ADDENDUM TO THE *METHODOLOGY FOR ASSESSING HEALTH RISKS ASSOCIATED WITH INDIRECT EXPOSURE TO COMBUSTOR EMISSIONS*

NOTICE

Exposure Assessment Group
Office of Health and Environmental Assessment
U.S. Environmental Protection Agency
Washington, D.C.

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FOREWORD

The Exposure Assessment Group (EAG) within the Office of Health and Environmental Assessment of EPA's Office of Research and Development has three main functions: (1) to conduct exposure assessments, (2) to review assessments and related documents, and (3) to develop guidelines for exposure assessments. The activities under each of these functions are supported by and respond to the needs of the various EPA program offices. In relation to the third function, EAG sponsors projects aimed at developing or refining techniques used in exposure assessments.

In response to increasing concerns over the potential impacts of emissions from combustion devices through indirect exposure routes, the Agency formed a multidisciplinary working group to review and update Agency guidance on conducting indirect exposure assessments. The Workgroup identified the 1990 EPA report, *Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions* (EPA/600/6-90/003, January, 1990) as the best existing guidance in this area. The Workgroup decided that this document is still generally appropriate for current needs, although some updates would be needed. These updates have been compiled in this Addendum to the 1990 document. Hopefully, this effort will assist assessors evaluate combustor emissions and ensure that the most current tools and information are used.

Michael A. Callahan
Director
Exposure Assessment Group

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PREFACE

In response to increasing concerns over the potential impacts of emissions from combustion devices through indirect exposure routes, the Agency formed a multidisciplinary working group to review and update Agency guidance on conducting indirect exposure assessments. The most complete Agency document on this topic is the 1990 EPA report, *Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions* (EPA/600/6-90/003, January, 1990). This document was initially drafted in 1986 and reviewed by the Agency's Science Advisory Board in 1987. The 1990 document incorporated comments of the SAB as well as other additional reviewers. The workgroup decided that this document is still fundamentally sound and appropriate for current needs, although changes would be needed.

The working group was divided into three sub-groups to deal with specific technical issues. The first subgroup focussed on modeling emissions, air dispersion, and deposition. Another subgroup reviewed the food chain modeling, including fate and transport modeling methodology and input parameters. The final group focussed on the remaining issues of human exposure and contact rates.

The approach used by the working group was to review the 1990 report and to identify and resolve issues. This addendum is formatted following this approach. After each "Issue" is presented, this addendum then describes the workgroup's "Conclusions/Recommendations" concerning that issue. The workgroup did, however, decide that some sections required more attention than just issue identification and resolution. Two sections replace the Indirect Exposure Document material currently in Chapter 3, Air Dispersion and Deposition of Emitted Pollutants, and Section 9.2. Surface Water, of Chapter 9. This addendum has undergone several revisions and has been reviewed by the workgroup as well as other individuals in EPA.

As a final note, it should be emphasized that this document was crafted as an Addendum to the 1990 EPA report *Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*, and, as such, should be used in combination with that report in conducting indirect exposure assessments.

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AUTHORS

This document was developed by the Indirect Exposure Assessment Workgroup, cochaired by Alec McBride of the Office of Solid Waste and John Schaum of the Office of Research and Development. The principal authors are listed below:

Office of Research and Development:
Robert Ambrose
Michael Callahan
David Cleverly
Matthew Lorber
Glen Rice
John Schaum
Donna Schewede

Office of Solid Waste:
David Layland
Alec McBride

Office of Air Quality Planning and Standards:
Joe Touma

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REVIEWERS

This document went through a series of reviews by the Indirect Exposure Assessment Workgroup (see below) as part of the development process. The progress of this Work Group was monitored by an Office Director's Oversight Group consisting of Peter Preuss (OSPRE), Sylvia Lowrance (OSW), Mark Greenwood (OPPT), John Seitz (OAQPS), Jeffrey Dennit (OSW), and William Farland (OHEA).   In addition, the final draft was circulated for Agency-wide internal review.

INDIRECT EXPOSURE ASSESSMENT WORKGROUP

Air Modeling and Emissions	Food Chain/Fate and Transport	Human Exposure and Contact Rates
Joe Touma, CHAIR, OAQPS Glen Rice, ORD Diane Byrne, OAQPS Gary Victorine, Region 5 Dave Guinnep, OAQPS Pam Blakely, Region 5 Fred Talcott, OPPE Bob Holloway, OSW Dave Cleverly, ORD Sonya Sasseville, OSW Stan Durkee,ORD Bill Petersen, ORD Dona Schewede, ORD David Layland, OSW	Matt Lorber, CHAIR, ORD Chuck Maurice, Region 5 Carol Braverman, Region 5 Rick Mattick, OPPTS Glen Rice, ORD Bob Ambrose, ORD Mark Mercer, OSW Norma Whetzel, OW Tom Murray, OPPTS Alec McBride, OSW	John Schaum, CHAIR, ORD Chuck Maurice, Region 5 Carol Braverman, Region 5 Rick Mattick, OPPTS Glen Rice, ORD Larry Burnes, ORD Steve Kroner, OSW Fred Talcott, OPPE Dave Cleverly, ORD Stan Durkee, ORD Dave Jaquith, OPPTS Don Rodier, OPPTS Al Rubin, OW Warren Peters, OAQPS Dorothy Canter, OSW Christine Dibble, OSW

ORD: Office of Research and Development
OSW: Office of Solid Waste
OAQPS: Office of Air Quality, Planning and Standards
OPPTS: Office of Prevention, Pesticides and Toxic Substances
OPPE: Office of Policy, Planning and Evaluation
OW: Office of Water
OSPRE: Office of Science, Planning and Regulatory Evaluation
OHEA: Office of Health and Environmental Assessment
OPPT: Office of Pollution Prevention an Toxics

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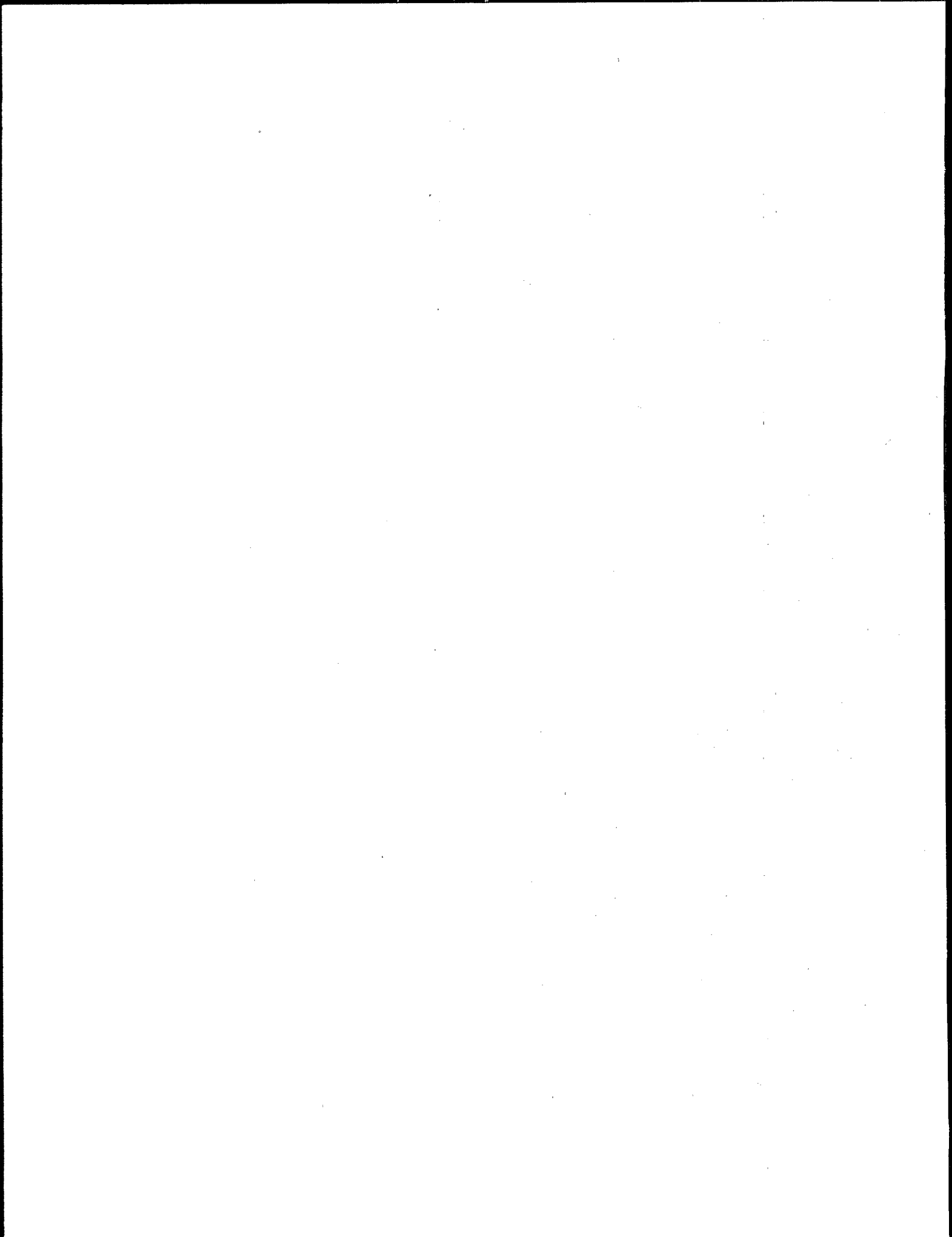
I. Introduction

As discussed in the Preface, this "Addendum" represents the deliberations of a working group established to review Agency guidance on conducting indirect exposure assessments. The workgroup decided that the document *Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions* (EPA, 1990a; available through the Center for Environmental Research Information at 513-569-7562; this document will hereafter be referred to as the Indirect Exposure Document) is largely appropriate for current needs, although updates are needed in some areas. The purpose of this Addendum is to detail those changes.

The most significant modifications that are being recommended to the 1990 report are in the following areas:

- Air dispersion and deposition modeling. The workgroup recommends that Chapter 3 of the Indirect Exposure Document, Air Dispersion and Deposition of Emitted Pollutants, be replaced with a revised Chapter 3 given in this Addendum. This chapter describes the use of an updated version of the COMPDEP model.

- Surface water impacts. The workgroup recommends that Section 9.2 of Chapter 9, titled Surface Water, be replaced with a revised Section 9.2 given in this Addendum. This revised section describes a single framework for evaluating surface water impacts to replace the three-tier approach given in the Indirect Exposure Document.

- Incorporation of Agency risk assessment policies. This Addendum includes the policies described in the February 26, 1992, Deputy Administrator memorandum "Guidance on Risk Characterization for Risk Managers and Risk Assessors" (Habicht, 1992) to identify high end and central tendency exposures be followed in conducting indirect exposure assessments.

In addition to the major changes noted above, there are other recommended changes, some of which may have significant effects on the exposure assessment results for different constituents.

I.1. Use of the Addendum as a Screening Tool

The workgroup recognized the need for a "screening" level methodology so that individuals assessing stack emissions can get a rapid evaluation which can simply answer the question as to whether or not a more detailed site-specific assessment is warranted. For example, if an incinerator is expected to be operating for only a number of months rather than years, it may be possible that indirect impacts are negligible. Similarly, if there are no farm sites (where animals are raised for food, e.g.) for tens to hundreds of miles from the incinerator, it may also be possible that farm-related indirect exposures are negligible. A screening tool could begin to more clearly define the focus of a site-specific indirect exposure assessment.

The 1990 Indirect Exposure Document as well as this addendum were not developed for purposes of this type of simple screening. The workgroup does recommend that efforts should be undertaken to develop screening tools.

This addendum does, however, provide some generalized guidance on limiting the scope of an assessment. Section 3.2 in the revised Chapter 3 of this addendum presents a comprehensive list of contaminants to consider for indirect impacts, and then provides generalized guidance on narrowing this list by considering, for example, feedstock materials, emissions from surrogate incinerators, availability of health-related parameters, estimated emission rates, potential for bioaccumulation, and so on.

While this guidance for contaminant selection can assist in narrowing the scope of an assessment, a second objective for a screening level tool is to reduce the complexity of the modeling procedures. Some additional thoughts on how to reduce this complexity include:

1) Use simplified atmospheric transport models to determine an air concentrations and depositions at a site where indirect exposures could occur, such as a farm.

2) Apply concentrations and depositions to a "screening scenario". This scenario could contain all the fate, transport, and transfer algorithms that are in this Addendum and the 1990 Indirect Exposure Document. It one were to use all the algorithms in these two documents, one would have to carefully consider all parameter selections. A host of parameters are involved in estimating exposure media concentrations, and a second group considers patterns of human exposure. Depending on the intended user or audience of this "screening scenario", all parameter assignments could adhere to a "high end" or "bounding" objective. If the final estimated risk passes one or more "screens", then there may be technical grounds to conclude that further evaluations pertinent to those screens are unnecessary.

I.2. Implementation of the Guidance

This guidance focusses on providing appropriate site-specific procedures for conducting indirect exposure assessments of emissions from combustion sources. The material also includes some information on individual parameter assumptions and other specific factors to consider. However, a number of the assumptions needed to complete an indirect exposure assessment may vary depending on the specific application or program involved. Therefore, decisions are still required in applying this guidance in different situations.

Also, given the long chain of calculations and accompanying parameter assumptions needed to evaluate some of the indirect exposure routes, it is very important that the exposure assessment include a detailed description of all of the uncertainties involved and how they may affect the final results.

I.3. Future Guidance Documentation

The workgroup also discussed long term goals pertaining to guidance for indirect exposure assessments. One is to update the 1990 IED with the information in this addendum to produce a single methodology document. This Addendum does not update the example calculations presented in the 1990 IED for cadmium and benzo-a-pyrene, and this updating would occur for the next full version of the IED. A second is to produce an

accompanying parameter guidance document. While the 1990 IED and this Addendum do contain a substantial amount of information on parameter assignment, the workgroup still recognizes a need for additional guidance, particularly for chemical-specific parameterization. Finally, the workgroup recognizes the need for a computer software tool to accompany the atmospheric modeling tools, such as the COMPDEP model. Key aspects of such a software tool are discussed in Part III of this Addendum. A parameter guidance document would be the companion to such a software tool.

I.4.   Addendum Format

The remainder of this Addendum is structured as follows. The section following this introduction is titled, "II. Indirect Exposure Document Discussions by Chapter". This section reviews each of the 15 chapters of the 1990 Indirect Exposure Document, providing replacements for Chapters 3 and Section 9.2 of Chapter 9. Other than these replacements, the section headings were numbered to exactly correspond to the 1990 document. For example, "2.4 Defining the Exposed Individual" below discusses issues with material in Section 2.4. Defining the Exposed Individual in the 1990 Indirect Exposure Document. The title of the third major section of this Addendum describes its purpose, "III. Recommendations for Long-Term Improvment of Multimedia Risk Modeling". Appendix A derives the calculation for estimating population risks for food consumption pathways.

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II. Indirect Exposure Document Discussions by Chapter

2. HUMAN EXPOSURE SCENARIOS

[Note: The following issue and associated conclusions/recommendations apply broadly to all Sections of Chapter 2.]

Issue   Since the Indirect Exposure Document was published, the Agency has issued new Exposure Guidelines (EPA, 1992a) which establish a new set of definitions and development strategy, for exposure scenarios. Therefore, updates are needed to achieve consistency with these Guidelines.

Conclusions/Recommendations

General Approach

A risk assessment should provide several different descriptors of risk, including both individual and population risks. Individual risks should be presented as both central tendency and high end estimates (see EPA, 1992a,1992c) for the population affected by the combustor. In addition, the number of people at various exposure/risk levels should be presented. Population risks should be expressed in several ways, also. For carcinogens, risks may be presented as the potential number of health effect cases in the affected population (either yearly, or over a longer period such as the projected life of the combustor). For non-carcinogens, long-term population risk can be presented as a number of persons whose exposure or dose exceeds the RfD, or number of persons whose exposure might exceed an acute effect threshold (if known). For both carcinogens and non-carcinogens, specific subgroups of the population should be highlighted, either because they are of interest (e.g., schoolchildren), or because of potentially high exposure/risk (e.g., subsistence farmers).

Defining the Population

Because Agency guidance on exposure/risk assessment calls for characterization of "high end" individual exposure/risk (EPA, 1992a), it is critical that the population be

defined appropriately. Since the "high end" is defined as roughly the top ten percent of the population in terms of exposure or risk, inclusion of large numbers of non-exposed persons in the population can skew the high-end (and mean) value downward, while ignoring lesser-exposed persons can have the opposite effect.

On the other hand, it is very important that the population be defined in such a way that it is clear whether any given individual is "in" or "out" of the population being considered. Defining the population as "anyone exposed to any chemicals from the combustor" is not particularly useful, since for any given individual, it is unclear whether they are "in" or "out," and therefore, it is very difficult to arrive at a population size. Geographical boundaries and activity-related criteria can serve a useful purpose here. If the population is defined as "all those who live or work within [some specific] boundaries," these are relatively straightforward criteria that can be used to define the size of the population being evaluated.

One option for setting boundaries for the study area is to set a fixed distance from the combustor, such as 20 km or 50 km, and draw a circle around the combustor with the specified radius. This is not the optimum method for defining the population, however. Although it may be quick and easy for a mathematical model to handle (an advantage), it is crude. Not only can this procedure result in inclusion of many unexposed or negligibly exposed persons in the study population (or exclude relevant population), but it can result in a great deal of unnecessary work. When detailed land-use and population-activity data are collected, it is important to avoid collecting information for wide geographical areas where little or no exposure occurs.

A second option for setting boundaries is to focus on an area for which individual risks may be above some specified level of concern. This has the advantage of excluding persons outside the boundary from the study (with some important exceptions noted below). This may save considerable time as the risk assessment is being done, since data collected for land use, personal activities, etc. inside the boundary would all be important to the assessment. A potential disadvantage of this method is that the "study area" may be misinterpreted as the "area at risk." Since the boundary is not circular (i.e., geographically arbitrary), but corresponds to a site-specific concentration/deposition

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isopleth from a model, the meaning of the boundary requires explanation. The area circumscribed by the boundary is the area for which further study will be done concerning those who live and work, and not a "high risk zone." Although this option may involve some additional "upfront" work to set up the analysis (relative to the first option), it should save work later, and result in a more useful risk assessment. When defining the "study area", one must be aware that different constituents and/or exposure pathways could result in different "study areas". A problem which may result with this approach, is that each constituent/pathway could result in a different "study area."

It is generally best to define the population potentially affected by the combustor rather than those in an arbitrary circle. Defining the study population as those potentially affected by the combustor can be done by looking at the persons living and working within the isopleth boundary, and then adding other persons outside the boundary who are potentially affected by water-related and other exposures.

Determining the Boundary of the Study Area for Individuals Potentially Exposed as a Result of Deposition/Dispersion

Until more experience with indirect exposure modeling is gained, a trial and error approach is recommended for defining the boundaries of the study area. The first step in this approach is to run the dispersion/deposition models out to a distance of 20 to 50 km. Then examine the risks at the outer isopleth based on the pathway and activities thought to pose the highest potential for risk. If the risk exceeds a level of concern, then extend the modeling out further and recheck the risks. (Note: Extending the study area beyond 50 km may require the application of long-range atmospheric transport models.) Eventually the isopleth corresponding to the specified level of concern will be determined and this will define the study area. The final decision on how to most efficiently conduct this trial and error procedure is probably best determined by the modeler who can evaluate the costs/time of running the model for various amounts of output. If risks in the outer ring are estimated to be above the concern level during the subsequent detailed analysis (considering all chemicals and pathways), the study area will need to be expanded.

Establish Isopleth Rings Within the Outer Boundary Isopleth Ring

Several rings or just a few additional isopleth rings can now be established within the outer boundary isopleth ring. Further analysis (as will be described below) now can focus on activities and individuals between isopleth rings. The width between these rings around the combustor stack depends on several things. First, the difference in concentration/deposition values between isopleths should be meaningful. Second, the ability of the computer software to quickly and conveniently draw isopleths may limit the number of isopleths mapped. In general, it may be helpful to construct isopleths at a somewhat more detailed level than necessary for the ensuing exposure analysis.

Figure 2-1 is a simple representation the outer boundary of a hypothetical study area and the isopleth rings within the study area. The individuals who lie within the study area as defined by the outer isopleth ring form the basic segment of the population to be evaluated, and will generally be evaluated for all appropriate pathways. Certain individuals who live outside the study area boundary should be added. These are discussed below.

Additional Individuals Potentially Exposed Through Intermittent Presence Within the Study Area Boundary

Individuals who work, attend school, or otherwise spend significant amounts of time within the study area boundary, even though they do not live within the boundary, should also be evaluated and included in the basic population studied. These include individuals potentially exposed by water-related routes and individuals potentially exposed through food ingestion.

Defining the Population for Study

In summary, addition of the various segments noted above will result in a population "potentially affected by the combustor" (hereafter called the **study population**). The study population consists of:

- persons living, working, or otherwise spending significant amounts of time
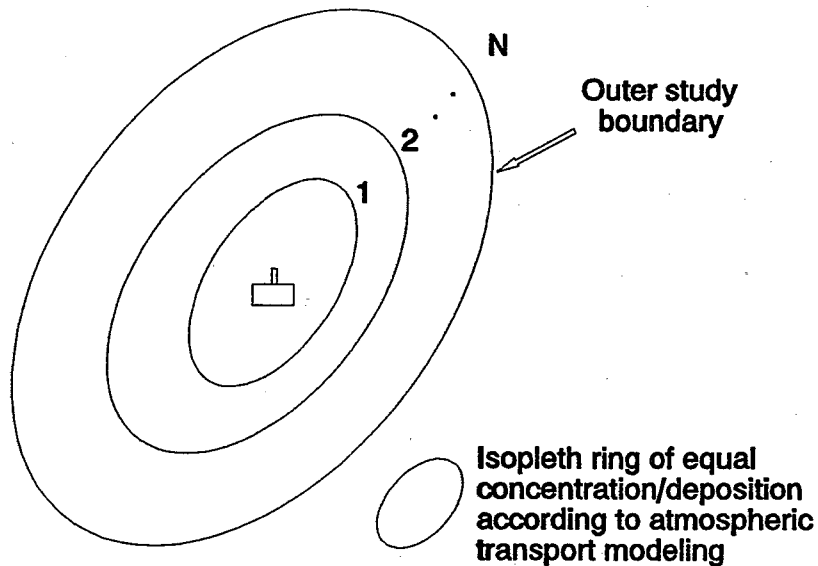
Figure 2-1. Simple representation of outer isopleth ring defining study area and isopleth rings within study area.

within the "study area boundary" defined through dispersion/deposition modeling;

- persons potentially exposed to non-negligible amounts of chemicals (emitted from the combustor) by water-related means; and

- persons potentially exposed to foodstuffs contaminated by the combustor emissions with non-negligible concentrations.

Developing Distributions of Individual Risk

The goal of this step is to assign an exposure (and risk) to the individuals within the

study population. This is done by considering exposure concentrations and activities. By the combination of concentration and activities, along with other appropriate dose-response or toxicological information, individual risk estimates can be made. The full procedure described below can become quite complex and resource intensive. Therefore, the assessor should attempt to reduce the scope of this effort in terms of chemicals and pathways. One way to do this is to make bounding type assessments using maximum exposure parameters applied at points of maximum concentrations or depositions. If these bounding assessments demonstrate risks below a concern level, then the associated chemicals and pathways can be safely eliminated from further study.

One can start in this process of assigning risk estimates by using isopleths of constant concentration/deposition, and differentiating among activities (e.g., starting with one isopleth and grouping the individuals by activity, such as farmers, residents with home gardens, residents without home gardens, non-resident workers, etc.). The following list of suggested steps in assigning risk estimates assumes constant concentration/deposition isopleths will be used as a basis (if emission rates and resulting concentration/deposition isopleths are likely to be changing over time, then these steps can be applied to time periods during which the emissions are relatively constant and summed to get the total exposure):

1. First, using the methodology presented in this document, compute contaminant levels in media of concern (e.g., air, water, soil, groundwater, beef, fruit/vegetables, milk, etc) for each ring. This information can be conveniently summarized on a table such as Table 2-1, or kept in a spreadsheet. To the extent possible the model inputs should be based on local information. Considerable uncertainty is likely to be associated with these estimates. See Chapter 15 for further information on how to assess this uncertainty.

2. Next, overlay isopleths onto aerial photographs, population maps, land use maps, etc. to identify the types of activities and numbers of people in each

Table 2-1. Example table for media levels.					
	Ring 1	Ring 2	Ring 3	Ring 4	Ring 5
Air (μg/m^3)					
Soil (μg/g)					
Surface water (mg/L)					
Beef (mg/kg)					
Milk (mg/L)					
Fish (mg/kg)					
Vegetables (mg/kg)					
Others					

ring. Several PC based models are available for generating populationdensity maps based on Census data including the Human Exposure Model from the Office of Air Quality Planning and Standards and the Geographic Exposure Modeling System from the Office of Prevention, Pesticides and Toxic Substances. Geographic Information Systems (GIS) could be used to identify land use, complex terrain, and population centers. Some of these systems use old Census data and it would be more accurate to use the TIGER files from the most recent census. Satellite photographs may provide the most recent information. Local surveys may also help locate farms and home gardeners.

3.   For each isopleth ring, estimate the number of farmers, residents with home gardens, other residents, and other groups defined in the study population (such as intermittently-exposed non-resident workers). Also, for each ring locate schools, fishing areas and other areas where unusual exposure may occur. Also estimate the number of school children (and where they go to school), and the number of people in any other special interest group like subsistence fishermen, developments for retired people, etc. This information could also be kept in a spreadsheet.

4.   For each isopleth ring and population group, determine which exposure pathways apply. Characterize behavior parameters for each pathway, e.g., ingestion rate, exposure duration, etc. This information can be summarized in a table such as Table 2-2, or stored in a spreadsheet. The level of detail used in characterizing behavior is dictated by the amount of data which is available or could be collected. Theoretically, each person in the ring could be surveyed and behavior identified, but this is clearly impractical in most situations due to the size of the population and resources available. However, even a limited (statistically-based) local survey can be quite informative and is highly recommended. Some options in order of increasing detail level are offered below for how to approach this problem:

   a.   Select the parameter values that represent best judgement of central values for current conditions of the groups identified above.

   b.   Divide each group into a low, medium or high exposure level and select the parameter values for each. The number of people in each subgroup should also be identified.

   c.   Assume statistical distributions for the parameter values in each group.

5.   The next step is to compute exposures and compile results. The results can

Table 2-2. Example exposure parameters for an isopleth ring within the study area.

	Gardeners	Other Residents	Farmers	School Children
Population size				
Residence time (yr)				
Soil ingestion: RATE (mg/d) FREQ (d/yr)				
Inhalation: RATE (m^3/d) FREQ (hr/d)				
Water ingestion: RATE (L/d) FREQ (d/yr)				
Beef Ingestion: RATE (g/d) FREQ (d/yr) percent local				
Milk Ingestion: RATE (g/d) FREQ (d/yr) percent local				
Fish Ingestion: RATE (g/d) FREQ (d/yr) percent local				
Vegetable ingestion: RATE (g/d) FREQ (d/yr) percent local				

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be displayed in a variety of ways. Cumulative distributions (exposure or risk vs number of people) are useful for identifying central and high end exposure levels. A frequency distribution showing number of people exposed at various exposures or risk levels is a particularly effective way to communicate the results of the analysis. These distributions can be based on the entire study population or individual special interest groups such as farmers, gardeners, school children, etc. A variety of options are available for creating these distributions. If exposure parameters can be expressed as distributions, then a Monte Carlo simulation is probably the best approach. This approach would involve using a frequency histogram of number of people in each ring (based on information generated in Steps 2 and 3) to select a location and associated media concentrations for each iteration. It is important to separate uncertainty and variability in the assessment and to clearly show support for all distributions selected. Further guidance on these issues and other aspects about how to conduct Monte Carlo analysis is provided in Chapter 15 of this document. If it is not feasible to conduct a Monte Carlo analysis, a series of point estimates can be used to approximate the distribution. As discussed in Step 4, local surveys could be used to characterize consumption rates of local grown foods, frequency and duration. For example if the surveys support generation of a low, medium and high consumption rate for farmers and the isopleth construction generates 5 rings, then 15 point estimates of exposure could be made and plotted vs number of farmers. This yields an approximation of the distribution. Since three consumption rates do not represent the full range of variability, upper percentiles will be underestimated and lower percentiles will be overestimated to some degree. Judgement will need to be decide if this uncertainty is acceptable.

6.   In addition to presenting the distributions of exposure, the assessor should highlight individual exposure/risk estimates

for several locations (i.e. maximum deposition, place where most people exposed, schools, etc.) and subpopulations of interest (i.e. subsistence farmers, recreational and subsistence anglers, nursing infants, ethnic groups or any other population segment with unusually high exposures). These scenarios could be charaterized using a central or range of exposure values combined with an estimate of the number of people in the group.

This effort should first focus on characterizing behavior describing exposure that occurs at a person's residence. A second step is to consider exposure that occurs outside his residence. Certain activities may involve exposure from a ring different than his residence. For example, a child may attend school in a different ring or an adult may eat food grown in a different ring or fish in a different ring. In later refinements, evaluation of how these parameter values and group sizes may change in future may be desired.

Note: Issues associated with characterizing population risk are discussed in association with Chapter 15, Risk Characterization.

2.3 Defining the Length of Time of Emissions

Issue There are no procedures suggested for addressing short term exposures from upset or intermittent emissions.

Conclusions/Recommendations

Occassional short-term releases are generally not an issue for indirect exposure analyses, since long-term buildup in the food chain is the principal concern for indirect exposure. The accumulation of short-term releases can be averaged and added to the continuous emissions if data are available to do so. However, short-term releases should be evaluated for potential acute effects as part of the direct exposure assessment. The highest inhalation exposures are associated with periods of highest air concentrations. Inversions or other unusual meteorologic conditions causing stable air minimize dispersion and can lead to unusually high air concentrations. Increases in emission rates also

increase air concentrations. As discussed in Chapter 3, the air model can estimate the highest daily air concentration expected to occur during a year. The model output is normalized by emission rate. So the highest expected emission rate can be combined with daily high model output to estimate the highest short term exposure level. This short term exposure level can be compared with acute exposure standards.

2.4 Defining the Exposed Individual

Issue   The Indirect Exposure Document suggests that impacts from combustors are negligible outside a 50 km radius. This is somewhat arbitrary and should be considered on a site-specific basis.

Conclusions/Recommendations

As previously discussed, the study area should be defined by calculating risks from the most important exposure route out to a distance where those risks are no longer of concern. The beef pathway could be the most sensitive for dioxin, but, if emissions of mercury are the main concern, then the fish and shellfish pathway may be the important one.

Issue   Section 2.4.4 of the Indirect Exposure Document discusses the use of mobility and length of residency statistics to select the duration of exposure. The discussion points out that more than half (about 60 percent) of the moves recorded by the Census Bureau were local moves within the same county. Therefore, many individuals who move may remain within the study area and continue to be exposed. The discussion also points out that different populations are characterized by different residency times in a single dwelling, e.g. farmers vs. homeowners vs. tenants. However, the Indirect Exposure Document does not discuss the recommendation in the Exposure Factors Handbook (EPA, 1989b) to use a central tendency estimate for exposure duration of 9 years and a high end estimate of 30 years based on mobility statistics. More discussion is needed about whether these estimates need revising on the basis that many of the moves may be within the study area.

Conclusions/Recommendations

Local census data may be used to determine appropriate values of the duration of exposure for the local population and population subgroups of concern, particularly when supplemented with site-specific surveys. Otherwise, the recommendation is to continue to use the 9 year and 30 year default values. Shorter time periods may be applicable in consideration of the expected life of the facility or duration of the burn (in the case of a mobile incinerator). However, the assessor should consider that indirect exposures may continue after emissions stop due to accumulation of contaminants in soil and other media.

2.5 Pathways of Human Exposure

Issue The Indirect Exposure Document does not address exposure through breast milk.

Conclusions/Recommendations

Procedures have been developed for estimating contaminant levels in human breast milk on the basis of the contaminant intake by the mother. Such procedures have been developed by Smith (1987) and Sullivan et al. (1991) and are also presented in the Dioxin Exposure Document (EPA, 1992c). The approach by Smith assumes that the concentration in breast milk fat is the same as in maternal fat and can be calculated as:

$$C_{milkfat} = \frac{m\ h\ f_1}{0.693\ f_2} \qquad [2\text{-}1]$$

where:

$C_{milkfat}$	=	concentration in maternal milk (pg/kg of milk fat)
m	=	average maternal intake of dioxin (pg/kg of body weight/day)
h	=	half-life of dioxin in adults (days)
f_1	=	proportion of ingested dioxin that is stored in fat
f_2	=	proportion of mother's weight that is fat (kg maternal fat/kg total body weight)

Although this procedure was developed for application to dioxin, it would be

applicable to other lipophilic organics if the chemical specific inputs can be established. This steady-state model assumes that the contaminant levels in maternal fat remain constant. Though not described here, Smith (1987) also presents more complex approaches which account for changes in maternal fat levels during breast feeding. The model developed by Sullivan et al. (1991) is a variation of the models proposed by Smith (1987). The Sullivan model considers changes in maternal fat levels and predicts chemical concentrations in milk fat as a function of time after breast feeding begins. The model proposed by Smith assumes that infant fat concentration at birth is zero, whereas Sullivan assumes that the infant fat concentration at birth is equal to the mother's fat concentration.

By way of illustration, the half-life of 2,3,7,8-TCDD in humans is estimated to be 5 to 7 years, as discussed in the Dioxin Exposure Document (EPA, 1992c). For the purpose of this preliminary analysis, it is assumed that a 7-year half-life applies to all of the dioxin-like compounds. Smith (1987) suggests values of 0.9 for f_1 and 0.3 for f_2. Using these assumptions and a background exposure level of 1 to 3 pg of TEQ/kg-d (derived from diet analysis, see EPA, 1992c), the concentration in breast milk fat is predicted to be about 10 to 30 ppt of TEQ, which agrees well with the measured values.

Using the estimated contaminant concentration in breast milk, the dose to the infant can be estimated as follows:

$$ADD_{infant} = \frac{C_{milkfat}\ f_3\ f_4\ IR_{milk}\ ED}{BW_{infant}\ AT} \qquad [2\text{-}2]$$

where:

ADD_{infant}	=	average daily dose to the infant (pg/kg/d)
IR_{milk}	=	ingestion rate of breast milk (kg/d)
ED	=	exposure duration (yr)
BW_{infant}	=	body weight of infant (kg)
AT	=	averaging time (yr)
f_3	=	fraction of fat in breast milk (dimensionless)

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f_4 = fraction of ingested contaminant which is absorbed (dimensionless)

This approach assumes that the contaminant concentration in milk represents the average over the breast feeding time period. If the dynamic models mentioned above are used, the dose can be estimated using an integration approach to account for the changes in concentration over time.

