.93E-02 <sup>l</sup>	U.S. EPA 1993o	1.93E-03 <sup>r</sup>	Beyer et al. 1994

**TABLE 5-1**  
**INGESTION RATES FOR EXAMPLE MEASUREMENT RECEPTORS**

Measurement Receptor	Example Food Web <sup>a</sup>								
		Body Weight (kg)	Reference	Food IR <sup>e</sup> (kg WW/kg BW-day)	Reference	Water IR (L/kg BW-day)	Reference	Soil/Sed IR <sup>m</sup> (kg DW/kg BW-day)	Reference
Mourning Dove	F, SS, TG, SG	1.50E-01 <sup>c</sup>	U.S. EPA 1993o	3.49E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	1.09E-01 <sup>k</sup>	U.S. EPA 1993o	7.01E-03 <sup>o</sup>	Beyer et al. 1994
Muskrat	BR, FW	1.09E+00	U.S. EPA 1993o	2.67E-01 <sup>j</sup>	U.S. EPA 1993o; Nagy 1987	9.82E-02 <sup>l</sup>	U.S. EPA 1993o	6.41E-04	Beyer et al. 1994
Northern Bobwhite	SG, SS	1.50E-01	U.S. EPA 1993o	3.49E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	1.09E-01 <sup>k</sup>	U.S. EPA 1993o	1.20E-02 <sup>l</sup>	Beyer et al. 1994
Northern Harrier	SW	9.60E-01	U.S. EPA 1993o	1.85E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	5.99E-02 <sup>k</sup>	U.S. EPA 1993o	9.95E-03 <sup>n</sup>	Beyer et al. 1994
Red Fox	SW	3.94E+00	U.S. EPA 1993o	1.68E-01 <sup>i</sup>	U.S. EPA 1993o; Nagy 1987	8.63E-02 <sup>l</sup>	U.S. EPA 1993o	1.51E-03	Beyer et al. 1994
Red-tailed Hawk	F	9.60E-01 <sup>d</sup>	U.S. EPA 1993o	1.85E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	5.99E-02 <sup>k</sup>	U.S. EPA 1993o	9.95E-03 <sup>n</sup>	Beyer et al. 1994
Salt-marsh Harvest Mouse	SW	9.10E-03	U.S. EPA 1993o	7.41E-01 <sup>g</sup>	U.S. EPA 1993o; Nagy 1987	1.58E-01 <sup>l</sup>	U.S. EPA 1993o	1.78E-03 <sup>q</sup>	Beyer et al. 1994
Short-tailed Shrew	F	1.50E-02	U.S. EPA 1993o	6.20E-01 <sup>h</sup>	U.S. EPA 1993o	1.51E-01 <sup>l</sup>	U.S. EPA 1993o	1.36E-02 <sup>o</sup>	Beyer et al. 1994
Spotted Sandpiper	SW, BR, FW	4.00E-02	U.S. EPA 1993o	5.69E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	1.74E-01 <sup>k</sup>	U.S. EPA 1993o	4.15E-02 <sup>u</sup>	Beyer et al. 1994
Swift Fox	SG	1.40E+00	U.S. EPA 1993o	1.93E-01 <sup>i</sup>	U.S. EPA 1993o; Nagy 1987	9.34E-02 <sup>l</sup>	U.S. EPA 1993o	1.73E-03 <sup>r</sup>	Beyer et al. 1994
Western Meadow Lark	TG	9.00E-02	U.S. EPA 1993o	4.21E-01 <sup>f</sup>	U.S. EPA 1993o; Nagy 1987	1.31E-01 <sup>k</sup>	U.S. EPA 1993o	1.39E-02 <sup>o</sup>	Beyer et al. 1994

**TABLE 5-1**  
**INGESTION RATES FOR EXAMPLE MEASUREMENT RECEPTORS**

Measurement Receptor	Example Food Web <sup>a</sup>								
		Body Weight (kg)	Reference	Food IR <sup>e</sup> (kg WW/kg BW-day)	Reference	Water IR (L/kg BW-day)	Reference	Soil/Sed IR <sup>m</sup> (kg DW/kg BW-day)	Reference
White-footed Mouse	SS	1.00E-02	U.S. EPA 1993o	6.14E-01 <sup>g</sup>	U.S. EPA 1993o; Nagy 1987	1.52E-01 <sup>l</sup>	U.S. EPA 1993o	2.70E-03	Beyer et al. 1994

Notes: IR- Ingestion Rate; WW- Wet weight; DW-Dry Weight; BW- Body Weight; kg - kilogram; L - Liter

- a = Food Webs: BR - Brackish/Intermediate Marsh; F - Forest; FW - Freshwater/Wetland; SG - Shortgrass Prairie; SS - Shrub/Scrub; SW - Saltwater Marsh; TG - Tallgrass Prairie.
- b = The body weight reported for the mallard is used as a surrogate value for the canvas back.
- c = The body weight reported for the northern bobwhite is used as a surrogate value for the morning dove.
- d = The body weight reported for the red-tailed hawk is used as a surrogate value for the northern harrier.
- e = Food ingestion rate (IR) values are reported in Table 5-1 as kg WW/kg BW-day. To convert IR from a dry weight (as calculated using allometric equations) to a wet weight basis, the following general equation is used:  
  

$$\text{IR kg WW/kg BW-day} = (\text{IR kg DW/BW-day}) / (1 - \% \text{ moisture}/100)$$
- f = Ingestion rate values provided in Table 5-1 are calculated based on assumed percent moisture content of food items of measurement receptors specified. For herbivores, the moisture content of ingested plant matter is assumed to be 88.0 percent (Taiz et al. 1991). For carnivores, the moisture content of ingested animal matter is assumed to be 68.0 percent (Sample et al. 1997). For omnivores, an equal fraction of plant and animal matter is assumed ingested with an overall average moisture content of 78.0 percent  $[(88.0 + 68.0)/2]$ .
- f = Food ingestion rates generated using the following allometric equation for all birds:  $\text{IR (g/day)} = 0.648 \text{ Wt}^{0.651} \text{ (g)}$ .
- g = Food ingestion rates generated using the following allometric equation for rodents:  $\text{IR (g/day)} = 0.621 \text{ Wt}^{0.564} \text{ (g)}$ .
- h = Allometric equations reported in U.S. EPA (1993o) do not represent intake rates for shrews; therefore, measured field values from the referenced sources are presented.
- i = Food ingestion rates generated using the following allometric equation for all mammals:  $\text{IR (g/day)} = 0.235 \text{ Wt}^{0.822} \text{ (g)}$ .
- j = Food ingestion rates generated using the following allometric equation for herbivores:  $\text{IR (g/day)} = 0.577 \text{ Wt}^{0.727} \text{ (g)}$ .
- k = Water ingestion rates generated using the following allometric equation for all birds:  $\text{IR (L/day)} = 0.059 \text{ Wt}^{0.670} \text{ (kg)}$ .
- l = Water ingestion rates generated using the following allometric equation for all mammals:  $\text{IR (L/day)} = 0.099 \text{ Wt}^{0.900} \text{ (kg)}$ .
- m = Soil and sediment ingestion rates calculated based on percent soil in diet as reported in Beyer et al. 1994.
- n = Percent soil in diet reported for the bald eagle is used as a surrogate value for the american kestrel, northern harrier, and red-tailed hawk.
- o = Percent soil in diet is assumed as 10.0 percent of diet based on range presented in Beyer et al. 1994.

p	=	Percent soil in diet reported for the mallard is used as a surrogate value for the canvas back.
q	=	Percent soil in diet reported for the white-footed mouse is used as a surrogate value for the deer mouse and salt-marsh harvest mouse.
r	=	Percent soil in diet reported for the red fox is used as a surrogate value for the long-tailed weasel, mink, and swift fox.
s	=	Percent soil in diet is assumed as 2.0 percent of diet based on range presented for herbivores.
t	=	Percent soil in diet reported for the wild turkey is used as a surrogate value for the northern bobwhite.
u	=	Percent soil in diet reported for the western sandpiper is used as a surrogate value for the spotted sandpiper.

### 5.3.2 COPC Concentrations in Food Items of Measurement Receptors

Determination of COPC concentrations in food items is required for calculating the daily dose of COPC ingested for each class-specific guild measurement receptor being evaluated. Since the risk assessment considers potential future exposure that may occur as a result of facility emissions over time, these concentrations are generally expected to be estimated mathematically. The following subsections provide guidance for estimating COPC concentrations in the following groups of food items:

- Invertebrates, phytoplankton, and rooted aquatic plants;
- Terrestrial plants;
- Fish; and
- Mammals, birds, reptiles, and amphibians.

