

AD-A150 767 THE PRELIMINARY POLLUTANT LIMIT VALUE APPROACH:  
PROCEDURES AND DATA BASE(U) ARMY MEDICAL BIOENGINEERING  
RESEARCH AND DEVELOPMENT LAB FORT. M J SMALL JUN 84  
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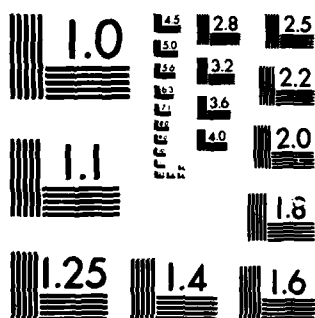
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TECHNICAL REPORT 8210

THE PRELIMINARY POLLUTANT LIMIT VALUE APPROACH:  
PROCEDURES AND DATA BASE

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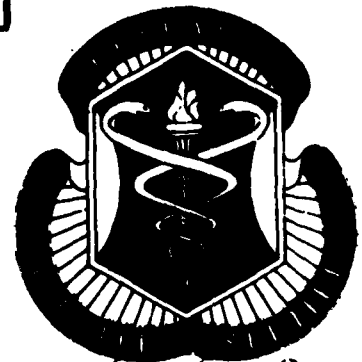
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20. Abstract (continued)

are presented. The approach requires data inputs from diverse disciplines such as toxicology, nutrition and physical chemistry. Useful literature sources are presented as well as representative values for many variables that are not pollutant-specific.

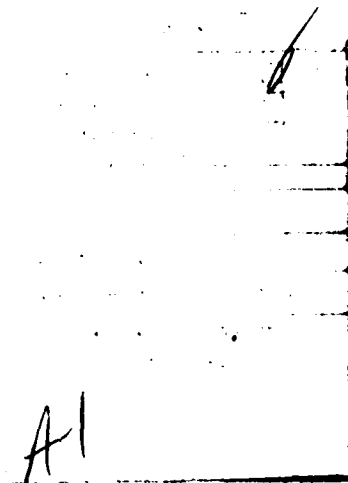
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## PREFACE

This report is intended for joint issue by the US Army Medical Bioengineering Research and Development Laboratory and by the US Army Engineer Waterways Experiment Station (WES), Vicksburg, MS. Funding to prepare this report was provided in part by WES, from account 96X3123596223.

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## PART I: INTRODUCTION

1. The US Army controls real estate that may have land or water contamination from discontinued chemical agent or explosives production, demilitarization, or associated training activities. These properties may still be in active use or under consideration for sale to non-Federal Government entities. Such land should not have residual chemical contaminants at levels that might be harmful in current or projected land-use situations. Decisions need to be made as to whether such land needs to be renovated, and if so, the extent of renovation required. In some cases, the intended land use will be known; in other cases, several options may have to be addressed. Land renovation costs will depend upon the extent of clean-up. Decisions will have to be made with a limited knowledge of the toxic properties of the contaminants, the extent of contamination, or the environmental mechanisms by which the contaminant could be a hazard to man.

2. The Preliminary Pollutant Limit Value (PPLV) approach has been developed by the US Army Medical Bioengineering Research and Development Laboratory (USAMBRDL) to provide the decision-maker with guidance to the general question:

Soil or water (or both) are contaminated with a chemical. If the land or water is intended to be used for one or more functions, what concentration of the chemical should be allowed to remain?

The approach was first advanced in 1976 in response to a groundwater pollution problem at Rocky Mountain Arsenal, CO,<sup>1</sup> and subsequently presented in the open literature.<sup>2,3</sup> It has been applied to several other installations; see Table 1.

3. The studies cited in Table 1 cover a 7-year period. In this time, advances in theory, research and empirical approaches, and scientific opinion have improved the ability to estimate environmental pollution limits. This report revises earlier PPLV approach presentations<sup>2,3</sup> of such advances. It also describes in enhanced detail PPLV data requirements and the ways that such data can be researched, deduced, or estimated. Where such data are not pollutant-specific, representative values and their sources are presented. Where pollutant-specific data must be located, documents that may readily provide needed information are listed. Consideration has been given to documents that are well-known in an attempt to reduce the need for protracted literature searches. In short, this report is intended to serve as a reference book for PPLV approach applications. Moreover, it should also be a useful document for related procedures that seek to estimate environmental pollution limits.

4. The PPLV approach should be kept in proper perspective; see Table 2. The approach incorporates reasonable treatment of toxicological data and pathways for human exposure into a computational framework whereby acceptable soil (or other environmental media) contaminant levels may be derived. Involved mathematical models are avoided when the available data do not support them. Toxicological data are derived from studies that may vary widely in relevance to humans and in scientific credibility. The analysis requires several types of data other than toxicity that are averaged, safe-sided, or scenario-specific. Some numerical inputs are well established,

while others are based on scanty documentation, interpretation, or guesswork. Since there is considerable reliance on "judgment calls," the temptation to endow a PPLV with an absolute and inviolate nature should be avoided. On the other hand, the PPLV approach can provide a useful framework in which to construct answers to environmental problems. Each new application in Table 1 has presented the USAMBRDL staff with situations which would have not been resolved with previously used methods. Additional concepts and procedures have been developed, evaluated, and incorporated into the approach. The author expects that future applications will present similar challenges, which will lead to further expansion and elaboration of the approach.

Table 1  
Summary of PPLV Approach Studies Undertaken or In Progress

Location/Reference	Problem	Hazards
Rocky Mountain Arsenal, CO <sup>1</sup>	Groundwater off-post is polluted by chemicals from past on-post production activities.	Groundwater is used for farming and drinking.
Alabama Army Ammunition Plant, AL <sup>4</sup>	Land is contaminated by chemicals from World War II explosives production.	Some land was sold for industrial use; retained land may be sold for unrestricted use.
Bangor Naval Submarine Base, WA <sup>5</sup>	Runoff with explosives is planned for diversion to an on-base pond.	Fish and shellfish from pond and pond's tidal outlet can be eaten by people.
Savanna Army Depot Activity, IL <sup>6</sup>	Explosives are found in sediments of slough and dry lagoons in Mississippi River flood plain.	Slough is a source for commercial fish. Washout from lagoons during floods may contaminate river.
Gratiot County Landfill, MI <sup>7</sup>	Polybrominated biphenyls are found in soil at landfill and at nearby farms.	Farms may be sold for industrial purposes or for unrestricted development.
Camp Sims, DC <sup>8</sup>	Riot gas may still remain in a disposal pit.	Land with pit is a possible building site.
Badger Army Ammunition Plant, WI <sup>8</sup>	Propellant in sediment might migrate to Wisconsin River.	River could become a drinking water supply in the future.
Fort McClellan, AL <sup>9</sup>	Chemical warfare decontamination by-products may be present in soil at 12 training ranges.	Unrestricted troop activities are proposed at these ranges.

Table 2

The PPLV Approach: Concepts and Features

Each use situation involves one or more pathways by which man is exposed to a pollutant. Initially, each pathway for transfer of a pollutant from the environment to man is treated as if it involved either (a) one environmental compartment or (b) a series of successive compartments containing the pollutant at equilibrium. Transfer from the final compartment to humans is considered a non-equilibrium process occurring at an assumed rate. A PPLV is that concentration of the pollutant in the first compartment that is calculated to result in reception by a target person of an acceptable daily dose via one or more pathways. The basic concept may be modified as the situation requires.

PPLVs

ARE

Essentially parsimonious but capable of elaboration

Based on available information, reasonable assumptions and some common sense

Flexible

Subject to update

Site- and situation-specific

Dependent on some degree of judgment

ARE NOT

Absolute

Sacred

Regulatory

Forever

The last word in court

Always possible to derive

Source: From Rosenblatt.<sup>10</sup>

THE PPLV APPROACH: AN OVERVIEW

5. The PPLV approach presumes that human life is to be safeguarded from the adverse effects of pollutants. Proposed environmental limits for pollutants are based on existing information and on a series of models reflecting the means by which man and pollutants interact. As noted in Table 2, these interactions are first processed in terms of individual exposure pathways. The PPLV is based on the limits computed for each pathway. The method was initially developed for pollutants in soil;<sup>1</sup> in this section, soil is considered as the repository for pollutants.

6. The decision-maker must first determine the pollutants and pathways to be considered. While such a determination appears to be an elementary exercise, it involves considerable thought. The author's experience is that the initial determination of pollutants is based on "laundry lists" of parent chemicals employed during active production. Certain of these, such as gases

or volatile liquids, can be ruled out of concern easily. Other compounds may be added by consideration of the environmental fate of parent compounds. When substances are elemental or ubiquitous, their levels need to be addressed in relation to background levels before one may conclude that an actual contamination problem exists. The prudent approach is to sample and analyze for suspected pollutants in the soil so that perceptions can be validated.

7. The decision-maker generally has in mind projected land-use scenarios; each scenario will be associated with one or more pathways. Pathway selection is based on how a pollutant in soil can eventually reach man by ingestion or inhalation. As examples of pathways, consider the following: groundwater in contact with contaminated soil may enter a municipal water supply; surface runoff over such soil may enter a lake with game fish; or, contaminated groundwater may irrigate crops grown for the purpose of raising livestock. The decision as to how many pathways to consider should be tempered by the realization that additional investments of time and money are incurred by the gathering of pathway information. cursory consideration of certain proposed pathways can indicate that they might not be particularly meaningful; see paragraphs 88-91.

8. A second step is to identify the data required for computations. One datum common to any PPLV computation is  $D_T$ , the acceptable daily dose to humans, expressed as mg pollutant/kg body weight/day.\*  $D_T$  is conceptually a "no-effects" threshold dose for human exposure to a pollutant not considered as a potential or proven carcinogen.\*\* For a potential or proven carcinogen,  $D_T$  is conceptually an "acceptable risk" dose. Appendix B discusses these concepts in detail. Methods of computing  $D_T$  based on the literature are presented in Part II of this report.

9. The equations that relate pollutant concentration in soil to  $D_T$  by each pathway are derived concurrently with the data definition process. The attitude at this point is that each pathway is the only pathway through which a contaminant in soil reaches man. That soil concentration is given the name "Single-Pathway Preliminary Pollutant Limit Value" or SPPPLV. In the PPLV approach, each pathway involves a linear compartmental model through which a pollutant passes. For example, a "livestock consumption" pathway can involve the hypothetical transfer of pollutant from soil to plant and thence from plant to animal. In the absence of refined information, each such transfer is characterized by a partition coefficient. The final transfer (meat consumption by humans) is characterized by an estimate of the nominal daily meat intake by humans.

10. SPPPLV relations have two general forms corresponding to the two transfer routes described in Table 2. If the pollutant reaches man without an intermediate compartment (such as direct ingestion of soil by children), the form is

$$C_{si} = IF_i \times D_T \quad (1)$$

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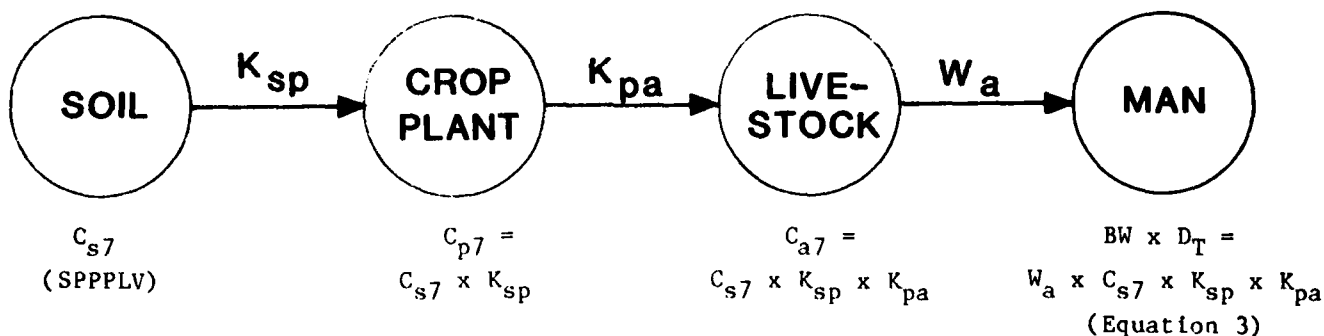
\* For convenience, symbols and unusual abbreviations are listed and defined in the Notation (Appendix H).