Smith (1987) reports that a study in Britain found that the breast milk ingestion rate for 7 to 8 month old infants ranged from 677 to 922 mL/d and that a study in Houston measured the mean production of lactating women to range from 723 to 751 g/d. Smith (1987) also reports that breast milk ingestion rates remain relatively constant over time while the infant is breast feeding, that the milk can be assumed to have a 4 percent fat content, and that 90 percent of the ingested contaminant is absorbed. The National Center for Health Statistics (1987) reports the following mean body weights for infants:

6-11 mo:	9.1 kg
1 year:	11.3 kg
2 yr:	13.3 kg

Using Equation [2-2] to evaluate the importance of breast feeding and assuming that an infant breast feeds for one year, has an average weight during this period of 10 kg, ingests 0.8 kg/d of breast milk and that the dioxin concentration in milk fat is 20 ppt of TEQ, the ADD to the infant over this period (i.e., AT = 1 yr) is predicted to be about 60 pg of TEQ/kg-d. This value is much higher than the estimated range for background exposure to adults (i.e., 1 to 3 pg of TEQ/kg-d). However, if a 70 yr averaging time is used, then the LADD (Lifetime Average Daily Dose) is estimated to be 0.8 pg of TEQ/kg-d which is near the lower end of the adult background exposure range. On a mass basis, the cumulative dose to the infant under this scenario is about 210 ng compared to a lifetime background dose of about 1700 to 5100 ng (suggesting that 4 to 12 percent of the lifetime dose may occur as a result of breast feeding). Traditionally, EPA has used the

LADD as the basis for evaluating cancer risk and the ADD (i.e., the daily exposure per unit body weight occurring during an exposure event) as the more appropriate indicator of risk for noncancer endpoints.

The simplified procedure described above contains a number of uncertainties. A tendency toward overestimates of the dose to the infant is caused by the assumption that reductions do not occur in maternal fat levels during breast feeding. Sullivan et al. (1991) estimates that the steady-state assumption may lead to overestimates of 20 percent. Uncertainty is also introduced by the assumption that the assumed half-life rate and partitioning factors apply to all the dioxin related compounds. Although these properties are likely to be similar among the various congeners, some variation is expected. It is unknown whether the net effect of these uncertainties would lead to over or under estimates of dose. However, the simple model appears to provide reasonable predictions of background levels found in breast milk and was judged adequate for purposes of a preliminary analysis.

Travis et al. (1988) presented an alternative approach to estimating breast milk contaminant levels. They proposed a biotransfer approach:

$$C_m = B_m I \qquad [2\text{-}3]$$

where:

C_m = contaminant concentration in breast milk (mg/kg)

B_m = biotransfer factor for breast milk (kg/d)

I = maternal intake of contaminant (mg/d)

They also argue that the biotransfer factor is primarily a function of the octanol-water partition coefficient (K_{ow}) and developed the following geometric mean regression:

$$B_m = 6.2*10^{-4} \ Kow \qquad [2\text{-}4]$$

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This regression was derived from data on 6 lipophilic compounds (log K_{ow} range: 5.16 to 6.5), but did not include any dioxins or furans. Assuming a log K_{ow} of 6.6 for 2378-TCDD, a B_m of 3700 kg/d is predicted. Combing this value with a maternal intake of 10 pg/d (or 10^{-7} mg/d), a breast milk concentration of 37 ppt is predicted. This prediction is about 10 times higher than what has been measured in the U.S. Thus, this approach does not appear to work as well as the earlier approach suggested by Smith et al (1987). It is recommended that assessors first try to apply the Smith approach and if model inputs cannot be found then use the approach developed by Travis et al. (1988).

Issue Placental transfers are not addressed in the Indirect Exposure Document.
Conclusions/Recommendations

This is an area which requires research to develop a methodology.
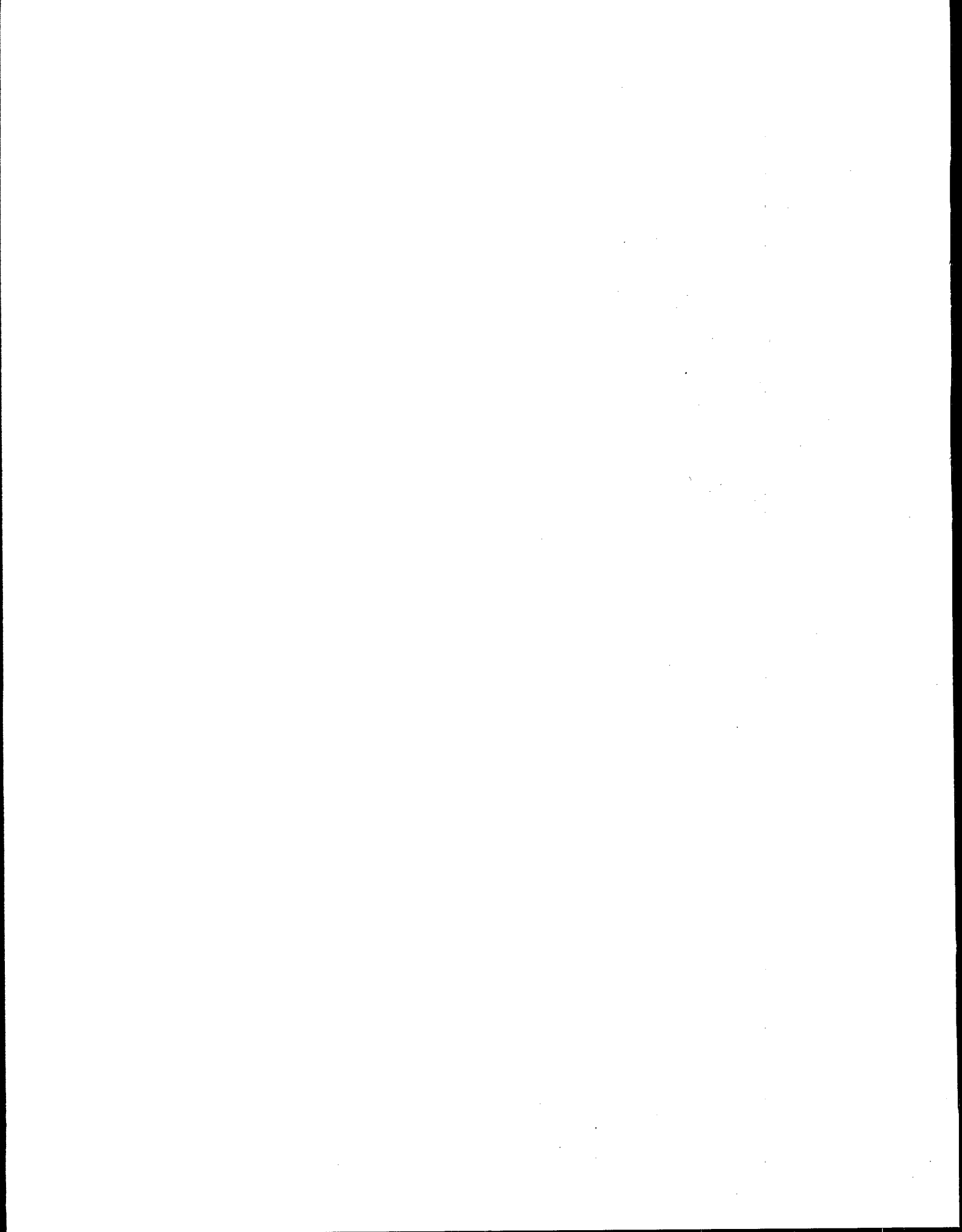
[The following is offered as a replacement for Chapter 3 of the Indirect Exposure Document. This alternative has been developed by David Cleverly of the Exposure Assessment Group, and Donna Schwede and Bill Peterson of the Atmospheric Research and Exposure Assessment Laboratory. Care has not been taken to make the units or parameter names consistent with other chapters of the Indirect Exposure Document. However, the units are internally consistent.]

3. AIR DISPERSION AND DEPOSITION MODELING OF THE POLLUTANT STACK EMISSIONS

3.1. BACKGROUND AND PURPOSE

Estimation of human health risks associated with exposures to air releases of contaminants from combustors requires estimates of the atmospheric concentrations and annual deposition rates of the emitted materials in the areas around the combustion facility. It has been customary for EPA to use air dispersion/deposition models to estimate the atmospheric transport, the surface deposition flux, and the ambient air concentrations of specific compounds attributable to smokestack emissions from an industrial combustion source. Air dispersion models are mathematical constructs that approximate the physical and chemical processes occurring in the atmosphere that directly influence the dispersion of gaseous and particulate emissions from the stack of a combustion source. These models are computer programs encompassing a series of partial differential and algebraic equations that calculate the dispersion and deposition of the emissions. Concentration and deposition isopleths of the contaminants discharged from the stack are computed at specified distances from the source. These quantities are used to estimate the magnitude of potential exposures to the human receptor, and to estimate the potential human health risks in populations living and working in the vicinity of the stationary combustion source.

The Agency's Guideline on Air Quality Models (EPA, 1993a) has identified numerous air dispersion/deposition models that may be applied to the analysis of source emissions. This chapter focuses on the COMPDEP model, which is recommended by the Working Group as a currently available air model appropriate for use in the analysis of

indirect exposures from combustor emissions. Efforts are currently underway to create an updated air transport model, which will be called ISC-COMPDEP. This model is a merger of parts of the ISC2 and COMPLEX 1 model. Further model development is discussed is Part III of this Addendum.

COMPDEP was first described in the Indirect Exposures Document. Recent revisions to the computer code have been made, creating an updated version. A principal change that was made allows the user to define up to 10 particle size categories in the analysis of the surface deposition of contaminants that are bound to particulates in the emissions.

The purposes of this Chapter are to: a) compile a comprehensive list of pollutants which may potentially occur in the stack emissions from the incineration and combustion of waste materials, b) present a hierarchical approach for determining contaminants to evaluate in a site-specific indirect exposure assessment, c) derive representative emission rates of the pollutants for air modeling purposes, including long-term average emissions, and short-term emissions that may result from perturbations, upset conditions, and startup and shutdown in operations, d) describe the COMPDEP model and associated wet and dry deposition algorithms, and, e) to describe procedures for applying the COMPDEP model using vapor phase and particulate phase partitioning of the emitted pollutants, and a specific particle size distribution of particulate matter.

3.2   SELECTING TOXIC AIR POLLUTANTS

The first step in the analysis of indirect exposures is the identification and selection of pollutants that may be emitted to the air during the combustion of anthropogenic waste materials. This selection process should focus on chemicals that are potentially toxic to humans, and that have a definite propensity for bioaccumulating or bioconcentrating in the human and ecological food chains.

As the initial step in the selection process, a comprehensive list of compounds that have been detected in combustor emissions is shown in Tables 3-1, 3-2, and 3-3. These tables list potentially toxic organic and inorganic contaminants that may be subject to the human health risk assessment associated with direct and indirect exposures to the

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Table 3-1. Initial list of dioxin-like compounds identified in emissions from the incineration and combustion of anthropogenic wastes.

Chlorinated Dibenzo-p-dioxins (CDDs)	Chlorinated dibenzofurans
2,3,7,8-TCDD	2,3,7,8-TCDF
1,2,3,7,8-PentaCDD	1,2,3,7,8-PentaCDF
1,2,3,4,7,8-HexaCDD	2,3,4,7,8-PentaCDF
1,2,3,6,7,8-HexaCDD	1,2,3,4,7,8-HexaCDF
1,2,3,7,8,9-HexaCDD	1,2,3,6,7,8-HexaCDF
1,2,3,4,6,7,8-HeptaCDD	1,2,3,7,8,9-HexaCDF
1,2,3,6,7,8,9-OctaCDD	2,3,4,6,7,8-HexaCDF
Other TetraCDDs	1,2,3,4,6,7,8-HeptaCDF
Other PentaCDDs	1,2,3,4,7,8,9-HeptaCDF
Other HexaCDDs	1,2,3,4,6,7,8,9-OctaCDF
Other HeptaCDDs	Other TCDFs
	Other PentaCDFs
	Other HexaCDFs
	Other HeptaCDFs

Table 3-2. Initial list of organic compounds identified in emissions from the incineration and combustion of anthropogenic wastes (key follows).

Organic compounds	RfD[a]	RfC[b]	Carc[c]	Ref.
Acetonitrile	+;L	+;L	-	1,2
Acrylonitrile	+	+ +	B1;O/l	1,2
Anthracene	+	-	D	1,2
Azobenzene	-	-	B2;O/l	1,2
Benzaldehyde	+;K	-	-	1,2
Benzene	UR	UR	A;O/l	1,2
Benz(a)anthracene	-	-	B2;O	1
Benzo(a)pyrene	-	-	B2;O	1
Benzo(b)fluoranthene	-	-	B2;O	1
Benzo(e)pyrene	-	-	UR	1
Benzo(g,h,i)perylene	-	-	D	1
Benzo(j)fluoranthene	-	-	UR	1
Benzo(k)fluoranthene	-	-	B2;O	1
Benzyl chloride	-	IA	B2;O	1,2
1,1-Biphenyl	+ +;K	IA	D	1,2
Bis(2-chloroethoxy) methane	-	-	D	1
Bis(2-chloroethyl) ether	-	IA	B2;O/l	1
Bis(2-ethylhexyl) phthalate	-	+;L	B2;O/l	2
Bis(chloromethyl) ether	-	IA	A;O/l	1,2
Bromochloromethane	-	-	D	1
Bromodichloromethane	+ +;K	-	B2;O	1
Bromomethane	+ +;Ne	+ + +;Ne	D	1,2
1,3-Butadiene	-	-	B2;l	1
Butyl benzyl phthalate	+;L	-	C;O	1,2
Captan	+ + +;De	UR	UR	1
Carbon disulfide	+ +;De	UR	-	1
Carbon tetrachloride	+ +;L	-	B2;O/l	1,2
Chlorobenzene	+ +;L	UR	D	1
Chlorocyclopentadiene	-	-	D	1
Chloroform	+ +;L	UR	B2;O/l	1,2
Chloromethane	UR	UR	UR	1
Chrysene	-	-	B2;l	1
Cumene	+;K	+;Ne	-	1,2
Di(2-ethylhexyl)phthalate	+ +;L	-	B2;O	1
Dibenzofuran	-	UR	D	1,2
Dibenzo(a,e)fluoranthene	-	-	UR	1
Dibenzo(a,h)fluoranthene	-	-	B2;l	1
1,2-Dibromo-3-chloropropane	-	+ +;Rsp	UR	1
Dibutyl phthalate	+	IA	D	1
1,2-Dichlorobenzene	+;L	-	D	1,2
1,3-Dichlorobenzene	UR	-	D	1,2
1,4-Dichlorobenzene	-	UR	-	1,2

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Table 3-2. (continued)

Organic compounds	RfD[a]	RfC[b]	Carc[c]	Ref.
1,1-Dichloroethane	UR	UR	C;O	1,2
1,2-Dichloroethane	-	-	B2;O/I	1
1,1-Dichloroethylene	++;L	UR	C;O/I	1,2
Dichloromethane	++;L	UR	B2;O/I	1
2,4-Dichlorophenol	+;Im	-	-	1,2
Dimethyl phthalate	UR	IA	D	1
1,4-Dioxane	-	-	B2;O	1
Ethyl benzene	+;LK	+;De	D	1,2
Fluoranthene	+;L	-	D	1
Formaldehyde	++;L	-	B1;I	1
Hexachlorobenzene	++;L	IA	B2;O/I	1,2
Hexachlorobutadiene	+;L	-	C;O/I	1,2
Hexachloroethane	++;K	UR	C;O/I	1,2
Methyl mercury	++;Ne	-	-	1
Methylene bromide	+	-	-	2
Methyl ethyl ketone	+;De	+;De	D	1,2
Naphthalene	UR	-	D	1,2
Pentachlorobenzene	+;LK	-	D	1,2
Pentachlorophenol	++;LK	UR	B2;O/I	1,2
Phenol	+;De	IA	D	1,2
Polychlorinated biphenyls	-	-	B2;O	1
Polycyclic organic matter	-	-	UR	1
Pyrene	+;K	-	D	1,2
Styrene	++;L	++;Ne	UR	1,2
1,2,4,5-Tetrachlorobenzene	+;K	-	-	1,2
1,1,1,2-Tetrachloroethane	+;K	-	C;O/I	1
1,1,2,2-Tetrachloroethane	UR	-	C;O/I	1
Tetrachloroethylene	++;L	-	UR	1,2
Toluene	++;LK	++;Ne	D	1,2
1,2,4-Trichlorobenzene	++;R	UR	D	1,2
1,1,1-Trichloroethane	WD	UR	D	1,2
1,1,2-Trichloroethane	++	UR	C;O/I	1,2
Trichloroethylene	UR	UR	WD	1
2,4,5-Trichlorophenol	+;L	IA	UR	1,2
2,4,6-Trichlorophenol	-	IA	B2;O/I	1,2
Vinyl chloride	-	-	A;O/I	1,2
m-Xylene	+	UR	-	1,2
o-Xylene	+	UR	-	1,2
p-Xylene	+	UR	-	1,2
Xylenes	++;De	UR	D	1,2

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Table 3-3. Initial list of inorganic contaminants identified in emissions from the incineration and combustion of anthropogenic wastes (key follows).

Inorganic contaminants	RfD[a]	RfC[b]	Carc[c]	Ref.
Antimony	+	-	-	1,2
Arsenic, inorganic	+ +	-	A;I	1,2
Barium	+ +;De	UR	-	1,2
Cadmium	+ + +	UR	B1;I	1,2
Chromium (III)	+	UR	UR	1,2
Chromium (VI)	+	UR	A;I	1
Lead + compounds	+ + +	-	B2,I	1
Manganese	+;Ne	+ +;Rsp	D	1
Mercury, inorganic	UR	UR	D	1,2
Mercuric chloride	UR	UR	-	2
Nickel, soluble salts	+ +;De	UR	D	1,2
Selenium + compounds	+ + +	-	D	1,2
Silver	+	-	D	1
Zinc + compounds	+ +	-	D	1,2

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Key to Tables 3-2 and 3-3

a. RfD is the reference dose defined as the daily ingestion exposure of a contaminant that is likely to be without appreciable risk during a portion of the lifetime.
b. RfC is the reference concentration defined as the daily inhalation exposure of a contaminant that is likely to be without appreciable risk during a portion of a lifetime.
c. Carc. is an abbreviation for carcinogen.
L = Adverse effects on the liver.
K = Adverse effects on the kidney.
De = Adverse developmental effects.
Im = Adverse effects on the immune system.
R = Adverse reproductive effects.
Ne = Adverse effects on the central nervous system.
Rsp = Adverse effects on the respiratory system.
IA = Inadequate data.
UR = Currently under review.
WD = Withdrawn
+ = Low confidence weighing of the supporting scientific information.
+ + = Medium confidence weighing of the supporting scientific information.
+ + + = High confidence weighing of the supporting scientific information.
- = No information.
Group A carcinogen: Human carcinogen (sufficient evidence of carcinogenicity in humans).
Group B carcinogen: Probable human carcinogen (B1 - limited evidence of carcinogenicity in humans; B2 - sufficient evidence of carcinogenicity in animals with inadequate or lack of evidence in humans).
Group C carcinogen: Possible human carcinogen (limited evidence of carcinogenicity in animals and inadequate or lack of human data).
Group D carcinogen: Not classifiable as to human carcinogenicity (inadequate or no evidence).
I = Carcinogenic by the inhalation route.
O = Carcinogenic by the oral route.
Reference 1 = EPA's Integrated Risk Information System (IRIS) on-line database as described in the Federal Register (58 FR 11490) February 25, 1993.
Reference 2 = EPA, 1989d.

combustor emissions. This list includes chemicals identified as most frequently detected and measured in stack emissions from incinerators, boilers, and industrial furnaces combusting hazardous waste, sewage sludge, municipal solid waste, biomass, automobile tires, and medical and hospital waste (Dempsey and Oppelt, 1993; CARB, 1990a,b; CARB, 1991; CAPCOA, 1991; EPA, 1986; EPA, 1988b). To the extent possible, chemical speciation of the various forms of these compounds should be identified. Using these Tables as a starting point, the assessor can narrow the number of compounds of concern for a particular combustor using the following three steps:

STEP 1. Consider the Feed Material Being Combusted

The selection of the chemicals for site-specific analysis will largely depend on the type of waste materials that will routinely be accepted and incinerated at the combustion facility. If chlorine is present in the feed, then it is imperative that chlorinated dioxins and dibenzofurans be evaluated in the exposure assessment. Even if chlorine is not specifically identified in the waste feed, it is recommended that this class of compounds be addressed in the assessment. It may be that only an extremely small concentration of chlorine in the waste is sufficient to participate in the formation of CDDs/CDFs. In addition, combustion air may contain precursor compounds and halides that may cause dioxins to be thermalytically formed. Therefore, it is generally suggested that assessments of waste incineration sources include dioxin-like compounds in the analysis of emissions. Products of incomplete combustion (PICs) will form in the stack gas emissions as a consequence of the incomplete destruction of all organic species leaving the combustion chamber. Therefore, the polycyclic aromatic hydrocarbons (PAHs), i.e. benzo(a)pyrene, will need to be routinely considered. Finally, to the extent a combustion facility accepts and incinerates metal-bearing materials and wastes, the heavy metals having significant toxicologic properties will need to be addressed in the exposure analysis, i.e., lead, mercury and mercury compounds, chromium, cadmium and nickel.

STEP 2. Consider the Availability of Appropriate Toxicological Information

Risk assessments cannot be completed for compounds which lack verified dose-

response relationships for specific health endpoints. Accordingly, such compounds can be eliminated from consideration in an exposure/risk assessment. Tables 3-2 and 3-3 contain information which can assist in a toxicological evaluation, including availability of Reference Doses (RfD), Reference Concentrations (RfC), a confidence rating for RfD and RfC information, characterization of the health impact (impact to liver, kidney, developmental effect, etc.), and the current carcinogenic rating (A through D). The assessor should review the latest version of IRIS to confirm if new chemicals have been added, if additional RfDs, RfCs have been verified, and if the carcinogenicity group classification has been added or updated.

STEP 3. Narrow the List with a Quantitative Ranking Scheme

After following the first two steps above, the long list in Tables 3-1 through 3-3 may be substantially narrowed. However, it may not be necessary to conduct full assessments on the remaining chemicals. Say, for example, a credible ranking scheme could be developed which would rank a list of 50 chemicals (and there are over 90 chemicals listed in Tables 3.1-3.3) from most to least concern. If the detailed site-specific assessment on the 20 chemicals of most concern indicated that chemicals 15 through 20 on the list resulted in negligible indirect health risk, than there would be credible grounds to conclude that chemicals 21 through 50 do not require further indirect assessment. Likewise, if the assessment indicated a health risk of potential consequence for chemicals 15 through 20, then evaluation of more chemicals on the list of 50 would be required. The Risk Assessment Guidance for Superfund (RAGS; EPA, 1989c) suggests a simple linear ranking scheme for focusing on the "most significant" chemicals. This ranking scheme multiples a quantitative toxicity value (slope factor, e.g.) times a quantitative concentration of the contaminant in the exposure media (soil, e.g.). For combustor emissions, the "concentration" term should be replaced with the emission rate of the chemical. Procedures to estimate emission rates are given in Section 3.3 below. A third factor that should be considered is the potential for the chemical to bioaccumulate. Factors indicating bioaccumulation potential include persistence in the environment - more persistence translates to more bioaccumulation - and partitioning tendencies - more

partitioning onto soils and sediments translates to more bioaccumulation. A surrogate factor which can be used for bioaccumulation potential is the logarithm of the octanol-water partition coefficient, denoted as log Kow. The higher the value of the log Kow, the greater is the possibility for partitioning onto soils and sediments. Longer persistence is correlated to tighter sorption to soils/sediments, which is why the log Kow can capture both persistence and partitioning tendencies appropriately.

3.3   ESTIMATING THE STACK EMISSION RATE OF THE TOXIC AIR POLLUTANTS

For the purposes of chemical selection as described above, and for air modeling and exposure assessment, the release rate of pollutants from the combustor stack is expressed in metric units of mass of the pollutant emitted per unit time (e.g., grams/s). The release rate used in indirect exposure assessments should generally be reflective of the expected average emissions from the facility over the long-term (e.g., over the engineered life of the combustion facility).   However, if acute exposures are of concern in the risk assessment, the release rate should be reflective of maximum short-term emissions (e.g., as a result of equipment malfunction, start-up and shut-down, or possible accidental releases). Although mass emission rates can be estimated in any of a number of ways, the following hierarchical order of preference is recommended:

A. *For facilities that are built and operational*, it is preferred that direct stack measurements be used, using EPA recommended chemical-specific (and, wherever possible, species or congener-specific) stack sampling, analytical, and quality control, quality assurance protocols and procedures. Stack monitoring should provide information on the concentrations of the pollutants (e.g., ng/dscm), the actual velocity of stack gas release (m/s), and stack gas temperature (K). In addition, based on the characteristics and heat value of the waste feed, the temperature of combustion, and stoichiometric conditions, the volume of flue gases evolved per unit of time should be estimated (in metric units of dry standard cubic meters per minute at 12% CO_2 or 7% O_2). To calculate a mass emission rate of the pollutant, it is necessary to multiply the estimated dry flue gas volume (m^3) per minute associated with combustion by the measured in-stack

concentration of the contaminant that are in units of g/dscm. (It should be noted that concentrations reported on an equivalent oxygen or carbon dioxide basis or on a dry volume basis must be adjusted to the actual stack gas conditions in order to determine the actual, in-stack concentrations.) The product of this calculation (g/min) is then divided by 60 s/min to give the grams per second emission rate needed as an input into the COMPDEP model. In cases were there are multiple stack tests from the same facility, care should be taken to ensure that the emissions characterization reflects a wide range of operating conditions and also accounts for any expected deterioration in facility performance which would affect the facility's emissions over its useful life. In arriving at the final estimate of emissions of the contaminant, the average value is considered representative of long-term emissions, taking into consideration the average yearly operating hours of the combustion facility.

B. *For facilities that have been constructed, but not yet operational, or are in the planning stages of development*, the following approach is recommended. Reports of stack tests which have measured the emissions of the pollutants of interest should be collected and reviewed from facilities that are most similar in technology, design, operation, capacity, auxiliary fuels used, waste feed types and composition, and air pollution controls as the facility under consideration. The stack test reports should be evaluated to determine if EPA recommended protocols, or equivalent, were used for stack sampling and analysis that are appropriate for the specific pollutants being measured. When combining data from test results for a number of facilities, care should be taken to convert concentrations and stack gas parameters to a common basis (and consistent units of measurement) that is appropriate for the facility under consideration, considering process feed rates and other facility-specific operating conditions. For purposes of exposure assessment and risk characterization, ranges and average values should be developed in order to address uncertainties inherent in the emissions estimates. However, the average emission rate of the contaminant is the value used to represent long-term, and expected emissions from the combustor under study.

C. *If no data exist relevant to a specific facility*, then the Office of Air Quality Planning and Standards's AP-42, *Compilation of Air Pollution Emission Factors* (EPA, 1985a), can be used. Care should be taken to select emission factors which were developed for technologies that best match the facility under consideration. The basic limitation of these data is the fact that emission factors are not usually reflective of specific emission control equipment. Also, information is available for only a limited number of pollutants.

Specifically, the AP-42 document provides guidance on emission factors for Municipal Waste Combustors, Sewage Sludge Incinerators, and Medical Waste Incinerators. At this time, emissions from Hazardous Waste Incinerators are not addressed in AP-42. Emission factors presented in AP-42 are designed for estimating emissions from a large number of sources over a wide area. The use of AP-42 emission factors to estimate emissions from any one facility should be done with great care. Whenever possible, emissions measured from the facility in question should be used in preference to the emission factor. In the absence of site specific emission test data, emissions measured at an identical or similar facility combusting the same or similar material should be used. AP-42 emission factors should be the last alternative because they are averages of values determined at one or more individual facilities. The individual values which are used to develop the average may vary considerably (for example the extreme values used for the emission factor for mercury from municipal mass burn combustors vary by over a factor of five from the value presented in AP-42). Emission factors for the following compounds will be available for the following types of incineration systems:

Municipal Waste Combustors: arsenic, cadmium, chromium, mercury nickel, lead, total tetra through octa chlorinated dibenzo-p-dioxin and furans.

Sewage Sludge Incinerators: antimony, arsenic, cobalt, beryllium, cadmium, chromium, lead, manganese, mercury, nickel, selenium, various chlorinated dibenzo-p-dioxin and furans.

Medical Waste Incinerators: antimony, arsenic, beryllium, cadmium, chromium, manganese, mercury, nickel, chlorobenzene, chlorophenol, total tetra through octa chlorinated dibenzo-p-dioxin and furans, total PCB.

D. *In the absence of suitable AP-42 emission factors*, clearly documented engineering evaluations may be used. Documentation should include copies of emission test reports used to derive the emission estimates, any assumptions made, and the rationale for the conclusions that are made.

3.4 INCREASES IN EMISSIONS DURING EQUIPMENT MALFUNCTIONS; STARTUP; AND SHUTDOWN

One of the more difficult aspects in deriving pollutant emission rates from incineration sources is the accounting for temporary increases in emissions that may occur as a result of startup and shutdown in operations, malfunctions or perturbations in the combustion process or changes in the removal efficiency of the air pollution control equipment. In deriving a quantitative measure of the magnitude and duration of increased emissions associated with these events, it is recommended that a procedure similar to the one used to derive estimates of routine emissions be applied. In this context the following sources of information, in order of preference, should be reviewed:

● The assessor should review stack emission testing and engineering reports on the performance and operations of combustion technologies, furnace designs, and air pollution control devices that are most similar in every respect to the facility under review. Often the emissions testing is accompanied by records that may give a gross indication of whether the system is functioning according to design specifications. Most facilities routinely monitor carbon monoxide (CO) in the stack to provide a general indication of combustion efficiency. Carbon monoxide inversely correlates with combustion efficiency, and a sudden increase in concentration could imply that an upset in the quality of the burn may have occurred. The engineering analysis in the test report may summarize these data, and qualitatively discuss upset conditions, and the length of time upset conditions were

maintained. Most facilities also routinely monitor furnace temperature. Furnace temperature is directly related to combustion efficiency and gives a qualitative measure of whether incineration of the wastes are occurring according to the design of the combustion chamber. Temperatures outside the prescribed envelope of routine operations may signal a temporary malfunction or upset in the quality of the burn. This may be due to the delivery of a highly combustible and/or wet material into the combustion chamber. During these conditions, temporary excursions in emissions of pollutants from the stack may occur, and this may have been recorded in the engineering test report.

● A second area of information regarding temporary increases in the emissions during equipment malfunctions are tests designed to determine the removal efficiency of the air pollution control devices (APCD). More specifically, some facilities may have been required by state air pollution control agencies to provide information on the longer-term performance of the APCD. In most cases such performance tests involve determining the variability in the efficiency of removal of particulate matter from the combustion gases, and/or the removal of acid gases such as sulfur dioxide and hydrogen chloride. In some rare instances the engineering evaluation may have been undertaken to determine the extent mercury was being reduced, or to what extent dioxins were controlled with the APCD. These engineering analysis may be public documents, and it may be possible to obtain copies from the appropriate state agency, or the EPA Regional office. In any case, these data may be helpful in establishing a quantitative basis for estimating the magnitude and duration, and frequency of occurrence of higher emissions than what is expected if the APCD were performing according to the design specifications.

In the event these sources of information do not provide a quantitative, e.g., numerical, basis for estimating the magnitude and duration of increase of the pollutant during upset conditions, then the procedure required by the State of California Air Resources Board (CARB, 1990) in the evaluation of toxic air contaminant emissions from waste incinerators can be applied. In this procedure, defaults for estimating emissions representative of emergency operating conditions and poor operating conditions at the

facility are provided, as follows:

- Emergency operating conditions. Estimation of stack emissions of the contaminants representative of emergency operating conditions should be based on uncontrolled emissions over a one-hour period. For example, if dioxin is assumed to be controlled by the APCD at a rate of 99 % relative to the uncontrolled concentration, then, under the emergency operating conditions scenario, the stack concentration would be assumed to be 100 times higher during a 1-hr period. The CARB has defined this emergency condition as a sudden upset in which case the air pollution control device (APCD) is by-passed to a waste stack, and uncontrolled emissions occur until the facility is completely shutdown. These operating conditions include such events as: a turbine trip, blown boiler tubes, failure in the APCD, feed system failure, fire, etc. However if the source could demonstrate that the APCD would never be by-passed during an emergency event, then use of the uncontrolled emissions would not realistically reflect the potential emissions from the facility. CARB gives no guidance on an alternative approach, but does indicate that the evaluation of potential health impacts resulting from acute exposures should represent a range of operating conditions. These operating conditions should reflect poor operation of the equipment and total equipment failure. For these operating conditions the increase in emissions should be estimated resulting from reduced control efficiency, and the duration of the event should be noted.

- Poor operating conditions. To represent stack emissions during operating conditions that are less than normal, CARB recommends, as a default, multiplying the average emissions (found from the source test database) by ten. This factor is incorporated into the annual emission rate of organic and metal emissions. CARB further recommends using a default value for the fraction of the time a facility operates under poor conditions on an annual basis. For organic contaminants, it is assumed that the facility operates normally 80% of the time and operates poorly for the other 20% of the time. For metal emission estimates, CARB recommends the default assumption that the facility operates normally 95% of the time, and under poor conditions for the other 5% of the time during the course of the year.

3.5   SHORT TERM IMPACTS DUE TO METEOROLOGIC CONDITIONS

As discussed above, short term increases in emission rates can lead to higher atmospheric concentrations than would occur during normal operations. Even during normal operations, fluctuations in atmospheric concentrations occur due to changing meteorologic conditions. During times of stable air conditions, i.e. atmospheric inversions, the dispersion of emissions is reduced and higher than normal air concentrations result. As discussed in Chapter 2, these short term increases are unlikely to significantly affect indirect exposures, but may be important to consider in evaluating acute effects from inhalation. The COMPDEP model can provide the daily high concentration expected over a one year period. Since the model assumes a constant emission rate, this high would occur as a result of stable air conditions. In order to evaluate the maximum short term exposure scenario, the assessor should judge whether the increases in emission rates due to upset conditions (as discussed in section 3.4) could combine with the effects of stable air to further increase this estimated daily high concentration from the model.