#### 5.3.2.1 COPC Concentration in Invertebrates, Phytoplankton, and Rooted Aquatic Plants

COPC concentrations in invertebrate, phytoplankton, and rooted aquatic plants can be calculated by rearranging the mathematical expression for a bioconcentration factor (*BCF*). Equation 5-2 is the mathematical definition of a *BCF*, which is the ratio, at steady-state, of the concentration of a compound in a food item to its concentration in a media. Equation 5-3 is the same equation expressed in terms of a COPC concentration in a food item.

$$BCF = \frac{C_i}{C_M} \quad \text{Equation 5-2}$$

$$C_i = C_M \cdot BCF \quad \text{Equation 5-3}$$

where

$BCF$	=	Bioconcentration factor (unitless [soil, sediment], or L/kg [water])
$C_i$	=	COPC concentration in <i>i</i> th plant or animal food item (mg COPC/kg)
$C_M$	=	COPC concentration in media (mg/kg [soil, sediment], or mg/L [water])

Equation 5-3 estimates a COPC concentration in an invertebrate, phytoplankton, and rooted aquatic plant to evaluate dose ingested to the measurement receptor. Calculation of COPC concentrations in media is further discussed in Chapter 3 and Appendix B. Media-to-receptor *BCFs* are receptor- and media-specific, and values along with supporting discussion are provided in Appendix C. Appendix F provides specific equations and supporting discussion for calculating COPC concentrations in plant and animal food items.

### Equilibrium Partitioning (EqP) Approach

When adequate site-specific characterization data is available, specifically organic carbon fraction data for soil and sediment, the permitting authority may elect in some cases to allow the calculation of COPC concentrations in soil invertebrate (Connell and Markwell 1990) or sediment invertebrate (U.S. EPA 1993q) using the equilibrium partitioning (EqP) approach. However, the EqP approach is not preferred over use of measured BCF values multiplied by the COPC concentration in the media (i.e., sediment or soil), following the approach previously discussed.

The EqP approach utilizes the correlation of the concentrations of nonionic organic compounds in sediment, on an organic carbon basis, to their concentrations in the interstitial water, to determine the observed biological effects on sediment invertebrate (U.S. EPA 1993q). The EqP approach is only applicable for (1) hydrophobic nonionic organic compounds, (2) soil- and sediment-invertebrates, and (3) COPCs with empirical water bioconcentration factors (U.S. EPA 1993q). Also, the EqP approach assumes that the partitioning of the compound in sediment organic carbon and interstitial water are in equilibrium, and the sediment—interstitial water equilibrium system provides the same exposure as a water-only exposure (U.S. EPA 1993q).

To calculate the COPC concentration in an invertebrate using the EqP approach, the soil or sediment interstitial water concentration should be multiplied by the *BCF* determined from a water exposure for a benthic invertebrate:

$$C_I = C_{IW} \cdot BCF_{WI} \quad \text{Equation 5-4}$$

where

$C_I$	=	COPC concentration in soil or benthic invertebrate (mg/kg)
$C_{IW}$	=	COPC concentration in soil or sediment interstitial water (mg/L)
$BCF_{WI}$	=	Bioconcentration factor for water-to-invertebrate (L/kg)

Equation 5-5 is used to calculate the COPC concentration in soil or sediment interstitial water for this approach:

$$C_{IW} = \frac{C_M}{f_{oc} \cdot K_{oc}} \quad \text{Equation 5-5}$$

where

$C_{IW}$	=	COPC concentration in soil or sediment interstitial water (mg/L)
$C_M$	=	COPC concentration in media (mg/kg [soil, sediment])
$f_{oc}$	=	Fraction of organic carbon in soil or sediment (unitless)
$K_{oc}$	=	Organic carbon partitioning coefficient (L/kg)

### 5.3.2.2 COPC Concentration in Terrestrial Plants

The COPC concentration in terrestrial plants ( $C_{TP}$ ) is calculated by summing the plant concentration due to direct deposition ( $Pd$ ), air-to-plant transfer ( $Pv$ ), and root uptake ( $Pr$ ). Equation 5-6 should be used to compute a COPC concentration in terrestrial plants:

$$C_{TP} = Pd + Pv + Pr \quad \text{Equation 5-6}$$

where

$C_{TP}$	=	COPC concentration in terrestrial plants (mg COPC/kg WW)
$Pd$	=	COPC concentration in plant due to direct deposition (mg/kg WW)
$Pv$	=	COPC concentration in plant due to air-to-plant transfer (mg/kg WW)
$Pr$	=	COPC concentration in plant due to root uptake (mg/kg WW)

Calculation of  $Pd$ ,  $Pv$ , and  $Pr$  is presented in Chapter 3 and Appendix B. Calculation of  $C_{TP}$  is further discussed in Appendix F.

### 5.3.2.3 COPC Concentration in Fish

The COPC concentration in fish is calculated by multiplying a COPC-specific  $BCF$  and trophic level-specific  $FCM$  by the dissolved water concentration, as follows:

$$C_F = BCF \cdot FCM \cdot C_{dw} \quad \text{Equation 5-7}$$

where

$C_F$	=	COPC concentration in fish (mg/kg)
$BCF$	=	Bioconcentration factor for water-to-fish (L/kg)
$FCM$	=	Food-chain multiplier (unitless)
$C_{dw}$	=	Dissolved phase water concentration (mg/L)

The COPC concentration in fish is calculated using dissolved phase water concentrations, since bioconcentration, or estimated bioaccumulation, values are typically derived from studies based on dissolved phase water concentrations. The  $FCM$  used to calculate a COPC concentration in fish should be appropriate for the trophic level of the fish ingested by a measurement receptor. Development of  $FCM$  values is discussed in the following subsection, and actual recommended values are provided in Table 5-2. The dissolved phase water concentration is calculated as discussed in Chapter 3 and Appendix B. Values for bioconcentration factors for water-to-fish, and discussion on their determination, can be found in Appendix C. Calculation of  $C_F$  is further discussed in Appendix F.

### Food-Chain Multipliers

$FCMs$  presented in Table 5-2 were adopted directly from U.S. EPA (1995k), which determined them for  $K_{ow}$  values ranging from 3.5 through 9.0 using the Gobas (1993) model. U.S. EPA determined  $FCMs$  to develop water criteria protective to wildlife of the Great Lakes (U.S. EPA 1995j). As presented in Equation 5-8, U.S. EPA (1995k) calculated trophic level specific  $FCMs$  (see Table 5-2) utilizing  $BAF$  values obtained from the Gobas (1993) model and compound specific  $K_{ow}$  values.

$$FCM = \frac{BAF_l}{K_{ow}} \quad \text{Equation 5-8}$$



where

$FCM$	=	Food-chain multiplier (unitless)
$BAF_l$	=	Bioaccumulation factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
$K_{ow}$	=	Octanol-water partition coefficient (L/kg)

$BAF$  values predicted using the Gobas (1993) model were based on chemical concentrations in both the water column and surface sediment. Bioaccumulation values for fish were determined from the rate of chemical uptake, the rate of chemical depuration (including excretion), metabolism, and dilution due to growth. As reported in U.S. EPA (1995k), data on physicochemical parameters and species characteristics reported by Oliver and Niimi (1988), Flint (1986), and Gobas (1993) were used.

For each  $K_{ow}$  value, the Gobas (1993) model reported correlating  $BAF_l$  values specific to each organism in the food web. U.S. EPA (1995k) determined trophic level-specific  $FCMs$  by calculating the geometric mean of the  $FCM$  for each organism in each respective trophic level. The  $FCMs$  were developed assuming no metabolism of a compound. Thus, for compounds where metabolism may occur (i.e., some PAHs), the COPC concentration in fish ingested by a measurement receptor may be overestimated. This information should be noted as an uncertainty in risk characterization. It should also be noted that the  $FCM$  values presented in Table 5-2 were developed using  $K_{ow}$  values reported in U.S. EPA (1995k); which may differ from  $K_{ow}$  values specified in Appendix A-2 of this guidance.

Using the U.S. EPA (1995k) assumption that a compound's  $\log K_{ow}$  value approximates its  $BCF_l$ , Equation 5-8 for determining  $FCM$  values can also be expressed as follows:

$$FCM = \frac{BAF_l}{BCF_l} \quad \text{Equation 5-9}$$

where

$FCM$	=	Food-chain multiplier (unitless)
$BAF_l$	=	Bioaccumulation factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
$BCF_l$	=	Bioconcentration factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)

Equation 5-9 can also be written to demonstrate the relation of a *BCF* multiplied by a *FCM* to estimate a *BAF*, as shown in the following equation:

$$BAF = BCF \cdot FCM \quad \text{Equation 5-10}$$

where

<i>BAF</i>	=	Bioaccumulation factor (L/kg)
<i>BCF</i>	=	Bioconcentration factor (L/kg)
<i>FCM</i>	=	Trophic level-specific food-chain multiplier (unitless)

*FCMs* are specified for use in this guidance to model a COPC concentration in fish, and also mammalian and bird food items, that are ingested by a measurement receptor. The *BCF-FCM* approach accounts for the uptake or bioaccumulation of COPCs into organisms, typically represented in equations as a *BAF* (U.S. EPA 1995j). The availability of data allows the *BCF-FCM* approach to be more consistently applied across class-specific guilds within food webs being evaluated.