\*\* More correctly, a proven oncogen in man or in test mammals, see paragraph 17.

Here  $C_{s1}$  is the SPPPLV for pathway "1" in mg pollutant/kg dry soil, and  $IF_1$  is an "intake factor" that typically includes information about the human weight and the rate of pollutant uptake. If one or more intermediate compartments is involved, the SPPPLV relation has the form:

$$C_{s1} = IF_1 \times D_T / K_1 \quad (2)$$

$K_1$  is a composite partition coefficient for transfers of the pollutant in soil to the matter consumed by man. As an example, Figure 1 represents the model for the "livestock consumption" pathway discussed above, therein called pathway 7.  $C_{s7}$  is the SPPPLV to be computed.  $C_{p7}$  and  $C_{a7}$ , the corresponding pollutant concentrations in plant matter and livestock respectively, are expressed in terms of  $C_{s7}$  and the appropriate partition coefficients  $K_{sp}$  (soil to plant) and  $K_{pa}$  (plant to animal). Equation 3 in Figure 1 expresses the daily human intake of the pollutant in meat,  $BW \times D_T$ , in terms of  $C_{s7}$ , the accumulated partition coefficients, and  $W_a$ , the daily intake of meat. The forms of  $IF_7$  and  $K_7$  are readily found.  $IF_7$  involves factors that are pollutant-unrelated while  $K_7$  involves pollutant-related factors. The expression for  $C_{s7}$  in terms of  $D_T$  corresponding to Equation 2 format is readily formed. Equations derived in this manner are presented in Part III of this report. Information concerning intake factors appear in Part IV of this report. Information concerning partition coefficients is discussed in Part V of this report.



$BW$  = Human body weight

$W_a$  = Daily meat diet

$IF_7 = BW / W_a$

$K_7 = K_{sp} \times K_{pa}$

$C_{s7} = (IF_7 / K_7) \times D_T$

Figure 1. Model to derive SPPPLV for pathway 7 (meat consumption, livestock raised on crops grown in contaminated soil).

11. Once equations are derived and data needs established, the literature is searched for relevant information.

12. The final step is to compute a scenario PPLV (symbolized for the case of soil as  $C_{sf}$  with units of mg pollutant/kg dry soil) based on component SPPPLVs. The relation

$$C_{sf} = 1 / \sum (1 / C_{si}) \quad (4)$$

is derived below.\* First, Equations 1 and 2 have the general form

$$C_{si} = R_i \times D_T \quad (5)$$

where  $R_i = IF_i$  (Equation 1) or  $R_i = IF_i / K_i$  (Equation 2). In a scenario, the dose to man is to be limited to  $D_T$  when the pollutant concentration in soil ( $C_s$ ) is  $C_{sf}$ . If  $D_{Ti}$  is the dose delivered through a component pathway when  $C_s = C_{sf}$ ,

$$D_T = \sum D_{Ti} \quad (6)$$

where summation is only for scenario pathways of interest.  $D_{Ti}$  values cannot be selected arbitrarily; by analogy to direct-current parallel circuitry,\*\*

$$C_{sf} = R_i \times D_{Ti} \quad (7)$$

Equations 6 and 7 are combined to produce the relation

$$C_{sf} = D_T / \sum (1/R_i) \quad (8)$$

Substitution of Equation 5 ( $1/R_i = D_T/C_{si}$ ) into Equation 8 leads to Equation 4.

#### REPORT ORGANIZATION

13. Four subsequent parts of this report have been referred to above, namely:

Part II:  $D_T$  Estimation Techniques. Various procedures are presented to convert unassessed toxicological information, recommended allowances, or criteria to  $D_T$ .

Part III: Environmental Pathway Relations. This section includes various SPPPLV relations derived in studies to date in a manner similar to that presented for pathway 7 in paragraph 10 and Figure 1.

\* The derivation presents equations that are used in later sections of the text and in several appendixes.

\*\* In this analog,  $D_T$  represents a "current" to be delivered by parallel branches.  $C_{sf}$  represents a "potential" and the  $R_i$  "resistance" in each branch. Equation 8 is the analog of Ohm's Law.

Part IV: Reference Data. This section presents representative values not related to chemical properties for use in  $D_T$  and SPPPLV equations. The bases for these values are discussed, along with suggested documents from which alternative values can be found when required.

Part V: Partition Coefficient Estimation Techniques. A presentation of methods for estimating partition coefficients.

Part VI, which has not been previously mentioned, discusses adjustments to the derivation of a PPLV from SPPPLVs (see Equation 4) when factors other than the avoidance of undue toxic effects to humans are involved. Part VI also presents a method for predicting which  $R_1$  values and thus, which pathways, are most important in determining a PPLV. The ability to do this can often reduce resource requirements. Finally, Part VII, presents a flow-chart of the PPLV approach with cross-references to text.

14. Eight appendixes are also included:

- \* Appendix A. Extended Reference Tables
- \* Appendix B. Technical Discussion of  $D_T$  Estimation Techniques
- \* Appendix C. Technical Discussion of SPPPLV Pathways
- \* Appendix D. Technical Discussion of Partition Coefficients
- \* Appendix E. Plant Pollutant Uptake From Soil - An Initial Assessment
- \* Appendix F. Treatment of a Ubiquitous Substance by the PPLV Method
- \* Appendix G. Population Factors for Scenarios
- \* Appendix H. Notation

Parts II, III and V present material for a user who wishes to do computations or seeks reference information. Appendixes B, C, and D are parallel sections that present the background and a critical review of information presented in the main text. Users not familiar with toxicological and environmental considerations are advised to read relevant parts of the main text and the corresponding appendixes.

15. Where practical, symbol notation of this text is consistent with that presented previously by Rosenblatt et al.<sup>1-3</sup> The report format is generally consistent with that of the US Army Engineers Waterways Experiment Station.<sup>11</sup> However, the author has used a numerical, sequential system for references. The author believes that this procedure is better suited to the types and number of references. Appendix figures, tables, and equations include the alphabetical appendix designation to distinguish them from those of the main text. Appendix references to paragraphs in the main text are designated with "m.t."



## PART II: $D_T$ ESTIMATION TECHNIQUES

### SELECTED REFERENCES

16.  $D_T$  estimation methods involve processing information derived from the toxicological literature. Fortunately, there are comprehensive references that provide summaries of toxicological studies, and they should be consulted before embarking on a source document search.

a. Registry of Toxic Effects of Chemical Substances (RTE), 1980.<sup>12</sup> This document has summary information concerning toxicological, mutagenic, and carcinogenic studies, along with citations. The RTE also provides compound synonyms, which may be required if extensive literature searching is planned.

b. Documentation of the Threshold Limit Values (DTLV), fourth edition.<sup>13</sup> Information on toxicological studies for over 600 compounds is presented in this document along with recommended air concentration limits (threshold limit values or TLVs) to protect workers against adverse health effects.

c. Patty's Industrial Hygiene and Toxicology, 1981.<sup>14</sup> Long considered a standard reference in the field, this edition is greatly expanded in scope and is a good starting point for information on many compounds.

d. The Chemical Regulation Reporter, a subscription service of the Bureau of National Affairs, provides a weekly digest of developments of chemical testing and regulation as well as an update of important Federal Regulations.

It is helpful to have access to the computerized Chemical Abstracts Service (CAS). The CAS number system for compound identification is widely used for entry into the CAS data base as well as other computerized data bases.

### POLLUTANT CLASSIFICATION PROCEDURES

#### Classification Criteria

17. In paragraph 8, a conceptual distinction was drawn between the significance of  $D_T$  for non-carcinogenic substances and of  $D_T$  for potential or proven carcinogens. Prior to a search for information from which to estimate  $D_T$ , substances should be so classified. The following criteria have been used to classify a substance as a potential or proven carcinogen for the purpose of  $D_T$  estimation:

a. There is strong evidence that the substance causes cancer in humans.

b. There is statistical evidence that a positive dose-level tumor-incidence (dose-response) relation exists for at least one mammalian species

studied in a period of time approaching the species' lifetime as part of a bioassay feeding or inhalation study.

c. The following criterion has been applied provisionally at USAMBRDL<sup>4</sup> and others may wish to consider it for use as a safe-sided approach; see Appendix B, paragraph 7. The "Ames Test," a bacterial mutant reversion test of the substance on strains of Salmonella typhimurium, demonstrates positive results with at least one strain in the presence or absence of a rat-liver activation system. Positive results are obtained when both a positive dose-reversion count relation can be derived and the number of revertants at the highest dose level used in the relation is at least twice the number of revertants of the control sample. This criterion should only be used in the absence of mammalian bioassay tests.

#### Information Sources

18. There are certain check lists and periodic reports that can be reviewed to screen a compound for an indication that it should be processed as a carcinogen:

a. It is cited as such in the RTE<sup>12</sup> or the DTLV.<sup>13</sup>

b. A substance is considered a carcinogen in Federal Occupational Regulations on toxic and hazardous substances.<sup>15</sup> For convenience, these substances are:

4-Nitrobiphenyl  
alpha-Naphthylamine  
Methyl chloromethyl ether  
3,3'-Dichlorobenzidine  
Bis-Chloromethyl ether  
beta-Naphthylamine  
Benzidine  
4-Aminodiphenyl  
Ethyleneimine  
beta-Propiolactone  
2-Acetylaminofluorene  
4-Dimethylaminoazobenzene  
N-Nitrosodimethylamine  
Vinyl chloride  
Inorganic arsenic compounds  
1,2-Dibromo-3-chloropropane  
Acrylonitrile

c. It is considered a potential carcinogen in the U.S. Environmental Protection Agency (EPA)-issued "Notice of Water Quality Criteria Documents" (NWQCD).<sup>16</sup> Table 3 lists these compounds along with D<sub>T</sub> estimates relative to an acceptable risk level (ARL) of 10<sup>-5</sup>; see paragraph 19.

d. It is identified as such in the U.S. Public Health Service "Annual Report on Carcinogens." The most recent report (December 1981)<sup>17</sup> lists 88 substances.

Table 3

D<sub>T</sub> Estimates for Selected "Priority Pollutants"<sup>a</sup>

Substance	D <sub>T</sub> , mg/kg/day
Acrylonitrile	1.8 x 10 <sup>-5</sup>
Dieldrin	3.1 x 10 <sup>-7</sup>
Aldrin	3.3 x 10 <sup>-7</sup>
Arsenic (III)	7.2 x 10 <sup>-7</sup>
Benzene	1.9 x 10 <sup>-4</sup>
Benzidine	4.4 x 10 <sup>-8</sup>
Beryllium salts	1.2 x 10 <sup>-6</sup>
Carbon tetrachloride	1.2 x 10 <sup>-4</sup>
Chlordane	3.2 x 10 <sup>-6</sup>
Hexachlorobenzene	7.6 x 10 <sup>-6</sup>
1,2-Dichloroethane	2.7 x 10 <sup>-4</sup>
1,1,2-Trichloroethane	1.7 x 10 <sup>-4</sup>
1,1,2,2-Tetrachloroethane	4.9 x 10 <sup>-5</sup>
Hexachloroethane	6.9 x 10 <sup>-4</sup>
2,4,6-Trichlorophenol	5.0 x 10 <sup>-4</sup>
Bis(chloromethyl)ether	1.1 x 10 <sup>-9</sup>
Bis(chloroethyl)ether	8.8 x 10 <sup>-6</sup>
Chloroform	5.5 x 10 <sup>-5</sup>
3,3'-Dichlorobenzidine	5.9 x 10 <sup>-6</sup>
1,1-Dichloroethylene	9.6 x 10 <sup>-6</sup>
2,4-Dinitrotoluene	3.2 x 10 <sup>-5</sup>
1,2-Diphenylhydrazine	1.3 x 10 <sup>-5</sup>
Halomethanes <sup>b</sup>	5.5 x 10 <sup>-5</sup>
Heptachlor	3.2 x 10 <sup>-6</sup>
Hexachlorobutadiene	1.3 x 10 <sup>-4</sup>
alpha-Hexachlorocyclohexane	3.7 x 10 <sup>-6</sup>
beta-Hexachlorocyclohexane	6.6 x 10 <sup>-6</sup>
"gamma-HCH" (lindane)	7.6 x 10 <sup>-6</sup>
n-Nitrosodimethylamine	4.0 x 10 <sup>-7</sup>
n-Nitrosodiethylamine	2.3 x 10 <sup>-7</sup>
n-Nitrosodi-n-butylamine	1.9 x 10 <sup>-6</sup>
n-Nitrosodiphenylamine	2.0 x 10 <sup>-3</sup>
n-Nitrosopyrrolidine	4.6 x 10 <sup>-6</sup>
Benz(a)pyrene	8.8 x 10 <sup>-7</sup>
Tetrachloroethylene	2.5 x 10 <sup>-4</sup>
Trichloroethylene	8.0 x 10 <sup>-4</sup>
Toxaphene	7.4 x 10 <sup>-6</sup>
Vinyl Chloride	5.7 x 10 <sup>-4</sup>

a. Restricted to potential or known carcinogens.