3.6   CONDENSED DESCRIPTION OF THE COMPDEP MODEL

The COMPDEP model was developed to provide estimates of the air concentrations and wet/dry deposition fluxes of the stack emissions of contaminants from industrial sources in varied topography (e.g, from simple to complex terrain). COMPDEP uses standard meteorological data to produce estimates of ambient air concentration, dry deposition and wet deposition at individual receptor sites. COMPDEP was basically derived as a combination of the Industrial Source Complex (Short Term) model (Bowers et al, 1979) and the COMPLEX I, an EPA recommended screening model for use in complex terrain (EPA, 1993). To account for pollutant deposition, the concentration algorithms in COMPLEX I were replaced with those from the Multiple Point Source Algorithm with Terrain Adjustments Including Deposition and Sedimentation (MPTER-DS) model (Rao and Satterfield, 1982). The MPTER-DS algorithms are based on the gradient transfer theory described in Rao (1981) and are extensions of the traditional Gaussian plume algorithms. The routines developed by the California Air Resources Board (CARB, 1986) were included for determining deposition velocity. The Industrial Source Complex - Short Term (ISCST)

(Bowers et al, 1979) algorithms for accounting for building wake effects were included. COMPDEP also contains algorithms for modeling wet deposition which are based on Slinn (1984) and PEI and Cramer (1986).

In accordance with a recent review of the existing operating computer code, COMPDEP was modified, and an updated version is currently available. In order to eliminate any confusion, the current version has been assigned the number 93252. In this numbering system, 93 refers to the year, the 252 refers to the day (September 9) of the most recent modifications. COMPDEP is available to users through a electronic bulletin board system known as the Support Center for Regulatory Air Models (SCRAM). This electronic bulletin board is maintained by EPA's Office of Air Quality Planning and Standards in Research Triangle Park, North Carolina through the Technology Transfer Network. The COMPDEP model can be accessed within SCRAM under the topic, "other models." SCRAM permits the user to download the computer code, and provides instructions on operating the COMPDEP model and for accessing meteorological data. User's may receive information on accessing the SCRAM by calling the systems operator by phone at (919) 541-5384 in Durham, North Carolina during normal business hours EST.

Because of recent refinements and modifications in the COMPDEP model, EPA has not printed a users manual. However, instructions on performing dispersion and deposition analysis with COMPDEP are on the SCRAM system. The following subsections are a review of the key algorithms employed within the program for estimating dispersion and deposition of contaminant emissions.

3.6.1 Dispersion Parameters

The standard deviation of the lateral and vertical concentrations are applied in the calculation of the ambient air concentrations of the contaminants released from the stack of stationary industrial sources. Point estimates are used in COMPDEP to calculate the dispersion parameters, σ_y and σ_z, for all terrain heights. Point estimates of σ_y and σ_z are used by ISCST for calculating concentrations in simple terrain. These point estimates are inserted in Equation [3-1] for calculating the ambient air concentration or the contaminant $(\mu g/m^3)$.

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$$\chi = \frac{Q \; K \; V}{2 \; \pi \; u_s \; \sigma_y \; \sigma_z} \; exp\left(-0.5 \left(\frac{y}{\sigma_y}\right)^2\right) \qquad \text{[3-1]}$$

where:

χ	=	ambient air concentration ($\mu g/m^3$)
Q	=	pollutant emission rate (g/s)
K	=	units conversion factor
V	=	vertical term (dimensionless)
u_s	=	wind speed (m/s)
σ_y, σ_z	=	standard deviation of lateral and vertical concentration distributions (m)
y	=	crosswind distance (m)

COMPLEX I uses the point estimate for σ_z, but uses sector averaging to calculate the horizontal dispersion instead of calculating a σ_y. Equation [3-2] is used in COMPLEX I to calculate ambient air concentrations.

$$\chi = \frac{Q \; K \; V}{\sqrt{2\pi} \; R \; \Delta\theta' \; u_s \; \sigma_z} \qquad \text{[3-2]}$$

where:

Q	=	pollutant emission rate (g/s)
K	=	units conversion factor
V	=	vertical term (dimensionless)
R	=	radial distance from source to receptor (m)
$\Delta\theta'$	=	sector width in radians (dimensionless)
u_s	=	wind speed (m/s)
σ_z	=	standard deviation of vertical concentration distribution (m)

The algorithms for calculating air concentrations were modified in COMPDEP so that predicted concentrations match those from ISCST for receptors below plume height and those from COMPLEX I for receptors above stack top.

3.6.2. Treatment of Terrain

COMPDEP is a merger of ISCST and COMPLEX I, and uses the method appropriate to the elevation of the receptor being modeled. ISCST calculates an effective plume height based on the relative difference in elevation between the stack base and the receptor. In the ISCST component, any terrain heights above stack top are not considered in the dispersion calculations. COMPLEX I calculates an effective height based on the relative difference in elevation between the stack and the receptor, but applies a stability class dependent correction factor to this adjustment. In this manner, terrain above stack top is considered.

3.6.3. Stack-Tip Downwash

Stack-tip downwash refers to the modification of the physical stack height when the stack gas exit velocity is less than 1.5 times the wind speed. In COMPDEP, the stack-tip downwash and building wake effects options can be selected simultaneously. The stack-tip downwash calculation can be used in determining the final plume height. However, the actual stack height is used to determine the plume rise when building wake effects are important.

3.6.4. Transitional/Final Rise

COMPDEP calculates both a final plume rise and a distance-dependent (transitional plume rise). Users have the option of selecting which plume height will be used in calculating concentrations. However, when building wake effects are being included, the distance-dependent rise is always used (even if final rise is selected by the user).

3.6.5. Buoyancy Induced Dispersion

Users can choose to include the effects of buoyancy induced dispersion which enhances the dispersion parameters as follows:

$$\sigma_{ze} = \left(\sigma_z^2 + \left(\frac{\Delta h}{3.5}\right)^2\right)^{1/2} \qquad [3\text{-}3]$$

$$\sigma_{ye} = \left(\sigma_y^2 + \left(\frac{\Delta h}{3.5}\right)^2\right)^{1/2} \qquad [3\text{-}4]$$

where:

σ_{ye}, σ_{ze}	=	effective standard deviation of lateral and vertical concentration distributions (m)
σ_y, σ_z	=	standard deviation of lateral and vertical concentration distributions (m)
Δh	=	plume rise (m)

Buoyancy induced dispersion can be used with the Huber-Snyder building effects algorithms in ISCST. Δh in the above equations is the distance-dependent (transitional) rise, if the receptor is located between the stack and the distance to final rise, or the final rise, if the receptor is located beyond the distance to final rise.

3.6.6. Calms Processing

No concentrations are computed for hours that are identified as calms. Users have the option of choosing to activate the calms processing routine. When this option is selected, the ambient air concentration at a receptor is calculated by dividing the total concentration for the period by the number of hours in the period less the number of calm hours. In COMPDEP, the model subtracts the number of calm hours from the number of hours in the period.

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3.6.7. Building Wake Effects

The method used in COMPDEP for determining building wake effects is the Huber-Snyder method used in ISCST. Wake effects are important if the plume height, calculated from the sum of the distance-dependent plume rise at a distance of two building heights and the stack height (without stack-tip downwash effects), is greater than (a) 2.5 times the building height or (b) the sum of the building height and 1.5 times the building width. If, using these criteria, the plume is affected by the building wake, the dispersion parameters are adjusted to account for the building effects and the distance dependent plume rise is used in calculating concentrations at individual receptors. Because COMPLEX I does not include building wake effects, COMPDEP does not allow the use of the ISCST algorithms for building wake effects when modeling complex terrain receptors.

3.6.8. Dry Deposition

The dry deposition flux is calculated from the product of the air concentration (for the fraction of the hour during which there was no precipitation) and the deposition velocity. The code incorporated into COMPDEP is essentially the same as the original CARB code (CARB, 1986) which is based on the work of Sehmel (1980) and Sehmel and Hodgson (1978). The CARB algorithms represent empirical relationships for transfer resistances as a function of particle size, density, surface roughness, and friction velocity. In the CARB model, integrated resistances to mass transfer are computed within two layers. In the first layer, which extends from one centimeter to one meter above the surface, atmospheric turbulence dominates mass transfer. In the second layer, which lies within one centimeter of the surface, the resistance to mass transfer is derived from particle deposition measurements that were taken in a wind tunnel over various surfaces using monodispersed particles.

The overall deposition velocity is given by Sehmel and Hodgson (1978) as:

$$v_d = \frac{v_g}{1 - exp\left(\dfrac{-v_g \ (I_{12} + I_3)}{u_*}\right)} \qquad [3\text{-}5]$$

where:

v_d =   deposition velocity (cm/s)

v_g =   gravitational settling velocity (cm/s)

I_{12} =   atmospheric resistance integral (dimensionless)

I_3 =   surface resistance integral (dimensionless)

u_* =   atmospheric surface layer friction velocity (cm/s)

The gravitational settling velocity is calculated as:

$$v_g = \left(1 + \frac{0.00973 \ \sqrt{T}}{d_p}\right)\left(\frac{(\rho_p - \rho_a) \ g \ d_p^2 \ 10^{-8}}{18 \ \mu}\right) \qquad [3\text{-}6]$$

where:

v_g =   gravitational settling velocity (cm/s)

T =   absolute air temperature (°K)

d_p =   particle diameter (μm)

ρ_p =   particle density (g/cm^3)

ρ_a =   air density (g/cm^3)

g =   acceleration of gravity (cm/s^2)

μ =   air viscosity (g/cm/s)

10^{-8} =   units conversion factor

The atmospheric resistance integral is based on surface flux profile relationships. For neutral and stable conditions,

$$I_{12} = \frac{1}{k}\left(ln\left(\frac{z_1}{z_2}\right) + \frac{4.7\,(z_1 - z_2)}{L}\right)$$ [3-7]

where:

k	=	von Karman's constant
z_1	=	upper limit of atmospheric resistance integral (i.e., 100 cm)
z_2	=	lower limit of atmospheric resistance integral (i.e., 1 cm)
L	=	Monin-Obukhov length (cm)

For unstable conditions,

$$I_{12} = \frac{1}{k}\left(ln\left(\frac{(A_{z1} - 1)(A_{z2} + 1)}{(A_{z1} + 1)(A_{z2} - 1)}\right) + 2\left(\frac{1}{tanA_{z1}} - \frac{1}{tanA_{z2}}\right)\right)$$ [3-8]

where:

$$A_{z1} = \left(1 - \frac{15\,z_1}{L}\right)^{0.25}$$

and

$$A_{z2} = \left(1 - \frac{15\,z_2}{L}\right)^{0.25}$$

The surface resistance integral is based on a least-squared empirical fit to the wind tunnel data. For particles with diameters $\geq 0.01\ \mu m$,

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$$I_3 = exp\left(-378.051 + 16.498\ lnSc + B\ lnt^+ - 12.804\ ln\left(\frac{d_p\ 10^{-4}}{z_0}\right)\right) \qquad [3\text{-}9]$$

where:

$$B = -11.818 - 0.2863\ lnt^+ + 0.3226\ ln\left(\frac{d_p\ 10^{-4}}{z_0}\right) - 0.3385\ ln\left(\frac{D}{z_0\ u_*}\right)$$

$$Sc = \frac{v}{D}$$

$$t^+ = 3.156x10^{-13}\ (d_p\ u_*)^2$$

and

Sc	=	Schmidt number (dimensionless)
v	=	air kinematic viscosity (cm ^{2}/s)
D	=	Brownian diffusion coefficient (cm ^{2}/s)
t^+	=	relaxation time (dimensionless)
d_p	=	particle diameter (μm)
z_0	=	surface roughness length (cm)
u_*	=	friction velocity (cm/s)
10^{-4}	=	units conversion factor

The Brownian diffusion coefficient is expressed as:

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$$D = \left(7.868x10^{-10}\ \frac{T}{d_p}\right)\left(1 + \left(\frac{0.02632}{d_p}\right)(6.32 + 2.01\ exp(-8.322\ d_p))\right) \qquad [3\text{-}10]$$

where:

D	=	Brownian diffusion coefficient (cm^2/s)
T	=	absolute temperature (°K)
d_p	=	particle diameter (μm)

Dry deposition velocities calculated by COMPDEP were compared with those calculated by the Fugitive Dust Model (FDM) (Winges, 1990) which also uses the CARB algorithms. There were no differences detected between the deposition velocities calculated by the two models, so no modifications were made to the COMPDEP code. The CARB algorithms were developed for application in flat terrain. These "flat terrain" algorithms have not been specifically modified for handling deposition in complex terrain.

3.6.9 Wet Deposition

COMPDEP calculates the annual wet deposition flux according to a method developed by Slinn (1984) and later modified by PEI and Cramer (1986). The wet deposition flux is represented by Equation [3-11]:

$$Dyw = \frac{f\ K\ Q}{\sqrt{2\pi}\ \sigma_y\ u_s} \sum_{n=1}^{n} \left[\Lambda(n,j)\ \phi_n\ exp\left[-\Lambda(n,j)\ \frac{x}{u_s}\right]\right]\ exp\left[-0.5\left[\frac{y}{\sigma_y}\right]^2\right] \qquad [3\text{-}11]$$

where:

Dyw	=	wet deposition flux of pollutant (g/m^2/s)
f	=	fraction of the hour during which precipitation occurs
$\Lambda(n,j)$	=	fraction of material removed per unit time in the nth particle size category and jth precipitation intensity category (s^{-1})

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$\phi(n)$ = fraction of total source material in the nth particle size category

K = units conversion factor

Q = pollutant emission rate (g/s)

σ_y = standard deviation of the crosswind concentration distribution (m)

u_s = wind speed (m/s)

x = downwind distance from source to receptor (m)

y = crosswind distance from source to receptor (m)

Table 3-4 provides examples of scavenging coefficients (s^{-1}) based on an analysis of precipitation data from Central Illinois and Miami, Florida, (PEI and Cramer, 1986). These values were default values in the previous version of COMPDEP, in which case the model user could not specify scavenging coefficients. However, in the current version of COMPDEP the scavenging coefficient for each particle size and precipitation category, $\Lambda(n,j)$, is input by the user. As with the building wake effects and dry deposition algorithms, this algorithm contains no specific adjustments for use in complex terrain.

3.7 MODEL INPUT PARAMETERS

There are three input files associated with COMPDEP:

1) control file that includes model option settings, source parameters, and receptor locations;

2) file of hourly meteorological data;

3) file of hourly precipitation data.

3.7.1. Control File

This file includes settings for program options, source location, emission parameters, and receptor locations. The control file includes the specific parameters listed in Table 3-5. The maximum number of particle size categories in COMPDEP is 10 and the maximum number of receptors is 500.

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Table 3-4. Examples of precipitation scavenging coefficients (per s) in COMPDEP.			
Precipitation	Particle size category (μM)		
Intensity	Less than 2	2 to 10	Greater than 10
Heavy	1.46E-03	4.64E-03	9.69E-03
Moderate	5.60E-04	8.93E-04	9.69E-03
Light	2.20E-04	1.80E-04	9.69E-03

3.7.2. Meteorological Data Files

There are two meteorological files used by COMPDEP. The first is a file consisting of hourly values for the wind speed, wind direction, stability class, mixing height, and ambient air temperature, as shown in Table 3-6.

Each array contains 24 values, one for each hour. The file can be created using either RAMMET (Catalano et al, 1987) or MPRM (Irwin and Paumier, 1990), which are EPA meteorological preprocessors. These preprocessors use surface data (CD-144 file), twice daily mixing heights, and on-site data . Both the CD-144 and mixing height files are available from the National Climatic Data Center (NCDC).

The second file used by COMPDEP contains precipitation data (which is required only if wet deposition is being calculated). Information contained in this file includes:

1. Date: described in terms of Julienne day and year

2. Hourly Precipitation data: Exact hourly quantities of hourly precipitation can be obtained from the National Climatic Data Center TD3240 file. What is required for COMPDEP, however, is hourly rainfall described in terms of intensity and precipitation type. The intensity categories are: 1) none = 0.0 in/hr; 2) light = trace to 0.10 in/hr; 3) moderate = 0.11 to 0.30 in/hr; and 4) heavy = greater than 0.30 in/hr. Precipitation type

Table 3-5. Parameters in the COMPDEP control files.

For Each Run	For Each Run
Starting year	Source east coordinate (user units)
Starting Julienne day	Source north coordinate (user units)
Starting hour	Stack height (m)
Horizontal scale factor to convert user units to kilometers	Stack temperature ($^\circ$K)
	Stack diameter (m)
Vertical scale factor to convert user units to meters	Stack gas exit velocity (m/s)
	Stack ground elevation (user units)
Pollutant half-life (s)	Number of particle size categories (maximum of 10)
Test option	Particle density (g/cm ^{3})
Terrain adjustment option	Emission rate (g/s)
Stack-tip downwash option	
Transitional plume rise option	
Buoyancy induced dispersion option	Fraction of emission in each particle size category
Calms processing option	
Dry deposition option	
Wet deposition option	For Each Receptor
Building wake effects option	
Anemometer height (m)	Receptor east coordinate (user units)
Array of wind speed profile exponents (by stability class)	Receptor north coordinate (user units)
	Receptor height above local ground (m)
Array of terrain adjustment factors (by stability class)	Receptor ground elevation (user units)
Distance limit for plume centerline above ground (m)	
Building height (m)	
Building width (m)	
Array of particle sizes (μm)	For Each Particle Size Category
Surface roughness length (m)	Scavenging coefficients for each precipitation intensity (s $^{-1}$)

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Table 3-6. Parameters in the meteorological data file for COMPDEP	
For Each Station	For Each Day
5 digit station ID of surface data	Last 2 digits of year
Last 2 digits of beginning year of surface data	Month of year
5 digit station ID of mixing height data	Day of month
Last 2 digits of beginning year of mixing height data	Array of Pasquill stability classes
	Array of wind speed (m/s)
	Array of ambient temperatures (°K)
	Array of wind directions (to nearest 10 degrees)
	Array of randomized wind directions (to nearest degree)
	Array of mixing heights (m)

is described using a numerical indicator termed F, as: 1) steady --- F = 1; 2) showers --- F = 0.50; 3) thunderstorm or squall --- F = 0.25; 4) snow, ice, or none ---F = 0.0.

3.8 MODEL OUTPUT

COMPDEP creates one output file that contains a verification of the model input including options selected, source information, and receptor locations. The output of the COMPDEP model for both surface deposition and ambient air impacts is a concentration array of ground-level receptors in all directions around the source. It is recommended that the minimum distance of the receptors be at 200 m from the stack, and that the maximum distance be 50 km from the stack. It is recommended that this array include a minimum of 160 ground-level receptors consisting of 10 receptor points along each of 16 wind

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directions every 22.5° on the polar azimuth. (Modeling experience has shown that most of the exposures associated with stack emissions from a typical incineration process occurs within 10 km, and that the maximum concentration is likely to occur within 1.0 km from the source.) In specifying the radial distances of the receptors from the incinerator stack, it is recommended that receptors be spaced every 200 m until 1 km is reached. It is recommended that the receptors be spaced every 1 km between 1 km distance from the source out to 5 km, and every 10 km between 10 km distance to 50 km from the source. The printed output also includes tabulations of annual average and period (e.g. multi-year) average values of dry deposition flux (g/m^2-yr), wet deposition flux (g/m^2-yr), combined dry and wet deposition flux, and annual average ambient air concentration ($\mu g/m^3$) at each modeled receptor in all directions along the compass. In addition to the long-term average concentration, the ISCLT portion of the COMPDEP model can produce concentrations corresponding to hourly, daily and monthly time scales. These time-scales are: highest concentration in 1-hr, 3-hrs, 8-hrs, and 24-hrs. These shorter time-frames are applicable to the analysis of human health effects associated with acute exposures.

3.9   COMPDEP MODEL APPLICATIONS

3.9.1. Recommended Application of the COMPDEP Model

At the point of stack emission and during the atmospheric transport, partitioning of the contaminants occurs between two physical phases: vapor and particle-bound phases. Pollutants with higher vapor pressures increase the vapor phase fraction. A vapor-to-particle ratio (V/P) needs to be established for each contaminant of interest. The V/P ratio represents the ratio of the concentration of the contaminant in the vapor phase to the concentration of that contaminant in the particulate phase, usually expressed in terms of percentage with V plus P adding to 100 %, e.g., 60 %/ 40 %.

Particle-bound contaminants can be removed from the atmosphere by both wet deposition (i.e., precipitation scavenging) and dry deposition (i.e., gravitational settling, Brownian diffusion). The contaminants can directly deposit onto soil surfaces, plant surfaces, in water bodies, and onto surrounding land. With respect to assessing potential contamination of the food chain, there are two processes important to estimating above

ground vegetation contamination: airborne vapor phase absorption into plants, and airborne particle deposition onto soils and plant surfaces.

The analysis of human exposures via direct inhalation and contact with contaminated soils and food requires certain outputs from the COMPDEP model to estimate exposure media concentrations. At a minimum, these outputs should include:

1. An estimation of vapor-phase concentrations of the contaminants (in units of μg/m^3). The vapor phase concentration is used to estimate absorption into plants and human exposure via direct inhalation of vapors.

2. An estimation of the wet and dry deposition flux of contaminated particles (units of g/m^2/yr). Deposition estimates are used for: plant concentrations (vegetations for animal and human consumption), soil concentrations (soil contact exposures and crop uptakes), and surface water concentrations (water and fish; via runoff and erosion of watershed soils and direct depositions).

3. An estimation of the ambient air concentration of contaminants bound to particles (units of μg/m^3). This is important in estimating direct inhalation exposures to the portion of the contaminants that is particle bound, and when added to the portion that exists as vapor (from #1 above), will give a value relative to total inhalation exposures (vapor-phase concentration <u>plus</u> the particle bound phase concentration).

It is apparent from these output requirements that air modeling must consider the physical state of the pollutants, e.g., the portion of the emission that is vapor-phase and the portion of the emission that is bound to particles. This ratio is likely to change from the point of release at the stack to any point distant from the stack. In some instances, as with semivolatile organics, the vapor fraction decreases as the gases cool and condense onto particulates. In other instances, as with volatile elemental mercury, the contaminant may continue to predominate as a vapor. With the current air model, it is not possible to model changes in the physical state of contaminants (the V/P ratio) with distance from the

source. Instead, it is recommended that users assume that the V/P ratio of the pollutant as it is emitted from the stack is equal to the V/P ratio of the contaminant as it may exist in ambient air at ground-level. This assumption is recommended because: 1) for most contaminants, the physical/chemical processes that may occur to transform this ratio in the atmosphere from the point of release from the stack to the ground-level receptor are largely unknown, 2) the model does not include procedures to address this phenomena, and 3) ambient conditions are more representative of exposure conditions than stack conditions.

In order to provide estimates of ambient air concentrations of vapors and estimates of ambient air concentrations of particles combined with estimates of wet/dry particle deposition flux, it is necessary that <u>users run the COMPDEP model twice</u>. Both model runs should assume a "unit emissions release rate", e.g., 1 g/s. Results from these unit runs can easily be transformed to final outputs given assumptions on emissions in vapor and particle forms. This will be illustrated below.

The recommended modeling procedure that will provide necessary outputs for further exposure modeling is:

● Run 1: To estimate vapor-phase concentration of the contaminant in ambient air.

COMPDEP should be run with the <u>wet/dry deposition switches turned to the "off" position</u>. This is to isolate the ambient air concentration of the contaminant in vapor-phase from the calculation of wet and dry particle deposition flux. This inactivates a plume depletion equation that subtracts out losses in ambient air concentration due to particle deposition. What is left are the Gaussian dispersion algorithms.

With the "unitized" emission rate, one can reconstruct the actual predicted ambient air concentration (μg/m^3) of vapors by multiplying the "actual" vapor-phase emission rate (g/s) by the "unitized" modeling result. For example, let the actual stack gas emission rate of total (vapor plus particle components) contaminant be 1×10^{-5} g/s, and the V/P ratio (expected under ambient conditions) be 60%V/40%P. Then the "actual" emission rate of the vapor-phase portion of the contaminant is calculated to be 6×10^{-6} g/s (1×10^{-5} g/s * 0.6). If the "unitized" ambient air concentration at the ground-level receptor is estimated

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by the COMPDEP model to be 1×10^{-8} $\mu g/m^3$ (i.e., this concentration is predicted with a unit emission rate of 1 g/s), then the "actual" predicted air concentration at that receptor can be estimated as:

$$(6\times10^{-6} \text{ g/s} \div 1 \text{ g/s}) * 1\times10^{-8} \text{ } \mu g/m^3 = 6\times10^{-14} \mu g/m^3$$

• **Run 2:   To estimate wet and dry particle deposition flux, and the ambient air concentration of the contaminant that is particle-bound.**

COMPDEP should be run with the <u>wet/dry particle deposition switches turned to the "on" position</u>, and using a "unit emission rate" of 1 g/s. This second run is considered a simulation of particle-bound contaminant only. Outputs of this run include unitized deposition rate and unitized ambient air concentrations of particles.

Like the vapor-phase run, the "actual" deposition flux (g/m^{-2} -yr) and "actual" particle-phase airborne concentrations can then be determined by multiplying the "actual" emission rate (g/s) of the particle-bound portion of the total contaminant emissions by the "unitized" modeling result at the ground receptor. For example, let the "actual" emission rate of the particle-bound portion of the contaminant be 4×10^{-6} g/s, and the "unitized" dry deposition flux at the ground receptor be 1×10^{-5} g/m^2-yr. Then the "actual" predicted dry deposition flux is 4×10^{-11} g/m^2 (4×10^{-6} g/s $\div$ 1 g/s * 1×10^{-5} g/m^2-yr). Using this same procedure, this second run provides the airborne concentration of contaminants bound to particles ($\mu g/m^3$).

• **To estimate total ambient air concentrations of the contaminant that is vapor phase and particle-bound to the contaminants.**

Inhalation exposures will include both the concentration in vapor-phase, and the concentration that is bound to particles in the ambient air. To make this estimate it is necessary to add together the ambient air concentration of vapors ($\mu g/m^3$) from the step 1 together with the ambient air concentration of particles ($\mu g/m^3$) estimated in step 2.

3.9.2 Source Characteristics

After running COMPDEP with unitized vapor and particle emission rates, calculation of the ambient air concentration and the wet/dry deposition flux of the contaminants at points distant form the stack emission requires that the following be specified:

1. Emission rate of the vapor portion of the contaminant
2. Emission rate of the particle-bound portion of the contaminant
3. Particle size distribution of the particulate matter emissions.

The following subsections give guidance on making these estimations.

3.9.2.1. Vapor Phase/Particle Bound Phase Partitioning of Semivolatile Organic Compounds

In the previous section it was noted that the COMPDEP model is run twice with a unit emission rate of 1 g/s for all the contaminants: 1) to derive the ambient air concentration of the vapors, and 2) to derive the ambient air concentration of particles and the estimates of wet and dry deposition flux of the particles. Reconstruction of the actual concentrations of the contaminants requires multiplication of the unitized result by the actual emission rate (g/s) of the contaminant assumed to be in the vapor-phase or that is bound to particles under ambient conditions. This requires prior determination of the partitioning of the total emission rate of the contaminant according to this same V/P ratio.

Bidleman (1988) has suggested a theoretical construct for estimating the V/P ratio of semivolatile organic compounds in ambient air. Bidleman presents the theory that a portion of the semivolatile organic compounds found in ambient air are freely exchangeable between the vapor and particle phases. Bidleman defines a second portion, the nonexchangeable fraction, as the quantity that is strongly and irreversibly adsorbed to particulate matter, and is not at equilibrium with a corresponding vapor phase. Bidleman cites an earlier model by Junge (1977), a theoretical model based on adsorption theory. Junge's model mathematically describes the exchangeable fraction of the semivolatile organic compound adsorbed to aerosol particles as a function of solute saturation vapor

pressure and total surface area of atmospheric aerosol particles available for adsorption. This is given by Equation [3-12].

$$\varnothing = c \, S_T / (p + c \, S_T) \qquad\qquad [3\text{-}12]$$

where:

$\varnothing$ = adsorbed fraction, unitless

c = constant developed by Junge, 1.7 E-4 atm-cm

S_T = total surface area of atmospheric aerosols in relation to total volume of air, cm^2/cm^3

p = solute saturation vapor pressure, atm^{-1}

Equation [3-12] requires an estimate of S_t, which is the total surface area of aerosol particles in the ambient air. Bidleman (1988) provides estimates of average total surface areas of aerosol particles relative to average total volume of air (cm^2/cm^3) citing a study by Whitby (1978). In addition , Whitby estimated the average total volume of aerosol particles per volume of air ($V_T = cm^3$ particles/cm^3 of air). Whitby's (1978) calculations varied according to the density of aerosol particles in the ambient air in different air sheds. These were as follows (units of S_T of cm^2/cm^3, V_T of cm^3/cm^3):

- Clean continental background S_T = 4.2 E-7 V_T = 6.5 E-12
- Average background S_T = 1.5 E-6 V_T = 3.0 E-11
- Background plus local sources S_T = 3.5 E-6 V_T = 4.3 E-11
- Urban S_T = 1.1 E-5 V_T = 7.0 E-11

For purposes of calculating the fraction of the semivolatile organic compound that adsorbed (using Junge's equation) onto the surface of aerosol particles in ambient air, Whitby's values for S_T (above) are recommended. For incinerators located in urban areas, S_T corresponding to the air-shed classification "Background plus local sources" should be appropriate. The fraction adsorbed to the surface of particles is subtracted from 1 (100 %) to derive the fraction existing in the vapor phase under ambient conditions. In this

manner, the vapor phase/particle-bound phase of the semivolatile organic compound is derived. This method is most appropriate for organic compounds with low vapor pressures, e.g., dioxins, PCBs, chlorinated benzenes, chlorinated phenols).

This approach is applied only in the context of providing a reasonable estimate of the V/P partitioning in ambient air. As discussed earlier, the V/P ratio of the contaminant estimated in ambient air is assumed to be equal to the V/P ratio of the contaminant at the point of emission from the stack. Therefore the recommended procedure is to apply the Bidleman (1988) approach to estimate the V/P ratio of the contaminant in ambient air, then apply this same V/P ratio at the stack to partition emission the emission rate of the contaminant between the two phases. Each phase of the contaminant, then, is modeled independently. An area of uncertainty with respect to this simplified approach is that it does not account for any changes in the V/P ratio from the point of release to the ground as contaminants disperse through the atmosphere.

With regard to the more volatile compounds (e.g., volatile organics and elemental mercury), based on the Henry's Law constant and saturated vapor pressures, one can infer that the compounds will partition primarily into the vapor phase.

3.9.2.2. Estimation of the In-Stack Particulate Matter Particle-Size Distribution

The COMPDEP air model contains algorithms to compute the rate at which dry and wet removal processes may deposit particulate matter emitted for the stack of the combustor to the surface of the Earth. This requires an initial estimation of the distribution of particulate differentiated on the basis of particle diameter before the COMPDEP program can predict deposition flux.

The diameters of small particles comprising particulate matter in stack emissions are usually measured in units of one millionth of a meter (micrometer, commonly called micron), abbreviated by the letters μm. The distribution of particulate matter by particle diameter will differ from one combustion process to another, and is greatly dependent on such factors as: the type of furnace and design of the combustion chamber; the composition of the feed/fuel; the particulate matter removal efficiency and design of the air pollution control equipment; the amount of air in excess of stoichiometric amounts that is

used to sustain combustion; and the temperature of combustion. Given these variables, the particle size distribution cannot be calculated, it can only be directly measured and inferred from prior data. Unfortunately few studies have been performed to directly measure particle size distributions from a variety of stationary combustion sources. Stack measurements over a wide range of particle diameters on a site-specific basis is preferred. These data should reflect a wide range of operating conditions, and the expected performance of the air pollution control equipment in removing the mass of particulates generated during combustion. In recognition of the fact that accurate and direct measurements of particle-size distributions at a combustion facility under study often times will be lacking, it is necessary to resort to a "generalized" assumption of the distribution for purposes of deposition analysis using the air model. The following procedure is recommended as a 'default' assumption of the particle size distribution to be applied only in situations where site-specific measurements are not available. In addition to this 'default' distribution, a procedure for apportioning the emission rate of the contaminant that is particle-bound to the particle size distribution is given.

The generalized particle size (diameter) distribution in Table 3-7 may be used as a default for combustion facilities equipped with either electrostatic precipitators (ESPs) or fabric filters (FFs), because the distribution is fairly typical of particle size arrays that have been measured at the outlet to advanced equipment designs (Buonicore and Davis, 1992). In terms of data preference, however, site-specific particle size distributions are highly recommended over use of the default.

When using either the default assumption or the actual distribution, the emission rate of the particle-bound portion of the total stack emission of the contaminant is apportioned to the particulate distribution. In high-temperature combustion processes characteristic of hazardous waste incinerators and municipal waste combustors, the contaminates will leave the combustion zone in the vapor phase. In other situations, molecules leaving the furnace area will undertake chemical reactions in the combustion gas stream to reform new molecules in the vapor phase. Once the combustion gases have cooled after passing through a boiler, a heat economizer, or a dry/wet scrubber device, condensation of the vapor phase chemicals may occur. The pollutants will then condense

Table 3-7. Generalized particle size distribution (μm), and proportion of available surface area, to be used as a default in deposition modeling if site-specific data is unavailable.

Particle Diameter (μm)[a]	Particle Radius (μm)	Surface Area/ Volume	Fraction of Total Weight	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

Sum: 3.4423

Notes: a. Geometric mean diameter in a distribution from EPA (1980).

to the surface of particles entrained in the combustion gas. By this paradigm, the apportionment of emissions by particle diameter becomes a function of surface area of the particle that is available for chemical adsorption. Therefore the first step to this apportionment is to calculate the proportion of available surface area of the particles. If particle density is held constant (i.e., 1 g/m^3), then the proportion of available surface area of aerodynamic spherical particles is the ratio of surface area to volume as follows:

(a) Assume aerodynamic spherical particles.

(b) Specific surface area of a spherical particle with a radius, r:

$$S = 4 \pi r^2$$

(c) Volume of a spherical particle with a radius, r:

$$V = 4/3 \pi r^3 \text{(d) The ratio of surface area (S) to volume (V) is:}$$

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$$S/V = 4 \pi r^2 / (4/3 \pi r^3)$$

$$S/V = 3/r$$

The following uses the particle size distribution in Table 3-7 as an example of apportioning the emission rate of the particle-bound portion of the contaminant to the particulate array. This procedure can be followed for apportioning actual emissions to the actual particle size distribution as measured at the stack. In Table 3-7, a spherical particle having a diameter of 15 μm (column 1) has a radius of 7.5 μm (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 12.8 % (by weight) of the total mass of particles is 15 μm. Multiplication of column 3 by column 4 gives an approximate calculation of the relative proportion of total surface area based on the percent of particles that are 15 μm diameter. Summation of column 4, relative proportion of surface area, gives an estimate of the total surface area of all the particles in the particle size distribution. In this example the sum is 3.44 μm^2 of total surface area available for chemical adsorption. The last column 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 for a given diameter (column 4) by the total surface area (3.44 μm^2). In the example of the 15 μm diameter particle, the fraction of total surface area available for adsorption is 0.0149 (0.0512 μm^2/3.4423 μm^2). Multiplication of the emission rate of the contaminant that is particle-bound (μg/s) by the fraction of total surface area for a given particle diameter gives an estimate of the emission rate of the contaminate apportioned to that particle diameter. For example, if it is assumed that the total emissions of 2,3,7,8-TCDD = 1 x 10$^{-5}\mu$g/s, and 45% of this emission rate, or 4.5 x 10^{-6} μm, is particle-bound, then approximately 6.7 x 10$^{-8}\mu$g 2,3,7,8-TCDD/s is apportioned to the 15 μm diameter particles (4.5 E-6 μm/s x 0.0149). This procedure is then repeated for all particle sizes in the array.