U.S. EPA OSW recognizes the limitations and uncertainties of applying *FCMs* derived from aquatic food web data to terrestrial receptors, as well as all top level consumers, whether their food is chiefly aquatic or not. However, the *BCF-FCM* approach is recommended in this guidance because (1) evaluation of multiple food chain exposure pathways is typically required to estimate risk to multiple mammalian and avian guilds in several food webs, (2) screening level risk assessment results are intended to support development of permits and focus risk management efforts, rather than as a final point of departure for further evaluation, and (3) U.S. EPA OSW is aware of no other applicable multipathway approaches for consistently and reproducibly estimating COPC concentrations in prey ingested by upper-trophic-level ecological receptors, considering current data limitations. Therefore, U.S. EPA OSW believes the *BCF-FCM* approach is the best available quantitative method for estimating COPC concentrations in upper trophic level food items ingested by measurement receptors, considering data availability and the objectives inherent to a screening level risk assessment.

**TABLE 5-2**  
**FOOD-CHAIN MULTIPLIERS**

Log $K_{ow}$	Trophic Level of Consumer		
	2	3	4
2.0	1.0	1.0	1.0
2.5	1.0	1.0	1.0
3.0	1.0	1.0	1.0
3.1	1.0	1.0	1.0
3.2	1.0	1.0	1.0
3.3	1.0	1.1	1.0
3.4	1.0	1.1	1.0
3.5	1.0	1.1	1.0
3.6	1.0	1.1	1.0
3.7	1.0	1.1	1.0
3.8	1.0	1.2	1.0
3.9	1.0	1.2	1.1
4.0	1.0	1.3	1.1
4.1	1.0	1.3	1.1
4.2	1.0	1.4	1.1
4.3	1.0	1.5	1.2
4.4	1.0	1.6	1.2
4.5	1.0	1.8	1.3
4.6	1.0	2.0	1.5
4.7	1.0	2.2	1.6
4.8	1.0	2.5	1.9
4.9	1.0	2.8	2.2
5.0	1.0	3.2	2.6
5.1	1.0	3.6	3.2
5.2	1.0	4.2	3.9
5.3	1.0	4.8	4.7
5.4	1.0	5.5	5.8
5.5	1.0	6.3	7.1
5.6	1.0	7.1	8.6

**TABLE 5-2**  
**FOOD-CHAIN MULTIPLIERS**

Log $K_{ow}$	Trophic Level of Consumer		
	2	3	4
5.7	1.0	8.0	10
5.8	1.0	8.8	12
5.9	1.0	9.7	14
6.0	1.0	11	16
6.1	1.0	11	18
6.2	1.0	12	20
6.3	1.0	13	22
6.4	1.0	13	23
6.5	1.0	14	25
6.6	1.0	14	26
6.7	1.0	14	26
6.8	1.0	14	27
6.9	1.0	14	27
7.0	1.0	14	26
7.1	1.0	14	25
7.2	1.0	14	24
7.3	1.0	13	23
7.4	1.0	13	21
7.5	1.0	13	19
7.6	1.0	12	17
7.7	1.0	11	14
7.8	1.0	10	12
7.9	1.0	9.2	9.8
8.0	1.0	8.2	7.8
8.1	1.0	7.3	6.0
8.2	1.0	6.4	4.5
8.3	1.0	5.5	3.3
8.4	1.0	4.7	2.4
8.5	1.0	3.9	1.7
8.6	1.0	3.3	1.1

**TABLE 5-2**  
**FOOD-CHAIN MULTIPLIERS**

Log $K_{ow}$	Trophic Level of Consumer		
	2	3	4
8.7	1.0	2.7	0.78
8.8	1.0	2.2	0.52
8.9	1.0	1.8	0.35
9.0	1.0	1.5	0.23

Source: U.S. EPA. 1995k. "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation factors." EPA-820-B-95-005. Office of Water. Washington, D.C. March.

#### 5.3.2.4 COPC Concentration in Mammals, Birds, Amphibians, and Reptiles

The COPC concentration in mammals and birds, as food items ingested by measurement receptors, are estimated using equations specific to each guild (i.e., herbivores, omnivores, and carnivores), and based on the plant and animal food items, and media ingested. Similar to calculating the COPC concentration in fish, a *BCF-FCM* approach is used to account for bioaccumulation. However, the contribution of COPC concentrations from each food item ingested must be accounted for directly for wildlife, whereas, the derivation of *BCF-FCM* values already accounts for the COPC contributions from all pathways for fish. Also for wildlife, a ratio of *FCMs* is applied to each animal food item ingested to account for the increase in COPC concentration occurring between the trophic level of the prey item (TL<sub>n</sub>) and the trophic level of the omnivore (TL<sub>3</sub>) or carnivore (TL<sub>4</sub>).

General equations for estimating COPC concentrations of food items in each guild, including use of a *FCM* ratio to estimate biomagnification, are described in the following subsections using mammals and birds as examples. Specific equations and discussion of associated parameters are provided in Appendix F. It should be noted that due to limited availability of biotransfer and toxicity data for reptiles and amphibians, the equations in the following subsections and in Appendix F have not been specifically described for use to model exposure to these receptors. However, if site-specific conditions and data warrant evaluation of reptiles and amphibians, the permitting authority may elect to utilize the same generic equations presented.

**Herbivorous Mammals and Birds**

As indicated in Equation 5-11, the COPC concentration in herbivorous mammals and birds is calculated by summing the contribution due to ingestion of contaminated plant food items and media. The general equation for computing COPC concentration in herbivores is as follows:

$$C_H = \sum ( C_{Pi} \cdot BCF_{Pi-H} \cdot P_{Pi} \cdot F_{Pi} ) + ( C_{s/sed} \cdot BCF_{S/BS-H} \cdot P_{S/BS} ) + ( C_{wctot} \cdot BCF_{W-H} \cdot P_W )$$

Equation 5-11

where

- $C_H$  = COPC concentration in herbivore (mg/kg)
- $C_{Pi}$  = COPC concentration in *i*th plant food item (mg/kg)
- $BCF_{Pi-H}$  = Bioconcentration factor for plant-to-herbivore for *i*th plant food item (unitless)
- $P_{Pi}$  = Proportion of *i*th plant food item in diet that is contaminated (unitless)
- $F_{Pi}$  = Fraction of diet consisting of *i*th plant food item (unitless)
- $C_{s/sed}$  = COPC concentration in soil or bed sediment (mg/kg)
- $BCF_{S/BS-H}$  = Bioconcentration factor for soil-to-plant or bed sediment-to-plant (unitless)
- $P_{S/BS}$  = Proportion of soil or bed sediment in diet that is contaminated (unitless)
- $C_{wctot}$  = Total COPC concentration in water column (mg/L)
- $BCF_{W-HM}$  = Bioconcentration factor for water-to-herbivore (L/kg)
- $P_W$  = Proportion of water in diet that is contaminated (unitless)

Media-to-herbivore *BCF* values are COPC and receptor-specific and provided in Appendix C. As discussed in Appendix D, plant-to-herbivore *BCF* values are receptor-specific and determined from biotransfer factors. Calculation of COPC concentrations in plant food items and media is further discussed in previous sections of Chapter 5, and in Chapter 3 and Appendix B. The variables representing the diet fraction and proportion of diet contaminated are discussed in Section 5.3 and Appendix F. Appendix F also provides specific equations and supporting discussion for calculating the COPC concentration in herbivores.

**Omnivorous Mammals and Birds**

As indicated in Equation 5-12, the COPC concentration in omnivorous mammals and birds is calculated by summing the contribution due to ingestion of contaminated animal and plant food items, and media.