ARL of 10<sup>-5</sup> assumed.

b. Several chloro-, bromo-, mixed bromo- and chloro-, and chlorofluoro isomers included. D<sub>T</sub> based on value for chloroform.

e. It is in Category I or II of the National Institute of Occupational Safety and Health (NIOSH) Preliminary Suggested List of Carcinogens<sup>18</sup> for inclusion in the Federal Regulation 29CFR1990.<sup>19</sup> As of this writing, the listed substances have not been incorporated into the regulation.

f. It has been identified as potentially mutagenic or carcinogenic by a proposed manufacturer's "substantial risk notice" in conformance with Section 8e of the Toxic Substances Control Act.<sup>20</sup> Summary annotated listings are available for notices submitted through October 1979<sup>21</sup> and from November 1979 to July 1981.<sup>22</sup>

#### Acceptable Risk Levels

19. In past studies,<sup>4,7,9</sup> an acceptable risk level of  $10^{-5}$  has been selected in conjunction with  $D_T$  estimates for carcinogens. This level corresponds to an additional case of cancer in the lifetimes of 100,000 hypothetically exposed persons. This was an ad hoc decision; a specific policy for selecting an ARL has not been adopted by the Army. Appendix B, paragraph 3, explains briefly the societal ramifications of selection of an ARL, while information in Appendix G should assist in determining populations at risk.

#### $D_T$ ESTIMATION PROCEDURES FOR NON-CARCINOGENS

20. The approaches presented here are ordered roughly in terms of preference. If several approaches can provide information from which to compute a  $D_T$ , the first is preferred.

#### Acceptable Daily Intake (ADI)

21. ADIs have been recommended by the Joint FAO/WHO Expert Committee on Food Additives.\* This committee is comprised of well-recognized toxicological and nutritional experts. The committee meets periodically to consider additional substances for ADI recommendations or to update past valuations. The results of each meeting are published by the WHO in its Technical Reports and the toxicological data involved are included in numbered "Food Additive Series" publications. No consolidated ADI list has, to the author's knowledge, been published. A user is advised to consult the most recent Report and work back in time to determine if a substance has been proposed or assigned an ADI. Table 4 lists recent reports. ADI values may be used directly as  $D_T$  estimates.

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\* The Food and Agriculture Organization (FAO) and the World Health Organization (WHO) are United Nations agencies. Their respective headquarters are in Rome, Italy and Geneva, Switzerland.

Table 4

WHO Reports Issued Since 1970 Involving Acceptable Daily  
Intake Recommendations

a) Reports of the Joint FAO/WHO Expert Committee on  
Food Additives (Technical Report number and date)

445	1970
462	1971
488	1972
505	1972
539	1974
557	1974
576	1975
617	1978
631	1978
648	1980

b) WHO Food Additive Series Containing Toxicological Reviews  
(Volume and date)

1	1972
5	1974
6	1974
8	1975
12	1977
13	1978
14	1980

Water Quality Criteria

22. The Clean Water Act of 1977<sup>23</sup> specified 129 substances (individual compounds or groups of related compounds) as being toxic pollutants. These substances are commonly referred to as "priority pollutants" for which water quality criteria were to be established. These criteria were summarized in the NWQCD.<sup>16</sup> Table 5 indicates priority pollutants considered non-carcinogenic and their water quality criteria-based  $D_T$  estimates. Appendix B, paragraphs 14-15, discusses the procedures used to estimate  $D_T$  from criteria. The Act's provisions are not limited to these substances, and others may be considered in the future.

Table 5

D<sub>T</sub> Estimates for Selected "Priority Pollutants"<sup>a</sup>

Substance	D <sub>T</sub> , mg/kg/day
Acrolein	0.016
Antimony Salts	4.2x10 <sup>-3</sup>
Dichlorobenzenes(mixed)	0.014
Dichloropropenes(mixed)	2.5x10 <sup>-3</sup>
Endosulfan	4.0x10 <sup>-3</sup>
Ethylbenzene	0.070
Fluoranthene	5.0x10 <sup>-3</sup>
Isophorone	0.15
Nickel Salts	4.4x10 <sup>-4</sup>
2,4-Dinitro-o-cresol	3.9x10 <sup>-4</sup>
Dinitrophenol	2.0x10 <sup>-3</sup>
Dimethyl phthalate	10
Diethyl phthalate	12
Dibutyl phthalate	1.2
Di-2-ethylhexyl phthalate	0.61
Thallium salts	5.0x10 <sup>-4</sup>
Toluene	1.43
1,2,4,5-Tetrachlorobenzene	5.0x10 <sup>-3</sup>
Pentachlorobenzene	0.016
1,1,1-Trichloroethane	0.54
Bis(2-chloroisopropyl) ether	1.0x10 <sup>-3</sup>

a. Not included are substances for which drinking water standards exist, substances for which criteria are based on carcinogenicity considerations, and substances for which criteria are based on organoleptic considerations.

## Threshold Limit Value Recommendations

23. TLVs were developed by the American Conference of Governmental Industrial Hygienists as recommended limits to protect working populations from the adverse occupational health effects of vapors, fumes, and dusts. In 1975, a large number of TLVs were incorporated into Federal occupational safety regulations.<sup>15</sup> The Conference periodically reviews existing TLVs for readjustment on the basis of new information and also considers TLVs for heretofore unaddressed substances.

24. The DTLV<sup>13</sup> should be reviewed first; a TLV is not valid for D<sub>T</sub> estimation if it is based on skin or nasal irritation, offensive odors, or the prevention of suffocation. If these conditions do not apply, Equation 9 estimates D<sub>T</sub> in terms of a TLV

$$D_T = TLV \times RB' \times (5/7) \times (AA / AO) / (SF \times BW) \quad (9)$$

where the TLV is in mg substance/cubic meter of air,  $RB'$  is the volume of air inhaled by a worker in an 8-hour day, which is presumed to be  $10\text{ m}^3$  for this specific purpose,<sup>16</sup> (5/7) adjusts from a 5-day work week to a 7-day calendar week, AA and AO are efficiency factors for absorption of pollutant from inhaled air to the bloodstream and from ingested matter to the bloodstream via the gastrointestinal tract respectively, and BW is the model adult body weight (70 kg); see paragraph 49.

25. In Equation 9, SF is a "safety factor" that is intended to account for the exposure of a general population (which may be more sensitive to exposure than a worker population) and for the involuntary nature of a general population exposure. SF may be assigned from an evaluation of the TLV data base for the "quality" of information present. The author suggests the following guidepost values:

a.  $SF = 10$ . The TLV was based on a well-conducted inhalation study concerning humans over a prolonged period (one or more years). The ambient air concentration of the substance was reasonably constant throughout the study period. The study indicated that at one concentration, no observable effects on human subjects could be detected and that at a higher concentration, observable effects could be so detected.

b.  $SF = 100$ . The TLV was based on a shorter term of exposure than in the above case, but in excess of 90 days. Alternatively, the TLV was based on a well-conducted 2-year feeding study of two or more mammalian species. As in the above case, both a no-observable effect and an observable effect daily dose level were attained. Alternatively, the TLV was based on effects data from long-term occupational exposure at concentrations that were highly variable or not well measured. As a third alternative, the TLV was based on an inhalation study of several animal species conducted for a 3- to 6-month period.

c.  $SF = 1,000$ . The study on which the TLV is based was of a shorter time frame than that discussed above, did not demonstrate a no-observable effect level, or involved a small number of human or animal subjects. Alternatively, the TLV was based on observations of homologous compounds.

Intermediate SF values (30 or 300) may be applied if the TLV basis appears intermediate between two of the above guideposts. AA and AO estimates require pharmacokinetic information. In the absence of such information, AA / AO should be assumed equal to one.

#### Mammalian Toxicological Studies

26. These studies are typically retrieved by suitable combination of manual and computerized literature searches. In some cases, starting references may be found in RTE,<sup>12</sup> DTLV,<sup>13</sup> or Patty.<sup>14</sup> The preferred type of information comes from the chronic mammalian study of 2-years duration. The animals ingest the substance of concern at selected dose feeding levels, expressed in mg/kg/day. A no-toxicant control group is included. From such a test protocol, one of three outcomes can be expected; see Table 6. This table supplies the appropriate dose feeding level, FL, and safety factor keyed to each outcome for use in Equation 10 below.

$$D_T = FL / SF \quad (10)$$

Table 6

Selected Dose Levels and Safety Factors for Use in Equation 10

Test Outcomes	Selected Dose Level (FL)	SF <sup>a</sup>
At all dose feeding levels, no effects are detected on test animals.	Use highest dose level	100-300
At one dose level, no effects are detected on animals. However, at a higher dose feeding level, effects are detected.	Use highest no-observed effects level	100-300
At all dose feeding levels, effects are detected on test animals.	Not recommended unless preference literature sources are unavailable. Use lowest dose level.	1,000-3,000

- a. A factor range is given to include considerations for the quality of the study; see Appendix B, paragraph 10 for details. The factors listed apply when  $D_T$  is estimated from a chronic study; see paragraph 26. If the study involved is a sub-chronic or 90-day study, these factors should be increased by a factor of ten.

27. Next in preference is the subchronic or 90-day study. Such a study may be performed when a substance is not suspected of being oncogenic. Table 6 and Equation 10 may be used to process study information; however, the safety factors adopted should be tenfold higher than those advanced in Table 6.

28. The least desirable study is the acute (single-dose) ingestion study on laboratory mammals. The animals are administered the substance of concern at selected dose levels and then observed 14 days for untoward effects. The test observations can be used to estimate the statistic LD50, i.e., the dose in mg/kg expected to kill 50 percent of dosed animals. A rather large number of compounds for which LD50 data exist are compiled in the RTE.<sup>12</sup>  $D_T$  can be estimated by Equation 11, which was derived<sup>1</sup> from relations advanced by Handy and Schindler,<sup>24</sup> see Appendix B, paragraph 17 for details of their approach.

$$D_T = 1.16 \times 10^{-5} \times \text{LD50} \quad (11)$$

## Other Standards, Official or Quasi-Official Recommendations, and Criteria

29. Several other sets of standards and recommendations may be available to the user. The author has encountered some such sets and here



presents his opinions as to their usefulness. No attempt has been made to place them in order of precedence.

a. Pesticide tolerances. These are included in Federal Regulation 40CFR180,<sup>25</sup> and specify the limiting content of selected pesticides in foods for livestock and human consumption. Whether these tolerances can be extrapolated to a  $D_T$  is doubtful.

b. Suggested no adverse response levels (SNARL)\* have been issued by the Office of Drinking Water, EPA, Washington, DC 20460 for unregulated drinking water pollutants. Normally, a SNARL is provided for three time periods; 1 day, 10 days, and indefinite. SNARLs are advisory to interested parties. The methods for SNARL formulation are similar to those for  $D_T$ ; however, SNARL values are expressed in terms of pollutant concentration in water. The SNARL documents that have been reviewed by the author<sup>26-29</sup> have been designed for a "worst case" target individual weighing 10 kg who drinks 1 L/day of water.  $D_T$  can be estimated from the indefinite period SNARL for such an individual; if the SNARL is in mg/L,  $D_T = 0.1 \times \text{SNARL}$ .

c. Drinking water standards. The author suggests that these be avoided; see Appendix B, paragraph 13.

d. Union of Soviet Socialist Republics maximum permissible concentrations in workroom air have been established for numerous chemicals. The author has not investigated the procedures by which concentrations are derived from toxicological information. However, in comparison with United States occupational standards,<sup>14</sup> corresponding USSR maximum permissible concentrations are generally more stringent; see Derr et al.<sup>30</sup> Equation 9 may be used to estimate a  $D_T$  from such a concentration; a SF = 30 is suggested. As in paragraph 24, this does not apply in cases where irritation, odor, or suffocation effects are involved.