3.10 METEOROLOGICAL DATA

The Guideline on Air Quality Models (EPA, 1993a) recommends the use of five years of meteorological data for making long-term estimates of ambient air concentrations.

However, it is recognized that 5 years of continuous meteorological measurements may not be available in all cases. In those situations, it is recommended that a minimum of one year of preprocessed meteorological data be used. It is important that the meteorological data be representative of local conditions nearest the site. Therefore the data should have been collected from the general vicinity of the combustor, and hourly data should be used. Additionally, if meteorological data are not available from the general vicinity of the combustor, then data from the nearest meteorological station should be used. This data should be representative of site conditions both spatially and climatologically (i.e., temporally). Meteorological data that are available from the National Weather Service may be suitable, although on-site meteorological data is preferred. The required types of data and appropriate measurement techniques for collecting site-specific meteorological data are discussed in "On-Site Meteorological Program Guidance for Regulatory Modeling Applications" (EPA, 1987a). Meteorological data includes measurements of wind speed, wind direction, ambient temperatures, cloud cover, ceiling heights, mixing heights, sky cover, atmospheric stability, atmospheric turbulence, hourly precipitation amounts, intensity of precipitation events and any other data needed in the air modeling exercise. When on-site data are used, the following information should be included: a) identification of the meteorological station site, and who maintains the station; b) the threshold for wind speed measurements; c) the method for collating and reducing the data; d) details on the the number and percentage of missing values in the meteorologic record; e) if applicable, details on the statistical methods applied to fill-in data gaps and missing values. In all cases, the EPA Regional staff meteorologist should be consulted when selecting meteorological data for dispersion and deposition modeling or when developing or evaluating a meteorological monitoring program.

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4. CALCULATING SOIL CONCENTRATIONS

4.1. Introduction

Issue   Indoor soil/dust concentrations may be different than outdoor soil levels.
Conclusions/Recommendations

Contaminants from sources outside the home may be brought into the home by airborne dust or tracking.   The resulting contaminant levels may be diluted with other indoor dusts.   Contaminants which degrade outdoors due to photolysis or biological processes, may be more persistent indoors.   Exposure may result via mouthing of objects with dust residues, dermal contact with dust residues or inhalation of suspended dusts. Procedures for assessing such exposures are not well established. Recommendations can be made to measure indoor dust to monitor contaminant levels. Cleaning procedures can be implemented to reduce exposures. For assessing impacts to indoor dust, it is recommended that the assumption be made that indoor dust originated as outdoor soil. Therefore, soil concentrations as estimated for outdoor conditions should be used as indoor dust concentrations. Furthermore, the soil concentration that should be used are the ones pertinent to the 1-cm "untilled" depth.

4.2.1. Calculating Cumulative Soil Concentration

Issue   The soil concentration algorithm considers deposition of particle-bound contaminants but does not consider vapor phase depositions or diffusions.

From the Indirect Exposure Document:

$$Sc = \frac{(Dyd + Dyw)\ [1.0 - exp(-ks\ Tc)]\ 100}{Z\ BD\ ks} \qquad [4\text{-}1]$$

where:

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Sc = soil concentration of pollutant after total time period of deposition (µg pollutant/g soil)

Dyd = yearly dry deposition rate of pollutant (g pollutant/m^2/yr)

Dyw = yearly wet deposition rate of pollutant (g pollutant/m^2/yr)

ks = soil loss constant (yr^{-1})

Tc = total time period over which deposition occurs (yrs)

100 = units conversion factor

Z = soil mixing depth (cm)

BD = soil bulk density (g/cm^3)

(Note that the units for soil concentration in Equation [4-1] have been changed from mg/g to µg/g, with a corresponding change in the units conversion factor.)

Conclusions/Recommendations

Volatilization loss is considered in the overall soil loss constant, with the rate constant due to volatilization equal to an equilibrium coefficient multiplied by a gas phase mass transfer coefficient (cm/s); see Equations (4-4) through (4-7) in the IED. Although the derivation for this rate constant was not given in IED, it has been independently verified as accurately representing volatilization loss (although the equation for the gas phase mass transfer coefficient, Kt of Equation (4-6), appears to be an empirical fit to data and is not referenced; it will be assumed to be appropriate for this application). If one assumes that the diffusive loading is driven by the same gas phase mass transfer coefficient (K_t) as volatilization, than one can solve for the loading term as:

$$L_{DIF} = 0.31536 \, K_t \, C_{va} \qquad \qquad [4\text{-}1]$$

where:

L_{DIF} = atmospheric diffusion flux to soil (g/m^2-yr)

K_t = gas phase mass transfer coefficient (cm/s; see Eq [4-6], IED)

C_{va} = gas phase air concentration (µg/m^3)

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The vapor phase air concentration that is appropriate for this formulation is the vapor phase concentration predicted by application of the air dispersion model. Chapter 3 of this Addendum further details application of the COMPDEP model to estimate vapor phase concentrations.

It is recommended that this diffusive term be added to the overall soil concentration equation as:

$$Sc = \frac{(Dyd + Dyw + L_{DIF})\ [1.0 - exp(-ks\ Tc)]\ 100}{Z\ BD\ ks} \qquad [4\text{-}1]$$

Finally, it should be noted that this formulation pertains to diffusive flux into the soil and does not address entry of vapor-phase contaminants via wet deposition. It is also not clear as to what extent this treatment of diffusive entry addresses the issue of "dry deposition" of vapors onto soils. The issue of vapor-phase impacts to soils remains a topic for future recommended research, as discussed in Part III of this Addendum.

4.2.2 Calculating the Soil Loss Constant

Issue The soil loss constant, ks of Equation [4-2] of the Indirect Exposure Document, does not include pollutant losses from soil erosion and surface runoff. For a small land area within a watershed, it could be argued that the soil loss constant does not need to consider such losses if whatever erodes or runs off in the downgradient direction from a site of concern (i.e., a farm where indirect exposures occur) is matched by an equal amount which erodes or runs onto it from upgradient areas. On the other hand, for the study region as a whole, as well as individual watersheds, losses due to soil erosion and surface runoff are important and need to be accounted for. These losses are incorporated in Chapter 9 in the soil erosion loss constant, kse, and the surface runoff constant, ksr (see Eq [9-4], Eq [9-6], and Eq [9-7] of this addendum).

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From the Indirect Exposure Document:

$$ks = ksl + ksg + ksv \qquad [4\text{-}2]$$

where:

ks = *soil loss constant due to all processes* (yr^{-1})

ksl = *loss constant due to leaching* (yr^{-1})

ksg = *loss constant due to degradation (abiotic and biotic)* (yr^{-1})

ksv = *loss constant due to volatilization* (yr^{-1})

Conclusions/Recommendations

It should be remembered that the soil concentration discussed in Chapter 4 of the Indirect Exposure Document is specific to a site where exposures occur, whereas for Chapter 9, the soil concentration is for the watershed as a whole. A watershed is likely to have subareas that are highly eroded such that erosion is a significant loss, subareas that are depositional where soil erosion is in fact a source term rather than a dissipation term, and subareas where, as the Issue discussion notes above, there may be little net loss via runoff or erosion. There will be a net loss via erosion to "average" watershed soils, hence the consideration of these terms for soil concentration in the surface water algorithm.

An assessor can use the current formulation in Chapter 4, but the exposure site soil concentration estimated in this way should be considered "worst case" or "hot spot", because the loss terms of runoff and erosion will not be considered. Alternately, the soil loss constant due to all processes, ks, can include both a soil erosion loss constant and a surface runoff loss constant. This is consistent with the approach taken in Chapter 9 of this addendum, and best represents average soil concentrations within a watershed:

$$ks = ksl + kse + ksr + ksg + ksv \qquad [4\text{-}2]$$

where:

ks	=	soil loss constant due to all processes (yr^{-1})
ksl	=	loss constant due to leaching (yr^{-1})
kse	=	loss constant due to soil erosion (yr^{-1})
ksr	=	loss constant due to surface runoff (yr^{-1})
ksg	=	loss constant due to degradation (yr^{-1})
ksv	=	loss constant due to volatilization (yr^{-1})

<u>Issue</u> The loss constant due to leaching, ksl of Equation [4-3] in the Indirect Exposure Document, does not properly account for surface runoff.

From the Indirect Exposure Document:

$$ksl = \frac{P + I - E_v}{\Theta\, Z\, [1.0 + (BD\, Kd_s\, /\Theta)]} \qquad [4\text{-}3]$$

where:

ksl	=	*loss constant due to leaching (yr^{-1})*
P	=	*average annual precipitation (cm/yr)*
I	=	*average annual irrigation (cm/yr)*
Ev	=	*average annual evapotranspiration (cm/yr)*
θ	=	*soil volumetric water content (mL/cm^3)*
Z	=	*soil depth from which leaching removal occurs (cm)*
BD	=	*soil bulk density (g/cm^3)*
Kd_s	=	*soil-water partitioning coefficient (mL/g)*

<u>Conclusions/Recommendations</u>

There is a need to include a runoff term, R, in the numerator of Equation [4-3] for calculating the loss constant due to leaching, ksl, as follows:

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$$ksl = \frac{P + I - R - E_v}{\Theta \ Z \ [1.0 \ + \ (BD \ Kd_s \ /\Theta)]} \qquad\qquad [4-3]$$

An annual runoff amount can be estimated given isopleths of surface runoff available in the "Water Atlas of the United States" (Gerahty, et al, 1973). The water atlas' isopleths give annual surface water contributions, which include interflow and ground water recharge, and they would need to be adjusted downward to reflect surface runoff only. Another approach for estimating surface runoff is to use the Curve Number Equation developed by the U.S. Soil Conservation Service. Isopleths of mean annual cropland runoff corresponding to various curve numbers have been developed by Stewart et al (1975), as reported by U.S. EPA (1985b). Curve numbers are assigned to an area based on the soil type, land use or cover, and the hydrologic condition of the soil.

Issue   Soil concentration depletion due to volatilization is modeled as a means of limiting soil concentration. However, this mass flux never experiences rainout or washout and subsequent redeposition. The result is an underestimate of soil concentrations for volatile soluble compounds.

Conclusions/Recommendations

The reposition of volatilized residues of semi-volatile organic contaminants such as dioxin is very small, and can generally be ignored. This may not be the case for more volatile compounds, and more research is recommended. No changes to the soil concentration algorithm to include redeposition of volatilized residues are recommended at this time.

4.3.3 Soil Depth

Issue   The concept of two mixing depths, 20 cm for tilled soils and 1 cm for untilled soils, needs to be more fully explained.

Conclusions/Recommendations

Most literature has placed the untilled depth for atmospheric particles depositing

at 1 or 2 cm, with some literature on deposition of radionuclides in untilled situations at 5 cm. The tilled mixing depth of 20 cm is used in the dioxin exposure document (EPA, 1992c) and elsewhere. An "untilled" soil concentration is one where the soil is not disturbed, as in pasture grass or lawn settings. It is used for dermal exposures and soil ingestion exposures. "Tilled" soil concentrations are used for the soil-to-crop algorithms (i.e., vegetables/fruits for human consumption, or hay/silage in the beef/milk food chain algorithm). Using the untilled soil concentration for soil-related exposures is a conservative assumption. If instead, it is felt that dermal exposures or soil ingestion exposures occur in conjunction with gardening or agricultural field crop production, than the tilled soil concentration should be used.

For soluble compounds, leaching might lead to movement below 1 cm and perhaps justify a mixing depth greater than 1 cm. However, no change to account for this is recommended at this time.

Issue Soil/dust concentrations on hard surfaces may have an effective mixing depth of less than 1 cm.

Conclusions/Recommendations

Deposition on to hard surfaces may result in dust residues which have negligible dilution with other residues. Examples may include sidewalks, slides, swings and other play areas at schools. Exposure may result via mouthing of these objects or dermal contact. Estimates of the ingestion of such residues or amounts transferred to skin have not been well established. Thus, such exposures are difficult to assess quantitatively. Recommendations can be made to measure residue levels on surfaces to monitor contaminant levels. Cleaning procedures can be implemented to reduce exposures. If an exposure assessment is to include contact with dust that is on hard surfaces, it is recommended that the concentration of contaminants on that dust be assumed to be equal to soil concentrations that are estimated for the "untilled" depth, which is in this guidance is recommended to be 1 cm.

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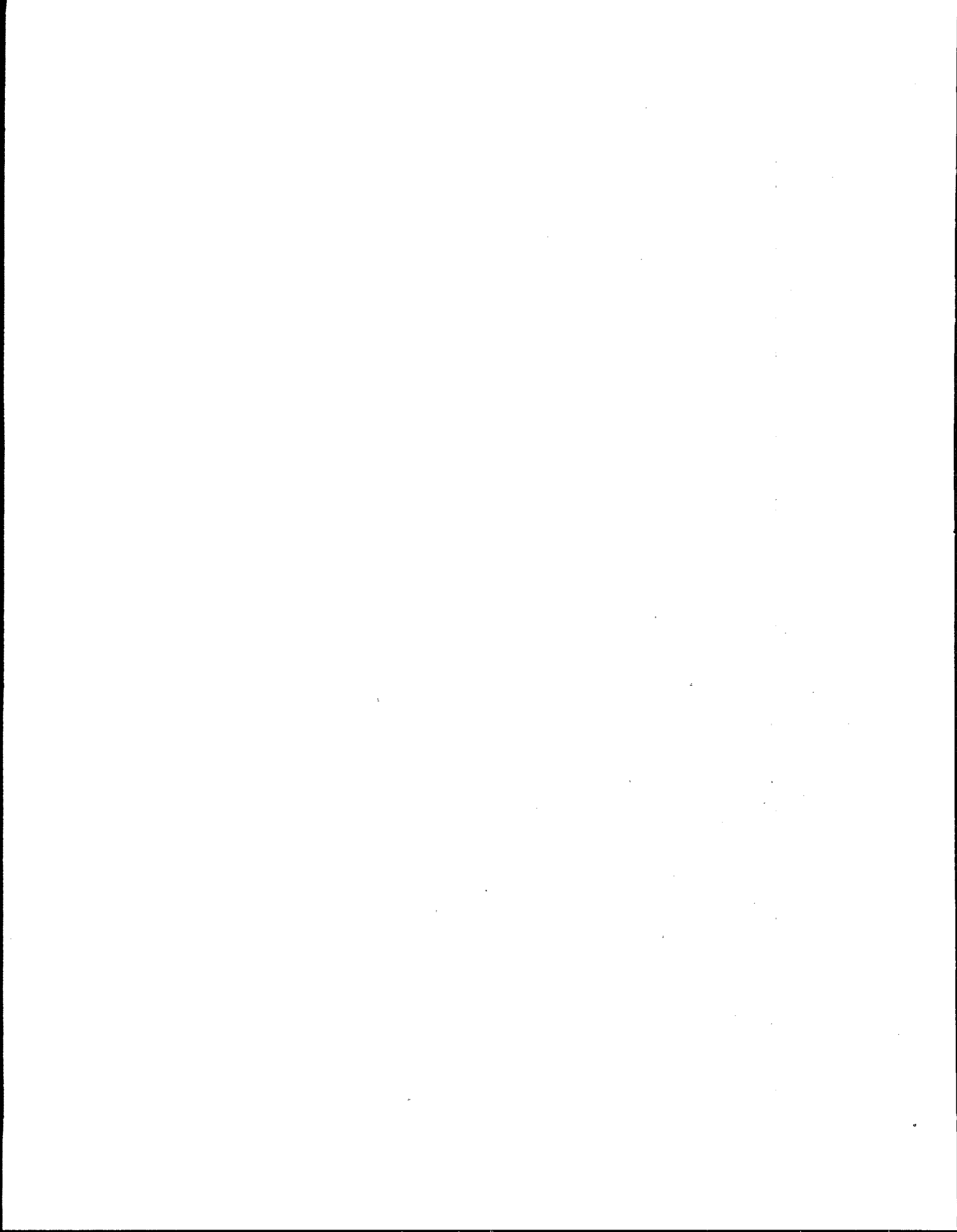
5. DETERMINING EXPOSURE THROUGH THE TERRESTRIAL FOOD CHAIN

5.2 Calculating Concentration of Pollutant in Plants

The approach which sums vapor transfers, particle depositions, and root uptake to estimate total plant concentrations is an appropriate one. However, there are issues with each pathway.

5.2.1 Plant Pollutant Concentration Due to Root Uptake

<u>Issue</u>   The Travis and Arms approach seems to be mixing and matching various chemicals and environmental settings to come up with an empirical transfer coefficient (Br). Lipophilic non-pesticidal compounds are included with soluble pesticides. The mechanisms for soil to plant transfers are different for the two classes of compounds. Also, for the process of root uptake, the characterization of potatoes and root vegetables as "protected" is inappropriate. The idea was that root vegetables were protected from vapor transfers and particle depositions. The Travis and Arms algorithm which assigns a value to Br (plant-soil bioconcentration factor) is inappropriate for potatoes and root vegetables. The Travis and Arms relationship is for soil to above ground plant transfers (e.g., translocation into shoots), not soil to below ground transfers (e.g., to roots and tubers).

From the Indirect Exposure Document:

$$Pr_i = Sc\ Br_i \qquad\qquad [5\text{-}2]$$

where:

Pr_i =   *concentration of pollutant in i^{th} plant group due to root uptake (µg pollutant /g plant tissue, dry weight [DW])*

Sc =   *soil concentration of pollutant after the total period of deposition (µg pollutant/g soil)*

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Br_i = plant-soil bioconcentration factor for the ith plant group

([µg pollutant/g plant tissue DW]/[µg pollutant/g soil])

The bioconcentration factor is given as:

$$\log B_r = 1.588 - 0.578 \log K_{ow} \qquad\qquad [5\text{-}3]$$

where:

K_{ow} = octanol-water partition coefficient

Conclusions/Recommendations

A better approach to vegetables for which roots are the edible portions, is to separate "above ground" and "below ground" vegetation, and state that below ground vegetation includes edible roots such as carrots, potatoes, radishes, etc. This is the approach taken in the dioxin exposure document (EPA, 1992c). It should be noted that concentrations of dioxin in carrots and potatoes are among the highest found in vegetables/fruits.

An approach developed by Briggs should be used in place of the Travis and Arms algorithm, for soil to below ground transfers to root vegetables. The Briggs approach uses a Root Concentration Factor (RCF) to estimate plant concentrations (Briggs, 1982). Recommended revisions to Equations [5-2] and [5-3] of the IED are:

$$Pr_{bg} = \frac{Sc\ RCF}{Kd_s} \qquad\qquad [5\text{-}2]$$

and:

$$\log (RCF - 0.82) = 0.77 \log K_{ow} - 1.52 \qquad\qquad [5\text{-}3]$$

where:

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Pr_{bg} = concentration of pollutant in below ground plant parts due to root uptake (μg pollutant/g plant tissue, fresh weight [FW])

Sc = soil concentration of pollutant (μg pollutant/g soil)

Kd_s = soil-water partition coefficient (mL/g)

RCF = ratio of concentration in roots to concentration in soil pore water ([μg pollutant/g plant tissue FW]/[μg pollutant/mL pore water])

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

The dioxin document (EPA, 1992c) uses an empirical correction factor, to reflect the fact that the barley roots of Briggs' experiments are different than bulky below ground vegetables such as potatoes or onions. Dioxin-like compounds will sorb to outer portions of below ground vegetation, but inner translocation is negligible. Therefore, the concentrations in the barley roots, for the lipophilic compounds used by Briggs in his experiments, would be higher on a whole plant basis than concentrations that would result from soil to root transfers for bulkier vegetation. In other words, the whole barley root concentrations would be similar to concentrations near the skin of a potato, but not a whole potato. The dioxin document uses an empirical reduction factor of 0.01, which was estimated using a surface area volume to whole plant volume ratio for a carrot. A similar fix would not be appropriate for an RCF developed for soluble compounds, which would have transpiration stream translocation and more uniform vegetative concentrations.

For the long-term, other approaches should be reviewed for root uptake of contaminants from soil. Also, for soil to above ground plant transfers, consideration might be given to the Transpiration Stream factor developed by Brigg's as a simple approach for more water soluble compounds as a possible alternative to the Travis and Arms algorithm. The principal cause for soluble pesticides to impact above ground parts of plants from soil contamination is through the transpiration stream.

The magnitude of transfer by lipophilic compounds has been shown to be much lower than soluble compounds. Given this, Travis' approach may be acceptable as the transfer factor does increase with decreasing Kow, i.e., it may appropriately reflect an observed trend for chemicals with increasing Kow. No change is therefore recommended,

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and one should use the Travis and Arms Br for soil to above ground transfers for all contaminants for which a Kow is known.

5.2.2 Plant Pollutant Concentration Due to Direct Deposition

Issue The basic framework given by Equation [5-4] is sound. However, the validity of including an "Fw" and its default assignment of 0.02 are questioned. This essentially zeroes out wet deposition impacts to plants.

From the Indirect Exposure Document:

$$Pd_i = \frac{1000 \ [Dyd \ + \ (Fw \ Dyw)] \ Rp_i \ [1.0 \ - \ exp(-kp \ Tp_i)]}{Yp_i \ kp} \qquad [5\text{-}4]$$

where:

Pd_i = concentration of pollutant due to direct deposition in the ith plant group (µg pollutant/g plant tissue DW)

1000 = units conversion factor

Dyd = yearly dry deposition rate (g pollutant/m^2/yr)

Fw = fraction of wet deposition that adheres to plant surfaces (dimensionless)

Dyw = yearly wet deposition rate (g pollutant/m^2/yr)

Rp_i = interception fraction of the edible portion of the plant tissue for the ith plant group (dimensionless)

kp = plant surface loss coefficient (yr^{-1})

Tp_i = length of the plant's exposure to deposition per harvest of the edible portion of the ith plant group (yrs)

Yp_i = yield or standing crop biomass of the edible portion of the ith plant group (kg DW/m^2)

Conclusions/Recommendations

Setting Fw at 0.02 greatly diminishes the impact of contaminants depositing via wet deposition. (The reference for this assignment is a memorandum which upon review has shown not to be technically rigorous.) The dioxin exposure document (EPA, 1992c) does not use an Fw value of 0.02 for estimating plant impacts; total deposition of contaminant onto plants is the sum of wet and dry deposition. Several other multimedia exposure assessments for dioxin include wet deposition in a "total" deposition term when estimating impacts to vegetation, using the same model as the Indirect Exposure Document. In effect, Fw is assigned a value of 1 for these dioxin exposure assessments. However, there is one dioxin exposure assessment which uses a parameter "b", which is the same as Fw and which was evaluated as having a value between 0.1 and 0.3 (McKone and Ryan, 1989).

A value of 1 for Fw is recommended when applying the methodology from the Indirect Exposure Document to hydrophobic contaminants such as dioxins, PCBs, or other organic contaminants whose log Kow exceeds 3.0. This is, at least, a conservative assumption taken by other researchers and justified by the strong sorptive tendencies of this class of organic chemicals to organic material. For metals and soluble organic chemicals, those with log Kow less than 3.0, it does make intuitive sense that they would not adhere significantly to vegetation while falling dissolved in rainwater. For these chemicals, an Fw of 0.10 is recommended.

Issue   From Equation [5-4], kp is usually described as a particle weathering factor and has been assigned a value of 18 yr^{-1}, equivalent to a half-life of 14 days.

Conclusions/Recommendations

The 14 day half-life value corresponds to physical processes which remove particles and does not consider chemical degradation. As such, a higher rate constant (i.e., a shorter half-life) may be justified to consider chemical degradation. In the Indirect Exposure Document, the value of 126.5 yr^{-1} for benzo(a)pyrene, corresponding to a 2 day half-life, appears to be based on an atmospheric degradation half-life. A value of 14 days is recommended for pollutants which do not degrade or degrade very slowly, such that kp

is based on physical processes removing particles from plants.

5.2.3 Plant Pollutant Concentrations Due to Air-to-Plant Transfer

Issue The algorithm for estimating vapor transfers to vegetations described in the IED as Equation [5-13] is problematic and should be replaced.

From the Indirect Exposure Document (p 5-16)

$$Pv_i = \frac{[(Fv \; Cy) + C_v] \; Bv_i}{\rho_a} \qquad [5\text{-}13]$$

where:

Pv_i = concentration of pollutant due to air-to-plant transfer in the ith plant group (μg pollutant/g plant tissue DW)

Fv = fraction of pollutant air concentration present in the vapor phase (dimensionless)

Cy = concentration of pollutant in air due to direct emissions (μg pollutant/m^3)

Cv = concentration of pollutant in air due to vaporization from soil(μg pollutant/m^3)

Bv_i = air-to-plant biotransfer factor for the ith plant group ([μg pollutant/g plant tissue DW]/[μg pollutant/g air])

ρ_a = density of air (g/m^3)

Conclusions/Recommendations

First, Fv is inappropriate and should be deleted from the equation, and Cy should be more precisely defined as, "vapor-phase concentration of pollutant in air due to direct emissions". Recall that the air dispersion modeling includes two computer runs, one which

generates vapor phase air concentrations, and one which generates particle phase concentrations and depositions. Therefore, an Fv is inappropriate for this framework since a vapor phase concentration will already be available. An Fv would be appropriate if air modeling assumed the *entire emissions* were in vapor phase and modeled air concentrations at exposure sites. In this case, a *total concentration* would need to be reduced to estimate only that amount in the vapor phase, and an Fv would be appropriate.

Second, the use of a vapor phase concentration which resulted from soil volatilization is inappropriate. Earlier in Section 5.2.1., it was discussed that the Travis and Arms relationship is only appropriate for soil to above ground plant transfers. It should be assumed that the Travis and Arms empirical factor, the Br_i, models all soil to above ground transfers, which includes transpiration stream translocation, dust resuspension followed by settling onto plants, and volatilization followed by vapor transfers. Including C_v while also using the Travis and Arms Br_i is double counting.

With these two changes, the plant concentration due to vapor transfers is simplified as:

$$Pv_i = \frac{Cy\ Bv_i}{pa} \qquad [5-13]$$

Issue Serious and legitimate concern has recently been raised in the use of the Bacci Algorithm for vapor transfers of dioxin. A recent article by in Environmental Science and Technology (McCrady and Maggard, 1993) demonstrated that the Bacci factor will significantly overestimate transfers of 2,3,7,8-TCDD vapor to grass leaves.

From the Indirect Exposure Document:

$$\log (Bv\ H) = -0.93 + 1.14 \log K_{ow} \qquad [5\text{-}15]$$

where:

Bv = air-to-leaf biotransfer ($[\mu g/g\ DW]/[\mu g/g]$)

H = Henry's Law constant ($Pa\text{-}m^3/mol$)

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

(Note: 1 atmosphere is equivalent to 9.87×10^{-6} Pascals.)

Conclusions/Recommendations

First, the Bacci empirical relationship given above was published in a 1990 article (Bacci, et al., 1990). It included the results of experimentation on 10 chemicals. A more recent publication by Bacci and coworkers (Bacci, et al., 1992) included results from four additional chemicals, for a total of 14 chemicals, and was also presented in a more generalized volume/volume transfer basis rather than mass/mass transfer basis:

$$\log B_{vol} = 1.065 \log Kow - \log \left(\frac{H}{R\ T} \right) - 1.654 \qquad [5\text{-}15a]$$

where:

B_{vol} = Bacci volumetric air-to-leaf biotransfer factor, unitless [(μg contaminant/L of wet leaf)/(μg contaminant/L air)]

Kow = contaminant octanol water partition coefficient, unitless

H = contaminant Henry's Constant, atm-m^3/mol.

R = ideal gas constant, 8.205×10^{-5} atm-m^3/mol-deg K

T = temperature, 298.1 K

-1.654 = empirical constant

Bacci, et al. (1990) showed that the volumetric transfer factor can be transformed to a

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mass-based transfer factor by assuming that 70% of the wet leaf is water, that the leaf density is 890 g/L, and given an air density is 1.19 g/L:

$$B_v = \frac{(1.19 \ g/L) \ B_{vol}}{(0.3) \ (890 \ g/L)}$$ [5-15b]

where:

B_v = mass-based air-to-leaf biotransfer factor, unitless [(μg contaminant/kg plant dry)/(μg contaminant/kg air)]

B_{vol} = Bacci volumetric air-to-leaf biotransfer factor, unitless [(μg contaminant/L of wet leaf)/(μg contaminant/L air)]

Bacci's experiments were conducted under conditions which would not account for photodegradation of his test chemicals from the leaf surfaces. A recent study by McCrady and Maggard (1993) which investigated the uptake and photodegradation of 2,3,7,8-TCDD sorbed to grass foliage suggests a significant difference in experimental B_{vol} for grass plants. The authors note that the log B_{vol} for 2,3,7,8-TCDD and azalea plants, using Bacci's empirical relationship, was estimated as 8.5. The experimental log B_{vol} for 2,3,7,8-TCDD and grass plants reported by McCrady was 6.9 when photodegradation was accounted for, and 7.5 in the absence of photodegradation. Since the photodegradation experiments by McCrady best represent outdoor conditions, their work suggests that the air-to-leaf transfer factor estimated by Bacci's algorithm may be 40 times too high for vapor-phase transfer of 2,3,7,8-TCDD onto grass leaves.

An issue discussed by McCrady is that the theoretical time for the grass tissue to reach a steady state is much shorter than that indicated in the Bacci experiments. Using Bacci's results, McCrady noted that the azalea leaves theoretically take greater than 400 days to reach equilibrium, in comparison to less than 20 days to reach equilibrium for the grass plants in their experiments. This difference is not entirely due to photodegradation. Thus, for estimating contaminant concentrations in animal feeds such as relatively short lived grass plants, the equilibrium B_{vol} from the Bacci azalea model may overestimate the

contaminant concentration in grass. On the other hand, McCrady (personal communication, J. McCrady, Corvallis Environmental Research Laboratory, EPA) suggests that the 50-day exposure time used in Bacci's experiments may allow for considerable diffusion into the newly formed plant surface wax. Thus, the sorbed TCDD residues may be trapped and unable to volatilize. If so, than the relatively high volatilization and photodegradation rates reported by McCrady may be higher than what might occur for the longer exposure times expected in real world situations.

These arguments are being presented to demonstrate the uncertainty in choosing either of the two reported B_{vol} values for estimating plant contaminant concentrations. McCrady's results pertaining to 2,3,7,8-TCDD cannot be generalized to other compounds or other contaminants in terms of commonly available contaminant parameters such as H or Kow. Therefore, a McCrady framework similar to Bacci's for estimating congener-specific B_v cannot be offered at this time. On the other hand, their work strongly suggests that the Bacci model may be inappropriate for food chain modeling, because of their experimental length of time, their use of an azalea leaf of high wax content, and lack of a artificial light source simulating photodegradation.

Based on work conducted for the dioxin exposure document, the following recommendation is made. The Bacci algorithm as more recently formulated (B_v of Equation [5-15b] above) should be used to estimate a chemical-specific air-to-leaf transfer factor. This algorithm is generalizable to any chemical for which a Henry's Constant, H, and an octanol water partition coefficient, Kow, is known. However, a value arrived at with this algorithm should be reduced by a factor of ten before use. The factor of ten reduction is suggested based on work conducted for the dioxin exposure assessment as an interim correction factor. Briefly, this work involved attempting to model the background concentrations of dioxin-like compounds in beef starting with a profile of air concentrations crafted to be typical of rural environments. This exercise demonstrated that use of the Bacci transfer factor without empirical adjustment would significantly overestimate concentrations, whereas use of the Bacci factor empirically reduced by a factor of 10 made predictions come in line with observations (note: the current draft of the dioxin exposure document is as yet unreviewed; this exercise does not appear in the 1992

released version of the dioxin exposure document - EPA, 1992c).

5.3 Calculating the Concentration of Pollutant in Animal Tissues

<u>Issue</u> The Travis and Arms biotransfer factor (Ba) is the only transfer factor in the methodology from the Indirect Exposure Document that uses mass ingestion of contaminants (mg/day) by animals and translates them to a tissue concentration (mg/kg whole concentration). Other approaches depend on a concentration in media to concentration in tissue bioconcentration/biotransfer factor.

<u>Conclusions/Recommendations</u>

The fact that Ba is based upon mass ingestion of contaminants doesn't invalidate the Travis and Arms approach by itself.   The approach does have the advantage that the transfers factors are based on the commonly available Kow. The dioxin exposure document (EPA, 1992c) uses a bioconcentration factor, which takes the ratio of the concentration of contaminant in cattle dry matter intake (mg/kg) and translates it to a concentration in cattle body and milk fat (mg/kg lipid based concentration). What the dioxin document also does, is to demonstrate that the 2,3,7,8-TCDD BCF (developed by Fries and Paustenbach) comes up with whole milk and whole beef concentrations that are actually fairly similar to whole milk and beef concentrations that would be estimated using the Travis and Arms approach. This exercise required assumptions on: dry matter intake by cattle (kg/day), beef and milk fat assumptions, and so on. This gives some validation of the Travis and Arms approach.

At this point, no changes should be made to the biotransfer factor, Ba. In addition to the benefit of it being generalizable based on Kow, factors were also compiled for metals in Table 5-4 of the Indirect Exposure Document.

<u>Issue</u> A concern is that some plants ingested by animals may not be contaminated.   This might call for an additional adjustment factor, F_{ij}, which would be included with $Qp_{ij}P_{ij}$ of Equation [5-19], and would be defined as the fraction of the ith plant group eaten by j^{th} animal which is grown on impacted soil (i.e., soil impacted at 5 km, average soil impact over 50 km, etc.). The implicit assumption in the current

framework is that this value is 1.00. A value less than 1.00 might be called for if cattle feed (or hog or chicken feed, etc.) were purchased by the farmer from a local distributor who gets it from a distant location.