However, unlike herbivores which are TL2 consumers, omnivores are TL3 consumers of animal food items and a ratio of *FCMs* is applied to each animal food item ingested to account for the increase in COPC concentration occurring between the trophic level of the prey item (TLn) and the trophic level of the omnivore (TL3). In general, the COPC concentration in omnivores depends on the COPC concentration in each food item ingested, and the trophic level of each food item, as follows:

$$C_{OM} = \sum (C_{Ai} \cdot \frac{FCM_{TL3}}{FCM_{TLn-Ai}} \cdot P_{Ai} \cdot F_{Ai}) + \sum (C_{Pi} \cdot BCF_{Pi-OM} \cdot P_{Pi} \cdot F_{Pi})$$

Equation 5-12

$$+ (C_{s/sed} \cdot BCF_{S/BS-OM} \cdot P_{S/BS}) + (C_{wctot} \cdot BCF_{W-OM} \cdot P_W)$$

where

- $C_{OM}$  = COPC concentration in omnivore (mg/kg)
- $C_{Ai}$  = COPC concentration in *i*th animal food item (mg/kg)
- $FCM_{TL3}$  = Food chain multiplier for trophic level 3 (unitless)
- $FCM_{TLn-Ai}$  = Food chain multiplier for trophic level of *i*th animal food item (unitless)
- $P_{Ai}$  = Proportion of *i*th animal food item in diet that is contaminated (unitless)
- $F_{Ai}$  = Fraction of diet consisting of *i*th animal food item (unitless)
- $BCF_{Pi-OM}$  = Bioconcentration factor for plant-to-omnivore for *i*th plant food item (unitless)
- $C_{Pi}$  = COPC concentration in *i*th plant food item (mg/kg)
- $P_{Pi}$  = Proportion of *i*th plant food item that is contaminated (unitless)
- $F_{Pi}$  = Fraction of diet consisting of *i*th plant food item (unitless)
- $C_{s/sed}$  = COPC concentration in soil or bed sediment (mg/kg)
- $BCF_{S/BS-OM}$  = Bioconcentration factor for soil- or bed sediment-to-omnivore (unitless)
- $P_{S/BS}$  = Proportion of soil or bed sediment in diet that is contaminated (mg/kg)
- $C_{wctot}$  = Total COPC concentration in water column (mg/L)
- $BCF_{W-OM}$  = Bioconcentration factor for water-to-omnivore (L/kg)
- $P_W$  = Proportion of water in diet that is contaminated (unitless)

Media-to-omnivore *BCF* values are COPC and receptor-specific and provided in Appendix C. The use of an *FCM* ratio to estimate biomagnification between trophic levels is discussed in a following subsection.

Calculation of COPC concentrations in animal food items is further discussed in previous sections of Chapter 5. Calculation of COPC concentrations in plant food items and media is further discussed in previous sections of Chapter 5, and in Chapter 3 and Appendix B. The variables representing the diet fraction and proportion of diet contaminated are discussed in Section 5.3 and Appendix F. Appendix F also provides specific equations and supporting discussion for calculating the COPC concentration in omnivores.

### Carnivorous Mammals and Birds

As indicated in Equation 5-13, the COPC concentration in carnivorous mammals and birds is calculated by summing the contribution due to ingestion of contaminated animal and media food items. In general, the equation for computing a COPC concentration for carnivorous food items is similar to the corresponding equation for omnivores; only without the component accounting for ingestion of plant food items. Similarly, a ratio of *FCMs* is applied to each animal food item ingested to account for the increase in COPC concentration occurring between the trophic level of the prey item (TLn) and the trophic level of the carnivore (TL4). The COPC concentration in carnivores depends on the COPC concentration in media, in each animal food item ingested, their respective trophic level, as follows:

$$C_C = \sum (C_{Ai} \cdot \frac{FCM_{TL4}}{FCM_{TLn-Ai}} \cdot P_{Ai} \cdot F_{Ai}) + (C_{s/sed} \cdot BCF_{S/BS-C} \cdot P_{S/BS}) + (C_{wctot} \cdot BCF_{W-C} \cdot P_W)$$

Equation 5-13

where

- $C_C$  = COPC concentration in carnivore (mg/kg)
- $C_{Ai}$  = COPC concentration in *i*th animal food item (mg/kg)
- $FCM_{TL3}$  = Food chain multiplier for trophic level 4 (unitless)
- $FCM_{TLn-Ai}$  = Food chain multiplier for trophic level of *i*th animal food item (unitless)
- $P_{Ai}$  = Proportion of *i*th animal food item in diet that is contaminated (unitless)
- $F_{Ai}$  = Fraction of diet consisting of *i*th animal food item (unitless)
- $C_{s/sed}$  = COPC concentration in soil or bed sediment (mg/kg)
- $BCF_{S/BS-C}$  = Bioconcentration factor for soil- or bed sediment-to-carnivore (unitless)



$P_{S/BS}$	=	Proportion of soil or bed sediment in diet that is contaminated (mg/kg)
$C_{wctot}$	=	Total COPC concentration in water column (mg/L)
$BCF_{W-C}$	=	Bioconcentration factor for water-to-carnivore (L/kg)
$P_W$	=	Proportion of water in diet that is contaminated (unitless)

Media-to-carnivore  $BCF$  values are COPC and receptor-specific and provided in Appendix C. The use of an  $FCM$  ratio to estimate biomagnification between trophic levels is discussed in the following subsection. Calculation of COPC concentrations in animal food items is further discussed in previous sections of Chapter 5. Calculation of COPC concentrations in plant food items and media is further discussed in previous sections of Chapter 5, and in Chapter 3 and Appendix B. The variables representing the diet fraction and proportion of diet contaminated are discussed in Section 5.3 and Appendix F. Appendix F also provides specific equations and supporting discussion for calculating the COPC concentration in carnivores.

### Use of Food Chain Multiplier Ratio to Estimate Biomagnification

Biomagnification involves the transfer of a chemical in food through successive trophic levels (Hamelink et al. 1971). Chemicals with greatest potential to biomagnify are highly lipophilic, have low water solubilities, and are resistant to being metabolized (Metcalf et al. 1975). To account for COPC biomagnification in the food chain, U.S. EPA OSW recommends the use of  $FCM$  ratios as derived by U.S. EPA (1995k).

$FCM$  ratios are used to estimate the increase in a COPC concentration resulting from the ingestion of TL2 prey (i.e., animal food item) by a TL3 measurement receptor (i.e., omnivore or carnivore), and the ingestion of TL2 and TL3 prey by a TL4 measurement receptor. Biomagnification, expressed as a biomagnification factor ( $BMF$ ), equals the quotient of the  $FCM$  of the measurement receptor divided by the  $FCM$  of the prey. It is important to note that the basic difference between the  $FCM$  and  $BMF$  is that the  $FCMs$  relate back to trophic level one, whereas  $BMFs$  always relate back to the preceding trophic level (U.S. EPA 1995k). This relation is entirely compatible, but confusion can result if the terms specific to trophic level are not used consistently and clearly (U.S. EPA 1995k). As presented in U.S. EPA (1995k), the following relation of  $FCM$  to  $BMF$  can be expressed as follows:

$$BMF_{TL2} = FCM_{TL2} \quad \text{Equation 5-14}$$

$$BMF_{TL3} = FCM_{TL3}/FCM_{TL2} \quad \text{Equation 5-14A}$$

where

$BMF_n$  = Biomagnification factor for  $n$ th trophic level  
 $FCM_{TLn}$  = Food chain multiplier for  $n$ th trophic level

#### 5.4 ASSESSMENT OF TOXICITY

Toxicity of a COPC is assessed by identifying toxicity reference values (*TRVs*) specific to a COPC and the measurement receptor being evaluated. As discussed in Chapter 6, *TRVs* are subsequently set as the denominator for computing COPC ecological screening quotients (*ESQs*) during risk characterization. The available *TRVs* used in risk characterization for lower trophic level communities are media specific; whereas *TRVs* for upper trophic level class-specific guilds are provided in terms of dose ingested. *TRVs* for community and class-specific guild measurement receptors are further described below:

- Community (lower trophic level) *TRVs* are media specific and used to screen ecological effects to receptors inhabiting soil, surface water, and sediment. Community *TRVs* are expressed on a concentration basis, such as milligrams of COPC per kilogram of soil, and generally either:
  - (1) a COPC media concentration that, based on its intended use by a regulatory agency, confers a high degree of protection to receptor populations or communities inhabiting the media (these include regulatory values such as federal ambient water quality criteria, state no-effect-level sediment quality guidelines, and sediment screening effect concentrations), or
  - (2) a laboratory-derived toxicity value representing a COPC media concentration that causes, over a chronic exposure duration, no adverse effects to a representative ecological receptor (e.g., no-observed-effect-concentration).
- Class-specific guild (upper trophic level) *TRVs* are used to screen ecological effects to wildlife, and expressed as a COPC daily dose ingested that causes, over a chronic exposure duration, no observed adverse effects to a measurement receptor. Class-specific guild *TRVs* are expressed in units of mass (e.g., milligrams or micrograms) of COPC per

kilogram body weight (wet weight) per day.

Guidance for selection of *TRVs* for community and class-specific guild measurement receptors is provided in the following sections. *TRVs* specific to example measurement receptors presented in the food webs in Chapter 4 are available in Appendix E.

#### 5.4.1 General Guidance on Selection of Toxicity Reference Values

Compound specific *TRVs* should be identified for each measurement receptor evaluated to characterize risk to a community or class-specific guild. U.S. EPA OSW recommends evaluation of the following sources of toxicity values, listed in order of general preference, in determining *TRVs* for use in a screening level risk assessment:

***Toxicity values developed and/or adopted by federal and/or state regulatory agencies; generally provided in the form of standards, criteria, guidance, or benchmarks.*** Toxicity values developed and/or adopted by federal or state regulatory agencies are generally media specific, and reported only for surface water and sediment. Examples include state or federal ambient water quality criteria (AWQC), National Oceanic and Atmospheric Administration (NOAA) effects range-low (ERL) values for sediment (Long et al. 1995), and State of Florida sediment quality guidelines (MacDonald 1993).