#### $D_T$ ESTIMATION PROCEDURES FOR CARCINOGENS

##### Water Quality Criteria

30. Table 3 lists estimates of  $D_T$  at a  $10^{-5}$  ARL for "priority pollutants."

##### Mammalian Bioassay Data

31. Data Sources. The author has found three consolidated sources of information on bioassay studies. The first is a listing of reports of completed studies sponsored by the National Toxicology Program (NTP).\*\* Reports

\* These documents are now called safe drinking health advisory opinions.

\*\* The NTP is a cooperative effort within the Department of Health and Human Services to coordinate and provide information about potentially toxic chemicals to regulatory and research agencies and to strengthen the science base in toxicology.<sup>31</sup> The NTP issues a quarterly bulletin on its activities at no charge. Contact Ms. Lois F. Juodeika, Editor, Landow Building, Room A306, 7910 Woodmont Avenue, Bethesda, MD 20205. The commercial

on about 280 substances have been issued. This list is available in quarterly management status reports<sup>32</sup> obtainable from the NTP. The author stresses that if a substance has been reported, it was not necessarily found to be an oncogen. A second source is a 1981 book by Sax<sup>33</sup> which has extracted the most recent information concerning chemicals from the RTE<sup>12</sup> along with annotative comments. The book has several very readable chapters dealing with known or suspected human carcinogens, the incidence of cancer, animal testing and epidemiological studies, and regulatory aspects of carcinogen control. The third source is the multi-volume "Survey of Compounds Which Have been Tested for Carcinogenic Activity." This document is collectively referred to as Public Health Service Publication 149. The individual volumes are listed below with alternate publication designation and years of literature covered:

Prior to 1947	Public Health Service Publication 149 (Proper)
1948-1953	Supplement 1 to the above Publication
1954-1960	Supplement 2 to the above Publication
1961-1967	DHEW Publication (NIH) 73-35 (in 2 volumes)
1968-1969	DHEW Publication (NIH) 72-35
1970-1971	DHEW Publication (NIH) 73-453
1972-1973	DHEW Publication (NIH) 75
1978	DHHS Publication (NIH) 80-453

The survey for 1974-1977 has not been issued. The earlier research (approximately before 1970) needs critical review for such aspects as the use of controls or the purity of tested substances.

32. The procedure given here (the "one-hit" model described by the EPA<sup>34</sup>) is appropriate when the results from only one positive dose-response level are to be compared to a control experiment. If several positive dose-response levels are available for analysis, a multistage model can be applied.

a. Separate tumor incidence data according to organ site or tumor type at each dose level.

b. For each organ or tumor category above, select the lowest dose where the incidence of tumors is significantly higher than that of controls, using the Fisher exact test at an  $\alpha < 0.05$ .

c. If needed, convert the feeding information to a dose unit basis.

For example, if the substance tested is reported as being a certain portion of food ( $C_{fd}$ ) in mg/kg or ppm units, this dose (DE) may be approximated as

$$DE = F \times C_{fd}$$

where  $F = 0.05$  for rats and  $0.13$  for mice.

d. Quantify the following variables:

---

telephone number is 301-496-1152.

$n_t$  = Number of animals with tumors at the selected lowest dose.

$NT$  = Number of animals in the group at the selected lowest dose.

$n_c$  = Number of animals with tumors in the control group.

$NC$  = Number of animals in the control group.

$L_e$  = Actual maximum lifespan of animals in the group at the selected lowest dose, in weeks.

$w$  = Average animal weight in kg at the selected lowest dose.

$L$  = Expected lifespan of animal species in study. If not specified, use 90 weeks for mice and 104 weeks for rats.

$l_e$  = Length of exposure to substance in test in weeks.

e. Compute the intermediate variables:

$$P_t = n_t / NT$$

$$P_c = n_c / NC$$

$$D = DE \times l_e / L_e$$

$$T_t = L_e / L$$

f. For each tumor type or organ site, compute  $B_A$ , which is a risk-dose proportionality factor,

$$B_A = -\ln [(1-P_t) / (1-P_c)] \times [1 / (D \times T_t^3)]$$

Choose the maximum value of  $B_A$  for subsequent computations ( $B_{Amax}$ ). Then,

g. Compute  $B_H$ , the scaled risk-dose factor for humans;

$$B_H = B_{Amax} \times (70 / w)^{1/3}$$

h.  $D_T$  is estimated as

$$D_T = ARL / B_H$$

Estimation of  $D_T$  from Non-Carcinogenic Data Base

33. The following procedure may be used when mammalian bioassay data is not available for processing or when the criterion of paragraph 17c applies. A hypothetical acceptable daily dose, to be called  $D_{Tn}$ , is computed from the most preferred of the procedures presented in paragraphs 21-29.  $D_{Tn}$  is used to compute a carcinogenic  $D_T$  by the relation

$$D_T = D_{Tn} \times K_{tn} \times ARL \quad (12)$$

where  $K_{tn}$  is a factor which is tentatively valued at 417. Appendix B, paragraphs 20-21 discusses how  $K_{tn}$  is derived.

### PART III: ENVIRONMENTAL PATHWAY RELATIONS

#### INTRODUCTION

34. This section presents equations that have been developed in past reports<sup>2-4</sup> for expressing a SPPPLV in terms of  $D_T$ . Paragraphs 35-39 involve pathways for which soil and water SPPPLV relations have been proposed.<sup>1-3</sup> Paragraphs 40-44 involve soil-specific pathways which were first considered in a study of land use options at Alabama Army Ammunition Plant.<sup>4</sup> The equations presented in this part can be derived in a manner similar to that presented in Figure 1 and paragraph 10. Appendix C presents equations for SPPPLVs which are not so derivable, and these illustrate novel extensions of the approach to new situations.

#### SOIL AND WATER PATHWAYS

Ingestion of pollutant in a water supply (Pathway 1).

35. For water, the basic equation is

$$C_{w1} = ( BW / W_w ) \times D_T \quad (13)$$

For pollutant-containing soil through which water has leached:

$$C_{s1} = ( BW / W_w ) \times ( K_{sw} )^{-1} \times D_T \quad (14)$$

where  $C_{w1}$  and  $C_{s1}$  are the water and soil SPPPLVs, respectively.  $C_{w1}$  has units of mg pollutant/L and  $C_{s1}$  has units of mg pollutant/kg dry soil. BW is an adult human body weight in kg, and  $W_w$  is the daily consumption of fluids in L/day.  $K_{sw}$  is the partition coefficient between soil and water, expressed in mg pollutant/L water per mg pollutant/kg dry soil; see paragraphs 72-73.

Consumption of Fish (Pathway 2)

36. Equations 15 and 16 are applicable when the primary source of pollutant to the fish is assumed to be from dissolved pollutant in water. Ingestion of polluted sediment or lower food chain life forms with accumulated pollutant is not expected. For this pathway,

$$C_{w2} = ( BW / W_f ) \times ( K_{wf} )^{-1} \times D_T \quad (15)$$

For pollutant-containing soil through which the above water has leached,

$$C_{s2} = ( BW / W_f ) \times ( K_{sw} \times K_{wf} )^{-1} \times D_T \quad (16)$$

where  $C_{w2}$  and  $C_{s2}$  are SPPPLVs as before.  $W_f$  is the consumption of fish in kg/day.  $K_{wf}$  is the partition coefficient between water and fish, expressed in mg pollutant/kg fish per mg pollutant/L water (see paragraph 74). A pathway applicable to bottom-feeding fish, which may accumulate pollutant directly from sediment, is presented in Appendix C, paragraph 15.

#### Consumption of Crops Irrigated with Contaminated Water (Pathway 3)

37. Equation 17 would apply to situations where the main concern is with water contamination; how the contaminant is delivered to the irrigation water is not of interest. Thus, the equation is valid for agricultural variants such as pond culture or hydroponics. For this water,

$$C_{w3} = ( BW / W_p ) \times ( K_{wp} )^{-1} \times D_T \quad (17)$$

If soil is the initial contaminant source and of concern, Equation 18 applies.

$$C_{s3} = ( BW / W_p ) \times ( K_{sw} \times K_{wp} )^{-1} \times D_T \quad (18)$$

where  $C_{w3}$  and  $C_{s3}$  are SPPPLVs as before.  $W_p$  is the consumption of plant matter in kg/day. Plant weight is reckoned on a dry weight basis.  $K_{wp}$  is the partition coefficient between water and plant matter, expressed in mg pollutant/kg plant weight per mg pollutant/L water; see paragraph 80.

#### Consumption of Livestock Fed Irrigated Crops (Pathway 4)

38. The soil-water situation of pathway 3 is presumed to apply. For water,

$$C_{w4} = ( BW / W_a ) \times ( K_{wp} \times K_{pa} )^{-1} \times D_T \quad (19)$$

If this water has leached contaminated soil, and a soil PPLV is sought,

$$C_{s4} = ( BW / W_a ) \times ( K_{sw} \times K_{wp} \times K_{pa} )^{-1} \times D_T \quad (20)$$

where  $C_{w4}$  and  $C_{s4}$  are SPPPLVs as before, and  $W_a$  is the consumption of the meat of livestock in kg/day.  $K_{pa}$  is the partition coefficient between plant and animal in mg pollutant/kg animal weight per mg pollutant/kg plant; see paragraph 75.

#### Consumption of Livestock Drinking Contaminated Water (Pathway 5)

39. Equations 21 and 22 apply; for water,

$$C_{w5} = ( BW / W_a ) \times ( K_{wa} )^{-1} \times D_T \quad (21)$$

If this water has leached contaminated soil, and a soil PPLV is sought,

$$C_{s5} = ( BW / W_a ) \times ( K_{sw} \times K_{wa} )^{-1} \times D_T \quad (22)$$

where  $C_{w5}$  and  $C_{s5}$  are SPPPLVs as before, and  $K_{wa}$  is the partition coefficient between water and livestock in units of mg pollutant/kg animal per mg pollutant/L water; see paragraph 75.

## SOIL-SPECIFIC PATHWAYS

### Consumption of Vegetables (Pathway 6)

40. The soil SPPPLV for this pathway is

$$C_{s6} = ( BW / W_p ) \times ( K_{sp} )^{-1} \times D_T \quad (23)$$

where  $K_{sp}$  is the partition coefficient between soil and plant matter in units of mg pollutant/kg plant weight per mg pollutant/kg dry soil; see paragraphs 78-80.

### Consumption of Livestock (Pathway 7)

41. The soil SPPPLV for this pathway is

$$C_{s7} = ( BW / W_a ) \times ( K_{sp} \times K_{pa} )^{-1} \times D_T \quad (24)$$

This equation is applicable to situations where the animals are expected to be fed with harvested plant matter (grass, silage, or grain) or allowed to graze on such plant matter. In the second case, the contribution of pollutant from direct ingestion of soil is not included. If the user wishes to include this contribution, a pathway can be devised; see Appendix C, paragraph 12.