From the Indirect Exposure Document:

$$A_j = [\sum_{i=1}^{n} (Qp_{ij} \, P_{ij}) + (Qs_j \, Sc)] \, Ba_j \qquad \qquad [5\text{-}19]$$

where:

A_j = concentration of pollutant in the jth animal tissue group (µg pollutant/g animal tissue DW)

QP_{ij} = quantity of ith plant group eaten by the jth animal each day (kg plant tissue DW/day)

P_{ij} = total concentration of pollutant in the ith plant group eaten by the jth animal (µg pollutant/g plant tissue DW)

Qs_j = quantity of soil eaten by the jth animal each day (kg soil/day)

Sc = soil concentration (µg pollutant/g soil)

Ba_j = biotransfer factor for the jth animal tissue group (d/kg)

Conclusions/Recommendations

A factor, F_{ij}, should be added to Equation [5-19] as follows:

$$A_j = [\sum_{i=1}^{n} (F_{ij} \, Qp_{ij} \, P_{ij}) + (Qs_j \, Sc)] \, Ba_j \qquad \qquad [5\text{-}19]$$

where:

F_{ij} = fraction of the ith plant group grown on contaminated soil and eaten by the jth animal (dimensionless) (other variables as above)

Default values of 1.00 should be assumed; values less than one should be based on information on the portion of cattle grain, silage, etc. that is transported from sites that are not impacted by the combustor.

5.3.2. Quantity of Soil Consumed by Animals

Issue A concern here is the Indirect Exposure Document's assuming no soil ingestion by pigs and poultry. Fries of USDA notes that pigs exhibit "rooting" behavior and assumes a maximum soil ingestion intake of 8 percent of dry matter based on a 2 to 8 percent range noted in his earlier PCB work. Chickens could also come in contact with soil and have soil ingestion.

Conclusions/Recommendations

A soil ingestion quantity of 8% should be assigned for pigs. No data could be found for free ranging poultry. It seems intuitively appropriate to assign a value for chickens less than that for pigs, and a value comparable for that of grazing cattle. Therefore, a value of 3% for free ranging chicken soil ingestion, the IED recommendation for cattle soil ingestion, is made here.

5.4 Calculating Human Daily Intake

Issue Further guidance is needed on how to estimate ingestion rates of home-grown foods.

Conclusions/Recommendations

The Indirect Exposure Document uses a two part procedure to estimate the consumption rate of locally produced foods. The first step uses national data to estimate total consumption rates of various food groups and then adjusts these using the fraction homegrown. Each of these issues is discussed below.

The total consumption rates are estimated primarily on the basis of the EPA's Office of Pesticide Program "Tolerance Assessment System" which was derived from the 1977-78 USDA Nationwide Food Consumption Survey (USDA, 1983). The data are conveniently summarized to provide consumption rates (normalized by body weight) for 1)

seven different plant groups and seven different animal groups, 2) various percentiles and 3) five different age groups. Such statistics are very useful in exposure assessments. However, when using these data the assessor should consider the following points:

● These data represent total ingestion rates of store-bought food. Obviously, what is of interest for a site-specific problem is the amount of food consumed which is locally grown within the study area. Ideally, local surveys would be used to directly determine ingestion rates of locally produced foods or (as a second choice) to estimate diet fractions needed to adjust the total ingestion rates.

● The USDA survey was conducted over a three day period. Thus, it does not represent long term behavior patterns which is the interest of exposure assessments used to support analysis of chronic health effects. This problem introduces uncertainty into the estimates of the median (50th percentile) and other percentiles. The data would be appropriate for estimating means.

● For purposes of assessing impacts of atmospheric deposition onto plants it is important to consider whether the edible portion is protected or not. However, even protected foods can be impacted if they take up contaminants via the roots after deposition on to soil.

The fraction of foods which are home-produced was also based on data from the USDA survey. Although these estimates are a potentially useful starting point to select site-specific values, ideally they should be refined on the basis of local surveys (as discussed above, it would be more useful to use local surveys to directly evaluate ingestion rates of locally produced food). The Workgroup was not able to agree on further recommendations in this area. Some of the diet fractions presented in the Indirect Exposure Document do not appear reasonable, i.e. 50% of the lima beans consumed by city residents are home produced. Clearly, the accuracy of these values need to be confirmed. The Workgroup recommended further analysis of these surveys before final recomendations are made. Additional considerations are noted below:

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● Chapter 2 recommends developing separate exposure estimates for various segments of the population such as farmers, home gardeners, nongardening residents, etc. These diet fractions were presented for city, suburban and nonmetropolitan areas. Thus, it is not clear how to apply these data to these population groups.

● The diet fraction listed for beef and dairy consumption in nonmetropolitan areas is 15% and 3% respectively. An earlier USDA study (USDA, 1966) of 900 rural farm households found that 44% of the beef and 40% of dairy products consumed were home-produced. Since this study was specific to farm households, it may be more accurate for this population segment. Similar issues would apply to the other food groups. The 1966 diet fractions sound high, but are based on fairly old data. EPA plans to evaluate whether a similar analysis can be made of the 1977-78 and the 1987-88 surveys.

● The USDA surveys estimated fraction home-grown by subtracting amounts of food purchased from total ingested. Some individuals may eat locally produced foods bought from neighbors or at farmer markets. Assessors should attempt to evaluate this practice on the basis of local information and adjust diet fraction assumptions accordingly.

EPA is in the process of evaluating new food ingestion data as part of the update to the Exposure Factors Handbook (EPA, 1989b) and may have a better basis for these recommendations soon.
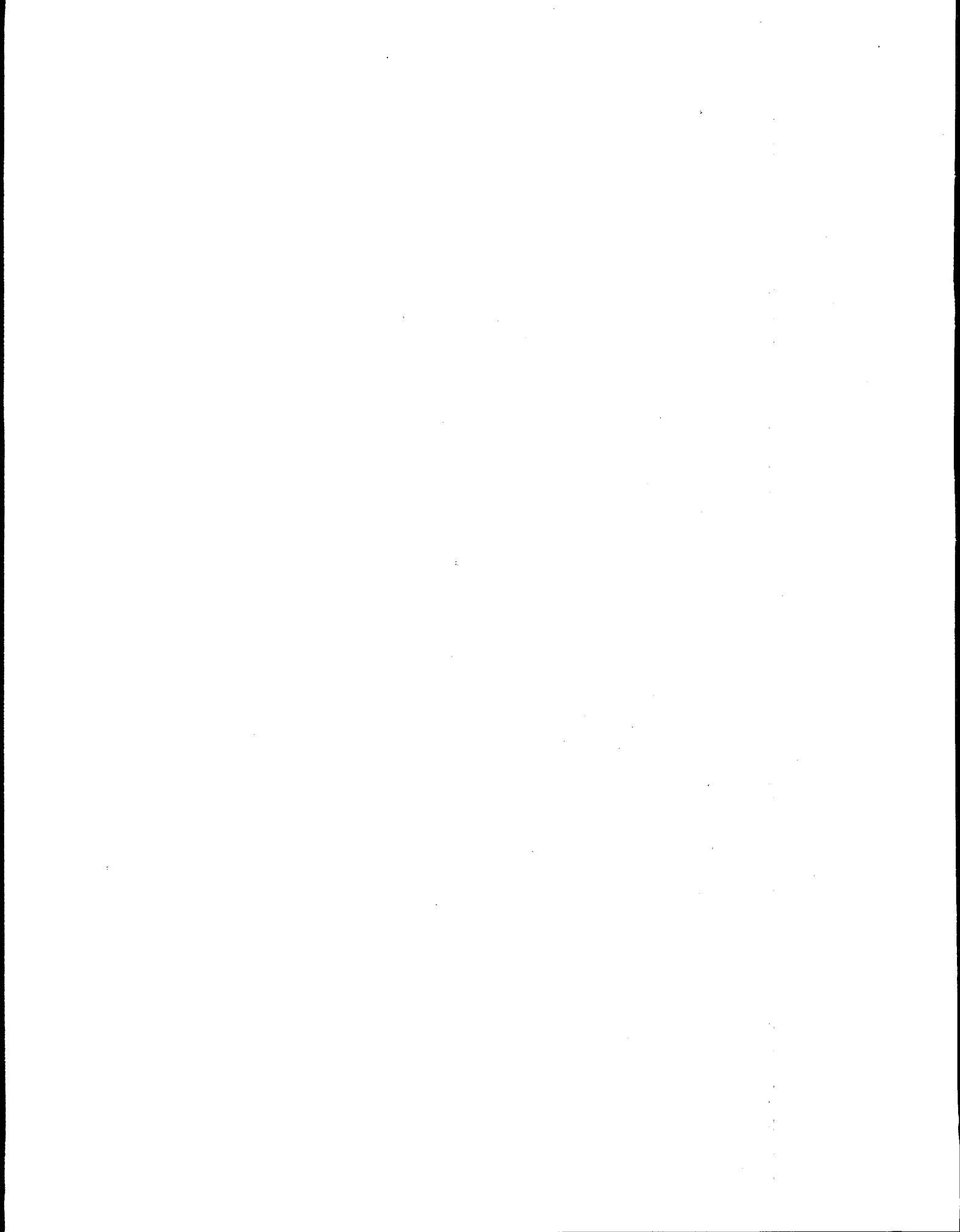
6. DETERMINING EXPOSURE FROM SOIL INGESTION

6.2 Human Daily Intake

Issue   There has been considerable discussion as to the appropriate soil ingestion assumptions.

Conclusions/Recommendations

It is recommended that for children ages 1 to 6, an ingestion rate of 0.1 g/day (as an average rate) and 0.2 g/day (as an upper estimate) and a body weight of 16 kg (see note below) should be used, while for adults an ingestion rate of 0.05 g/day (as an average) and 0.1 g/day (as an upper estimate) and a body weight of 70 kg should be used. These ingestion rate recommendations are based largely on the judgement of the Working Group. A number of soil ingestion studies (EPA, 1989b) have been conducted, but they do not provide a strong statistical basis for evaluating upper estimates of soil ingestion for children. These studies have been interpreted differently even within EPA. Note that EPA, 1989b identified the range 0.1 to 0.2 g/day as representative of the mean and recommended 0.8 g/day as an upper estimate. Virtually no reliable data are available for evaluating adult soil ingestion. The reasons that the existing studies on children are not well suited to deriving distributions or upper percentiles include: 1) they were conducted over 3-4 days and therefore do not represent usual behavior and 2) they involve substantial experimental error, i.e. the range of values seen in different children are likely to represent uncertainty more than true variability in behavior.

Although the 16 kg body weight assumption for children is generally adequate, a more accurate procedure is to use the average of the inverse body weights over this age range.

These recommendations apply to children with normal mouthing tendencies. Some children exhibit abnormal mouthing behavior or "pica" and would have much higher ingestion rates. The associated soil ingestion rates, frequency and duration of the behavior are not well established. Thus, no quantitative basis can be offered to evaluate this behavior.

EPA is in the process of evaluating new soil ingestion data as part of the update to

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the Exposure Factors Handbook (EPA, 1989b) and may have a better basis for recommendations in this area soon.

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## 7. DETERMINING EXPOSURE FROM DERMAL ABSORPTION VIA SOIL

<u>Issue</u>   The Indirect Exposure Document does not provide guidance for quantitative evaluation of dermal risks.

<u>Conclusions/Recommendations</u>

New quantitative procedures for dermal exposure have recently been published in Dermal Exposure Assessment: Principles and Applications (EPA, 1992b), and should be adopted here.

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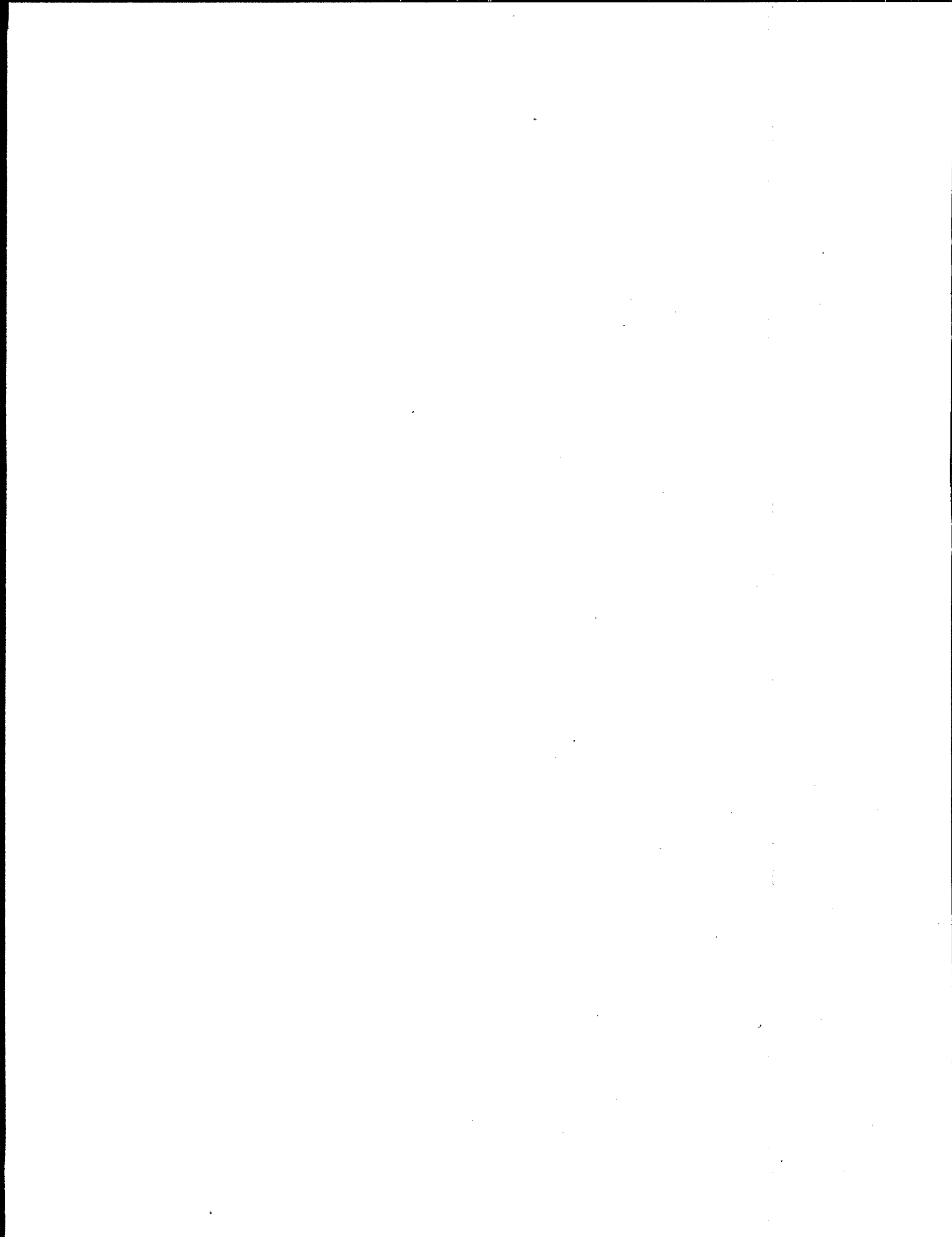
8. DUST RESUSPENSION

8.4 Example Calculations

<u>Issue</u> The expert panel which met in September, 1992, to evaluate the August, 1992 dioxin exposure document (EPA, 1992c), recommended a different model be adopted for evaluating suspensions of contaminated soil via wind erosion. The model used in the dioxin document is the same one used in Chapter 8 of the Indirect Exposure Document.

<u>Conclusions/Recommendations</u>

The model recommended by the expert panel was researched and it was not clear that it offered a substantial improvement over the one used and it might even be more data intensive. No change is recommended for the present.

<u>Issue</u> The Indirect Exposure Document only addresses dust resuspension due to wind erosion. However, "fugitive dust" generated from agricultural tilling and from vehicle traffic on paved and unpaved roads are much larger sources of resuspended particulate matter. Also, the IED does not present any algorithm for estimating dispersion of suspended dust.

<u>Conclusions/Recommendations</u>

The document, "Control of Open Fugitive Dust Sources" (EPA, 1988) includes algorithms for estimating emissions from agricultural tilling and paved and unpaved roads. A companion document, "User's Manual for the PM-10 Open Fugitive Dust Source Computer Model Package" (EPA, 1990b), is available which implements these techniques for use on a personal computer. The "Guideline on Air Quality Models (Revised)" (EPA, 1993a) contains information on dispersion models that can be used to estimate airborne concentrations downwind from fugitive dust sources. Specifically, the ISC2 model may be used for area and line sources, such as agricultural fields and roads. More simply, one can use a box model to estimate air concentrations near the source of fugitive emissions. Either of these two approaches will result in airborne concentrations of contaminants bound to particles at a site downwind from where fugitive emissions occur.

With care, there are ways to further use these estimated particle-bound contaminant concentrations. First, a portion of this concentration can reasonably be assumed to be 10 μm in diameter or less, and most of the fugitive emission models do distinguish emissions that are less than and greater than 10 μm. This portion can be added to air concentrations which are estimated for direct, inhalation exposures. Second, contaminants resuspended in dust can be resettled onto vegetations (above ground fruits/vegetables, pasture grass, cattle feed) or soils assuming a velocity of deposition - μg/m^3 * m/sec = a rate of deposition in units of μg/m^2-sec. Dry deposition velocities from the COMPDEP model can be used here as one option for dry deposition. Alternately, a velocity of dry deposition can be assumed based on an assumption of particle size and gravitational settling. An appropriate, estimated velocity of gravitational deposition for 10 μm size particles is 0.01 m/sec (1 cm/sec), as given in Seinfeld (1986). There still would need to be consideration of wet deposition of resuspended particles. A wet deposition amount can be estimated as a product of the air concentration times annual rainfall times a volumetric washout fraction for contaminants in airborne particles. This washout ratio is defined as: (mass contaminant/volume rain) $\div$ (mass contaminant/volume air). Bidleman (1988) discusses the washout ratio - saying it ranges between 10^3 and 10^6; is typically between 10^5 and 10^6, and uses a value of 2 * 10^5 for his further calculations. This is recommended as a reasonable value for first approximations if the impact of fugitive emissions are to be considered.

In summary, wet and dry depositions of resuspended airborne particulates are given as:

$$dry\ deposition = V_d\ C_{pa} \qquad [8\text{-}1]$$

$$wet\ deposition = R\ W_p\ C_{pa} \qquad [8\text{-}2]$$

where:

C_{pa} = contaminant air concentration estimated for resuspended particles,

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μg/m^3 (or comparable mass/volume units)

V_d = dry deposition velocity, m/sec (0.01 m/sec)

R = annual rainfall, m/yr

W_p = washout ratio, unitless (2*10^5)

However, depositing resuspended contaminants in dust particles should be done carefully. For example, if one is suspending dust due to agricultural tillage, one should not redeposit that suspended amount back onto the very same agricultural soil. That would be double counting. In the same vein, depositing resuspended dust due to agricultural tillage onto the field crops grown on that very same agricultural soil is also double counting. Recall that the Travis and Arms soil to above ground plant transfer coefficient, Br_i, is expected to estimate all causes for contaminants to transfer from soils to plants growing in the soils. Therefore, it would be invalid to resuspend dust due to agricultural tillage, deposit it onto agricultural crops, and then also use the Travis and Arms Br_i.

The only situation where resuspended impacts should be considered is when the site of impact of such particles is physically distinct from the site of origin of the resuspended dust. For example, dust resuspended from roadways onto soils or vegetations would be reasonable since roadway dust is a unique source to soils or vegetations. Another example would be the impact of agricultural tillage onto nearby residential settings. There again, the suspended dust is a unique source to the nearby residence.

As a final note, one should always compare the contaminant concentrations of dispersed, resuspended contaminated dust with air concentrations estimated by dispersion/deposition modeling from the stack to see if addition of resuspended dust adds significantly to the reservoirs predicted to occur from the stack. In the same way, one should compare the rate of deposition of contaminants in resuspended dust to that estimated by the atmospheric deposition modeling. If the air concentration and deposition rates are very small in comparison to those which are due to stack emissions, say 1% of concentrations and depositions due to direct emissions, they can be neglected.

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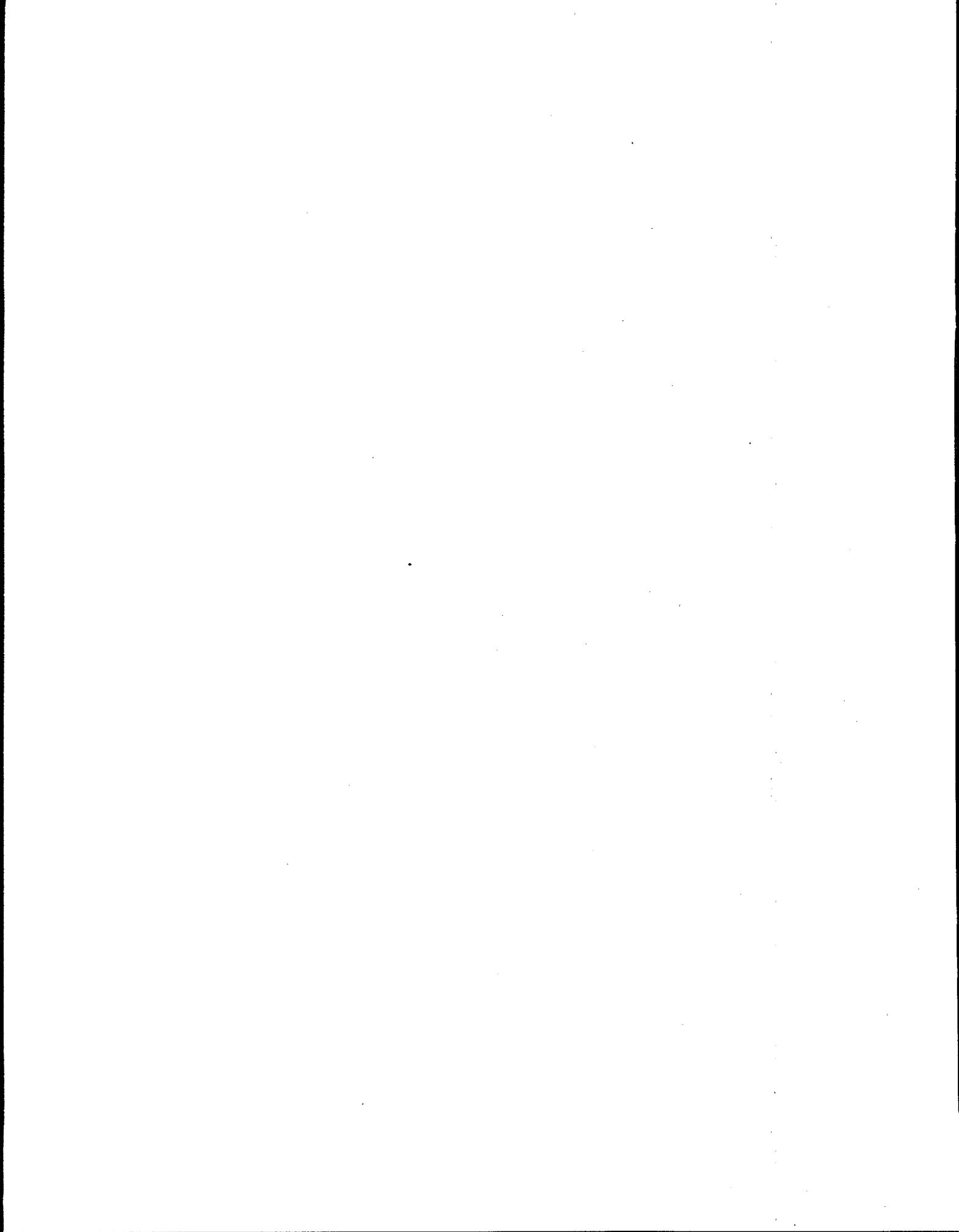
[The following is offered as a framework for estimating impacts to water bodies from combustors. It replaces the multiple frameworks offered in Section 9.2 of Chapter 9 of the Indirect Exposure Document. Sections 9.1, 9.3, and 9.4 of Chapter of the Indirect Exposure are still evaluated as being appropriate, except for issues as noted below. This alternative has been developed by Bob Ambrose of the Athens Environmental Research Laboratory and Matt Lorber of the Office of Health and Environmental Assessment. Care has not been taken to make the units or parameter names consistent with other chapters of the Indirect Exposure Document. However, the units are internally consistent.]

[Revised Section 9.2. begins here]

9.2. CALCULATING WATER CONCENTRATIONS

9.2.1 INTRODUCTION

The following framework for estimating surface water impacts from stack emissions estimates water column as well as bed sediment concentrations. Water column concentrations include dissolved, sorbed to suspended sediments, and total (sorbed plus dissolved, or total contaminant divided by total water volume). This framework also provides three concentrations for the bed sediments: dissolved in pore water, sorbed to bed sediments, and total. The model accounts for four routes of contaminant entry into the water body: 1) sorbed to soils eroding into the water body, 2) dissolved in runoff water, 3) direct deposition of particle-bound contaminant; and 4) direct diffusion of vapor phase contaminants into the water body. The model also accounts for four dissipation processes which remove contaminants from the water column and/or bed sediment reservoirs: 1) decay of total contaminants (sorbed + dissolved) within the water column, 2) decay of total contaminants (sorbed + dissolved) within the bed sediment, 3) volatilization of dissolved phase out of the water column; and 4) removal of total contaminant via "burial" from the surficial bed sediment layer. This burial rate constant is a function of the deposition of sediments from the water column to the bed; it accounts for the fact that much of the soil eroding into a water body annually becomes bottom sediment rather than suspended sediment. The impact to the water body is assumed to be

uniform. This tends to be more realistic for smaller water bodies as compared to large river systems. Key assumptions in the surface water impact algorithm are:

- Soil concentrations within a depositional area (which is distinct from a watershed; see discussion for WA_L below in Section 9.2.10) are assumed to be uniform within the area, and can be estimated by the following key parameters representing the area as a whole: dry and wet contaminant deposition rates, a soil dissipation rate, a soil bulk density, and a soil mixing depth;

- The partitioning of the contaminant within the soil/water matrices - surface soils, suspended solids in the water body, and bed sediments of the water body - can be described by partition coefficients;

- One route of entry into the surface water body will be direct deposition. A second route of entry is contaminant dissolved in annual surface runoff. This will be estimated as a function of the contaminant dissolved in soil water and annual water runoff. A third route of entry is via soil erosion. A sorbed concentration of contaminant in soil, together with an annual soil erosion estimate, a sediment delivery ratio, and an enrichment ratio, can be used to describe the delivery of contaminant to the water body via soil erosion. A sediment delivery ratio serves to reduce the total potential amount of soil erosion (i.e., the total potential equals a unit erosion rate as in kg/m^2 times a watershed area, in m^2) reaching the water body recognizing that most of the erosion from a watershed during a year deposits prior to reaching the water body. The enrichment ratio recognizes the fact that soils which erode tend to be lighter in texture, more abundant in surface area, and have higher organic carbon. All these characteristics lead to concentrations in eroded soils which tend to be higher in concentration as compared to in-situ soils. A fourth and final route of entry is via diffusion in the gaseous phase. The dissolved concentration in a water body is driven toward equilibrium with the vapor phase concentration above the water body. At equilibrium, gaseous diffusion into the water body is matched by volatilization out of the water body. Gaseous diffusion is estimated

with a transfer rate (determined internally given user inputs) and a vapor phase air concentration. This air concentration is specified by the user and is an output of the atmospheric transport model.

• For the surface water solution algorithm, it is assumed that equilibrium is maintained between contaminants within the water column and contaminants in bed sediments. Equilibrium is established when the dissolved phase concentration in the water column is equal to the dissolved phase concentration within the bed sediments. This condition is imposed by the water body equations.

• A rate of contaminant "burial" in bed sediments is estimated as a function of the rate at which sediments deposit from the water column onto the surficial sediment layer. This burial represents a permanent sink and recognizes that a portion of the soil, and contaminant sorbed to it, which erodes into a water body becomes bottom sediment while the remainder becomes suspended sediment. This solution assumes that there will be a net depositional loss, even though resuspension and redeposition of sediments is ongoing, particularly with moving water bodies. For cases where the net deposition rate is zero, there will be no burial loss calculated.

• Separate water column and benthic decay rate constants will allow for the consideration of decay mechanisms which remove contaminants from the water body. If a transformation yield coefficient is specified, the decay of one chemical is linked to the internal loading of a second chemical.

Figure 9.1 below displays the framework for this analysis, with a listing of the ten concentrations which are part of the solution algorithm, and the state equations which link the concentrations.

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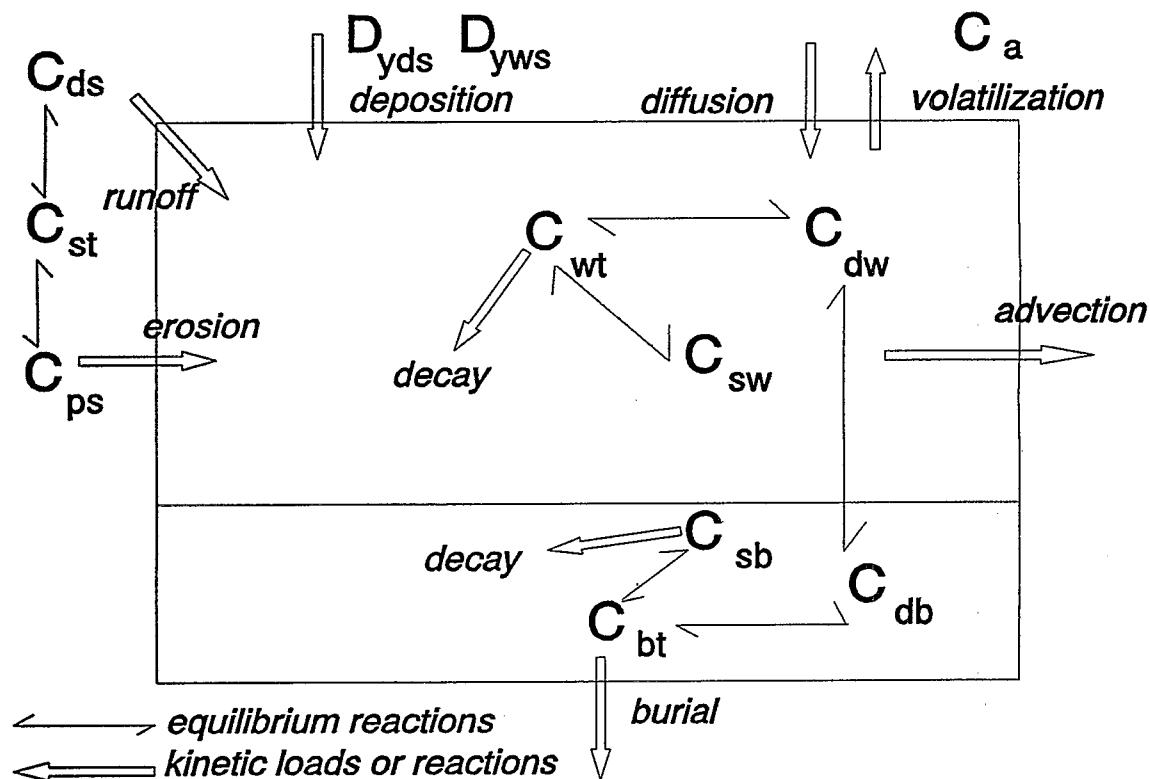
Figure 9.1. Basic structure of the water algorithm showing concentrations considered, relationships between concentrations, and routes of fate and dissipation

Definitions

C_{st}	total soil concentration	mg/L
C_{ds}	concentration dissolved in soil water	mg/L
C_{ps}	concentration sorbed to soil	mg/kg
D_{yds}	yearly dry deposition to surface water	mg/yr
D_{yws}	yearly wet deposition to surface water	mg/yr
C_a	vapor phase air concentration above water	$\mu g/m^3$
C_{wt}	total concentration in water column	mg/L
C_{wtot}	total water concentration in surface water system, including water column plus benthic sediment (not shown in Figure 1)	mg/L
C_{dw}	dissolved phase water concentration	mg/L
C_{sw}	sorbed phase water concentration	mg/kg
C_{bt}	bottom sediment total concentration	mg/L
C_{db}	concentration dissolved in bed sediment pore water	mg/L
C_{sb}	concentration sorbed to bottom sediments	mg/kg

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STATE EQUATIONS CORRESPONDING TO FIGURE 9.1

I. Soil

$$C_{st} = Sc \ BD$$

$$C_{st} = \theta_s \ C_{ds} + BD \ C_{ps}$$

$$C_{ps} = C_{ds} \ Kd_s$$

$$C_{ps} = \frac{Sc \ Kd_s \ BD}{\theta_s + Kd_s \ BD}$$

$$C_{ds} = \frac{Sc \ BD}{\theta_s + Kd_s \ BD}$$

$$Sc = \text{see Equation [9-2]}$$

II. Surface Water System

$$C_{wtot} = C_{wt} \cdot d_w/d_z + C_{bt} \cdot d_b/d_z$$

$$= \text{see Equation [9-1]}$$

$$f_{water} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 10^{-6}) \cdot d_w/d_z}{(1 + Kd_{sw} \cdot TSS \cdot 10^{-6}) \cdot d_w/d_z) + (\theta_{bs} + Kd_{bs} \cdot BS) \cdot d_b/d_z}$$

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$$f_{benth} = \frac{(\theta_{bs} + Kd_{bs} \cdot BS) \cdot d_b/d_z}{(1 + Kd_{sw} \cdot TSS \cdot 10^{-6}) \cdot d_w/d_z + (\theta_{bs} + Kd_{bs} \cdot BS) \cdot d_b/d_z}$$

III. Water Column

$$C_{wt} = f_{water} \cdot C_{wtot} \cdot d_z/d_w$$

$$C_{dw} = C_{wt} \cdot f_{dw} = C_{wt} \left[\frac{1}{1 + Kd_{sw} \cdot TSS \cdot 10^{-6}} \right]$$

$$C_{sw} = Kd_{sw} \cdot C_{dw}$$

IV. Bed Sediment

$$C_{bt} = f_{benth} \cdot C_{wtot} \cdot d_z/d_b$$

$$C_{db} = C_{bt} \cdot f_{db}/\theta_{bs} = C_{bt} \left[\frac{1}{\theta_{bs} + Kd_{bs} \cdot BS} \right]$$

$$C_{sb} = Kd_{bs} \cdot C_{db}$$

Note that by substituting the relationship between C_{wt} and C_{wtot} into the expression for C_{bt}, we can obtain benthic concentrations as a functions of water column concentrations:

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$$C_{bt} = C_{wt} \cdot \frac{\theta_{bs} + Kd_{bs} \cdot BS}{1 + Kd_{sw} \cdot TSS \cdot 10^{-6}}$$

$$C_{db} = C_{dw}$$

$$C_{sb} = C_{ps} \cdot Kd_{bs}/Kd_{sw}$$

where:

Sc	=	soil concentration (μg/g)
θ_s	=	volumetric soil water content (L_{water}/L)
θ_{bs}	=	bed sediment porosity (L_{water}/L)
Kd_s	=	soil/water partition coefficient (L/kg)
Kd_{sw}	=	suspended sediment/surface water partition coefficient (L/kg)
Kd_{bs}	=	bottom sediment/sediment pore water partition coefficient (L/kg)
BD	=	soil bulk density (g/cm^3)
TSS	=	total suspended solids (mg/L)
BS	=	bed sediment concentration (g/cm^3)
d_w	=	depth of the water column (m)
d_b	=	depth of the upper benthic layer (m)
d_z	=	total depth of water body, $d_w + d_b$ (m)
f_{water}	=	fraction of total water body contaminant concentration that occurs in the water column
f_{benth}	=	fraction of total water body contaminant concentration that occurs in the bed sediment
f_{dw}	=	fraction of water column contaminant concentration that is dissolved
f_{db}	=	fraction of bed sediment contaminant concentration that is dissolved

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9.2.2 CHEMICAL MASS BALANCE EQUATIONS

If Figure 9.1 is taken as a control volume for the water body, a steady-state mass balance equation can be written that balances chemical loadings with outflow and loss:

$$C_{wtot} = \frac{L_T}{Vf_x \, f_{water} + k_{wt} \, V_t} \qquad \text{[9-1]}$$

where:

$C_{wtot} =$ total water body concentration, including water column and benthic sediment (mg/L)

$L_T \quad =$ total chemical load into water body, including deposition, runoff, erosion, atmospheric diffusion, and internal chemical transformation (g/yr)

$Vf_x \quad =$ average volumetric flow rate through water body (m^3/yr)

$V_t \quad =$ total volume of water body or water body segment being considered, including water column and benthic sediment (m^3)

$k_{wt} \quad =$ total first order dissipation rate constant, including water column and benthic degradation, volatilization, and burial (yr^{-1})

$f_{water} \quad =$ fraction of total water body contaminant concentration that occurs in the water column

A similar mass balance equation can be written for the watershed soils, balancing areal deposition fluxes with chemical loss processes:

$$Sc = \frac{L_W}{ks \, Z \, BD} (1.0 - \exp(-ks \, Tc)) \, 100 + C_{sb} \qquad \text{[9-2]}$$

where:

$Sc \quad =$ average watershed soil concentration after time period of deposition (μg pollutant/g soil)

$L_W \quad =$ yearly average load of pollutant to watershed on an areal basis

(g pollutant/m^2-yr)

ks = total chemical loss rate constant from soil (yr^{-1})

Tc = total time period over which deposition has occurred (yr)

Z = representative watershed mixing depth to which deposited pollutant is incorporated (cm)

BD = representative watershed soil bulk density (g/cm^3)

100 = units conversion factor (μg-m^2/g-cm^2)

C_{sb} = background "natural" soil concentration (μg pollutant/g soil)

The major terms in Equations [9-1] and [9-2] are discussed in sections below.