***Toxicity values published in scientific literature.*** Appropriate values should be derived from a laboratory study which characterizes adverse effects on ecologically-relevant endpoints (e.g., growth, reproduction, mortality). As discussed in Section 5.4.1.3, toxicity values obtained from scientific literature may also require application of an uncertainty factor (UF) to account for extrapolation uncertainty.

***Toxicity values calculated for sediment using equilibrium partitioning (EqP) approach.*** The EqP approach is further described in Section 5.3.2.1. Calculating sediment toxicity values using the EqP approach requires determination of (1) an organic carbon content of the sediments, and (2) a corresponding surface water toxicity value.

***Toxicity values from surrogate compounds.*** Surrogate compounds are selected through evaluation of parameters such as chemical structure and toxicity mechanisms of action. For example, low molecular weight (i.e. those have two or less rings) polycyclic aromatic hydrocarbons (PAH's) could be grouped together and evaluated using the toxicity data from a PAH congener belonging to this group.

The evaluation of toxicity values published in scientific literature should consider (1) ecological relevance of the study, (2) exposure duration (e.g., chronic, acute), and (3) study endpoints (e.g., NOAEL, LOAEL). The identification of literature toxicity values used to derive *TRVs* should focus on toxicological data

characterizing adverse effects on ecologically relevant endpoints, such as growth, seed germination, reproduction, and survival. Study endpoints specified for reported toxicity values generally include the following:

- Soil, surface water, and sediment measurement receptors
  - No-observed-effect-level (NOEL) or no-observed-effect-concentration (NOEC)
  - Lowest-observed-effect-level (LOEL) or lowest-observed-effect-concentration (LOEC)
  - Median lethal concentration to 50 percent of the test population (LC50) or median effective concentration for 50 percent of the test population (EC50)
  
- Wildlife measurement receptors
  - No-observed-adverse-effect-level (NOAEL)
  - Lowest-observed-adverse-effect-level (LOAEL)
  - Median lethal dose to 50 percent of the test population (LD50)

Evaluation of toxicity test data is further discussed in Section 5.4.1.1.

When multiple studies are assessed equally under the criteria above, professional judgement can be applied to determine the most appropriate study and corresponding toxicity value to be selected as the *TRV* (see Section 5.4.1.2). As discussed in Section 5.4.1.3, toxicity values obtained from scientific literature may also require application of an UF to account for extrapolation uncertainty (due to differences in test endpoint and exposure duration) when considering use of the test value as a *TRV* in a screening level risk assessment.

#### 5.4.1.1 Evaluation of Toxicity Test Data

A *TRV* should represent a COPC concentration or dose that causes no observed adverse effects to an ecologically relevant endpoint of a receptor exposed for a chronic (long-term) duration. As noted above, evaluation of test data from ecologically relevant studies should be further assessed based on exposure duration and study endpoint.

The following hierarchy, in terms of decreasing preference, should be followed to assess exposure duration and study endpoint:

1. Chronic NOAEL
2. Subchronic NOAEL
3. Chronic LOAEL
4. Subchronic LOAEL
5. Acute median lethality point estimate
6. Single dose toxicity value

The following guidelines should be used to generally determine exposure duration:

- For fish, mammals, and birds:
  - A chronic test lasts for more than 90 days
  - A subchronic test lasts from 14 to 90 days
  - An acute test lasts less than 14 days
  
- For other receptors:
  - A chronic test lasts for 7 or more days
  - A subchronic test lasts from 3 to 6 days
  - An acute test lasts less than 3 days

The logic followed to identify the a toxicity value should be fully documented. Sources of toxicity values include electronic databases, reference compendia, and technical literature. Toxicity values identified from secondary sources should be verified, wherever possible, by reviewing the original study. If an original study is unavailable, or multiple studies of similar quality are available, best professional judgment should be used to determine an appropriate toxicity value.

#### 5.4.1.2 Best Professional Judgement for Evaluating Toxicity Values

If more than one toxicity study meets a set of qualifying criteria applicable for study endpoint and exposure duration, best professional judgement should be used to identify the most appropriate study and corresponding toxicity value for *TRV* selection. The most appropriate study is the one with the least uncertainty about the accuracy of the value of endpoint (i.e., NOAEL) that, ultimately, provides the greatest degree of protectiveness to the applicable measurement receptor. The most appropriate study

should be identified by reviewing the experimental design of each study. Discussed below are important aspects of experimental design that should be evaluated.

- ***Number of treatments, spread between treatments, and number of replicates per treatment.*** The number of treatments and the spread between exposure concentrations (or dose groups) will affect the accuracy of the test endpoint (such as the NOAEL). That is, the smaller the spread between the NOAEL and LOAEL, the less the uncertainty is about the true concentration or dose at which there is no adverse effect. The statistical power of a toxicity test (or any test for that matter) is dependent, in large part, on the number of replicates (or number of animals per dose). That is, the ability of a test to detect statistical differences (test sensitivity) increases as the number of replicates increase.
- ***Exposure route.*** The exposure route of the test should coincide with the applicable exposure route or pathway under consideration in the risk assessment. For example, the screening level risk assessment may evaluate the risk of contaminated soils to terrestrial plants due to exposure to bulk soil. Therefore, a terrestrial plant toxicity study that evaluated the effects of soil solutions on a plant species may be a less appropriate than a study based on effects of bulk soil.
- ***Exposure during sensitive life stage.*** Ideally, all toxicity studies would evaluate the effects of a toxicant on the most sensitive life stage, such as neonatal zooplankton and first instar larvae. Therefore, the exposure duration should be receptor- and toxicant-specific.
- ***Nominal or measured test concentrations.*** Measured test concentrations more accurately estimate the true concentration of a toxicant presented to a receptor. Nominal, or unmeasured, test concentrations do not account for potential losses of the toxicant (such as toxicant adsorbed to particulate material) or for inaccuracies in preparing test solutions. In addition, samples for measuring test concentrations should be collected from the exposure chamber, not the delivery system.
- ***Use, type, and performance of controls.*** A positive control (no toxicant) should be used in each toxicity study. The only difference between a positive control and a treatment is the absence of the toxicant from the control. Performance in a positive control should meet pre-existing performance criteria (such as acceptable survival). Treatment performance should be statistically compared to (or inferred from in some circumstances) to control performance to identify statistical endpoints (such as the NOAEL and LOAEL). In some situations, a negative control (toxicant with known toxicity, also called a performance control) may be appropriate. If a negative control is used, its results should be compared to standards to determine if test receptor sensitivity was acceptable.
- ***Method used to determine endpoint (i.e., NOAEL).*** Ideally, an acceptable number of replicates should be used so a test has statistical power. An appropriate statistical test should be performed to identify the NOAEL. In some cases, the NOAEL may have to be inferred because of insufficient number of replicates. While the latter is not unscientific, the former method provides a measure that the conclusion might be false. For example, if test results are statistically analyzed at a probability level of 95 percent, there is a 5 percent chance that the results of the statistical analysis are false.

### 5.4.1.3 Uncertainty Factors for Extrapolation From Toxicity Test Values to *TRVs*

Incomplete knowledge of the actual toxicity of a chemical leads to the use of UFs to reduce the likelihood that risk estimates do not underestimate risk. Historically, UFs have been used for various extrapolations, and their applications reflect policy to provide conservative estimates of risk (Chapman et al. 1998). As discussed below, UFs are used in the risk assessment to reduce the probability of underestimating ecological risk from exposures to combustor emissions. This is performed by multiplying a toxicity value by a UF to produce a *TRV* reflecting an NOAEL for a chronic exposure duration.

UFs should be used to convert a toxicity value to a chronic NOAEL-based *TRV*. In most cases, the UFs discussed below should be applicable to available toxicity values. In some cases, however, irregular toxicity data (such as, a subchronic LC50) may be the only available information. In these cases, the toxicity data should be thoroughly reviewed and professional judgment should be used to identify appropriate UFs that are consistent with those listed below. Special attention should be taken with toxicity values from single oral dose, intraperitoneal, and subchronic lethality tests.

Specifically, UFs should be used to account for extrapolation uncertainty due to differences in test endpoint and exposure duration:

- Test endpoint uncertainty—extrapolation from a non-NOAEL endpoint (e.g., LOAEL, LD50) to an NOAEL endpoint
- Duration uncertainty—extrapolation from a single dose, acute, or subchronic duration to a chronic duration

Except as noted above for irregular toxicity data, the following UFs (Calabrese and Baldwin 1993) should be used to convert a toxicity test endpoint to a *TRV* equivalent to a chronic NOAEL:

- A chronic LOAEL (or LOEL or LOEC) should be multiplied by a UF of 0.1 to convert it to a chronic NOAEL
- A subchronic NOAEL should be multiplied by a UF of 0.1 to convert it to a chronic NOAEL.
- An acute lethal value (such as an LC50 or LD50) should be multiplied by an UF of 0.01 to convert it to a chronic NOAEL.