### Consumption of Dairy Products (Pathway 8)

42. The soil SPPPLV for this pathway is

$$C_{s8} = ( BW / W_d ) \times ( K_{sp} \times K_{pa} \times K_{ad} )^{-1} \times D_T \quad (25)$$

Here,  $W_d$  is the consumption of dairy products in L/day and  $K_{ad}$  is a partition coefficient between animal tissue and milk, and has units of mg pollutant/L milk per mg pollutant/kg animal weight; see paragraph 76.

### Ingestion of Soil (Pathway 9)

43. This pathway presumes that young children ingest soil, either incidentally in the course of outside play, or compulsively; see Appendix C, paragraph 5. The soil SPPPLV is

$$C_{s9} = ( BW_c / W_{sc} ) \times D_T \quad (26)$$

where  $BW_c$  is a child's weight in kg and  $W_{sc}$  is the kg/day of soil involved.

### Inhalation of Raised Dust (Pathway 10)

44. This pathway presumes that outdoor workers would inhale dust raised from material-moving equipment (fork-lifts, tractors, trucks, bulldozers, etc.), as may be anticipated during construction or other industrial activities. The dust that is inhaled during non-work hours is neglected. Weather conditions may prevent the raising of dust during a certain fraction of work-days. The pathway equation is

$$C_{s10} = [( BW \times 10^6 ) / ( C_{ss} \times RB' )] \times ( 1.6 / F_w ) \times D_T \quad (27)$$

$C_{ss}$  is the dust concentration in air (mg/m<sup>3</sup>) when dust occurs.  $RB'$  is the volumetric air intake of a worker in an 8-hour period. The factor 1.6 represents the working day portion of the year (365 calendar days/225 working days).  $F_w$  is the factor to account for weather conditions, see paragraph 64. The factor  $10^6$  converts mg of dust to kg of dust.

#### Inhalation of vapors (Pathway 11)

45. This pathway's formulation presupposes that workers are engaged in underground labor and there is no effective barrier between the workers and vapors emanating from contaminated soil. Moreover, ventilation is poor, so that an appreciable build-up of pollutant vapors in the breathing airspace could occur; see Appendix C, paragraph 8. The applicable equation is

$$C_{s11} = ( BW / RB' ) \times K_{sv}^{-1} \times D_T \quad (28)$$

where  $K_{sv}$  is a partition coefficient relating pollutant vapor content in air to that in soil; see paragraph 77.  $K_{sv}$  has units of mg pollutant/m<sup>3</sup> air per mg pollutant/kg soil.

### PART IV: REFERENCE DATA

46. This section presents information concerning variables that are not pollutant-related. Most of these variables are included in the  $IF_1$  factor; see paragraph 10. A representative value is presented for each variable along with a discussion of how it was obtained. For ease of reference, Table 7 lists the variables, representative values, and other paragraphs of the report that employ them.

47. The representative values are intended for "default" use in PPLV equations. Unusual situations may justify different valuations to these data. For example, persons in a hot, dry climate would drink more water than at the representative 1.6 L/day rate (paragraph 53). The target human group of concern may be children of a specific age, such as is encountered in Appendix E. The discussion presented in conjunction with each value will help in the selection of alternative values. The author suggests that, unless wide departures from default conditions are involved in pathway scenarios, the representative values should be used. The accuracy associated with  $D_T$  and  $K_i$  inputs is usually "order of magnitude" at best; extensive efforts to fine-tune  $IF_1$  inputs are usually not warranted. One may wish to consider "worst case" situations, but while this may be morally satisfying, it can lead to bias in PPLV results, especially when several scenarios are involved. Moreover, the pathway may turn out to be unimportant in the valuation of the PPLV; see paragraphs 88-91.

Table 7

Cross-Reference of Representative Values to Paragraphs in Report

Variable	Representative Value	Paragraphs in Which Used
B <sub>w</sub>	70 kg	24,35-42,44-45
BW <sub>c</sub>	12 kg	43
RB	17 m <sup>3</sup> per 8-hour day	44-45
W <sub>w</sub>	1.6 L/day	35
W <sub>f</sub>	0.02 kg/day	36
W <sub>a</sub>	0.21 kg/day	39,41
W <sub>p</sub>	0.07 kg/day	37,40
W <sub>d</sub>	0.46 L/day	42
W <sub>sc</sub>	10 <sup>-4</sup> kg/day	43
C <sub>ss</sub>	10 mg/m <sup>3</sup>	44
F <sub>w</sub>	0.67	44
F <sub>f</sub>	0.076	74
F <sub>a</sub>	0.3 (cattle)	75
	0.5 (swine)	75
	0.037 (cow's milk)	75

## SELECTED REFERENCE SOURCES

48. Relatively little time need be spent in literature searches if the required information has been compiled. Several such compilations that are references in subsequent sections are mentioned here. Their selection does not imply that they are the only documents with useful data, nor that their data are necessarily more "valid" than those from other sources.

a. Scientific Tables (STAB)<sup>35</sup> is issued periodically by Geigy Pharmaceuticals and has extensive information on human physiology and biochemistry.

b. Biology Data Book (BDB)<sup>36</sup> has several studies summarized with respect to human weight and age data for many geographical areas, as well as information about animal weight and food consumption.

c. Agricultural Statistics (AGST)<sup>37</sup> is an annual statistical abstract publication of the U.S. Department of Agriculture. AGST has data on every important commercial farm activity in this country, including crop acreage, yields, livestock production, food consumption patterns, forestry, and on major Departmental Programs.

d. Standard Values in Nutrition and Metabolism (SVNM)<sup>38</sup> is somewhat dated, but has extensive information on nutrient needs for several animal species, composition of foodstuffs of animal origin, average yields of plants for human or livestock consumption, and the composition of feeds for livestock and poultry.



e. The Report on the Task Group on Reference Man (RTRM)<sup>39</sup> was prepared for the International Commission on Radiological Protection. RTRM has specific recommendations for typical values for a wide range of anatomical and physiological attributes of man as well as supporting commentary and sources.

f. Composition of Foods (AH8),<sup>40</sup> collectively known as "Agriculture Handbook No. 8" is an ongoing compilation of information pertaining to the composition of most common foods. Several updates to the original handbook have been prepared for specific food categories, viz:

Dairy and Egg Products	8-1
Spices and Herbs	8-2
Baby Foods	8-3
Fats and Oils	8-4
Poultry Products	8-5
Soups, Sauces and Gravies	8-6
Sausages and Luncheon Meats	8-7

#### BODY WEIGHTS

##### Adult Body Weight ( BW )

49. The representative value is 70 kg. This value is widely used in criteria and standards,<sup>16,41</sup> and is probably accurate to the nearest 10 kg as a representative value of most common adult male groups. The results from several studies are presented in BDB<sup>36</sup> and RTRM;<sup>39</sup> representative weight tables as a function of height and age are presented in STAB<sup>35</sup> and RTRM.<sup>39</sup> Data are also provided for adult women. BDB<sup>36</sup> can be consulted if specific racial, age, or national differentiations are required.

##### Child Body Weight ( BW<sub>c</sub> )

50. The representative value is 12 kg for the two-year-old child. BDB,<sup>36</sup> STAB,<sup>35</sup> and RTRM<sup>39</sup> provide either experimentally determined or statistical representations of child weight data. For a two-year old, which is the approximate age of concern for soil-ingestion, 12 kg is, to the nearest kg, representative of most populations. STAB<sup>35</sup> provides tables for weight by age or sex, while BDB<sup>36</sup> provides further break-down by racial or national categories.

#### INHALATION DATA

##### Air Inhaled by Workers ( RB' )

51. The representative value is 17 m<sup>3</sup> per 8-hour workday. This volume was based on the product of inspired air per breath x the breathing rate. Volumes are given in STAB<sup>35</sup> and RTRM.<sup>39</sup> RB' depends upon the classification of the work. RTRM<sup>39</sup> gives three classifications with some examples:

- a. "light" - office work, laboratory work, most hospital work or housework
- b. "moderate" - intermediate between "light" and "heavy"
- c. "heavy" - commercial fishing, foundry work, face work in mines, postal delivery on foot.

The representative value is intermediate between the highest value for "light" work ( $14.9 \text{ m}^3$ ) and the lowest for "heavy" work ( $20.6 \text{ m}^3$ ).<sup>39</sup>

52. If breathing data are desired for non-work situations, a value of  $9.6 \text{ m}^3$  is a typical inhaled volume during 8 hours of non-occupational waking activity;  $3.6 \text{ m}^3$  for 8 hours of rest.<sup>39</sup> A 24 hour-day volume can be computed on the basis of a composite hypothetical week of 40 hours work, 56 hours sleep, and 72 hours of non-occupational activity. For  $\text{RB}' = 17 \text{ mg/m}^3$ , the daily inhalation volume would be  $28 \text{ m}^3$ . Other daily volumes can be readily computed for females and children from data in STAB<sup>35</sup> or RTRM.<sup>39</sup>

#### ORAL CONSUMPTION FACTORS

##### Daily Intake of Water ( $W_w$ )

53. The representative value is 1.6 L/day. This value was derived from information presented in RCRM<sup>39</sup> for adult man liquid intake with deduction of that portion supplied from milk. Other information pertaining to water intake is discussed elsewhere.<sup>41</sup> A 2 L/day intake has been incorporated into water quality criteria<sup>16</sup> and drinking water standards.<sup>41</sup> Based on a discussion of several studies,<sup>41</sup> an averaged liquid intake of 1.63 L/day was computed. Thus, the 2 L/day is somewhat safe-sided. The sources of liquid intake can vary widely between individuals. A considerable portion of liquid intake can be from water sources that may not be of pathway 1 concern, particularly bottled beverages. Intake levels are also a function of ambient temperature or the level of work activity. RCRM<sup>39</sup> provides daily water intake estimates for women (1.2 L/day) and for 10-year-old children (1.0 L/day).

##### Daily Consumption of Fish ( $W_f$ ) and Meat ( $W_a$ )

54. Representative values are 0.020 kg/day fish and 0.21 kg/day meat. These consumption values are presented together since nutritional literature often discusses the "meat, fish, and poultry" category without breakdown as to constituents. This is in recognition of the interconvertability of these foodstuffs in the diet. There is a wide variation in the consumption of each constituent, but probably less variation in the overall category consumption.

55.  $W_f$  was based on per capita annual statistics in AGST<sup>37\*</sup> and information presented in RCRM.<sup>39</sup> Consumption patterns vary widely. Cordle et al.<sup>42</sup> present illustrative population vs. level of consumption data; about

\* AGST per capita data is reported in pounds/year, which the author has converted to a nominal daily intake (1 pound/year =  $1.24 \times 10^{-3}$  kg/day).

75 million U.S. consumers are estimated to eat in excess of an estimated national average value of 18.7 g/day and 400,000 consumers eat in excess of 150 g/day. Generally, most consumed fish is from oceanic locales.<sup>42</sup> For example, the fish consumption value used in Water Quality Criteria<sup>16</sup> was only 6.5 g/day, based on fish sources from fresh and estuarine water areas. The representative value given above does not differentiate between fish from these different waters. If a fresh water source only is involved and consumption patterns are projected to be "usual," an intake of 0.005 kg/day would be appropriate.

56.  $W_a$  was based on per capita statistics in AGST.<sup>37</sup> This consumption value may be broken down into sub-components by specific animal sources. Cattle and pigs predominate; 1974 estimates are that 173.4 pounds of a 188 pounds per capita annual meat consumption are from these two sources.<sup>37</sup> Per capita consumption of beef and pork in AGST<sup>37</sup> correspond to 0.135 and 0.077 kg/day, respectively. Although no pathway has involved poultry consumption, a per capita consumption rate of 0.063 kg/day is provided for future consideration.<sup>37</sup>

57. The representative values may somewhat understate consumption levels of the adult man in terms of "meat, fish, and poultry." Representative values of these three foodstuffs would sum to 0.293 kg/day. Table 764 in AGST<sup>37</sup> presents a "meat, fish, and poultry" suggested consumption level of 5.73 lb/week (0.371 kg/day) in a hypothetical moderate-cost diet of a 20-54 year old male. If one needs to estimate meat, fish, or poultry intake for other human groups, data presented in this table<sup>37</sup> can be used to pro-rate the composite consumption level. For example, AGST<sup>37</sup> presents a suggested consumption level of 3.32 lb/week (0.216 kg/day) for 12 to 19-year-old females on a moderate-cost diet. The pro-rated meat consumption for this female could be estimated at  $(0.216/0.293) \times (0.21 \text{ kg/day})$  or 0.155 kg/day.