9.2.3 SEDIMENT MASS BALANCE EQUATIONS

Before calculating chemical fate, a mass balance equation for sediments in the water body must be solved. First, we begin with the water column. Referring to Figure 9.2, the soil eroding into the water body, X_w, equals the sum of the amount depositing into the upper bed, X_d, and the advective loss from the water column, X_a. Solving for the suspended solids concentration in the water column:

$$TSS = \frac{X_e \ WA_L \ SD \ 10^3}{Vf_x + W_{dep} \ WA_w}$$

[9-3]

where:

TSS = suspended solids concentration (mg/L)

X_e = unit soil loss, calculated in the soils section from the USLE equation (kg/m^2-yr)

WA_L = watershed surface area (m^2)

SD = watershed sediment delivery ratio (unitless)

Vf_x = average volumetric flow rate through water body (m^3/yr)

W_{dep} = suspended solids deposition rate (m/yr)

WA_w = water body surface area (m^2)

10^3 = units conversion factor

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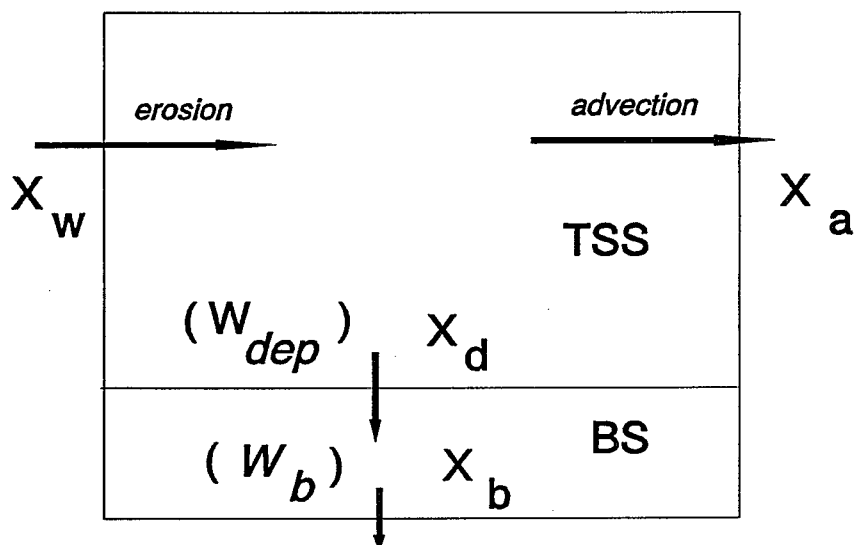
Figure 2. Steady state representation for sediments in water bodies.

DEFINITIONS

X_w	soil erosion input from depositional area	g/yr
X_a	advective loss from water body	g/yr
X_d	deposition onto bottom sediment	g/yr
X_b	burial below bottom sediment layer	g/yr
TSS	suspended solids concentration	g/L
BS	bottom sediments concentration	g/L
W_{dep}	rate of deposition onto bed sediment	m/yr
W_b	rate of burial	m/yr

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Often, the user will have data on average suspended solids, but not the deposition rate. In this case, the deposition rate can be calculated as:

$$W_{dep} = \frac{X_e \ WA_L \ SD \ 10^3 - Vf_x \ TSS}{WA_w \ TSS}$$ [9-4]

where terms are as defined above.

In the second part of the solids balance, the mass deposited to the bed, X_d, is set equal to the mass buried, X_b. Solving for the burial rate gives:

$$W_b = W_{dep} \ \frac{TSS \ 10^{-6}}{BS}$$ [9-5]

where:

W_b	=	burial rate (m/yr)
W_{dep}	=	deposition rate (m/yr)
TSS	=	suspended solids concentration (mg/L)
BS	=	benthic solids concentration (kg/L)
10^{-6}	=	conversion factor (kg/mg)

Finally, the benthic porosity, the volume of water per volume of benthic space, is calculated from the benthic solids concentration and sediment density:

$$\theta_{bs} = 1 - BS/\rho_s$$ [9-6]

where:

θ_{bs}	=	benthic porosity (L/L)
BS	=	benthic solids concentration (kg/L)
ρ_s	=	solids density, 2.65 kg/L

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For input benthic solids concentrations between 0.5 and 1.5 kg/L, benthic porosity will range between 0.8 and 0.4.

9.2.4. LOADS TO WATERSHED SOILS

The pollutant load term includes wetfall and dryfall fluxes, along with internal transformation loads:

$$L_W = Dydw + Dyww + L_{Is} + L_{DIF} \qquad [9\text{-}7]$$

where:

$Dydw$	=	yearly average dry depositional flux of pollutant (g/m^2-yr)
$Dyww$	=	yearly average wet depositional flux of pollutant (g/m^2-yr)
L_{Is}	=	internal transformation load of pollutant per areal basis (g/m^2-yr)
L_{DIF}	=	atmospheric diffusion flux to soil (g/m^2-yr)

Wet and dry depositional fluxes are determined by measurement or by air modeling and are specified as input to this model. Internal loading is due to chemicals that are transformed chemically or biologically into daughter products, which may be of interest in risk assessment. Transformation yields can be specified for the sequential reaction:

$$B \xrightarrow[ksg(B)]{Ys(BC)} C \qquad [9\text{-}8]$$

where:

B	=	parent compound
C	=	daughter compound (or reaction product)
$ksg(B)$	=	first order transformation rate constant (yr^{-1})
$Ys(BC)$	=	reaction yield coefficient (mg of C/mg of B)

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The internal loading generated by this transformation reaction is given by:

$$L_{Is} = k_{sg}(B) \; Ys(BC) \; Sc(B) \; BD \; Z \; 10^{-2} \qquad\qquad [9\text{-}9]$$

where:

L_{Is} = internal transformation load of pollutant per areal basis (g/m^2-yr)

$ksg(B)$ = first order transformation rate constant (yr^{-1})

$Ys(BC)$ = reaction yield coefficient (mg of C/mg of B)

$Sc(B)$ = soil concentration of B (μg/g)

BD = bulk density of soil, g/cm^3

Z = representative watershed mixing depth to which deposited pollutant is incorporated (cm)

10^{-2} = units conversion factor

This loading is added to chemical C. If the yield coefficient is set to zero, then the compounds are treated as independent.

The load due to vapor diffusion is given as:

$$L_{DIF} = 0.31536 \; K_t \; C_{va} \qquad\qquad [9\text{-}10]$$

where:

L_{DIF} = atmospheric diffusion flux to soil (g/m^2-yr)

K_t = gas phase mass transfer coefficient (cm/s; see Eq [4-6], IED)

C_{va} = gas phase air concentration (μg/m^3)

9.2.5 LOSS PROCESSES IN WATERSHED SOILS

The total chemical loss rate ks in equation [9-2] is due to several physical and chemical processes:

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$$ks = ksl + kse + ksr + ksg + ksv \qquad \text{[9-11]}$$

where:

ks	=	soil loss constant due to all processes (yr^{-1})
ksl	=	soil loss constant due to leaching (yr^{-1})
kse	=	soil loss constant due to erosion (yr^{-1})
ksr	=	soil loss constant due to runoff (yr^{-1})
ksg	=	soil loss constant due to chemical transformation/ degradation (yr^{-1})
ksv	=	soil loss constant due to volatilization (yr^{-1})

The degradation constant, ksg, is derived by the user. The other four constants are given by:

$$ksl = \frac{P + I - R - EV}{\theta_s \, Z \, [1.0 + (BD \, Kd_s / \theta_s)]} \qquad \text{[9-12]}$$

$$kse = \frac{0.1 \, X_e \, SD \, ER}{BD \, Z} \left(\frac{Kd_s \, BD}{\theta_s + Kd_s \, BD} \right) \qquad \text{[9-13]}$$

$$ksr = \frac{R}{\theta_s \, Z} \left(\frac{1}{1 + (Kd_s \, BD/\theta_s)} \right) \qquad \text{[9-14]}$$

$$ksv = Ke \, Kt \qquad \text{[9-15]}$$

where:

P	=	average annual precipitation (cm/yr)

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I	=	average annual irrigation (cm/yr)
R	=	average annual runoff (cm/yr)
Ev	=	average annual evapotranspiration (cm/yr)
θ_s	=	volumetric water content (dimensionless; cm^3/cm^3)
Z	=	watershed mixing zone depth (cm)
BD	=	soil bulk density (g/cm^3)
SD	=	sediment delivery ratio
ER	=	contaminant enrichment ratio
Kd_s	=	soil-water partition coefficient (cm^3/g)
X_e	=	unit soil loss ($kg/m^2/yr$; see Eq [9-3], IED)
Ke	=	equilibrium coefficient (s/cm/yr); see Eq [4-5], IED)
Kt	=	gas phase mass transfer coefficient (cm/s; see Eq [4-6], IED)
0.1	=	units conversion factor

Sc is the concentration resulting from contaminated particles depositing on and mixing with surface soils. For strongly hydrophobic contaminants such as dioxins or PCBs, where Kd_s are very large, Sc will be essentially equal to the "total" soil concentration, C_{st}, as well as the sorbed concentration, C_{ps}, and the dissolved phase concentration, C_{ds}, will be vanishingly small. (See the state equations above.) However, for a generic solution where a contaminant may not be as hydrophobic, contaminants depositing as particles are assumed to reequilibrate in the soil/soil water system. In the listing of state equations, the reequilibrated sorbed phase concentration, C_{ps}, and the dissolved phase concentration, C_{ds}, are now used to estimate loads due to soil erosion and loads due to surface runoff, respectively.

9.2.6 LOADS TO THE WATER BODY

Total chemical loading to the water body is comprised of five inputs:

$$L_T = L_{Dep} + L_{RI} + L_R + L_E + L_{Dif} + L_I \qquad \text{[9-16]}$$

where:

L_T	=	total contaminant load to the water body (g/yr)
L_{Dep}	=	deposition of particle bound contaminant (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_{Dif}	=	diffusion of vapor phase contaminant (g/yr)
L_I	=	internal transformation load (g/yr)

The runoff and erosion loads require estimation of average contaminant concentration in watershed soils that comprise the depositional area. This will be discussed first.

9.2.6.1 Load due to direct deposition

The load to surface waters via direct deposition is solved as:

$$L_{Dep} = (Dyds + Dyws) \, WA_w \qquad \text{[9-17]}$$

where:

L_{Dep}	=	direct deposition load (mg/yr)
$Dyds$	=	representative yearly dry deposition rate of pollutant onto surface water body (g pollutant/m^2/yr)
$Dyws$	=	representative yearly wet deposition rate of pollutant onto surface water body (g pollutant/m^2/yr)
WA_w	=	water body area (m^2)

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9.2.6.2 Load due to impervious surface runoff

A fraction of the chemical wet and dry deposition in the watershed will be to impervious surfaces. Dry deposition may accumulate and be washed off during rain events. If the impervious surface includes gutters, the pollutant load will be transported to surface waters, bypassing the watershed soils. The average load from such impervious surfaces is given by:

$$L_{RI} = (D_{yww} + D_{ydw})\ WA_I \qquad [9\text{-}18]$$

where:

L_{RI} =   impervious surface runoff load (g/yr)

WA_I =   impervious watershed area receiving pollutant deposition (m^2)

D_{yww} =   yearly wet deposition flux onto the watershed ($g/m^2/yr$)

D_{ydw} =   yearly dry deposition flux onto the watershed ($g/m^2/yr$)

9.2.6.3 Load due to pervious surface runoff

Most of the chemical deposition to a watershed will be to pervious soil surfaces. These loads are accounted for in the soil mass balance equation. During periodic runoff events, dissolved chemical concentrations in the soil are transported to surface waters as given by:

$$L_R = R\ (WA_L - WA_I) \left[\frac{Sc\ BD}{\theta_s + Kd_s\ BD} \right] 10^{-2} \qquad [9\text{-}19]$$

where:

L_R =   pervious surface runoff load (g/yr)

R =   average annual runoff (cm/yr)

Sc =   pollutant concentration in watershed soils ($\mu g/g$; Eq [9-2])

BD =   soil bulk density (g/cm^3)

θ_s =   volumetric soil water content (cm^3/cm^3)

Kd_s = soil-water partition coefficient (L/kg or cm^3/g)

WA_L = total watershed area receiving pollutant deposition (m^2)

WA_I = impervious watershed area receiving pollutant deposition (m^2)

10^{-2} = units conversion factor (g^2/kg-μg)

9.2.6.4 Load due to soil erosion

During periodic erosion events, particulate chemical concentrations in the soil are transported to surface waters as given by:

$$L_E = X_e \ (WA_L - WA_I) \ SD \ ER \left[\frac{Sc \ Kd_s \ BD}{\theta_s + Kd_s \ BD} \right] 10^{-3} \qquad [9\text{-}20]$$

where:

L_E = soil erosion load (g/yr)

X_e = unit soil loss (kg/m^2/yr)

Sc = pollutant concentration in watershed soils (μg/g; Eq [9-2])

BD = soil bulk density (g/cm^3)

θ_s = volumetric soil water content (cm^3/cm^3)

Kd_s = soil-water partition coefficient (L/kg or cm^3/g)

WA_L = total watershed area receiving pollutant deposition (m^2)

WA_I = impervious watershed area receiving pollutant deposition (m^2)

SD = watershed sediment delivery ratio (unitless)

ER = soil enrichment ratio (unitless)

10^{-3} = units conversion factor (g-cm^2/μg-m^2)

9.2.6.5 Load due to gaseous diffusion

The change in the total water concentration over time due to volatilization is given by:

$$\frac{\partial C_{wtot}}{\partial t}\bigg|_{volat} = -\frac{K_v}{D}\left(f_{water}f_{dw}C_{wtot} - \frac{C_a\,10^{-6}}{H/(RT_k)}\right)$$

[9-21]

where:

C_{wtot} = total water body contaminant concentration (mg/L)

K_v = overall transfer rate (m/yr)

D = depth of water body (m)

f_{water} = fraction of total water body contaminant concentration that occurs in the water column

f_{dw} = fraction of water column contaminant concentration that is dissolved

C_a = vapor phase air concentration over water body ($\mu g/m^3$)

H = contaminant Henry's Constant (atm-m^3/mole)

R = universal gas constant, $8.206*10^{-5}$ atm-m^3/mole-K

T_k = water body temperature (K)

10^{-6} = units conversion factor

The right hand side of Equation [9-21] contains two terms. The first term constitutes a first order loss rate of aqueous contaminant, and is covered in more detail in section 9.2.8.2 below. The second term in Equation [9-21] describes diffusion of gas-phase contaminant from the atmosphere into the water body. Because this term is independent of water body contaminant concentration, it can be treated as an external load. As formulated above, this term has units of mg/L-yr. It must be converted to loading units by multiplying by the water column volume, V. Noting that V/D is equal to the surface water area WA_w, the atmospheric diffusion load is given as:

$$L_{Dif} = \frac{K_v\,C_a\,WA_w\,10^{-6}}{H/RT_k}$$

[9-22]

where:

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L_{Dif} = diffusion of vapor phase contaminant (g/yr)

K_v = the overall transfer rate (m/yr)

WA_w = surface water body area (m^2)

C_a = vapor phase air concentration over water body ($\mu g/m^3$)

H = contaminant Henry's Constant (atm-m^3/mole)

R = universal gas constant (= 8.206×10^{-5} atm-m^3/mole-°K)

T_k = water body temperature (°K)

10^{-6} = units conversion factor

9.2.6.6 Load due to internal transformation

Chemicals may be transformed chemically or biologically into daughter products, which may be of interest in risk assessment. A transformation yield can be specified for the sequential reaction:

$$B \overset{Y(BC)}{\underset{k(B)}{\rightarrow}} C \qquad \text{[9-23]}$$

where:

B = parent compound

C = daughter compound (or reaction product)

k(B) = first order transformation rate constant (yr^{-1})

Y(BC) = reaction yield coefficient (g of C/g of B)

The internal loading generated by this transformation reaction is given by:

$$L_I = \left[k_{dw}(B) \quad C_{wt}(B) \quad V_w \quad + \quad k_{db}(B) \quad C_{bt}(B) \quad V_b \right] \; Y(BC) \qquad \text{[9-24]}$$

where:

L_I = the internal transformation load to C (g/yr)

$k_{dw}(B)$ = water column transformation rate constant from B to C (yr^{-1})

$k_{db}(B)$ = benthic transformation rate constant from B to C (yr^{-1})

$C_{wt}(B)$ = total water column concentration of B (mg/L)

$C_{bt}(B)$ = total benthic concentration of B (mg/L)

V_w = water column volume (m^3)

V_b = benthic volume (m^3)

$Y(BC)$ = reaction yield coefficient (g of C/g of B)

This loading is added to chemical C. If the yield coefficient is set to zero, then the compounds are treated as independent.

9.2.7 ADVECTIVE FLOW FROM THE WATER BODY

The first term in the denominator of Equation [9-1] accounts for advective flow from the water body. It is the product of the average annual volumetric flow rate, Vf_x, and the fraction of the chemical in the water body that is present in the water column, f_{water}. An impacted water body derives its annual flow from its watershed, or effective drainage area. Flow and watershed area, then, are related, and compatible values should be specified by the user. Given the area of drainage, one way to estimate annual flow volume is to multiply total drainage area (in length squared units) by a unit surface water runoff (in length per time). The *Water Atlas of the United States* (Geraghty et al., 1973) provides maps with isolines of annual average surface water runoff, which is defined as all flow contributions to surface water bodies, including direct runoff, shallow interflow, and groundwater recharge. The range of values ranged from 5 to 40 in/yr in various parts of the U.S.

9.2.8 CHEMICAL DISSIPATION WITHIN THE WATER BODY

The second term in the denominator of Equation [9-1] accounts for dissipation within the water body. It is the product of the water body volume, V_t, and the total first order dissipation rate constant, k_{wt}. The water body volume, in units of m^3, together with the annual flow rate, in m^3/yr, determines the average residence time of a pollutant

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traveling through the water body. The residence time for Lake Erie is about 10 years, for example, while for the larger Lake Superior, it is estimated to be 200 years. For a swiftly moving river, on the other hand, the residence time can be on the order of hours (1 hour = 0.00011 yr). Larger volumes and residence times allow the internal dissipation processes to have a larger effect on pollutant concentration, while smaller volumes and residence times lessen the effect. The user should take care to specify reasonable volumes for the type of surface water body being represented. In addition, the user should specify compatible values for related water body parameters, such as surface area, WA_w. The water body volume divided by the surface area gives the average depth, which can vary from a fraction of a meter for small streams to a few meters for shallow reservoirs to tens of meters for deep lakes.

The total dissipation rate constant, k_{wt}, applies to the total water body concentration, C_{wtot}, and includes processes affecting any of the chemical phases -- dissolved or sorbed in the water column or benthic sediments. Volatilization, water column and benthic degradation, and burial are considered:

$$k_{wt} = f_{water}\, k_{gw} \;+\; f_{benth}\, k_{gb} \;+\; f_{water}\, k_v \;+\; f_{benth}\, k_b \qquad [9\text{-}25]$$

where:

k_{wt}	=	overall total water body dissipation rate constant (yr^{-1})
k_{gw}	=	water column degradation or transformation rate constant (yr^{-1})
k_{gb}	=	benthic degradation or transformation rate constant (yr^{-1})
k_v	=	water column volatilization rate constant (yr^{-1})
k_b	=	benthic burial rate constant (yr^{-1})
f_{water}	=	fraction of total water body contaminant concentration that occurs in the water column
f_{benth}	=	fraction of total water body contaminant concentration that occurs in the benthic sediment

These processes are described below.

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9.2.8.1. Chemical/Biological Degradation

Contaminants can be degraded by a number of processes in the water column or in the benthic sediment. The major chemical and biological processes include hydrolysis, photolysis, oxidation, and biodegradation. Each of these processes have been studied and are incorporated in a mechanistic way in advanced water quality models. In this methodology, the overall first-order water column and benthic degradation rate constants are user input variables, and should be based on knowledge about the contaminant behavior in similar surface water systems.

9.2.8.2 Volatilization

Volatile chemicals can move between the water column and the overlying air, as described by Equation [9-21]. The right hand side of this equation contains two terms. The second term describes diffusion into the water from the atmosphere, and is treated in Section 9.2.6.5 as an external load. The first term, $(K_v f_{water} f_{dw} C_{wtot}/D)$, constitutes a first order loss rate of aqueous contaminant. This term includes the quantity $f_{water} f_{dw} C_{wtot}$, which is equal to the water column dissolved phase concentration C_{dw} and which is subject to volatilization loss. The rate constant for volatilization from the water column, k_v, is given as:

$$k_v = \frac{K_v f_{dw}}{D}$$

[9-26]

where:

k_v	=	water column volatilization loss rate constant (yr^{-1})
K_v	=	overall transfer rate, or conductivity (m/yr)
f_{dw}	=	fraction of contaminant in the water column that is dissolved
D	=	water body depth (m)

The overall transfer rate, K_v or conductivity, is determined by the two-layer resistance model. The two-resistance method assumes that two "stagnant films" are

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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, it is obvious that the same mass must pass through both films, thus the two resistances combine in series, so that the conductivity is the reciprocal of the total resistance:

$$K_v = (R_L + R_G)^{-1} = \left(K_L^{-1} + \left(K_G \frac{H}{R\,T_K} \right)^{-1} \right)^{-1} \qquad [9\text{-}27]$$

where:

R_L = liquid phase resistance (year/m)

K_L = liquid phase transfer coefficient (m/year)

R_G = gas phase resistance (year/m)

K_G = gas phase transfer coefficient (m/year)

R = universal gas constant (atm-m^3/mole-$^\circ$K)

H = Henry's law constant for the pollutant (atm-m^3/mole)

T_k = water body temperature ($^\circ$K)

The value of K_v, the conductivity, depends on the intensity of turbulence in a water body and in the overlying atmosphere. As the Henry's Law coefficient increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. As the Henry's Law coefficient decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

Because Henry's Law coefficient generally increases with increasing vapor pressure of a compound and generally decreases with increasing solubility of a compound, highly volatile low solubility compounds are most likely to exhibit mass transfer limitations in water and relatively nonvolatile high solubility compounds are more likely to exhibit mass transfer limitations in the air. Volatilization is usually of relatively less magnitude in lakes and reservoirs than in rivers and streams.

The estimated volatilization rate constant is for a nominal temperature of 20 $^\circ$C. It

is adjusted for the actual water temperature using the equation:

$$K_{v,T} = K_{20} \; \theta^{(T-20)} \qquad\qquad [9\text{-}28]$$

where:

θ =   temperature correction factor, set to 1.026.

T   =   water body temperature (°C)

There have been a variety of methods proposed to compute the liquid (K_L) and gas phase (K_G) transfer coefficients. The particular method that is recommended here is the O'Connor method.

The liquid and gas film transfer coefficients computed under this option vary with the type of water body. The type of water body is specified as one of the surface water constants and can either be a flowing stream, river or estuary or a stagnant pond or lake. The primary difference is that in a flowing water body, the turbulence is primarily a function of the stream velocity, while for stagnant water bodies wind shear may dominate. The formulations used to compute the transfer coefficients vary with the water body type, as shown below.

9.2.8.2.1. Flowing Stream or River

For a flowing system (type 0), the transfer coefficients are controlled by flow induced turbulence. For these systems, the liquid film transfer coefficient (K_L) is computed using the O'Connor-Dobbins (1958) formula:

$$K_L = \left(\frac{10^{-4} \; D_w \; u}{D_z} \right)^{1/2} (3.15 \times 10^7) \qquad\qquad [9\text{-}29]$$

where:

K_L =   liquid phase transfer coefficient (m/year)

u = current velocity (m/s)

D_w = diffusivity of the chemical in water (cm^2/s)

D_z = water depth (m)

10^{-4} = units conversion factor

3.15×10^7 = units conversion factor

The gas transfer coefficient (K_G) is assumed constant at 36500 m/yr for flowing systems.

9.2.8.2.2. Quiescent Lake or Pond

For a stagnant system (type 1), the transfer coefficients are controlled by wind induced turbulence. For stagnant systems, the liquid film transfer coefficient (K_L) is computed using the O'Connor (1983) equations:

$$K_L = u^* \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_w^{-0.67} (3.15x10^7) \qquad [9\text{-}30]$$

$$K_G = u^* \left(\frac{k^{0.33}}{\lambda_2}\right) Sc_a^{-0.67} (3.15x10^7) \qquad [9\text{-}31]$$

where:

$$u^* = C_d^{0.5} \ W$$

$$Sc_a = \frac{\mu_a}{\rho_a \ D_a} = \frac{\nu_a}{D_a}$$

$$D_a = \frac{1.9}{MW^{2/3}}$$

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$$v_a = (1.32 + 0.009 \ T_a) \times 10^5$$

$$Sc_w = \frac{\mu_w}{\rho_w \ D_w}$$

$$D_w = \frac{22 \times 10^{-5}}{MW^{2/3}}$$

$$\rho_w = 1 - 8.8 \times 10^{-5} \ T_w$$

$$\log(\mu_w) = \left[\frac{1301}{998.333 + 8.1855(T_w - 20) + 0.00585(t_w - 20)^2} \right] - 3.0233$$

and:

u^*	$=$	shear velocity (m/s)
C_d	$=$	drag coefficient ($= 0.0011$)
W	$=$	wind velocity, 10 m above water surface (m/s)
ρ_a	$=$	density of air corresponding to the water temperature (g/cm^3)
ρ_w	$=$	density of water corresponding to the water temperature (g/cm^3)
k	$=$	von Karman's constant ($= 0.4$)
λ_2	$=$	dimension-less viscous sublayer thickness ($= 4$)
Sc_a	$=$	air Schmidt number (dimensionless)
Sc_w	$=$	water Schmidt number (dimensionless)
D_a	$=$	diffusivity of pollutant in air (cm^2/sec)
D_w	$=$	diffusivity of chemical in water (cm^2/sec)
μ_a	$=$	viscosity of air corresponding to the air temperature (g/cm-s)

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μ_w = viscosity of water corresponding to the water temperature (g/cm-s)

v_a = dynamic viscosity of air (cm^2/sec)

MW = molecular weight

T_a = air temperature (°C)

T_w = water temperature (°C)

3.15×10^7 = units conversion factor

9.2.8.3 Deposition and Burial

The benthic burial rate, W_b, is determined as a function of user input variables as part of the sediment balance (see Section 9.2.3). This burial rate is used to determine the mass loss of contaminant from the benthic sediment layer. As seen in Figure 9.1, the burial loss rate is applied to the total benthic contaminant concentration, C_{bt}. The water body contaminant burial loss rate is solved by equating the mass loss rate of total water body chemical with mass loss rate of benthic chemical:

$$C_{wtot} \, V_t \, k_b \;=\; C_{bt} \, V_b \, \frac{W_b}{d_b} \qquad\qquad [9\text{-}32]$$

where:

C_{wtot} = total water body contaminant concentration, including water column and benthic sediment (mg/L)

V_t = total volume of water body or water body segment being considered, including water column and benthic sediment (m^3)

k_b = first order burial rate constant for total chemical (yr^{-1})

C_{bt} = total benthic contaminant concentration (mg/L)

V_b = volume of upper benthic sediment layer (m^3)

d_b = depth of the upper benthic sediment layer (m)

W_b = benthic burial rate (m/yr)

From the state equations given after Figure 9.1, it is seen that the total benthic

contaminant concentration, C_{bt}, can be expressed as a function of the total water body concentration, C_{wtot}. Solving for the total chemical burial rate gives:

$$k_b = f_{benth} \frac{W_b}{d_b}$$

[9-33]

where:

f_{benth} = fraction of total water body contaminant concentration that occurs in the bed sediment

d_b = depth of the upper benthic sediment layer (m)

W_b = burial rate (m/yr)

9.2.9 PEAK STORM EVENT CONCENTRATIONS

The previous equations together describe the long-term average water body concentrations of sediment and chemical. Short-term peak concentrations may also be of interest in assessing risk from some chemicals. The basic mass balance equations for determining peak storm event concentrations of sediment and chemical are:

$$TSS_{storm} = \frac{X_{storm}}{V_{storm}} 10^3$$

[9-34]

$$C_{storm} = \frac{L_{storm}}{V_{storm}}$$

[9-35]

where:

TSS_{storm} = peak suspended solids concentration during storm event (mg/L)

C_{storm} = peak chemical concentration during storm event (mg/L)

V_{storm} = peak water body volume during storm event (m^3)

X_{storm} = total load of sediment from the watershed during the storm (kg)

L_{storm} = total load of chemical from the watershed during the storm, including runoff and erosion (g)

10^3 = g/kg

First we calculate the water body volume during the storm assuming that the storm runoff volume is added to the average streamflow volume:

$$V_{storm} = \frac{Vf_x \, T_r}{365 \times 24} + Q_{RS}$$

[9-36]

where:

Vf_x = yearly average stream flow (m^3/yr)

T_r = duration of the storm event (hr)

Q_{RS} = total storm runoff volume (m^3)

365 = days/yr

24 = hours/day

The total storm runoff volume Q_{RS} is the sum of runoff from pervious and impervious areas of the watershed:

$$Q_{RS} = (WA_L - WA_I) \, D_R \, 10^{-2} + WA_I \, R_t \, 10^{-2}$$

[9-37]

where:

WA_L = total watershed surface area (m^2)

WA_I = impervious surface area on watershed (m^2)

R_t = depth of total rainfall for the storm event (cm)

D_R = depth of runoff from pervious areas of the watershed (cm)

10^{-2} = m/cm

The runoff depth D_R is estimated by the following equation:

$$D_R = \frac{(R_t + M_t - 0.2S)^2}{(R_t + M_t + 0.8S)} \qquad [9\text{-}38]$$

where:

D_R = depth of runoff from pervious areas of the watershed (cm)

R_t = depth of total rainfall for the storm event (cm)

M_t = depth of snowmelt during the storm event (cm)

S = watershed retention parameter (cm)

The watershed retention parameter S is calculated from the Soil Conservation Service (SCS) runoff curve number input by the user according to the following equation:

$$S = 2.54\ [(1000/CN) - 10] \qquad [9\text{-}39]$$

where:

CN = runoff curve number

Next, the mass of sediment eroded from the watershed to the receiving water during a storm event can be estimated with the Modified Universal Soil Loss Equation (MUSCLE):

$$X_{storm} = 2.04 \times 10^6\ (Q_{ps}\ q_p)^{0.56}\ K\ LS\ C\ P\ SD \qquad [9\text{-}40]$$

where:

X_{storm} = total load of sediment from the watershed during the storm (kg)

Q_{ps} = volume of runoff from pervious area, calculated below (km^2-cm)

q_p = peak runoff from pervious area, calculated below (m^3/sec)

K = erodibility factor (tons/acre)

LS = topographic or slope length factor (unitless)

C = cover management factor (unitless)

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P   =   supporting practice factor (unitless)

SD   =   sediment delivery ratio (unitless)

This equation is an empirical relationship and the units must be consistent with those shown above. Selection of K, LS, C, P, and SD is discussed in Wischmeier and Smith (1978) and EPA (1985b), and briefly reviewed in Section 9.2.10 below.