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# Chapter 6

## Risk Characterization

### What's Covered in Chapter 6:

- ◆ Risk Estimation
  - ◆ Risk Description
  - ◆ Uncertainty and Limitations of the Screening Level Risk Assessment
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- 

Risk characterization includes risk estimation and risk description (U.S. EPA 1992b). Risk estimation is an integration of the exposure assessment (see Section 5.1) and the toxicity assessment (see Section 5.4) to determine the potential risk to a community or guild from exposure to a COPC. Risk estimation is quantified using the quotient method to calculate an ecological screening quotient (*ESQ*) (Suter 1993). Risk description describes the magnitude and nature of potential risk for each community and guild, based on the quantitative results of the risk estimation and calculated *ESQ* values. Risk description also discusses the significance of the default assumptions used to assess exposure, because they affect the magnitude and certainty of the calculated *ESQ* value. The resultant risk characterization should consider any major uncertainties and limitations associated with results generated in performing the screening level risk assessment.

Section 6.1 discusses using the quotient method and calculation of *ESQs* to estimate potential ecological risk. Section 6.2 discusses various aspects of the risk description. Section 6.3 discusses consideration of uncertainties and limitations.

### 6.1 RISK ESTIMATION

To estimate potential ecological risk, an *ESQ* should be calculated specific to each measurement receptor, COPC, and exposure scenario location evaluated in the risk assessment. Also, dietary-variable *ESQs* should be computed for class-specific guild measurement receptors based on “equal diet” dose and “exclusive diet” dose, as discussed in Section 5.3. As expressed in Equation 6-1, an *ESQ* is the quotient of the COPC estimated exposure level (*EEL*) divided by the COPC and measurement receptor specific toxicity reference value (*TRV*), as follows:



$$ESQ = \frac{EEL}{TRV} \quad \text{Equation 6-1}$$

where

<i>ESQ</i>	=	Ecological screening quotient (unitless)
<i>EEL</i>	=	COPC estimated exposure level (mass COPC/mass media [communities] or mass daily dose COPC ingested/mass body weight-day [class-specific guilds])
<i>TRV</i>	=	COPC toxicity reference value (mass COPC/mass media [communities] or mass daily dose COPC ingested/mass body weight-day [class-specific guilds])

Care should be made to ensure that the units for the *EEL* value and the *TRV* are consistent, including correct use of corresponding wet and dry weights. *TRVs* specific to organic and inorganic compounds are typically expressed in units of  $\mu\text{g}/\text{kg}$  and  $\text{mg}/\text{kg}$ , respectively. General guidance for determining *TRVs* is provided in Chapter 5. Also, Appendix E provides compound specific *TRVs* for the example measurement receptors identified in the food webs in Chapter 4.

*ESQs* for community measurement receptors are calculated using *EELs* specific to the COPC concentration in the corresponding media. A COPC specific *ESQ* should be calculated for each community measurement receptor at each location evaluated, as appropriate for the food web being analyzed in the risk assessment. For calculating *ESQs* for class-specific guild measurement receptors, the *EEL* is the daily dose of COPC ingested. A COPC specific *ESQ* should also be calculated for each class-specific guild measurement receptor at each location evaluated, as appropriate for the food web being analyzed in the risk assessment. For class-specific guild measurement receptors, *ESQs* should be calculated specific to equal and exclusive diets (see Chapter 5).

To evaluate potential risk resulting from exposure of a measurement receptor to multiple COPCs at a specific location, each of the COPC-specific *ESQ* values should be summed to determine a total *ESQ*.

$$ESQ_{ReceptorTotal} = \sum ESQ_{COPC\ Specific} \quad \text{Equation 6-2}$$

where

$$\begin{aligned} ESQ_{Receptor\ Total} &= \text{Total ecological screening quotient for receptor (unitless)} \\ ESQ_{COPC\ Specific} &= \text{COPC specific ecological screening quotient (unitless)} \end{aligned}$$

As for COPC-specific *ESQ*s, total *ESQ*s for class-specific guild measurement receptors should be calculated specific to equal and exclusive diets (see Chapter 5).

## 6.2 RISK DESCRIPTION

Risk description considers the magnitude and nature of potential risk for community and class-specific guild measurement receptors evaluated, and provides information for the risk manager and permitting authority to evaluate the significance of an *ESQ* value. Also, Section 6.2.2 recognizes some of the default exposure assumptions that may affect the magnitude of an *ESQ* value.

### 6.2.1 Magnitude and Nature of Ecological Risk

The magnitude and nature of potential risk should be further considered for each measurement receptor with a COPC-specific *ESQ* value equal to or above risk target levels specified by the appropriate permitting authority. Interaction between the risk assessor and the risk manager and permitting authority has been noted throughout the process (See Figure 1 for Scientific Management Decision Points). At the risk characterization phase of the risk assessment, most of the interaction between the risk assessor and the risk manager and permitting authority is through description of the certainty of the resulting risk estimates. Consistent with the NCP and current U.S. EPA guidance (1998c), the risk manager and permitting authority with input from the risk assessor should also consider the need to collect additional information to refine risk estimates and/or implement permit requirements (i.e., operating conditions, use of APCDs, waste feed conditions, or environmental monitoring) at combustion facilities where an *ESQ* exceeds risk target levels for ecological communities or guilds that may reasonably be expected to be exposed.

The magnitude and nature of potential risk should also be further considered for each measurement receptor with a total *ESQ* value greater than or equal to the target risk levels. While the total *ESQ* provides the risk manager and permitting authority with useful information regarding potential risk resulting from exposure of a measurement receptor to multiple COPCs at a specific location, potential limitations and uncertainties

associated with the calculation of the total *ESQ* should be considered before its use. Specifically, the resulting total *ESQ* is determined by summing COPC-specific *ESQs* that will usually be calculated utilizing *TRVs* (see Chapter 5) based on different effects (e.g. growth, reproduction), toxicity endpoints (e.g., NOAEL, LOAEL) and/or exposure durations (e.g., chronic, acute). In considering usability of total *ESQs*, U.S. EPA OSW recommends that the risk manager and permitting authority focus on the highest contributing COPCs, or classes of COPCs which can appropriately be added across effects, toxicity endpoints and exposure durations, in further evaluating potential risks due to exposure to multiple COPCs.

Broad assessment endpoints rather than toxicologically-specific endpoints are recommended for performing a screening level ecological risk assessment (see Chapter 5). Therefore, the potential risk to each community and guild evaluated in the risk assessment should be described. Specifically, potential adverse effects should be described for each community and guild with a COPC-specific or total *ESQ* value equal to or above risk target levels. This should be performed for each selected food web and receptor location evaluated, and specific to equal and exclusive diets for applicable class-specific guilds. The description should characterize potential risk to the selected assessment endpoints, based on the measures of effect and measurement receptors. U.S. EPA OSW recommends that the risk description specific to a measurement receptor include, at a minimum, the contributing COPCs, emission sources, exposure pathways, and significant uncertainties.

### 6.2.1.1 Target Levels

Target levels are risk management based and set by the regulatory authority. Target values are not a discrete indicator of observed adverse effect. If a calculated risk falls within target values, a regulatory authority may, without further investigation, conclude that a proposed action does not present an unacceptable risk. A calculated risk that exceeds these targets, however, would not, in and of itself, indicate that the proposed action is not safe or that it presents an unacceptable risk. Rather, a risk calculation that exceeds a target value triggers further careful consideration of the underlying scientific basis for the calculation.

### 6.2.2 Fate and Exposure Assumptions

As noted throughout this guidance, the screening level ecological risk assessment is based on numerous conservative assumptions affecting the potential for a receptor to be exposed to a compound emitted from a facility and the numeric magnitude of the resulting estimated risk. These fate and exposure assumptions are required as a result of current data gaps and uncertainties associated with available scientific information and data required for risk evaluation. However, U.S. EPA OSW recommends that as information is available to address data gaps and reduce uncertainties specific to ecological risks identified at a facility by the screening level risk assessment, it should be provided to the permitting authority for approval to be incorporated into evaluation of risk. Some of the fate and exposure assumptions utilized in this guidance to conduct a screening level risk assessment are listed below:

- The estimated COPC concentration in soil and sediment is 100 percent bioavailable. This includes a COPC that is weakly or strongly adsorbed to particles and a COPC that is dissolved in interstitial water.
- The estimated dissolved COPC concentration in the water column is 100 percent bioavailable. For ingestion of water by wildlife, this includes a COPC that is freely dissolved as an ion or compound, and a COPC that may be adsorbed to another matrix, such as dissolved organic carbon.
- The total COPC mass estimated to be ingested by a measurement receptor is taken up across the gut and reaches the site of toxic action. This includes COPC concentrations in food items and abiotic media. This assumes that no fraction of the COPC mass is metabolized or otherwise depurated by an ecological receptor, and that there is no competition for available sites where the toxic action occurs.
- The chemical species present is the most toxic form, and is the form represented by the *TRV*.
- Community measurement receptors inhabiting an abiotic medium take up 100 percent of the COPC concentration to which they are exposed. All COPC mass taken up by a plant or animal food item of a measurement receptor is assimilated into edible biomass.
- An ecological receptor is continuously exposed during its entire life, including critical life stage(s).
- A measurement receptor's home range is 100 percent within the assessment area being evaluated in the risk assessment.
- A measurement receptor's food is 100 percent contaminated.