#### Daily Consumption of Plants ( $W_p$ )

58. The representative value is 0.070 kg/day, dry weight basis. Plants included here are usually considered as vegetables. Grain plants other than corn are not included, nor are melons, tree-borne fruits, and nuts. The literature is not consistent as to which plants are considered "vegetables" or "fruits," so cross-comparisons will reveal apparent disagreement among sources, typically of the order of  $\pm 20$  percent.

59. A representative value estimate involved selection of a diet and a dry-weight percentage to convert nominal plant weight to a dry-weight basis. The diet chosen was that of an 18-year-old male addressed by Kolybe et al.<sup>43</sup> For the food groups potatoes, leafy vegetables, legume vegetables, root vegetables, and garden fruits (tomatoes, cucumbers), the summed daily intake was 0.459 kg/day; see Table 3 in Kolybe et al.<sup>43</sup> Table 8 presents the data base involved to compute the dry-weight percentage estimate. Therein, daily intake values have been derived for heavily-consumed vegetable items based on data in Tables 263, 265, and 267 of AGST.<sup>37</sup> Corresponding to these items, dry-weight percentages have been taken from data presented in AH8.<sup>38</sup> A "weighted-average" basis was used to compute the dry-weight percentage 15.22 percent. The product  $0.1522 \times 0.459 \text{ kg/day}$  is the representative value above.

Table 8

Per Capita Daily Intakes and Dry Weight Contents of Selected Vegetables

Item	Per Capita Consumption, kg/day <sup>a</sup>	Dry Weight Percent <sup>b</sup>
Cabbage	0.013 (fresh produce and canned sauerkraut)	7.6
Carrots	0.011 (fresh, canned, frozen)	11.8
Celery	0.010 (fresh)	5.9
Corn	0.020 (fresh, canned, frozen)	27.3
Cucumber	0.014 (fresh and as pickles)	4.9
Lettuce	0.029 (includes escarole)	5.0 (averaged for several varieties)
Onions	0.011 (fresh only, includes shallots)	11.0 (excludes shallots)
Snap-beans	0.011 (fresh, canned, frozen)	9.9
Tomatoes	0.022 (fresh, canned, does not include items such as catsup or sauce)	6.5
White Potatoes	0.146	20.2
Totals	0.287	15.2 (computed weighted average)

a. Computed from AGST,<sup>37</sup> 1973 data.

b. Data from AH8,<sup>40</sup> raw useful plant matter basis.

Daily Consumption of Dairy Products (  $W_d$  )

60. The representative value is 0.46 L/day. This item of consumption (which includes milk and milk products such as cheese, butter, and ice cream) has been well-studied, and values are available in several references.<sup>37,39,43</sup> The representative value was derived from a suggested consumption of 3.38 quarts/week in Table 764 of AGST<sup>37</sup> for a moderate-cost diet for males aged 20 to 54 years. This reference may be consulted for values for women and different aged children. The proportion of liquid milk as a specific constituent of dairy products changes notably with age, as does the daily volume of dairy products. RTRM<sup>39</sup> can be consulted to provide milk intake data.

Daily Ingestion of Soil (  $W_{sc}$  )

61. A representative value is  $10^{-4}$  kg/day. Estimates of  $W_{sc}$  are highly speculative; a controlled study is virtually impossible to perform. The representative value was mentioned in a feature article in the Baltimore Sun<sup>44</sup> concerning lead exposures and is appropriate to incidental soil ingestion. If pica (the compulsive ingestion of non-food matter by young children) is to be considered, a value of  $5 \times 10^{-4}$  kg/day is suggested. This lies within the range of estimates provided in two references.<sup>44,45</sup>

## DUST FACTORS

### Dust Content in Air ( $C_{ss}$ )

62. The representative value is  $10 \text{ mg/m}^3$ . Few field or controlled studies have been done concerning this factor. Two of note are by Sutter<sup>46</sup> and by Nicholson and Cardinale.<sup>47</sup> Sutter was concerned with dust clouds from radioactive-contaminated soil handling operations. To simulate such operations, soil was delivered by a powder pump into a wind tunnel through which air was blown. Dust samples were collected in a plenum chamber 20 feet downwind of the point of application. At wind tunnel airspeeds of 3.2 to 20 miles/hour (5.1 to 32.2 km/hr), airborne soil concentrations of  $46\text{--}128 \text{ mg/m}^3$  were attained. These concentrations were in the range of dust levels found in the vicinity of previously-studied tractor operations in the field.<sup>47</sup> Nicholson and Cardinale were interested in dust levels experienced inside and outside of tanks and personnel carriers. In their study,<sup>47</sup> M60A1 tanks and M113A1 armored personnel carriers were deployed in simulated convoy or assault situations. Dust was collected on external samplers located at either the tank hatch height or the carrier deck height. Dust levels so measured ranged from 50 to  $220 \text{ mg/m}^3$ .

63. Certain factors would rule against a  $C_{ss}$  representative value of the order of  $100 \text{ mg/m}^3$ , which would be indicated from these studies.<sup>46,47</sup>

a. Not all dust would penetrate beyond the outer nasal passage by virtue of the dust particle size distribution.

b. Even with favorable weather conditions, equipment does not operate continuously.

c. If a  $100 \text{ mg/m}^3$  level of dust was attained for a sustained period of time, dust filters and eye protection would have to be employed. Moreover, Federal regulations limit dust levels to  $15 \text{ mg/m}^3$ <sup>315</sup> in the absence of such devices.

The author believes that the  $10 \text{ mg/m}^3$  is probably fairly representative of a time-weighted average dust concentration.

### Weather Condition Factor ( $F_w$ )

64. A representative value is 0.67. This value was derived from the number of days without measurable precipitation typical of many areas east of the Mississippi River (about 240 days/year). Some precipitation events involve either light rain or rain for a short time duration followed by rapid drying. Other events involve heavy rains or snows which can render the ground wet for several days after the precipitation has ended. These two factors tend to counterbalance each other.

## FAT CONTENTS OF FISH AND ANIMALS

65. For representative values, see paragraph 66. The fat content of fish,  $F_f$ , is used in conjunction with the estimation of  $K_{wf}$  discussed in paragraph 74. The fat content of animals,  $F_a$ , is used in conjunction with the estimation of  $K_{wa}$  or  $K_{pa}$  discussed in paragraph 75. Where livestock consumption is involved (pathways 4, 5, and 7),  $F_a$  values are representative of meat; where dairy ingestion is involved (pathway 8),  $F_a$  values are representative of milk.

66. Table 9 presents data for several animal species. Fish fat (or more properly lipids) content data are from AH8<sup>40</sup> quotations for raw, edible portions. A representative value of 0.076 is suggested, based on the pooled lipids content of several fish species; see paragraph 74. The milk fat content is a nationwide average value cited in AH8;<sup>40</sup> this reference can be consulted for contents in specific dairy items. County extension agents can be contacted to provide values for a given locale. As indicated in paragraph 75,  $F_a$  should be based upon overall animal weight composition. The representative value selected for beef is 0.30, which is the upper range reported for a "yield grade 3, low choice quality" animal.<sup>48</sup> Dressed carcass (the slaughtered animal less hide, head, feet, and viscera) weight data are available in AH8<sup>40</sup> for other quality beef, and 90 percent of the fat levels reported there can be used for  $F_a$ . \* Typical pork carcass fat levels range from 47 to 57 percent;<sup>40,49</sup>  $F_a = 0.5$  should suffice for most calculations. AH8<sup>40</sup> can also be consulted for information on fat contents in several alternative meat or poultry selections.

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\* The fat content in the dressed carcass is somewhat higher than that in removed parts.

Table 9

Fat Content in Fish, Animal, and Dairy<sup>a</sup>

Type	Fraction fat
Bass, freshwater	0.026-0.027
Carp	0.042
Soft clams, meat and liquid	0.010
Drum, freshwater	0.052
Crayfish	0.005
Catfish, freshwater	0.031
Oyster	0.018
Crabs (steamed)	0.015
Trout, brook	0.021
Trout, rainbow or steelhead	0.114
Lake trout	0.100
Lake herring (cisco)	0.023
Beef	0.3
Pork	0.5
Milk from cow	0.037
Venison	0.06

a. See text for reference citations and bases for estimates.

**PART V: PARTITION COEFFICIENT ESTIMATION TECHNIQUES****ANCILLARY PHYSICAL PROPERTIES**

67. Literature that directly provides PPLV partition coefficients is seldom encountered. Fortunately, procedures for estimating these constants from other physicochemical properties have been developed; see Appendix D, paragraph 5. The estimations presented in this part are generally restricted to organic compounds. Moreover, the following need to be assumed:

a. The pollutant is conserved in all compartments between the environmental source and man. There are no chemical reactions or metabolic processes to either create or destroy it.

b. Pollutant in soil is only found physically adsorbed on soil organic carbon ( SOC ).

c. Pollutant in water is dissolved.

d. Pollutant in fish is associated with lipids; that in terrestrial animals, with fat.

The physical properties discussed below are temperature-dependent; 25°C (298.2°K) is commonly chosen as the ambient environmental temperature of interest; this convention is followed here.

#### Octanol - Water Partition Coefficient ( $K_{ow}$ )

68.  $K_{ow}$  is the equilibrium ratio between the concentration of a compound in n-octanol and its concentration in water.  $K_{ow}$  is considered a key parameter from which to estimate other desired properties. Values of  $K_{ow}$  range from about 0.1 to 10,000,000; hence  $\log K_{ow}$  is often used in mathematical relations. Hansch and Leo provide an extensive listing of measured  $\log K_{ow}$  values.<sup>50</sup> They have also pioneered a methodology to estimate  $\log K_{ow}$  from compound structure. This methodology and other procedures are presented in Chapter 1 of the recently-published "Handbook of Chemical Property Estimation Methods" (CPEM).<sup>51</sup>

#### Compound Solubility in Water ( $C_{sol}$ )

69.  $C_{sol}$  is nominally the maximum concentration of dissolved compound in water that can be attained at equilibrium with the compound in its "normal state." In this report,  $C_{sol}$  has units of mg/L. Solubility information on many compounds can be found in standard chemical handbooks. DTLV<sup>13</sup> presents solubility information for reported compounds, while individual water quality criteria reports provide  $C_{sol}$  for "priority pollutants." In lieu of published data,  $C_{sol}$  can be estimated from  $\log K_{ow}$ ; see Chapter 2 of CPEM.<sup>51</sup>

#### Saturation Vapor Density ( $VD_o$ )

70.  $VD_o$  is strictly the maximum density of a compound in the vapor phase that can be attained at equilibrium with the compound in its "normal" state. The documents mentioned in paragraph 69 can be consulted for information on either the normal boiling temperature (the temperature at which the partial pressure of the compound in the vapor phase is 760 mm Hg [ $10^5$  Pa]) or some reduced boiling temperature with vapor pressure specified. In either case, the saturation vapor pressure at 25°C (  $P_o$  ) has to be estimated; procedures to do this are presented in Chapter 14 of CPEM.<sup>51</sup>  $VD_o$  is easily computed from  $P_o$  based on ideal gas law considerations. If  $P_o$  is in mm Hg (the usual reporting unit), for  $VD_o$  in  $\text{mg/m}^3$ ,

$$VD_o = 1.64 \times 10^4 \times P_o \times MW / T$$

where MW is the compound molecular weight and T is the temperature in °K.