The storm runoff volume from pervious areas is calculated from the runoff depth according to:

$$Q_{ps} = (WA_L - WA_I)\ D_R\ 10^{-6} \qquad\qquad [9\text{-}41]$$

where:

Q_{ps} =   volume of runoff from pervious area (km^2-cm)

WA_L =   total watershed surface area (m^2)

WA_I =   impervious surface area on watershed (m^2)

D_R =   depth of runoff from pervious areas of the watershed (cm)

10^{-6} = km^2/m^2

A trapezoidal hydrograph is assumed so that the peak runoff rate can be calculated as:

$$q_p = \frac{(WA_L - WA_I)\ D_R}{T_r} \left[\frac{R_t + M_t}{R_t + M_t - 0.2S} \right] \frac{10^{-2}}{3600} \qquad\qquad [9\text{-}42]$$

where:

q_p =   peak runoff from pervious area (m^3/sec)

WA_L =   total watershed surface area (m^2)

WA_I =   impervious surface area on watershed (m^2)

D_R =   depth of runoff from pervious areas of the watershed (cm)

R_t =   depth of total rainfall for the storm event (cm)

M_t =   depth of snowmelt during the storm event (cm)

S = watershed retention parameter (cm)

10^{-2} = m/cm

3600 = sec/hr

Finally, the mass of chemical load to the receiving water during the storm event is calculated:

$$L_{storm} = L_{sRI} + L_{sR} + L_{sE}$$ [9-43]

where:

L_{storm} = total load of chemical from the watershed during the storm, including runoff and erosion (g)

L_{sRI} = storm runoff load from impervious surfaces (g)

L_{sR} = storm runoff load from pervious surfaces (g)

L_{sE} = storm erosion load from pervious surfaces (g)

Runoff from impervious surfaces includes dryfall accumulated since the previous rainfall event and wetfall during the present rainfall event:

$$L_{sRI} = \left(\frac{D_{ydw} T_{acc}}{365} + \frac{D_{yww} T_r}{24 \times 365} \right) WA_I$$ [9-44]

where:

L_{sRI} = storm runoff load from impervious surfaces (g)

D_{ydw} = yearly dry deposition flux onto the watershed (g/m^2-yr)

D_{yww} = yearly wet deposition flux onto the watershed (g/m^2-yr)

WA_I = impervious surface area on watershed (m^2)

T_{acc} = time since previous rainfall event (days)

T_r = duration of rainfall event (hours)

24 = hours/day

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$$365 \quad = \quad \text{days/yr}$$

Runoff from pervious soil surfaces transports dissolved chemical concentrations in the soil to the water body:

$$L_{sR} = (WA_L - WA_I) \, D_R \, C_{ds} \, 10^{-2} \qquad [9\text{-}45]$$

where:

L_{sR} =   storm runoff load from pervious surfaces (g)

C_{ds} =   dissolved chemical concentration in soil, given by the state equations following Figure 9.1 (mg/L)

WA_L =   total watershed surface area (m^2)

WA_I =   impervious surface area on watershed (m^2)

D_R =   depth of runoff from pervious areas of the watershed (cm)

10^{-2} =   units conversion factor (m/cm)

The mass of chemical eroded from the watershed to the receiving water during a storm event can be calculated from the sediment loss and the particulate soil concentration:

$$L_{sE} = X_{storm} \, SD \, ER \, C_{ps} \, 10^{-3} \qquad [9\text{-}46]$$

where:

L_{sE} =   erosion load of chemical from the watershed during the storm (g)

C_{ps} =   chemical concentration sorbed to soil, given by the state equations following Figure 9.1 (mg/kg)

X_{storm} =   total load of sediment from the watershed during the storm (kg)

10^{-3} =   g/mg

For risk assessment purposes, the dissolved chemical concentration can be of interest. It may be assumed, for example, that the sorbed chemical fraction is removed in

a water treatment plant, and that the dissolved fraction is passed through to the user. The dissolved concentration in the river during the storm event is calculated by:

$$C_{dstorm} = C_{storm}\left[\frac{1}{1 + Kd_{sw}TSS_{storm}10^{-6}}\right]$$ [9-47]

where:

C_{dstorm}	=	dissolved concentration of chemical during storm event (mg/L)
C_{storm}	=	peak chemical concentration during storm event (mg/L)
TSS_{storm}	=	peak suspended solids concentration during storm event (mg/L)
Kd_{sw}	=	suspended sediment/surface water partition coefficient (L/kg)
10^{-6}	=	kg/mg

9.2.10 PARAMETER GUIDANCE

The following is offered as abbreviated guidance for all user input and internally solved terms for the water equations:

• **Dydw, Dyww, C_a, Tc:** Based on output from the atmospheric transport model, the user must specify the long-term, watershed average values for three loading parameters: dry and wet deposition of contaminants sorbed to particulates, and the vapor phase air concentration. In addition, the user must specify the duration of the atmospheric loading, Tc; this is set to the expected lifetime of the combustor, usually 30 years. Together, these parameters drive the watershed soil and water body contamination. The deposition fluxes are in units of g/m^2-yr, the air concentration is in units of $\mu g/m^3$, and the time of concentration is in yr.

• **ksg, Ys, C_{sb}:** The overall chemical degradation/ transformation rate constant, yield coefficient, and background concentration must be specified for the soil. The soil degradation rate constant, ksg, is specific to the contaminant and to environmental conditions, such as climate, soil type, and soil moisture. In the Indirect Exposure

Document, cadmium was assumed not to undergo soil degradation, and ksg was given a value of 0. The degradation rate constant for benzo(a)pyrene was set at 0.803 yr^{-1}. If chemical C is created by a transformation reaction of chemical B in soils, the yield coefficient Ys must be specified. One example is the methylation of inorganic mercury, represented as chemical B, into methyl mercury, represented as chemical C, with a yield coefficient of 1.0. If the yield coefficient is left at 0, no transformation will be calculated. The background concentration C_{sb} reflects the natural concentration in the soil prior to contaminant deposition. This value will be 0.0 for most organic contaminants. Nonzero values for the naturally-occurring metals, however, should generally be specified.

- k_{dw}, k_{db}, Y: Chemical degradation/transformation rate constants and a yield coefficient must be specified for the water column and benthic sediment. The degradation rate constants are specific to the contaminant and to environmental conditions, such as pH, bacterial levels, or light. If chemical C is created by a transformation reaction of chemical B in the water column or benthic sediment, the yield coefficient Y must be specified. If the yield coefficient is left at 0, no transformation will be calculated.

- H, T_w, T_a, u, W: Henry's Constant, H, water temperature, T_w, air temperature, T_a, water velocity, u, and wind speed, W, are required for estimating volatile losses and diffusive loads of contaminant into soils and the water body. Henry's constants are known for many contaminants of interest. They are expressed here in units of atm-m^3/mole. Average water and air temperatures should be specified by the user. Values generally range between 10 and 20 °C, and are converted internally to Kelvin units. Water velocity can vary from essentially 0 for stagnant ponds or lakes to 1.5 m/sec for fast-moving streams. Sustained average wind speeds may vary from close to 1 to 10 m/sec. Data may be obtained from local weather stations.

- P, I, R, EV: These are annual water balance quantities. Precipitation, P, is available from common meteorologic references. Irrigation, I, is a site-specific parameter and should not be zero if the watershed is comprised of irrigated farm lands. Runoff, R,

can be estimated using the *Water Atlas of the United States* (Geraghty et al., 1973). This reference provides maps with isolines of annual average surface-water runoff, which they define as all flow contributions to surface water bodies, including direct runoff, shallow interflow, and ground-water recharge. The range of values shown include 5 to 15 in/yr throughout the Midwest corn belt, 15 to 30 in/yr in the South and Northeast, 1 to 5 in/yr in the desert Southwest, and a wide range of 10 to 40 in/yr in the far West. Since these values are total contributions and not surface runoff, they need to be reduced to estimate surface runoff. A reduction by 50 percent should suffice if using the Water Atlas for the R term. Evapotranspiration, EV, can be estimated from pan evaporation data. A "potential evapotranspiration", PEV, can be estimated by an annual pan evaporation times 0.70 (or thereabouts), and is defined as the evapotranspiration that occurs when soil water is not limiting. "Actual" evapotranspiration, or EV, is about half of PEV. Site specific values for these terms should be obtained if possible.

- **Z:** The user must specify the mixing depth into which contaminant is incorporated for average watershed soils. If the watershed is dominated by soils that are not tilled, a value of 1 cm is recommended. This is a value commonly used for "non-tilled" situations, such as undeveloped land, pasture land, or residential properties. If the watershed is dominated by tilled agricultural land, than a value of 20 cm is recommended. This is a value commonly used for tilled soils including tilled agricultural fields and home gardens.

- **BD, θ_s:** These soil properties include the bulk density, BD, and the surface soil water content, θ_s. BD has a relatively narrow range of about 1.2 to 1.7 g/cm^3. A value of 1.50 g/cm^3 should suffice for most uses unless site specific data is available. Volumetric water content, θ, can be estimated as the midpoint between a soil's field capacity and wilting point, if a representative watershed soil can be ascertained for the combustor being evaluated. A reasonable range for θ is 0.10 (for very sandy soils) to 0.30 (for heavy loam/clay soils).

• BS, TSS, W_{dep}, ISS: These water body properties are analogous to the bulk density for soils noted above. The benthic sediment concentration, BS, should range between 0.5 and 1.5 kg/L. A value of 1.0 kg/L should be reasonable for most applications.

As described in the beginning of Section 9.2.3, either the TSS or W_{dep} must be known; one can be estimated from the other (and other parameters).

TSS concentrations can vary widely between water bodies and over time. Average values typically will range between 1 and 100 mg/L. Given similar soil erosion loads, values will be lower for standing water bodies such as ponds or lakes as compared with rivers and streams. The more turbulent flow in rivers will reduce the effective deposition rate and suspend sediments to a greater degree than a relatively calm lake. If site specific data are not available, the user should specify concentrations of 1 to 10 in ponds and lakes, and 10 to 20 in streams and rivers.

Net solids deposition is a complex process, and depends on the size of the particle and the shear stress near the bed. Deposition will be a fraction of the Stokes settling velocity, which varies from 117 m/yr for fine silt (2 micron diameter) to 3000 m/yr for medium silt (10 microns), to 73000 m/yr for fine sand (50 microns).

• WA_L, WA_I: These are the watershed surface areas for determining loading to the water body. WA_L is the total watershed surface area affected by deposition that drains to the body of water. WA_I is the impervious watershed area affected by deposition that is guttered and that drains to the water body.

Properly assigning values to WA_L and WA_I is non-trivial. The areas can be quite extensive, as the dispersion and deposition model may predict only gradual declines in deposition as a function of distance from the stack. What is also important to consider is the watershed hydrology in the absence of any deposition considerations. Total sediments in a water body may have originated from watershed soils which are (or have the potential to be) impacted as well as unimpacted by combustor depositions. If the combustor is depositing principally on a land area which feeds a tributary of a larger river system, then one should consider what might be termed an "effective" area. An "effective" drainage

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area will almost always be less than the total area of a watershed. A "watershed" includes all the land area which contributes water to a river system. For large river systems, this area is in the order of thousands of square miles and includes several tributaries and smaller streams feeding into the main branch of the river. Each stream and tributary has its own drainage area. If the deposition area can be ascertained to lie within that drainage area, than it would be appropriate to assign WA_L and WA_L' based on the drainage area size.

Another consideration for determining WA_L and WA_l is the location of the area affected by deposition fallout with respect to the point where water is extracted for drinking and fish are caught for consumption. If these points are significantly upstream in the river system in relation to the deposition area, there is no reason to conclude that sediments or water near where the water is extracted are impacted by the combustor. If these withdrawal points are downgradient of the deposition area, then there is reason to believe that sediments and water are impacted. However, if they are downgradient from the deposition area but not at the bottom of the watershed, then sediment and water quality further downgradient from the withdrawal points is not of concern and land draining into these downgradient portions would not be part of the "effective drainage area". One further possible consideration is how far upgradient in the watershed one should go when determining the size of the effective drainage area. While sediments introduced at the furthest points may eventually work their way down to the mouth of the watershed, this may take geologic time and not recent historic time. Therefore, sediment quality near a deposition area need not consider these far reaches.

For a standing water body such as a lake or a pond substantially fed by ground water recharge, an assumption that is made using the simple framework of this assessment is that all sediments within the lake/pond are completely mixed. Therefore, WA_L should equal all the area around the lake/pond contributing sediment, and, as in the above discussion on river systems, a part of the land area contributing sediments to streams or rivers which may feed the standing water body.

• WA_w, V_w, D_b, Vf_x: This set of parameters defines and characterizes the water

body or reach. WA_w is the water body surface area, in m^2. The volume of the water column, V_w in m^3, and the average flow volume, Vf_x in m^3/yr, determine the average residence time of a pollutant in the water body, which can vary from hours in streams to years in lakes. Average flows can be obtained from gaging stations, or from calculations using watershed area and average runoff coefficients as summarized in section 9.2.7. Flows may vary from 10^5 m^3/yr in small streams or ponds draining less than a square kilometer to 10^9 m^3/yr in large rivers the size of the Potomac. Volumes for a lake or pond can be calculated as the product of surface area and average depth. Volumes for a stream reach can be calculated as the product of reach length, average width, and average depth. The upper benthic sediment depth D_b, representing the portion of the bed in equilibrium with the water column, cannot be precisely specified. Values from 0.01 to 0.05 m would be appropriate.

• **R, K, LS, P, C, SD, ER:** These factors describe the erosion of soil and contaminant from the watershed to the water body. The first five terms are multiplied together to give the long-term average soil loss, X_e, in kg/m^2-yr. These are the terms for the Universal Soil Loss Equation, and are also described in Section 9.2.3. of the Indirect Exposure Document. Following are brief notes on the five terms needed for the Universal Soil Equation.

• **Rainfall/erosivity index, R:** The R term represents the influence of precipitation on erosion, and is derived from data on the frequency and intensity of storms. This value is typically derived on a storm-by-storm basis, but it has been compiled regionally for the development of average annual values (Wischmeier and Smith, 1978). Annual values range from < 50 for the arid western United States to > 300 for the Southeast. The value used in Indirect Exposure Document was 400.

• **Soil erodibility, K:** The soil erodibility factor reflects the influence of soil properties on erosion, with values ranging from <0.05 for non-erodible sandy soils to >0.50 for highly erodible silty soils. The value used in Indirect Exposure Document

is 0.21.

- **Length-slope factor, LS:** The topographic factor reflects the influence of slope steepness and length of the field in the direction of the erosion. Steeper slopes and longer lengths lead to higher LS values, with a range of 0.1 for slopes < 1.0 percent and lengths < 100 ft to > 2.0 for slopes generally > 10 percent. The two key considerations for its assignment, therefore, are the size of the field for which erosion estimates are being made, and the slope of that field. Indirect Exposure Document uses the USLE to estimate erosion losses off the edge of a unit area within a watershed, which might be an acre or a hectare, for example. The LS assigned in Indirect Exposure Document is 0.179, implying flat terrain and a small unit field. For example, a combination of slope length and slope of 200 meters and 2 percent respectively, gives an LS value of 0.20.

- **Support practice factor, P:** The support practice factor reflects the use of surface conditioning, dikes, or other methods to control runoff/erosion. P can be no greater than 1.0. However, values less than 1.0 should only be assigned when specific practices are employed which are designed to reduce erosion. P is assigned a value of 1.0 in Indirect Exposure Document.

- **Management practice factor, C:**   The final term in the USLE is the cover and management practice factor, C, which primarily reflects how vegetative cover and cropping practices, such as planting across slope rather than up and down slope, influences erosion. C values can be no greater than 1.0, with this value appropriate for bare soils. A C value of 1.0 is an appropriate choice for active landfills or sites of high soil contamination (like Superfund sites) mostly devoid of vegetation. For an inactive landfill with grass cover or any area with dense vegetative cover such as grass, a value of 0.1 or less is appropriate. Values greater than 0.1 but less than 0.7 are appropriate for agricultural row crops, which offer more protection than bare soil, but not as much protection as dense vegetation. The Indirect Exposure Document assigns a value of 0.5 for C.

- **Sediment Delivery Ratio, SD:** The sediment delivery ratio for a large land area (a watershed or part of a watershed) can be calculated based on the area of the watershed using an approach proposed by Vanoni (1975):

$$SD = a \ (WA_L)^{-b} \qquad\qquad [9\text{-}48]$$

where:

SD	=	watershed sediment delivery ratio (dimensionless)
WA_L	=	watershed area receiving fallout (m^2)
b	=	empirical slope coefficient (= -0.125)
a	=	empirical intercept coefficient (see below)

Based on various studies of sediment yields from watersheds, Vanoni concluded that the sediment delivery ratios vary approximately with the -(1/8) power of the drainage area. Inspection of the data presented by Vanoni suggests that the "a" parameter in the above equation varies with the size of the watershed. Although the Agency is currently evaluating methods for estimating sediment yields, the Vanoni equation along with the following values for "a" are recommended in the interim:

Watershed Area (square miles)	"a" Coefficient (-)
≤ 0.1	2.1
1	1.9
10	1.4
100	1.2
1000	0.6

Note: 1 square mile is equivalent to $2.59 \times 10^6 \ m^2$.

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For example, with WA_L given in the Indirect Exposure Document as 1.5×10^7 m^2, SD is estimated as 0.18.

- **Enrichment Ratio, ER:** Enrichment refers to the fact that erosion favors the lighter soil particles, which have higher surface area to volume ratios and are higher in organic matter content. Therefore, concentrations of organic contaminants, which are a function of organic carbon content of sorbing media, would be expected to be higher in eroded soil as compared to in-situ soil. While enrichment is best ascertained with sampling or site-specific expertise, generally it has been assigned values in the range of 1 to 5 for organic matter, phosphorous, and other soil-bound constituents of concern. The enrichment ratio would be expected to be higher in sandy soils as compared to silty or loamy soils because the finer silt particles which erode from a soil generally characterized as sandy are more a deviation from the norm compared to silt particles which erode from a soil generally characterized as silty or loamy. A value of three for organic contaminants would be a reasonable first estimate.

- **Kd$_s$, Kd$_{sw}$, Kd$_{bs}$:** These three adsorption partition coefficients describe the partitioning of a contaminant between sorbing material, in this case soil, surface water suspended solids and bed sediments, and water in a sorbing material/water mixture. For organic contaminants, this partition coefficient has been estimated as a function of the organic carbon partition coefficient and the fraction of organic carbon in the partitioning media:

$$Kd_{ij} = Koc_j \, OC_i \qquad\qquad [9\text{-}49]$$

where:

Kd_{ij} = partition coefficient for pollutant j associated with sorbing material characterized by organic carbon content, OC_i (L/kg or cm^3/g)

Koc_j = sorbing material independent organic carbon partition coefficient for contaminant j (L/kg or cm^3/g)

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OC_i =   fraction organic carbon content of sorbing material (dimensionless)

In the absence of measured values, the Koc can be estimated from a chemical's octanol water partition coefficient, Kow. Empirical equations relating Kow to Koc are listed in Lyman, et al. (1982). Of six different equations listed in that reference, the following derived by Karickhoff, et al. (1979) is recommended for use for chemicals with high Kow (highly sorbed, hydrophobic contaminants such as PCBs, dioxins):

$$log\ Koc = log\ Kow - 0.21 \qquad\qquad [9\text{-}50]$$

where:

Koc   =   organic carbon partition coefficient (L/kg)

Kow   =   octanol-water partition coefficient (dimensionless)

This equation was empirically developed from a limited number of hydrophobic contaminants ($n = 10$, $R^2 = 1.00$). It implies that Koc is very similar to Kow for strongly sorbed compounds such as the dioxin-like compounds.

For organic contaminants, what is also then required for assignment of Kd's are the organic carbon contents of solids and sediments of water bodies. Solids of water bodies are generally higher than organic carbon contents of the surrounding lands. Furthermore, organic carbon contents of suspended organic materials and solids are typically greater than those of bottom sediments. A significant sink for strongly hydrophobic contaminants such as dioxin-like compounds is thought to be suspended, or non-settling, organic material. In modeling 2,3,7,8-TCDD in Lake Ontario (EPA, 1990c) using the WASP4 model, a compartment separate from suspended solids termed "non-settling organic matter" served as a permanent sink. For the framework offered above, a single reservoir of suspended materials onto which incoming contaminants sorb is modeled.

Foth (1978) lists the organic nitrogen content of several soil types ranging from sand and sandy loam to clay. The range from that list is 0.0002 to 0.0024 on a fractional basis. Assuming a carbon to nitrogen ratio of 10 (Brady, 1984; who notes that C:N ratios

vary from 8 to 15, with the typical range of 10 to 12), organic carbon contents of soil generally might range from 0.002 to 0.024. A value that might be assumed to be 0.01 in order to estimate Kd_s for general purposes. The organic carbon content of bottom sediments will be higher given arguments that erosion favors lighter textured soils with higher organic carbon contents, and also that bottom sediments are partially comprised of detritus materials. A range of 0.03 to 0.05, given surface soil content at 0.01, might be reasonable. The organic carbon content of suspended materials can approach 0.20, but a range between 0.05 and 0.10 might be more reasonable given prior assignments of 0.01 and 0.03 to 0.05.

The Kd_s supplied in Indirect Exposure Document for benzo(a)pyrene and cadmium are 1.2×10^5 L/kg and 500 L/kg, respectively.

[Revised Section 9.2. ends here]

9.3. Precipitation

Issue   The procedure to estimate contaminant concentration in water of precipitation collection systems may lead to over estimates. The procedure divides the total deposition rate by the precipitation rate. Some of the contaminant in dry deposition may have low solubilities and settle out of suspension.

Conclusion/Recommendation

If the collection system causes turbulent mixing of the water, particulates could be suspended and the current approach would be appropriate. If such mixing does not occur, the current procedure is acceptable for bounding estimates. However, if more realistic estimates are desired, the assessor should limit the concentrations of all contaminants to their solubility limit. For organics further refinement may be possible through the use of equilibrium partitioning.

9.4. Groundwater

Issue   The conclusion that combustor emissions do not impact groundwater was based on an analysis of two combustors. Other combustors may have different conditions

which would exacerbate groundwater impacts and invalidate this conclusion.

Conclusion/Recommendation

The original examples covered a wide range of combustor types, chemicals and geohydrologic conditions. However, site-specific conditions may be encountered which would lead to greater groundwater impacts. In contrast to the original examples, conditions that might enhance groundwater impacts include higher deposition rates, more soluble compounds in the emissions and higher recharge rates. In these circumstances, site-specific groundwater modeling may be required before this pathway can be eliminated from consideration.

10. DETERMINING EXPOSURE FROM WATER INGESTION

<u>Issue</u> The water concentration proposed for use in estimating exposure is the total water concentration, which includes the dissolved and sorbed forms. This was recognized as conservative in the text.

<u>Conclusions/Recommendations</u>

The revised Chapter 9 does provide a model which calculates the dissolved phase concentration (along with the total concentration and sorbed phase concentration). It is most appropriate to use this dissolved phase concentration, termed C_{dw} in Chapter 9. The basis for this recommendation is that water treatment systems filter out particulates; hence what remains are the dissolved phase residues of the contaminant.
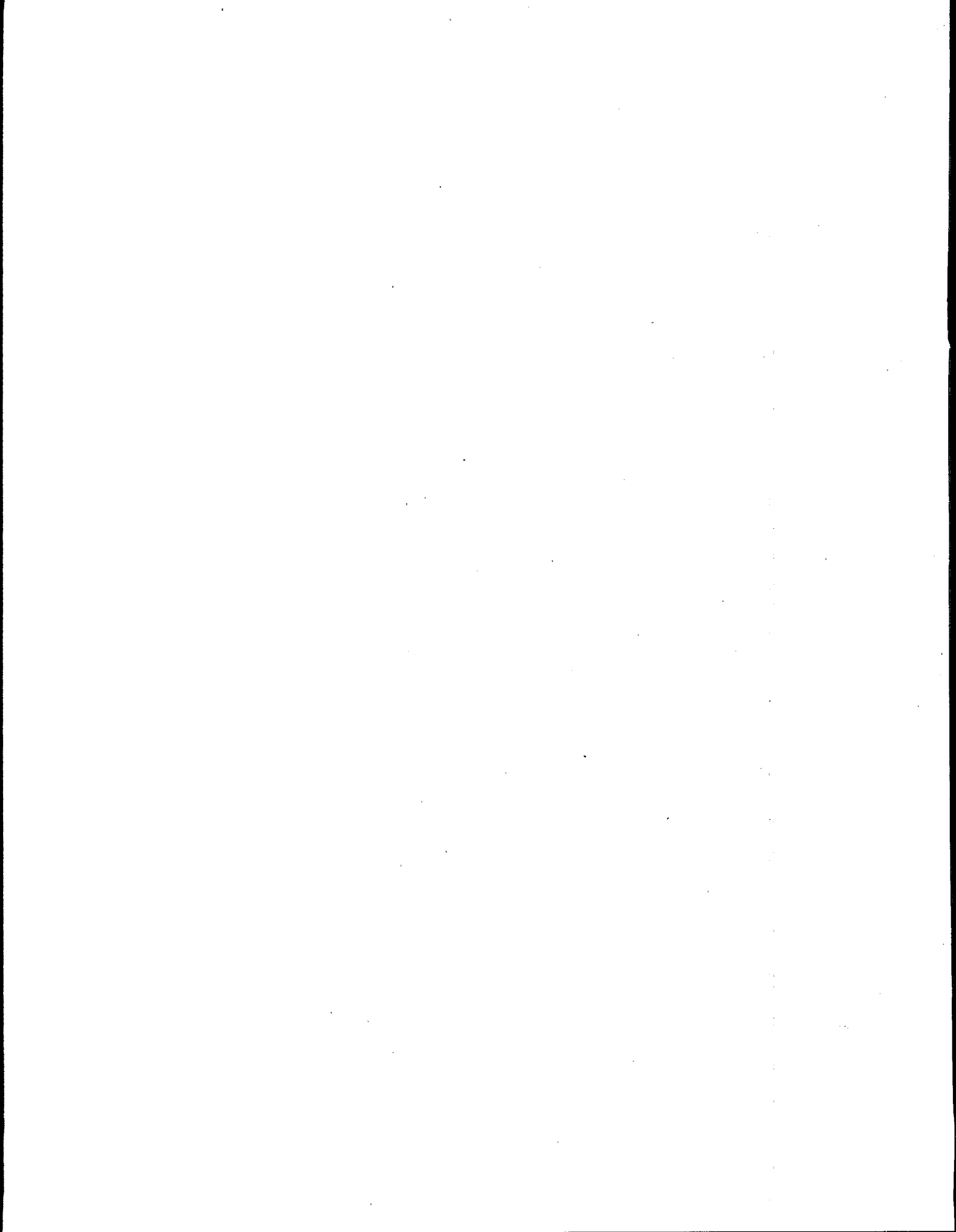
11. DETERMINING EXPOSURE FROM FISH INTAKE

11.2 Calculating Daily Intake from Fish

11.2.2 Bioconcentration Factor

Issue   The dioxin document promotes the use of a "Biota Sediment Accumulation Factor", or BSAF, for estimating fish lipid concentrations based on organic carbon normalized concentrations of contaminants on bottom sediments.

Conclusions/Recommendations

The use of the BSAF is recommended for dioxin-like compounds (i.e., dioxins and furans with dioxin-like toxicity). BSAF values for these compounds are proposed in the dioxin exposure reassessment document (EPA, 1992c). Also, some available literature on BSAFs for PCBs are discussed in that document. A more complete discussion on bioaccumulation approaches for 2,3,7,8-TCDD, including the BSAF and water-column based approaches, can be found in "Interim Report on Data and Methods for Assessment of 2,3,7,8-Tetrachloro-p-dioxin Risks to Aquatic Life and Associated Wildlife" (EPA, 1993c).

While this recommendation is made here, it should be noted that water column approaches for lipophilic compounds including the dioxins, are currently being used in the Agency and used appropriately. One such factor described in EPA's Water Quality Guidance for the Great Lakes Systems (EPA, 1993b) is termed the bioaccumulation factor, or BAF. This factor, multiplied by the total water concentration, gives a lipid-based fish tissue concentration. The afore-mentioned Water Quality Guidance contains a list of BAF values for a number of pollutants. Since the aquatic impact model described in Chapter 9 does predict water column concentrations (including total, dissolved, and sorbed concentrations), other approaches can easily be used.

Issue   Alternate approaches for estimation of aquatic bioconcentration and bioaccumulation may also be appropriate.

Conclusions/Recommendations

For estimating bioconcentration and bioaccumulation, there is a model known as the Food and Gill Exchange of Toxic Substances Model (FGETS). It is a product of ERL-Athens, GA and has been validated for a number of chemicals.

11.2.3 Fish Ingestion Rate

Issue Ingestion rates specific to the water bodies impacted by the combustor are needed. In addition to presenting the distributions of exposure, the assessor should use point- estimate based scenarios to highlight individual exposure estimates for several locations (i.e. maximum deposition, place where most people exposed, and areas of special interest, such as schools) . Separate ingestion rates for freshwater and estuarine fish and shellfish are needed, depending on the nature of the local surface water bodies. Generally, the ingestion of marine fish and shellfish is not of interest in indirect exposure estimates of single sources, such as combustors because, except possibly for anadromous species such as salmon, marine life is not expected to become contaminated to a significant extent.

Conclusion/Recommendations

The waterway impacted by the combustor should be identified and evaluations made of how much fish could be produced and caught. Ideally these estimates are made on the basis of local information. Table 11.1 contains ingestion rates for freshwater and estuarine fish and shellfish and are offered as a starting point to select site-specific values. These are based on an analysis of the results of the USDA 1977-78 National Food Consumption Survey. When using these data the assessor should consider the following points:

● The survey was conducted over a three day period. Thus, it does not represent long term behavior patterns which is the interest of exposure assessments used to support analysis of chronic health effects. This problem introduces uncertainty into the estimates of medians (50th percentile) and other percentiles. It can provide appropriate estimates of

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the average.

● Because most of the persons surveyed did not eat fish or shellfish during the survey period, the 50th percentile values are zero. The mean values are more appropriate to use as central tendency estimates of fish and shellfish consumption over a lifetime. However, these averages are on a per capita basis, ie. averaged across all survey participants (including fish eaters and nonfish eaters). The average fish consumed by fish eaters is probably a more relevant estimate of central exposures. This value would be higher than the per capita average.

● These data represent total ingestion rates of store-bought fish. Obviously, what is of interest for a site specific survey is the amount of fish consumed from waters within the study area. Assuming local surveys are not available EPA (1989b) recommends approaching this problem by using judgement to estimate the number of fish meals (100 to 200 g) per year that a person may reasonably consume from the water body of concern. By comparing these judgement based values to the national survey data the assessor can make some evaluation of their reasonableness. EPA (1989b) also presents studies that indicate that recreational anglers near large water bodies consume 30 g/d (as a mean) and 140 g/d (as an upper estimate). If evidence exists, that subsistence fishing occurs in the area of interest, then even higher levels may be warranted. Wolfe and Walker (1987) found subsistence fish ingestion rates up to 300 g/d in a study conducted in Alaska.

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Table 11-1. Fish consumption estimates from the USDA 1977-78 National Food Consumption Survey (consumptions were recorded for three day periods; N = 36249; units are grams/day/person.).