The relevance of fate and exposure assumptions specific to COPCs at a site, and their numerical bias to resulting *ESQ* values should be considered before application of results. Also, to facilitate the qualitative assessment of toxicokinetic and toxicodynamic factors (e.g., bioavailability, metabolism), toxicological profiles of numerous compounds often considered in combustion risk assessments (see Section 2.3) are included in Appendix H. U.S. EPA OSW prepared these profiles because it believes that these compounds (1) will be the principal compounds of ecological concern at combustion facilities, and (2) to promote consistency in presenting and evaluating relevant COPC-specific toxicity information.

### 6.3 UNCERTAINTY AND LIMITATIONS OF THE RISK ASSESSMENT PROCESS

This section describes how to interpret uncertainties associated with the risk assessment. The discussion of uncertainties in this section and in Section 6.3.1 was adopted from the U.S. EPA *1996 Risk Assessment Support to the Development of Technical Standards for Emissions from Combustion Units Burning Hazardous Waste* (EPA Contract Number 68-W3-0028), dated February 20, 1996.

Uncertainty can be introduced into a risk assessment at every step of the process outlined in this document. Uncertainty occurs, because risk assessment is a complex process, requiring the integration of the following:

- Release of pollutants into the environment
- Fate and transport of pollutants, in a variety of different and variable environments, by processes that are often poorly understood or too complex to quantify accurately
- Potential for adverse effects in receptors, as extrapolated from studies of differing species
- Probability of adverse effects in functionality of food web that is made up of species that are highly variable

Uncertainty is inherent in the process even if the most accurate data with the most sophisticated models are used. The methodology outlined in this document relies on a combination of point values—some conservative and some typical—yielding a point estimate of exposure and risk that falls at an unknown percentile of the full distributions of exposure and risk. For this reason, the degree of conservatism in risk estimates cannot be known; instead, it is known that the values combine many conservative factors and are likely to overstate actual risk (Hattis and Burmaster 1994). Therefore, a formal uncertainty analysis is

required to determine the degree of conservatism. This section discusses the types of uncertainty and the areas in which uncertainty can be introduced into an assessment. In addition, this section discusses methods for qualitatively and quantitatively addressing uncertainty in risk assessments.

It should also be noted, variability is often used interchangeably with the term “uncertainty,” but this is not strictly correct. Variability may be tied to variations in physical and biological processes, and cannot be reduced with additional research or information, although it may be known with greater certainty (for example, the weight distribution of a species may be known and represented by the mean weight and its standard deviation). “Uncertainty” is a description of the imperfect knowledge of the true value of a particular variable or its real variability in an individual or a group. In general, uncertainty is reducible by additional information-gathering or analysis activities (that is, better data or better models), whereas real variability will not change (although it may be more accurately known) as a result of better or more extensive measurements (Hattis and Burmaster 1994).

### **6.3.1 Types of Uncertainty**

Finkel (1990) classified all uncertainty into four types: (1) variable uncertainty, (2) model uncertainty, (3) decision-rule uncertainty, and (4) variability. Variable uncertainty and model uncertainty are generally recognized by risk assessors as major sources of uncertainty; decision rule is of greatest concern to the risk manager.

#### **6.3.1.1 Variable Uncertainty**

Variable uncertainty occurs when variables appearing in equations cannot be measured precisely or accurately, because of either (1) equipment limitations, or (2) spatial or temporal variances between the quantities being measured. Random, or sample, errors are common sources of variable uncertainty that are especially critical for small sample sizes. It is more difficult to recognize nonrandom, or systematic, errors that result from the basis for sampling, experimental design, or choice of assumptions. As stated in Section 6.3, true variability is something we can not do much about (except to know that it exists).

### 6.3.1.2 Model Uncertainty

Model uncertainty is associated with all models used in all phases of a risk assessment. For example, the use of a single species to represent several will introduce uncertainty into the risk assessment because of the considerable amount of interspecies variability in sensitivity to a COPC. Computer models are simplifications of reality, requiring exclusion of some variables that influence predictions but cannot be included in models because of (1) increased complexity, or (2) a lack of data for these variables. The risk assessor needs to consider the importance, in consultation with the modeler, of excluded variables on a case-by-case basis. In addition, a model which was developed to use “average” conditions as its inputs, could result in a large amount of uncertainty when “specific” conditions are used. Finally, choosing the correct model form is often difficult, because conflicting theories appear to explain a phenomenon equally well.

The models specified for use in this document were selected on the basis of scientific policy. Therefore, the air dispersion and deposition model (ISCST3) and the indirect exposure models (IEM) were selected, because they provide the information needed to conduct indirect assessments and are considered by U.S. EPA to be state-of-the-science models. This choice of models could also be considered under decision rule uncertainty. ISCST3—the air dispersion model recommended for use—has not been widely applied in its present form. Few data are available on atmospheric deposition rates for chemicals other than criteria pollutants, thereby making it difficult to (1) select input variables related to deposition, and (2) validate modeled deposition rates. Because dry deposition of vapor phase materials is evaluated external to the air dispersion model, the plume is not depleted and, as a result, mass balance is not maintained. The effect of this would be to overestimate deposition, but the magnitude of the overestimation is unknown. Mass balance is maintained for other forms of deposition (such as wet deposition and particle phase dry deposition). Long-range transport of pollutants into and out of the areas considered was not modeled, resulting in an underestimation of risk attributable to each facility.

In addition to air dispersion modeling, the use of other fate and transport models recommended by this guidance can also result in some uncertainty. For example, the models which estimate COPC concentrations in waterbodies may be particularly conservative for waterbodies located in estuarine environments with tidal influence. Because tidal influence is not considered in the models presented in Chapter 3, the resultant dilution of COPC concentrations in water and sediments likely caused by tidal

influence will not be considered in the risk assessment. Thus, the risk assessment results will likely be more conservative for tidally influenced waterbodies than for those waterbodies that are not tidally influenced. Permitting decisions based on risk estimates for estuarine environments should consider this uncertainty. The delineation of this uncertainty may be one area that could be addressed in a more refined site-specific risk assessment, if warranted.

### **6.3.1.3 Decision-rule Uncertainty**

Decision-rule uncertainty is probably of greatest concern to risk managers. This type of uncertainty arises, for example, out of the need to balance different social concerns when determining an acceptable level of risk. The uncertainty associated with risk analysis influences many policy and risk management decisions. Possibly the most important aspect for the risk estimates is the selection of constituents to be included in the analysis. Constituents identified by this guidance will include compounds that have the potential to pose the greatest risk to ecological receptors through exposure. For example, many PICs are highly lipophilic and tend to bioaccumulate, thereby presenting a potentially high risk to upper trophic level receptors through the consumption of contaminated food items.

### **6.3.2 Description of Qualitative Uncertainty**

Often, sources of uncertainty in a risk assessment can be determined but cannot be quantified. For example, this can occur when a factor is known or expected to be variable, but no data are available (e.g., presence of COPCs without toxicity data). In this case, default data may be available that can be useful in estimating a possible range of values. Uncertainty also often arises out of a complete lack of data. A process may be so poorly understood that the uncertainty cannot be quantified with any confidence. In addition, some sources of uncertainty (such as uncertainty in theories used to deduce models) are inherent qualifications reflecting subjective modes of confidence rather than probabilistic arguments. When uncertainty can be presented only qualitatively, the possible direction and orders of magnitude of the potential error should be considered.



### 6.3.3 Description of Quantitative Uncertainty

Knowledge of experimental or measurement errors can also be used to introduce a degree of quantitative information into a qualitative presentation of uncertainty. For example, standard laboratory procedures or field sampling methods may have a known error level that can be used to quantify uncertainty. In many cases, uncertainty associated with particular variable values or estimated risks can be expressed quantitatively and further evaluated with variations of sensitivity analyses. Finkel (1990) identified a six-step process for producing a quantitative uncertainty estimate:

- Define the measure of risk (i.e., assessment endpoint). More than one measure of risk may result from a particular risk assessment; however, the uncertainty should be quantified or reached individually.
- Specify “risk equations” that present mathematical relationships that express the risk measure in terms of its components. This step is used to identify the important variables in the risk estimation process.
- Generate an uncertainty distribution for each variable or equation component. These uncertainty distributions may be generated by using analogy, statistical inference techniques, expert opinion, or a combination of these.
- Combine the individual distributions into a composite uncertainty distribution.
- Recalibrate the uncertainty distributions. Inferential analysis could be used to “tighten” or “broaden” particular distributions to account for dependencies among the variables and to truncate the distributions to exclude extreme values.
- Summarize the output clearly, highlighting the important risk management implications. Address specific critical factors.
  - Implication of supporting a point estimate produced without considering uncertainty
  - Balance of the costs of under- or over-estimating risks
  - Unresolved scientific controversies, and their implications for research

When a detailed quantitative treatment of uncertainty is required, statistical methods are employed. Two approaches to a statistical treatment of uncertainty with regard to variable values are described here and were used in this analysis where appropriate. The first is to use an appropriate statistic to express all variables for which uncertainty is a major concern. For example, if a value used is from a sample (such as

yearly emissions from a stack), the mean and standard deviation should both be presented. If the sample size is very small, it may be appropriate to (1) give the range of sample values and use a midpoint as a best estimate in the model, or (2) use the smallest and largest measured value to obtain two estimates that bound the expected true value. Selection of the appropriate statistic depends on the amount of data available and the degree of detail required. Uncertainties can be propagated by using analytical or numerical methods.