#### Soil Organic Carbon Adsorption Coefficient ( $K_{oc}$ )

71. This is the ratio of the concentration of a compound physically adsorbed on soil organic carbon (SOC) to that in aqueous solution at equilibrium; see Appendix D, paragraph 1.  $K_{oc}$  relates to the leaching of a pollutant by water, which in many of the pathways is the first inter-compartmental transfer.  $K_{oc}$  can be used as an estimator of  $K_{gw}$  in lieu of data or better estimators. Other than for a few specific pesticide compounds, few measurements of  $K_{oc}$  have been reported. Estimation equations are provided in Chapter 4 of CPEM,<sup>51</sup> two of which are:



$$K_{oc} = \text{antilog} ( -0.55 \times \log C_{sol} + 3.64 )$$

$$K_{oc} = \text{antilog} ( 0.544 \times \log K_{ow} + 1.38 ) \quad (29)$$

#### PARTITION COEFFICIENT EVALUATION PROCEDURES

$K_{sw}$

72. As a first approximation,  $K_{sw}$  is inversely proportional to  $K_{oc}$  :

$$K_{sw} = ( F_{oc} \times K_{oc} )^{-1} \quad (30)$$

where  $F_{oc}$  is the soil fraction of SOC. In such case, an estimate of SOC is required. Some published assays may report the soil organic matter fraction instead;  $F_{oc}$  is approximately 0.58 times this fraction.<sup>51</sup> Table 10 includes some soil organic matter assays for different locales in the United States.

73. Soil adsorption isotherms are typically used to estimate  $K_{sw}$  or  $K_{oc}$  ; the Environmental Protection Agency has provided a suggested procedure.<sup>54</sup> The Freundlich isotherm often fits experimental data satisfactorily:

$$C_{se} = k_f \times C_{we}^{( 1 / n_f )}$$

where  $C_{se}$  and  $C_{we}$  represent the equilibrium concentrations of the compound in soil and water. The parameters  $k_f$  and  $n_f$  are determined from statistical or graphical analysis of experimental results. From the definition of  $K_{sw}$ , if  $n_f = 1$ ,  $K_{sw} = 1 / k_f$ . If not, within the limits of isotherm applicability,  $K_{sw}$  can be determined from experimental data for any specified  $C_{se}$  or  $C_{we}$ . Chapter 4 of CPEM<sup>51</sup> discusses this determination in detail, and Appendix D, paragraph 11 discusses its consequences relative to PPLV computations. Ideally, the soil assayed should be representative of the study area. This has two advantages:

a.  $K_{sw}$  is directly determined.

b.  $K_{oc}$  can be estimated from  $K_{sw}$  and subsequently can be used to provide estimates of  $K_{sw}$  in other soils.

$K_{wf}$

74.  $K_{wf}$  is similar in meaning and significance to the fish bioconcentration factor (BCF). A BCF is the ratio of the pollutant concentration in fish to that in the water in which the fish resides. BCFs have been experimentally obtained for many substances; those for "priority pollutants" are included in the specific water quality criteria documents. In lieu of experimental observation, an estimate of BCF can be derived from physicochemical properties. The following is one such equation that has been devised for such use:<sup>51</sup>

$$K_{wf} \approx BCF = \text{antilog} ( 0.76 \times \log K_{ow} - 0.23 ) \quad (31)$$

Table 10

Selected Soil Organic Matter Assays

Soil	Location	Percent Organic Matter	Reference
Powell silt loam	Lower Columbia River Basin (OR, WA)	3.8	52
Fort Collins loam	Colorado Great Plains	1.4	52
Pachappa fine sandy loam	Southern California	0.6	52
Miami silt loam	Glaciated areas of Ohio, Indiana	2.4	52
Brookston silty clay loam	Glaciated areas of Ohio, Indiana	5.4	52
Davidson clay loam	Southeast Piedmont (GA to VA)	3.6	52
Dunbar fine sandy loam	North Carolina coastal plain	2.2	52
Carroll Island soil (silty loam)	Chesapeake Bay, MD	0.73	52
Adirondack spodosol	Blue Mountain, NY	35	53
Lima-Honeoye silt	Aurora, NY (Lake Cayuga)	5.5	53
Crider	Gallatin County, IL	1.74	54
Maile	Tallamook County, OR	5.3	54
Walla Walla	Salt Lake County, UT	2.99	54
Sharpsburg	Tama County, IA	2.35	54
Bladen	Liberty County, GA	2.2	54
Malbis	Johnston County, NC	0.89	54
Houston Black	Collin County, TX	1.05	54

Other equations are presented in CPEM<sup>51</sup> for predictions from  $C_{sol}$  or  $K_{oc}$ . Equation 31 is specific for fish with a lipids content of about 7.6 percent.<sup>16,51</sup> If this equation is used for a situation where  $F_f$  is markedly different from 7.6 percent, a pro-rata adjustment should be included.\* For example, Equation 15 can be rewritten in terms of BCF :

$$C_{w2} = ( BW / W_f ) \times ( BCF \times F_f / 0.076 )^{-1} \times D_T \quad (32)$$

$K_{pa}$  and  $K_{wa}$

75.  $K_{pa}$  and  $K_{wa}$  may be estimated for equations derived by Kenaga<sup>55</sup> from feeding studies of cattle and swine. Presented equations<sup>55</sup> were in terms of an animal bioaccumulation factor, or the parts per million (ppm) of pollutant in animal fat per ppm of pollutant in the diet. Unlike the BCF above, this factor was "normalized" to a unit fat level base. Taking this into account, if the predictor variable is  $K_{ow}$ ,

$$K_{wa} \approx K_{pa} \approx F_a \times \text{antilog} (-3.457 + 0.500 \log K_{ow}) \quad (33)$$

If the predictor variable is  $C_{sol}$ ,

$$K_{wa} \approx K_{pa} \approx F_a \times \text{antilog} (-1.476 - 0.495 \log C_{sol}) \quad (34)$$

In Equations 33 and 34,  $K_{wa} \sim K_{pa}$  is implicitly assumed; livestock is expected to process pollutant from water in the same manner as pollutant from plant matter.

$K_{ad}$

76.  $K_{ad}$  is included to account for differences between a pollutant's concentration in milk as compared to other animal matter. To date, one numerical value of  $K_{ad}$  has been obtained, 1.44 for Arochlor 1254 in cow butterfat as compared with that in adipose tissue (Fries et al.).<sup>56</sup> In lieu of specific information,  $K_{ad}$  is recommended to be set as unity in Equation 25, i.e.

$$C_{s8} = ( BW / W_d ) \times ( K_{sp} \times K_{pa} )^{-1} \times D_T$$

$K_{pa}$  is determined from either Equation 33 or 34, and in these equations,  $F_a$  refers to the milk fat fraction.

$K_{sv}$

77.  $K_{sv}$  can be estimated by the following equation

$$K_{sv} = VD_o \times K_{sw} / C_{sol} \quad (35)$$

\* This conclusion is based on Equations 5-6 in CPEM,<sup>51</sup> which was used to estimate BCF for use in water quality criteria.<sup>16</sup> In these criteria,  $F_f = 0.03$ , and Equations 5-6 was pro-rated in the manner shown here. Equation 31 here and Equations 5-6 in CPEM<sup>51</sup> involved the same fish species (fathead minnows, bluegill sunfish, rainbow trout, and mosquito fish).

$VD_o$  and  $C_{sol}$  have units of  $mg/m^3$  air and  $mg/L$  water, respectively. Appendix D, paragraph 2 discusses the details and limitations of Equation 35.

$K_{sp}$  and  $K_{wp}$

78. At present, procedures to predict these coefficients are not well developed. Table 11 is a listing of default plant bioconcentration factors (PBF) that are suggested for general classes of organic compounds. These PBF values indicate a pollutant's concentration in plant matter (in terms of fresh or harvested plant weight in the Table) relative to that in the soil. To convert PBF to  $K_{sp}$ , adjustment for water content is required; data in Table 8 can be used for this purpose. In lieu of specific water content data,

$$K_{sp} \approx 6 \times PBF \quad (36)$$

79. Table 11 was condensed from a critical review by Dr. W. Dickinson Burrows of selected literature concerning the uptake of chemicals from the soil by plants. This review appears in Appendix E. Several presumptions were made in devising Table 11:

- a. Only whole plant studies were included.
- b. For each category of plant portion, the appropriate crop was given priority. For example, root crops of choice are carrots, sugar beets, etc. In the absence of information on a particular root crop, data for the root of some other plant was used. In the absence of information on a useful forage crop, any leafy matter reported was considered potential forage.
- c. Numbers were rounded off to a single digit.
- d. If PBF data were available for several compounds that fit in a chemical category, the largest PBF was used.

The PBFs listed in Table 11 are considered "worst case" in that given a choice of possible results with different plant/compound system data, the highest value was used.

80. Neither  $K_{wp}$  or  $K_{sp}$  values have been systematically collated. If  $K_{wp}$  is required, and no experimental information (i.e., hydroponic studies) are available, a suggested default value would be  $K_{sp} / K_{sw}$ . Conversely, if  $K_{sp}$  can be estimated on the basis of experimental information, but  $K_{sp}$  is required, a suggested default value would be  $K_{sw} \times K_{sp}$ . Both default procedures presume that

$$K_{sp} = K_{sw} \times K_{wp}$$

which may not necessarily reflect the actual mechanism of transfer of a pollutant in soil to the plant (see Equations 18 and 20 for applicable situations).

Table 11

Summary Values for Plant Bioconcentration Factors, Wet Weight Basis

Chemical Category	Crop Portion	PBF	Basis
High molecular weight polychlorinated hydrocarbons and simple derivatives: dieldrin, aldrin, PCB, DDT	Root	2	DDT, carrot
	Seed <sup>a</sup>	0.2	Endrin, soybean
	Fruit	0.1	Dieldrin/aldrin mix, pumpkin
	Leaf	0.3	Dieldrin/aldrin mix, kale
	Forage	3	Heptachlor, bromegrass
Moderately basic compounds, i.e., amines, anilines, urea	Root	1	Pyrazon, sugarbeet
	Leaf	8	Linuron, soybean
	Forage	8	Linuron, soybean
Non-ionic, moderately to highly water soluble compounds	Root	2	DIMP, <sup>b</sup> radish
	Seed <sup>a</sup>	4	Aldicarb, cotton
	Fruit	2	DIMP, tomato
	Leaf	5	DIMP, several plants
	Forage	5	DIMP, several plants
Non-ionic, sparingly water soluble	Root	3	Chlorphenvinphos, carrot
	Forage	2	BPMC, <sup>c</sup> rice
Acidic compounds, neutral pH	Root	8	2,4-D, barley
	Leaf	2	Trichloroacetic acid, wheat
	Forage	2	Trichloroacetic acid, wheat

a. Peanuts should not be considered as seeds.

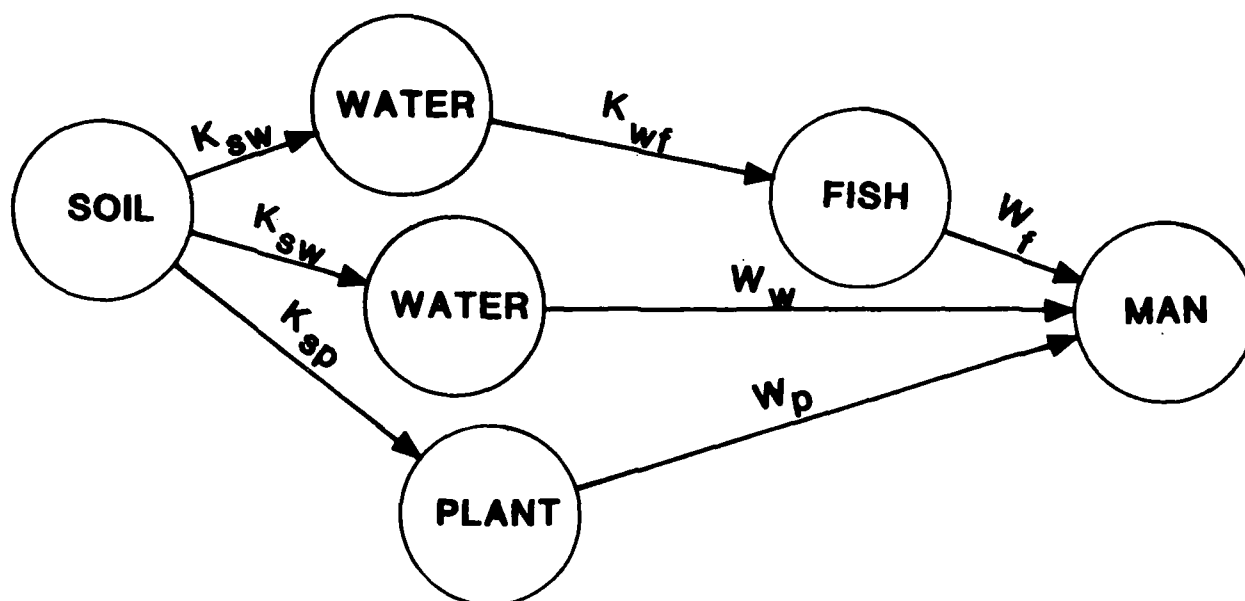
b. Diisopropyl ester of methylphosphonic acid.

c. O-sec-butylphenyl ester of methylcarbamic acid.