Estimate	Fresh No Shellfish	Fresh With Shellfish	Estuarine No Shellfish	Estuarine With Shellfish	Marine No Shellfish	Marine With Shellfish	Total No Shellfish	Total With Shellfish
Mean	1.64	1.64	2.50	4.27	7.72	8.23	11.85	14.15
50th %	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
90th %	0.00	0.00	4.73	9.80	28.33	30.00	42.07	51.04
95th %	5.29	5.29	14.50	28.35	48.37	51.17	66.15	75.60
99th %	38.00	38.00	56.00	80.00	93.33	97.07	128.00	146.17

Estimate	Fresh + Estuarine No Shellfish	Fresh + Estuarine With Shellfish	Estuarine + Marine No Shellfish	Estuarine + Marine With Shellfish
Mean	4.14	5.92	10.22	12.51
50th %	0.00	0.00	0.00	0.00
90th %	9.80	16.53	37.80	44.73
95th %	28.00	38.00	56.70	67.50
99th %	76.55	101.33	112.00	129.47

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12. DETERMINING EXPOSURE FROM DERMAL ABSORPTION FROM WATER

<u>Issue</u>   New Agency guidance is available for addressing dermal absorption exposures.
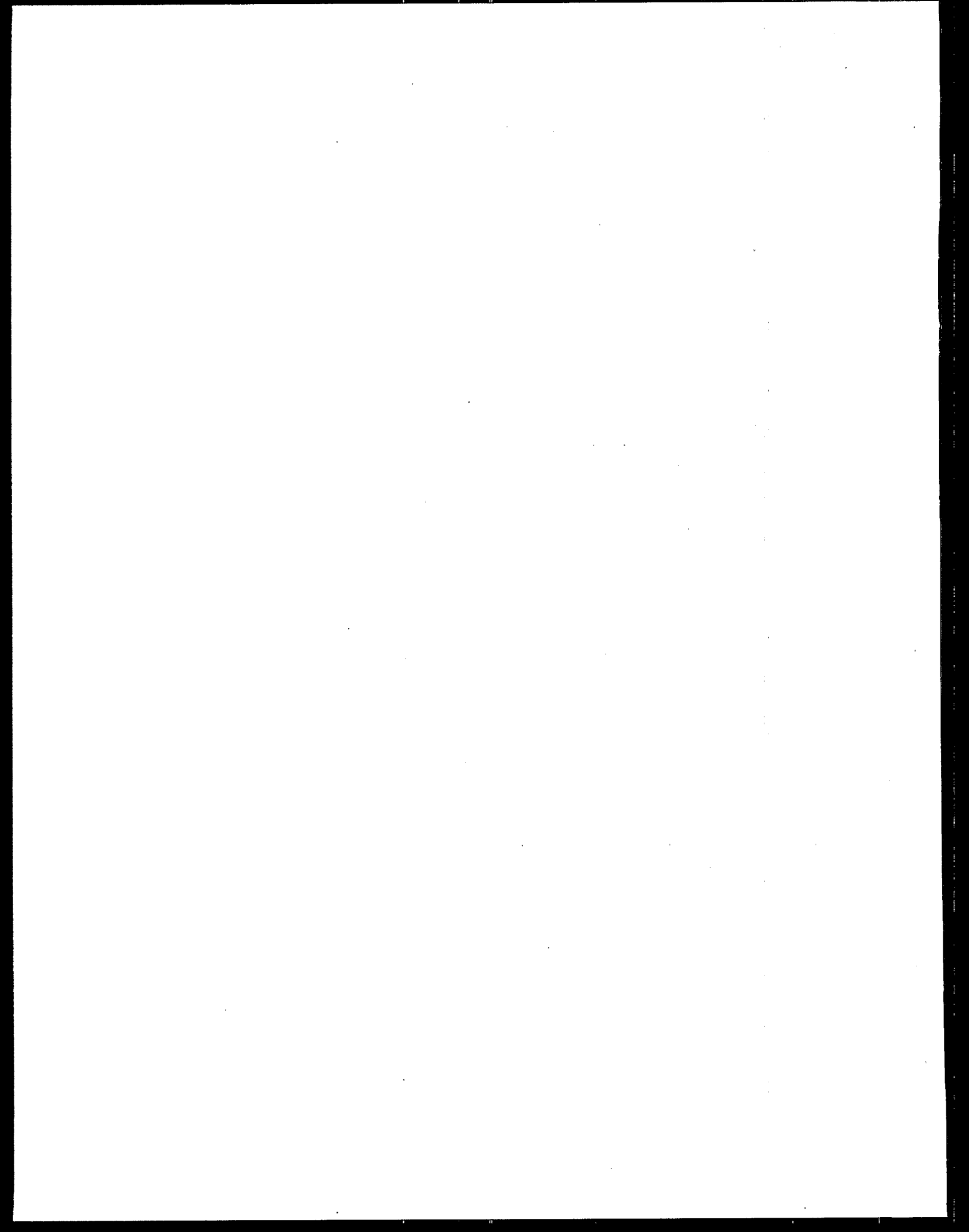
<u>Conclusions/Recommendations</u>

This chapter should be replaced by the appropriate sections of the report, "Dermal Exposure Assessment: Principals and Applications" (EPA, 1992b).
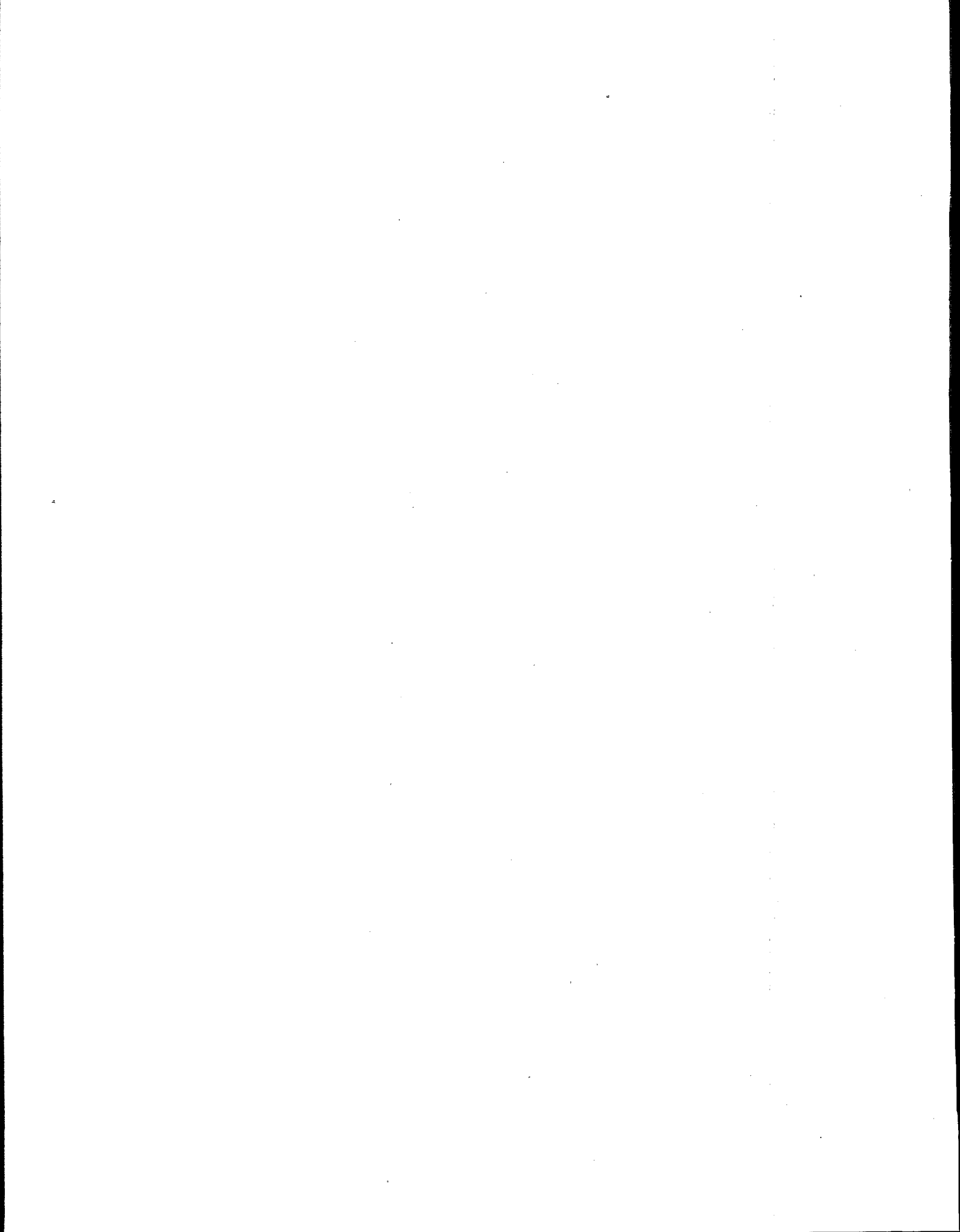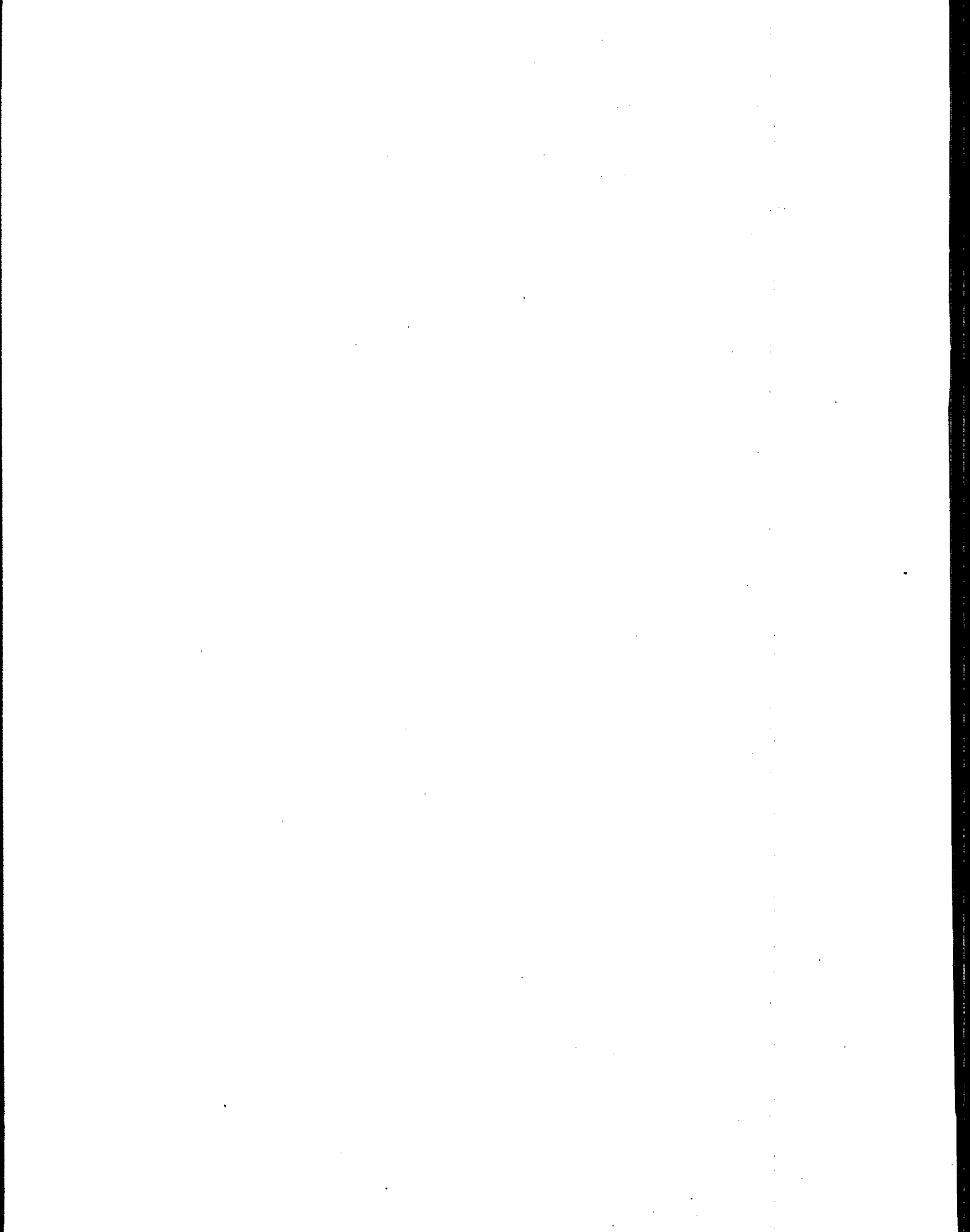
13. HAZARD IDENTIFICATION

Not relevant for this review.

14. DOSE-RESPONSE ASSESSMENT

Not relevant for this review.

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15. RISK CHARACTERIZATION

Section 15.2.3 Estimating Total Exposure by Each Route

Issue   The Indirect Exposure Document does not fully address how to add risks across pathways (for carcinogens vs. noncarcinogens) or how to add risks across chemicals.

Conclusions/Recommendations

Agency guidance for adding risks across pathways are contained in Chapter 8 of the Risk Assessment Guidance for Superfund: Volume I - Human Health Evaluation Manual (Part A) (EPA, 1989c). The guidelines for adding risks across chemicals are included in The Risk Assessment Guidelines of 1986 (EPA, 1987b), in the section titled "Guidelines for the Health Assessment of Chemical Mixtures" (51 FR 34014). In general, for carcinogens, risks should be added across chemicals. However, for systemic toxicants, risks should be added across chemicals only when they target the same organ. Also, risks should be added across pathways when it is reasonable to expect an individual to experience exposure by a given set of pathways.

Issue   The Indirect Exposure Methodology does not provide guidance on how to combine the results of the indirect exposure risk assessment with the results of a direct exposure risk analysis. Individuals will be exposed both directly through inhalation and indirectly through oral and dermal exposures.

Conclusions/Recommendations

Although the Indirect Exposure Methodology is intended to address only indirect exposures, in reality individuals will also receive direct inhalation exposures. The air models discussed in Chapter 3 calculate long-term average ambient air concentrations. For the purposes of estimating direct inhalation risk, it is important that the ambient air concentrations of the pollutant represent the sum of both the vapor phase and the fine particulate phase (i.e., the sorbed phases). This was discussed in the Revised Chapter 3 presented in this Addendum. Except as noted below, the combined vapor and particulate phase concentrations should generally be used directly for estimating risk.   For

carcinogens, the inhalation risk is best computed by multiplying the compound specific Unit Risk (m^3/mg) by the average (over the exposure period) concentration (mg/m^3) of the contaminant in air at the point of exposure. If Unit Risks are not available, a carcinogenic slope factor, q^*_i can be used if it can be demonstrated that it is appropriate for the inhalation pathway. This procedure involves first estimating the inhalation dose:

$$ADI_h = \frac{C_h \ IR \ ET \ EF \ ED \ 1000}{BW \ AT} \qquad [15-1]$$

where:

ADI_h	=	average daily intake of the hth pollutant (mg/kg/day)
C_h	=	ambient air concentration of the hth pollutant (μg/m^3)
IR	=	inhalation rate (m^3/hr)
ET	=	exposure time (hours/day)
EF	=	exposure frequency (days/yr)
ED	=	exposure duration (years)
BW	=	body weight (kg)
AT	=	averaging time (days)
1000	=	units conversion factor

Carcinogenic risk is calculated as follows:

$$Individual \ Risk_h = q^*_{i,h} \ ADI_h \qquad [15-2]$$

where:

$q^*_{i,h}$ = inhalation carcinogenic slope factor for the hth pollutant (mg/kg/day)$^{-1}$

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and the averaging time for the ADI is taken as a lifetime (e.g., 70 years). The hazard quotient for non-carcinogens is calculated as follows:

$$Hazard\ Quotient_h = \frac{C_h\ 0.001}{RfC_h}$$
[15-3]

where:

C_h	=	ambient air concentration of the hth pollutant ($\mu g/m^3$)
RfC_h	=	reference concentration of the hth pollutant (mg/m^3)
0.001	=	units conversion factor

In general, the ambient air concentration (which should include both particles and vapors, as stated before) should not be adjusted in order to calculate the inhalation risk, unless the particle sizes are above about 10 microns. Below this size, particles are considered inhalable and represent an inhalation exposure. In general, only fugitive dust emissions or resuspended dust (e.g., from mechanical disturbance of soil) would be expected to have a significant particle component in the size range larger than 10 microns. If significant exposures to particles much larger than 10 microns are projected to occur, the portion of the ambient air concentration represented by particles above 10 microns should be considered along with other oral exposures for the purpose of estimating risk.

15.3 Risk Estimation

Issue   The Indirect Exposure Document does not address population risk. The Agency's risk characterization guidance recommends that population risk be considered along with individual risk and that both types of risk descriptors be presented in Agency risk assessments.

Conclusions/Recommendations

Two approaches can be used to estimate population risks to carcinogens:

1. Simply add the risks based on individual exposures across the population of

concern, i.e., the entire impacted area, all farmers in impacted area, school children, etc. This is generally more conveniently estimated by multiplying the average individual risk by the population size.

2. Base the estimate on the amount of contaminant entering the food supply per year. This approach is probably most practical for the pathways involving ingestion of locally produced food. This would involve estimating the annual amount of food produced in each isopleth ring, computing the contaminant level in the food in each ring, and adding up the products of contaminant concentration and the amount of food produced for each ring. Then the population risk is computed as follows:

$$Population\ Risk = \frac{q^* \ ED}{BW \ LT} \sum_{i=1}^{n} FP_i \ C_i \qquad [15\text{-}4]$$

where:

q^*	=	cancer slope factor (kg-d/mg)
ED	=	exposure duration (yr)
BW	=	body weight (kg)
LT	=	lifetime (yr)
n	=	number of rings (dimensionless)
FP_i	=	average annual food production in ring i/365 days per year (kg/d)
C_i	=	contaminant concentration in food from ring i (mg/kg)

This approach assumes that all food produced in the study area is consumed (at any location inside or outside the study area) and that all resulting individual risks are in the linear range of the dose-response curve. For derivation of the population risk equation, see Appendix A. (A similar approach could also be followed for the dairy products ingestion and fish ingestion pathways, if dairy farming and fishing (recreational, subsistence, commercial) are important activities in the study area.)

Either of these approaches yields the number of incremental cancer cases occurring

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over a 70 year period. The second approach has the advantage that it accounts for exposure which may occur as a result of exporting food outside of the study area. However, neither approach accounts for the exposure/population risk which may occur due to contamination of food produced outside of the study area. Although the individual risks outside the study area are below levels of concern, the population risks could be important if significant long-range transport occurs. This issue can be evaluated by examining how much of the emitted contaminant is deposited in the study area. If 90 percent of the contaminant is deposited in the study area, then, for carcinogens, approximately 90 percent of the population risk is accounted for. However, the long range transport and impacts of incinerator emissions are not well understood and the local vs long range impacts may not be linearly proportional to the relative amounts deposited.

In the case of non-carcinogens, population risk could be characterized in terms of the number of individuals estimated to have a hazard quotient greater than one (1) during any portion of their lives, i.e., persons that are exposed to a dose greater than a reference dose (RfD).

15.4 Characterization of Uncertainty

Issue   A discussion of Monte Carlo type assessments of uncertainty is included in the Indirect Exposure Document. However, little guidance is given on how and when to use the technique.

Conclusions/Recommendations

As discussed in Chapter 2, using local surveys and a series of point estimates, one can develop approximations of exposure/risk distributions and estimate exposure levels for a variety of special interest scenarios. This approach may be sufficient for many situations. However, if more detailed information is needed on the distribution of exposure and risk, the assessor can consider using a Monte Carlo simulation analysis. The decisions about whether and how to conduct Monte Carlo assessments are quite complicated and cannot be fully addressed here. However, some general guidance can be provided.

It is critical in all uncertainty analysis and especially those based on Monte Carlo, to

distinguish between variability and uncertainty. Uncertainty results from lack of knowledge about the true value of a parameter and variability is the change in a parameter value across a population or situation. The same parameters can have elements of uncertainty and variability. For example the contaminant concentration in soil can be uncertain due to measurement or modeling error and spatially variable due to differences in deposition at various locations. Distinction between these elements can be made in a variety of ways.

In the framework of Monte Carlo simulation, the impacts of uncertainty and variability can be systematically addressed using a "double loop" or "nested" simulation approach. Under this approach the "outer loop" addresses the uncertain parameters, and applies user specified probability models to make random selections for these terms. For a given selection of the uncertain parameters, the "inner loop" allows all the population exposure variables to vary and a distribution of population exposure or risk is obtained. When this process is repeated for other selections of the uncertain variables a family of curves representing potential distributions of risk in the population is obtained. These results can then be applied, for example to estimate the fraction of the population with exposure above a specified level and to establish error bounds on this fraction. This approach requires developing distributions of uncertainties, in addition to population variability and can be quite difficult. In cases where statistically based survey or measurement data are available, statistical likelihood functions may be used to allow a non-subjective quantification of uncertainties. However, such data are frequently (generally?) lacking. Otherwise, it may be possible to select distributions via professional judgement, but the assessment should clearly state that the outcome is largely dependent on judgement used to develop the distributions.

An alternative to the double looping approach is to use sensitivity analysis to demonstrate uncertainty and approximate error bounds. The distinction between uncertainty and variability should be clearly shown in the final display of a distribution generated from a Monte Carlo simulation. As an example, uncertainty bands can be drawn around the distribution of variability.

Unless special provisions are made, all variables used in a Monte Carlo simulation

should be independent. In principle, it is possible to construct a multivariate probability distribution describing the dependence between two or more variables, however this is not commonly done due to the greater data requirements and increased complication of the analysis. None the less, when strong dependencies between variables are present, they may have an important impact on the conclusions of the analysis. This is particularly true when some individuals may have a tendency to have high end values for two or more variables. Where dependencies can be described, a useful approach is to determine a distribution for one and use values from this distribution to compute the second variable (using a conditional distribution for the second variable given knowledge of the first variable). The assessor must avoid situations where two or more values are assigned to a single variable where it appears in different places in a risk calculation. If multiple assignments are inadvertently made, they will inappropriately alter the shape of the resulting probability distribution.

Inconsistencies can arise between exposure and toxicity assessments because of fixed exposure assumptions imbedded in toxicity metrics. For example, RfCs, RfDs and cancer slope factors have assumptions built into them about breathing rates, life expectancy, etc.

It is often difficult to find appropriate distributions for use in Monte Carlo assessments.   Some general guidance for selecting distributions is presented below:

- Distributions derived from national data may not represent local conditions. To extent possible use distributions or frequency histograms derived from local surveys. When distributional data are drawn from a national or other surrogate population, it is important that the assessor address the extent to which local conditions may differ from the surrogate data. In addition to a qualitative statement of uncertainty, the representativeness assumption is appropriately addressed as part of a sensitivity analysis.
- Many surveys (both local and national) addressing issues such as food consumption were conducted over a short time period for each respondent and may not represent long term trends (the respondents usual behavior). Generally, environmental risk assessments for chronic health effects address risk as a function of the long term average exposures of

individuals, and thus are most appropriately conducted using data on long term average, "usual" behavior. Similar problems arise when distributions of concentration data arise from short term monitoring periods or when factors such as soil ingestion are measured using protocols of a duration of only several days.

■ Values near the tail of a distribution are very sensitive to the form of distribution selected. Tails of ideal distributions extend to infinity. Consider using empirical histograms when substantial data are available or truncating ideal distributions at reasonable bounding estimates.

Issue   The use of mass balance checks was not mentioned as a means of evaluating uncertainty. A mass balance would be violated, for example, if the mass of contaminant estimated to get into a media (for example soil) exceeds the mass being emitted from the stack.

Conclusion/Recommendations

The COMPDEP air emissions model is designed on mass balance principles and therefore should not lead to impossible air concentrations or deposition rates which exceed the emission rates. Depositions are substracted out of the airborne reservoir of particle-bound contaminants as the depositions occur. However, some of the media transfer models, which use the output from the air models, are based on simple transfer/partitioning approaches which do not have built in mass balances. If these models are properly parameterized, then the possibility of meaningful mass balance violations is minimized. This is discussed further below. However, it is generally recommended that assessors make mass balance checks to ensure that reasonable predictions are being made. These checks can be made in various ways. One way is to compare estimates of the amounts of contaminant in the various media (i.e. soil, vegetation and biota) within the study area (i.e., the area within the outer isopleth boundary, as described in Chapter 2 of this Addendum) to the amount emitted from the stack. Comparable time frames must be used for this type of comparison. For example, the amount of contaminant in the beef annually produced from the study area should not exceed the amount of contaminant emitted during the year (except in an unusual circumstance where a large cattle ranch

begins operation within the study area several years after incineration begins, and accumulation in the environment to that point could lead to large withdrawals by the cattle initially). In addition to fate, transport, and transfer mass balance transfer, one should also be aware of mass balance violations when it comes to estimating exposures given media concentrations. For example, the amount of impacted beef ingested by populations in the study area should not exceed the amount of beef produced in the study area.

Because the fate and transport, and food chains algorithms, do not contain built-in mass balance checks, mass balance violations could occur. Contaminants estimated to be deposited onto soils partition between a sorbed phase and a dissolved phase. Transfers occur into below ground and above ground vegetation with a biotransfer factor. Bioconcentration factors take concentrations in one media, water concentrations for example, and translate them to a concentration in another media, fish. In this simple framework, mass balances are considered but are not rigorously maintained. For example, soil to plant transfers are not explicitly modeled as a loss for soil concentration estimation. However, there is an overall loss constant for the soil concentration algorithm, which explicitly considers leaching, erosion, runoff, degradation, and volatilization. One could estimate the loss via plant uptake and add that to the degradation rate constant; otherwise, plant uptake loss is not explicitly considered.

There are other examples of this kind where exchanges between media and sinks are not rigorously modeled. However, this particular type of theoretical mass balance issue is not normally expected to be a fatal flaw for any contaminant evaluated. First, dissipation from key media is modeled with loss rate constants - these key media include soils, vegetation, and surface waters (water column and benthic sediments). Guidance has been presented for proper parameterization of these dissipation factors in the 1990 IED as well as this Addendum. Second, all transfer and bioconcentration parameters have been empirically developed from appropriate data sets - these key transfer factors include soil and air to plants, contaminant intake by terrestrial animals to contaminant concentrations in food products, and aquatic media concentrations (water or sediment) to fish. These empirical factors are, by design and definition, approximations of observed phenomena.

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Another type of mass balance violation could occur with improper parameterization. For example, the aquatic impact requires the methodology user to estimate the land area draining into an impacted water body as well as a contaminant deposition rate that represents depositions over that entire area. If one selects a deposition rate that would occur at the point of maximum deposition, within a few hundred meters of the stack emission, as representing deposition over a drainage basin that is millions of square meters in area, and/or one estimates a drainage basin size much too large for an impacted water body (which is defined in this methodology in terms of flow rates and volumes), one could very easily obtain results that obviously violate mass balance considerations - that an impacted surface water bodies receives more contaminant over a multi-year period in runoff, erosion, and direct deposition than is emitted from the stack over that multi-year period.

Proper parameterization of the model is the key to not violating principals of mass balance. The following is offered as pointers to consider for mass balance concerns:

1) <u>No parameter is trivial:</u> All parameters used in the modeling should be presented for others to scrutinize. Careful attention should be paid to the stack emission rate assumed for air transport modeling, as every subsequent media concentration is proportionally related to it. All fate, transport, and transfer parameters specific to the contaminant are the second most important model parameters. Insure that all parameters are in the proper units. If an air concentration is presented to the assessor in units of $\mu g/m^3$, and the food chain models require its units to instead be in pg/m^3, then an oversight in converting will result in all media concentrations related to air concentrations (i.e., plants, animal food products, and water and fish of the surface water body) to be overestimated by a factor of a million.

2) <u>Do reality checks with estimated media concentrations:</u> This is, of course, easier said than done. It means that assessors should evaluate their predicted concentrations with observed concentrations in the literature. If predicted concentrations exceed observations by an order of magnitude, for example, one should very carefully evaluate model input

parameters for mistakes.

While this addendum cannot offer a comprehensive tabular summary of media concentrations for key contaminants, the following is offered. As part of EPA's reassessment of dioxin-like compounds, exposure media concentrations were compiled for these compounds. In addition to a comprehensive survey of the literature, a principal purpose of this compilation was to estimate background exposures to dioxin-like compounds. Dioxin-like compounds are known to be ubiquitous in the environment, and concentrations are present where there is no immediate source of release. Literature reports of exposure media concentrations which were evaluated as best representing background conditions - not directly associated with a contaminated site or downwind of a incinerator known to be emitting dioxin-like compounds - were culled out and reviewed. Average concentrations of dioxin toxic equivalents (TEQ) were estimated for these exposure media:

Air	$0.095 \ pg/m^3$
Soil	8.0 ng/kg (ppt)
Fish	1.2 ng/kg (ppt whole fish of various lipid contents)
Water	0.0056 pg/L (ppq)
Milk	0.07 ng/L (ppt whole milk at 3.5% fat)
Beef/veal	0.48 ng/kg (ppt whole product assuming 19% fat)

After conducting an assessment for dioxin TEQs, assessors should compare their predicted exposure media with the above. Since the above values were selected to represent background levels, it may be possible that these levels are exceeded near a source. However, if predicted concentrations are significantly higher than these, then a careful review of input parameters and intermediate exposure media should occur. A first check would be on air concentrations predicted by the air transport model for dioxin TEQs. The above concentration at $0.095 \ pg/m^3$ was an average for urban/suburban areas in the United States. An evaluation of available air concentrations in rural areas where no source was immediately nearby indicated that air concentrations in these areas are about 5 times

lower than urban concentrations, or at about 0.020 pg/m^3. If an air prediction of TEQs is 1.0 pg/m^3, which is about an order of magnitude higher than average urban conditions and 50 times higher than rural conditions, one should carefully evaluate emission assumptions and all other air transport modeling parameters. If the air prediction of TEQs appears more in bounds, such as 0.01 pg/m^3, but the beef concentration is 5.0 ppt, which is an order of magnitude higher than 0.48 ppt, than again the assessor has to review his food chain input parameters for errors. Any other evaluations of model performance, such as further comparisons with literature data or sensitivity analyses, will assist in addressing concerns about mass balance violations.

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III. RECOMMENDATIONS FOR LONG-TERM IMPROVEMENT OF MULTIMEDIA RISK MODELING

1. Air Dispersion and Deposition

Although ISC-COMPDEP will be based on the EPA's ISC2 and COMPLEX I regulatory dispersion models, its application will be in a different context than required by the Clean Air Act. Therefore, the subgroup recommends that ISC-COMPDEP be peer reviewed for indirect exposure analysis.

The subgroup recommends longer term development (1 to 2 years) of the next generation of air dispersion models. This would involve various projects, most importantly:

1. the development of the modeling capability to make reliable predictions of the wet and dry deposition of chemicals that exist in the atmosphere in the vapor phase. The L_{DIF} term to revised Equation [4-1] of this Addendum is recommended for diffusive entry of vapor-phase contaminants into soil. This could answer the need for an algorithm for dry deposition of vapors into soils. Currently, there is no approach for wet deposition of vapors;

2. the development of a more sophisticated model for use in complex terrain;

3. the evaluation of algorithms for wet deposition of particles.

In the development of these models, consideration should be given to integrating the modules that estimate bioaccumulation in food chain, surface runoff in the receiving waters and other components of the indirect exposure methodology. This would combine all modeling efforts into one assessment tool.

It is important that air deposition modeling be kept current with the developments in the state-of-the-science. The short-term recommendations are not sufficient for developing the state-of-the-science deposition model. Therefore, the subgroup provides the following long-term recommendations.

1. There is a need to develop a suitable deposition algorithm for gases. Once developed and tested, such an algorithm can be put into the ISC2 model and a future version of ISC-COMPDEP.

2. The dry deposition algorithm in ISC2 was not intended for complex terrain applications. In order to determine if the algorithm is applicable to complex terrain, additional testing and, if necessary, modifications are needed.

3. It is necessary to develop and evaluate suitable wet deposition algorithms.

4. For national applications of the ISC-COMPDEP model, a species-dependent chemical data base is needed. For example, the dry deposition algorithm requires site specific data on particle sizes and densities and gas deposition algorithms require data on chemical properties. Such data are not readily available.

5. For national applications of ISC-COMPDEP, a workbook example guidance document to illustrate all the steps needed for indirect exposure analysis would be very useful.

6. If refined concentration estimates are desired for receptors in complex terrain, then there is a need to further update the ISC-COMPDEP model. COMPLEX I is a screening level model, and research by ORD/AREAL has identified a more refined model (i.e., CTDMPLUS). It is a major effort to modify this model to include a deposition algorithm.

7. Climatological models can be used to provide annual average estimates with lower costs than the models mentioned above which require on-site hourly data. However, research is needed for developing a climatological model for complex terrain that uses the CTDMPLUS state-of-the-science formulation, a suitable dry and

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wet deposition algorithm for this model.

2. Indirect Exposure Analysis - General

The procedures described in this Addendum and the Indirect Exposure Document are not currently compiled into a single integrated model. The COMPDEP model is an independent computer code. There is no computer tool, however, which takes the air concentrations and depositions from COMPDEP, and using algorithms of this Addendum and the Indirect Exposure Document, estimates exposure media concentrations and subsequent exposures. Such a model should have several software features.

First, it should be **interactive**. This could be accomplished by writing an indirect exposure methodology shell that would call various data input, process, and post-process modules. Options for such a shell include standard languages such as C++, or Windows. Second, it should be **integrated**. Calculated concentrations and fluxes in individual media modules should be transferred to other media modules via common blocks or arguments. The user should also have the opportunity to directly specify loadings to individual media. Third, it should be **modular**. Users should be able to substitute alternate modules for individual media quickly and easily. This would allow specialized applications (e.g., for mercury) as well as evolutionary improvement of the overall system with time. Finally, it should be linked to a **statistical driver**. This would facilitate such operations as automated sensitivity analysis, first-order error analysis, and Monte Carlo analysis. These operations should encourage users to explore what controls the uncertainty in the overall risk estimates.

Having such a software tool is the first step in the long term improvement of multimedia risk assessment. The proper parameterization of each application will always be a major issue. Supporting national databases should be made easily accessible to the user. For example, the interactive program DBAPE (Data Base and Parameter Estimation for Soils) is available to all users, distributed through the Center for Exposure Assessment Modeling. Eventually, such programs should be accessible through the multimedia shell, or through an accompanying geographical information system.

Some multimedia applications inevitably will have to be specialized for particular chemicals or locations. A linked set of more sophisticated mass balance and chemical speciation models should be available for these special applications, for testing and improving components of the nationwide multimedia model, and for parameterizing regional or nationwide applications.

Because mercury is presently an important and difficult contaminant, the development of state-of-the-art compartment mass balance models for mercury would be useful. Recommendations for such a model are being considered, but are considered beyond the scope of this document.

3. Animal Tissue Biotransfer Factors and Food Consumption Rates

The mass intake to whole body concentration approach used in the Indirect Exposure Document may not be the optimum approach for the determination of pollutant concentration in animal tissue. A concentration to concentration approach for the bioconcentration transfer factor should be considered for the long run. Also, recognizing the importance of the animal intake assumptions (fraction of the intakes in grain, forages, and silage, etc.) the assumptions made for the current draft should be reevaluated for accuracy.

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Appendix A: Approaches to Estimating Population Risk from Food Production

1. By definition:

$$Population\ Risk = \sum_{i=1}^{n} IndividualRisks \qquad [A\text{-}1]$$

2. Assuming all individual risks are in the linear dose-response range:

$$Population\ Risk = q^* \sum_{i=1}^{n} d_i$$
$$= n\ q^*\ d_{avg} \qquad [A\text{-}2]$$

where:

q^*	=	cancer slope factor (kg-day/mg)
d	=	dose (mg/kg-day)
n	=	population size (dimensionless)

3. For example, the total population risk from dioxin in each type of food supply in the U.S. is:

$$PopulationRisk = q^*\ n_{US}\ d_{USavg} \qquad [A\text{-}3]$$

where:

q^*	=	cancer slope factor (kg-day/mg)
n_{US}	=	U.S. population size (dimensionless)
d_{USavg}	=	U.S. average dose (mg/kg-day)

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4. Expanding the dose term:

$$\text{Population Risk} = \frac{q^* \; n_{US} \; C_{USavg} \; IR_{USavg} \; ED}{BW \; LT} \qquad \text{[A-4]}$$

where:

q^*	=	cancer slope factor (kg-day/mg)
n_{US}	=	U.S. population size (dimensionless)
C_{USavg}	=	U.S. average concentration of dioxin in the food (mg/g)
IR	=	ingestion rate of the food (g/d)
ED	=	exposure duration (yr)
BW	=	body weight (kg)
LT	=	lifetime (yr)

5. Assuming that all the food produced is consumed, then:

$$FP_{US} = n_{US} \; IR_{USavg} \qquad \text{[A-5]}$$

where:

FP_{US}	=	U.S. production of the food (g/d)
n_{US}	=	U.S. population size (dimensionless)
IR_{USavg}	=	U.S. average ingestion rate of the food (g/d)

6. Substituting FP_{US} into Equation [C-4] produces:

$$\text{Population Risk} = \frac{q^* \; C_{USavg} \; FP_{US} \; ED}{BW \; LT} \qquad \text{[A-6]}$$

where:

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q^* =   cancer slope factor (kg-day/mg)

C_{USavg} =   U.S. average concentration of dioxin in the food (mg/g)

FP_{US} =   U.S. production of the food (g/d)

ED =   exposure duration (yr)

BW =   body weight (kg)

LT =   lifetime (yr)

7. Assume one is interested in risks created by dioxin contaminated food produced in area X but potentially consumed anywhere in the U.S. The concentration term then becomes:

$$C_{USavg} = \frac{mass\ dioxin\ contaminated\ food\ produced\ within\ area\ X}{total\ U.S.\ food\ production}$$
$$= \frac{C_X\ FP_X}{FP_{US}} \qquad \text{[A-7]}$$

where:

C_{USavg} =   U.S. average concentration of dioxin in the food (mg/g)

C_X =   concentration of dioxin in the food from area X (mg/g)

FP_X =   production of the food in area X (g/d)

FP_{US} =   U.S. production of the food (g/d)

8. Substituting for C_{USavg} into Equation [C-6]:

$$Population\ Risk = \frac{q^*\ ED\ C_X\ FP_X}{BW\ LT} \qquad \text{[A-8]}$$

where:

q^* =   cancer slope factor (kg-day/mg)

ED =   exposure duration (yr)

C_X =   concentration of dioxin in the food from area X (mg/g)

FP_X =   production of the food in area X (g/d)

BW = body weight (kg)

LT = lifetime (yr)

9. Assume area X is divided into 5 rings with differing amounts of the food production and dioxin levels in the food:

$$Population\ Risk = \frac{q^* \ ED}{BW\ LT} \sum_{i=1}^{5} FP_i\ C_i \qquad [A\text{-}9]$$

where:

q^* = cancer slope factor (kg-day/mg)

ED = exposure duration (yr)

BW = body weight (kg)

LT = lifetime (yr)

FP_i = production of the food in the ith ring of area X (g/d)

C_i = concentration of dioxin in the food from the ith ring of area X (mg/g)