A second approach is to use the probability distributions of major variables to propagate variable value uncertainties through the equations used in a risk analysis. A probability distribution of expected values is then developed for each variable value. These probability distributions are typically expressed as either probability density functions (*PDF*) or cumulative probability density functions (*CPF*). The *PDF* presents the relative probability for discrete variable values, whereas the *CPF* presents the cumulative probability that a value is less than or equal to a specific value.

A composite uncertainty distribution is created by combining the individual distributions with the equations used to calculate the probability of particular adverse effects and points. Numerical or statistical methods are often used. In Monte Carlo simulations, for example, a computer program is used to repeatedly solve the model equations, under different selections of variable values, to calculate a distribution of exposure (or risk) values. Each time the equations are calculated, values are randomly sampled from the specified distributions for each variable. The end result is a distribution of exposure (or risk). These can again be expressed as *PDFs* or, more appropriately, as *CPFs*. The distribution enables the risk assessor to choose the value corresponding to the appropriate percentile in the overall distribution. For example, the risk assessor can select an exposure level or risk level that corresponds to the 95th percentile of the overall risk distribution rather than a point estimate of risk that is based on the 95th percentile values for each variable.

#### 6.3.4 Risk Assessment Uncertainty Discussion

The science of risk assessment is evolving; where the science base is incomplete and uncertainties exist, science policy assumptions must be made. It is important for risk assessments of facilities that burn hazardous waste to fully explain the areas of uncertainty in the assessments and to identify the key assumptions used in conducting the assessments. Toward that end, a table should be added to the end of each section (e.g., stack emissions, air modeling, exposure assessment, risk characterization) which lists the

key assumptions in that section, the rationale for those assumptions, their effect on estimates of risk (overestimation, underestimation, neutral), and the magnitude of the effect (high, medium, low). For example, it could explain that using a particular input variable, such as exit gas temperature, will under- or overestimate long-term emissions, and the resulting risks, by a factor of  $x$ . These tables can be used to evaluate the extent to which protective assumptions were used in the risk assessments. They can also help determine the nature of the uncertainty analysis to be performed. The assumptions listed in the risk characterization section, which synthesizes the data outputs from the exposure and toxicity analyses, should be the most significant assumptions from each of the previous sections.

Within this guidance, identification of uncertainties and limitations are also included with the discussion of specific technical issues (e.g., TOE, estimates of emission rates, COPC selection process, quantification of non-detects) as they are presented in their respective sections. Limitations associated with parameter values and inputs to equations are presented in the Appendices.

As an example discussion, the following summarizes some of the uncertainty involved in the air dispersion modeling component of the risk assessment process.

Although dispersion modeling is a valuable tool for estimating concentration and deposition impacts, it has many limitations. The accuracy of the models is limited by (1) the ability of the model algorithms to depict atmospheric transport and dispersion of contaminants, and (2) the accuracy and validity of the input data. For example, most refined models require input of representative meteorological data from a single measuring station. In reality, a release will encounter highly variable meteorological conditions that are constantly changing as it moves downwind. U.S. EPA's *Guideline on Air Quality Models—Revised* (Title 51 CFR Appendix W) describes two types of model uncertainty. Inherent uncertainty involves deviations in concentrations that occur even if all of the model input is accurate. Reducible uncertainty is associated with the model and the uncertain input values that will affect the results. Although it is important to accurately represent actual conditions by selecting the right model, and using accurate and representative input data, all model results are subject to uncertainty. Nevertheless, models are generally considered reasonably reliable in estimating the magnitude of highest concentrations resulting from a release, although they may not necessarily be time-and space-specific (Title 51 CFR Appendix W). When applied properly, air dispersion models are typically accurate to  $\pm 10$  to 40 percent and can be used to yield a "best estimate" of air concentrations (Title 51 CFR Appendix W).

Uncertainties specific to other technical components (e.g., TOE, quantification of non-detects) of the risk assessment process are further described in their respective chapters or sections of this guidance.

### **6.3.5 Limitations and Uncertainties Specific to a Screening Level Ecological Risk Assessment**

As a screening-level tool, the screening level ecological risk assessment has several inherent limitations. Some of these limitations are discussed in Section 6.3.5.1. After computing the *ESQs* and analyzing the risk assessment results, the risk assessor should evaluate the uncertainty associated with the screening level risk assessment. Section 6.3.5.2 provides a list of uncertainties that U.S. EPA OSW recommends should typically be evaluated, at least qualitatively, in a screening level risk assessment.

#### **6.3.5.1 Limitations Typical of a Screening Level Ecological Risk Assessment**

The approach used to select the measurement receptors is based, in part, on the premise that if key components of the ecosystem are protected, protection will be conferred to populations and, by extension, communities and the ecosystem. Although this approach is reasonable given the nature of the analysis and the availability of the data, protection of measurement receptors may not always adequately protect all ecologically significant assessment endpoints. Similarly, the selection process for ecological receptors relies on a modified trophic element approach. As a result, representative species may not be the most sensitive to particular compounds, but may have been chosen as a function of their ecological significance and the availability of natural history information.

COPCs were selected to provide a conservative representation of those compounds in hazardous waste combustion stack and fugitive emissions that have the highest potential to result in adverse ecological effects. Due to a lack of data on adverse ecological effects associated with combustion emissions through all exposure pathways, this list may not be all inclusive.

The toxicity of compounds varies with the measurement receptors and with the availability and form of a given compound. If a compound is more bioavailable to an organism for absorption or uptake (such as through increased solubility in the surface soil, surface water, or sediment), then the toxic potential of the compound increases. Availability and chemical form are affected by factors such as pH, temperature, alkalinity, seasonal variation, microbial activity, organic carbon content, and complexation with other

compounds. In the risk assessment, bioavailability of COPCs is assumed to be similar to that observed in the toxicity studies reported in the literature. Thus, toxicity may be over- or underestimated, depending in part on the extent to which site-specific compound bioavailability differs from those in studies reported in the literature.

Attempts to quantify and correct for uncertainty resulting from the use of surrogate species is common, but controversial. Calabrese and Baldwin (1993) discuss the use of uncertainty factors to adjust for extrapolations among taxa, between laboratory and field responses, and between acute and chronic responses. These multipliers are expected to adjust for differences in responses among taxa resulting from differences in physiology and metabolism. When extrapolating from laboratory to field settings, important considerations are differences in physical environment, organism behavior, and interactions with other ecological components. Extrapolation between responses will be necessary in some cases, particularly when data on relevant endpoints are not available (most commonly when extrapolating from a LOAEL to a NOAEL). The net effect of uncertainty factors on the accuracy of the risk assessment depends on the accuracy of the assumptions that underlie the factors themselves.

### 6.3.5.2 Uncertainties Typical of a Screening Level Ecological Risk Assessment

A screening level risk assessment is typically performed using at least some default parameter values in place of site-specific measured data (see Sections 3.12 and 6.2.2), and incorporating assumptions (see Section 6.2) as a result of data gaps. The absence of site-specific information and the need to use these assumptions may result in uncertainty associated with the calculation of *ESQs*. An understanding of the uncertainties associated with the *ESQs* is necessary for understanding the significance of the *ESQs*. After identifying the major uncertainties associated with the risk assessment results, their significance should be evaluated with respect to the computed *ESQs*. Uncertainties that generally should be evaluated in a screening level ecological risk assessment for a combustion facility are listed below:

- Changes in future COPC emissions compared with modeled emission rates used in the risk assessment.
- Quantification of emissions and evaluation of non-detects used in the risk assessment.
- The site-specific representativeness of food web(s) used in the risk assessment.

- The exposure potential of the measurement receptors.
- The representativeness of equal and exclusive diet assumptions for measurement receptors.
- The effect of COPC physicochemical properties on estimates of fate and bioavailability.
- The effect of site-specific environmental conditions affecting the fate, transport, and bioavailability of the COPCs.
- The assumption that once exposed, a measurement receptor does not metabolize or eliminate a COPC.
- The potential risk to measurement receptors of COPCs with no *TRVs*.

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