**PART VI: SPPPLV EQUATION REVIEW AND ADJUSTMENTS****EXTERNAL RESTRICTIONS**

81. The PPLV approach presented so far is primarily concerned with the avoidance of unacceptable long-term human health effects. The estimate of an acceptable pollutant dosage is  $D_T$  (see Part II). Relationships of the form of Equation 1 or 2 link  $D_T$  to respective SPPPLVs. Equation 4 is then used to compute a PPLV for a given scenario.

82. This may not necessarily complete the analysis. Consider Figure 2, which shows a scenario where pathways 1, 2, and 6 are involved and a soil PPLV is to be computed. Corresponding to  $C_{gf}$ , concentrations in the intermediate compartments (water, fish, and plant matter) can be computed:



Restriction and Example	Total Intake by Man	Concentrations in Compartments			
		Soil	Water	Fish	Plant
None	$BW \times D_T$	$C_{sf}$	$C_{wf}$	$C_{ff}$	$C_{pf}$
Type 1, $C_{wt} < C_{wf}^*$	Less than $BW \times D_T$	$C_{wt} / K_{sw}$	$C_{wt}$	$C_{wt} \times K_{wf}$	$C_{wt} \times K_{sp} / K_{sw}$
Type 2, $C_{sol} < C_{wf}$	$BW \times D_T$	$\left[ \frac{BW \times D_{Tr}}{W_p \times K_{sp}} \right]^{**}$	$C_{sol}$	$C_{sol} \times K_{wf}$	$\frac{BW \times D_{Tr}}{W_p}$

\*  $C_{wt}$  indicates concentration in water at which adverse fish effects may occur.

\*\*  $D_{Tr} = D_T - D_{Tl}$ , where  
 $D_{Tl} = (W_w \times C_{sol} + W_f \times C_{sol} \times K_{wf}) / BW$

Figure 2. Hypothetical scenario exposure pathways illustrating "Type 1" and "Type 2" restrictions.

$$C_{wf} = C_{sf} \times K_{sw} \quad (37)$$

$$C_{ff} = C_{sf} \times K_{sw} \times K_{wf} \quad (38)$$

or

$$C_{ff} = C_{wf} \times K_{wf} \quad (39)$$

$$C_{pf} = C_{sf} \times K_{sp} \quad (40)$$

Moreover, the following relation (based on Equation 6) is applicable

$$BW \times D_T = C_{wf} \times W_w + C_{ff} \times W_f + C_{pf} \times W_p \quad (41)$$

External restrictions may preclude the validity of these relations. For example, suppose that at  $C_{wf}$ , fish cannot survive, or if they do, they are inedible. From Equation 37,  $C_{sf}$  would have to be adjusted downwards. However, from Equations 38 and 40, this impacts on all other concentrations. This situation, where considerations other than human toxicity restrict the concentration to an intermediate component in a pathway, is called a "type 1" restriction.

83. A more complicated situation arises if the restriction is instead that  $C_{wf}$  exceeds  $C_{sol}$ . If this occurs,  $K_{sw}$  is not a valid partition coefficient; see Appendix D, paragraph 1. Equations 37 and 38 are invalid, but Equation 39 is still valid. If  $C_w = C_{sol}$ ,

$$BW \times D_T > W_w \times C_{sol} + W_f \times C_{sol} \times K_{wf} + W_p \times C_{pf}$$

Since pathway 6 does not include water, Equation 40 is still valid; the above inequality can be resolved by use of a higher  $C_{pf}$ , which in turn, leads to a higher  $C_{sf}$ . This type of restriction is called a "type 2" restriction and leads to an upwards adjustment in the PPLV. Note that the "type 2" restriction exists here only because pathway 6 is not dependent upon the value of  $C_{sol}$  relative to  $C_{sf}$ . Had this pathway not been included, the restriction due to  $C_{sol} < C_{wf}$  would have been a "type 1" restriction.

#### "TYPE 1" AND "TYPE 2" ADJUSTMENT PROCEDURES

84. The previous paragraphs can be expanded upon to provide a general approach to PPLV adjustment due to "type 1" and "type 2" restrictions. The procedure will differ depending upon whether a soil or water PPLV is to be determined; see Table 12.

- a. Draw the applicable pathway diagram for each PPLV situation similar to that in Figure 2.
- b. Write down the applicable analogs of Equations 37 to Equation 41.
- c. Consult Table 12, which summarizes specific restrictions identified to date and pathway equations involved in adjustments.

Table 12

Processing Instructions for Restrictions

Restriction	Instruction
Fish Toxicity (pathway 1)	This is a "type 1" restriction
Organoleptic effects in water (pathways 1 and 2)	This is a "type 1" restriction
Water solubility (pathways 1-5)	<p>If a water PPLV is to be computed (from Part III, one or more of the following pathway equations apply: 13, 15, 17, 19, 21), treat as a "type 1" restriction.</p> <p>If a soil PPLV is to be computed (the equations cited above must not be involved), treat as a "type 2" restriction. Compute <math>D_{TL}</math> based on pathway Equations 14, 16, 18, 20, or 22 (whichever are in the PPLV scenario). If pathway 11 is involved, <math>W_{11} \times C_{11} = RB' \times VDo</math>. Adjust other applicable pathway equations using <math>D_{Tr}</math>.</p>
$C_p$ is a constant (pathways 6-8)	<p>Pathway Equations 13, 15, 17, 19, and 21 must not be involved. Compute <math>D_{TL}</math> based on pathway Equations 23, 24 and 25 (whichever are in the PPLV scenario). Adjust other applicable pathway equations using <math>D_{Tr}</math> in lieu of <math>D_T</math>.</p>

d. If a "type 1" restriction is involved, recompute the value of the PPLV based on the restriction and appropriate partition coefficients. Figure 2 presents the sample problem adjustments applicable to pathways 1, 2, and 6, where the restriction is  $C_{wt} < C_{wf}$  ( $C_{wt}$  indicates pollutant concentration in water at which adverse fish effects occur).

e. If a "type 2" restriction is involved, the restricted pathways are addressed first. The format of the partition coefficients assists here; a pathway will be restricted if it includes a partition coefficient with a subscript representing the restricted compartment. For each such pathway, the concentration of pollutant in the compartment ultimately consumed by man is computed by consideration of equations analogous to 37-40. A partial dose for these pathways,  $D_{TL}$ , is computed

$$D_{TL} = (1/BW) \times \sum (W_i \times C_{iL}) \quad (42)$$



where  $W_i$  represents the human-consumed matter from pathway "i" (for example, if  $i=1$ ,  $W_i = W_w$ ).  $C_{i2}$  represents the adjusted concentration of pollutant in the consumed matter. In Figure 2,  $D_{T2}$  is computed in the footnote.\* For other pathways, a reduced  $D_T$ ,  $D_{Tr}$ , where

$$D_{Tr} = D_T - D_{T2} \quad (43)$$

is used to compute other SPPPLVs. Only these SPPPLVs (i.e., determined on the basis of  $D_{Tr}$ ) are used in the computation of the PPLV. Then,  $D_{Tr}$  is used to compute  $C_{s6}$  (the only difference between the soil concentration shown in Figure 2 and Equation 23 is the substitution of  $D_{Tr}$  for  $D_T$ ). Here, pathway 6 is the only restricted pathway, thus  $C_{s6}$  is the PPLV.

#### COMMENTS ON EXTERNAL RESTRICTIONS

85. The discussion of toxicity restrictions is limited here to fish, although other intermediate receptors (terrestrial animals, plants) could merit such a restriction. From a practical viewpoint, if toxicity data for a pollutant are to be found for non-human receptors, the data will be for fish. Consolidated data sources that may be consulted for fish toxicity data include the summarized Water Quality Criteria;<sup>16</sup> the somewhat dated California Water Quality Criteria;<sup>57</sup> the "CHRIS List"<sup>58</sup> and articles in the Journal of the Water Pollution Control Federation Annual Literature Review Issues (usually issued in June, of which the most recent is cited<sup>59</sup>). The most commonly reported indicator of fish toxicity is the 96-LC50, an estimated pollutant concentration that will cause a 50 percent mortality to a given fish species after 96 hours exposure.  $C_{wt}$  may be approximated as  $[(96-LC50) / 100]$ .

#### Organoleptic Effects

86. Type 1 restrictions are anticipated with pollutants that are organoleptic substances in water. Phenol and monochlorophenols are classic compounds. They impart such a disagreeable taste, color, or odor to water at some concentration that people are unable or reluctant to consume the water. Table A1 should serve as a "screen" to identify such substances. Substances not on these tables may be assumed not to be organoleptic. Table A1 includes "priority pollutants"<sup>16</sup> and substances that have been assigned maximum permissible water concentrations by the Ministry of Health of the USSR.<sup>60</sup> The values presented in this table should be considered suggestive. Humans can vary widely in response and preference to a substance at a given concentration. The organoleptic designation at a given concentration is often based on subjective judgement. Fish in organoleptic pollutant-contaminated water may not necessarily be inedible. The author suggests that in lieu of information about the transfer of an organoleptic pollutant from water to fish (pathway 2), an organoleptic pollutant in water should be considered capable of tainting fish at the same concentration at which it is capable of rendering water unpotable.

\* For the example in Figure 2,  $D_{T2}$  is expressed in the format of Equation 42.  $W_w \times C_{s01}$  represents the limited pollutant uptake in drinking water;  $W_f \times C_{s01} \times K_{wf}$ , that in ingested fish.

$C_p$  not related to  $C_s$

87. Lead contamination at AAAP<sup>4</sup> was the first situation for which this restriction was found. Here, the relation  $C_{pf} = C_{pi} = (\text{a constant})$  was involved. Lead provides an interesting problem; it is an ubiquitous substance. Even in the absence of higher-than-background pollution, some uptake of lead is expected to occur. However, once this ambient component is accounted for, a PPLV can be computed. Appendix F details how PPLVs for lead at AAAP were determined. In the procedure used, a "type 2" restriction existed with respect to the lead transferred via plant uptake by farm animals. The procedure also illustrates pathway formulations that involve more in-depth consideration of livestock than presented in Part III.

#### NUMERICAL COMPARISON OF SPPPLV EQUATIONS

88. Equation 4, namely

$$C_{sf} = 1 / \sum (1/C_{si}) \quad (4)$$

indicates that a PPLV will be lower than any of its component SPPPLVs.  $C_{si}$  is proportional to  $D_T$ ,

$$C_{si} = R_i \times D_T \quad (5)$$

Examination of Equation 5 shows that the SPPPLV with the lowest  $R_i$  is most important in determining the magnitude of the PPLV. Preliminary evaluation of  $R_i$  may allow a researcher to anticipate which pathways can be neglected; the value of  $R_i$  for such pathways would have to be relatively large compared to the pathway with minimum  $R_i$ . Presented here is an approach to  $R_i$  evaluation that may be useful in certain cases in reducing research efforts (see Part VII). It also demonstrates the magnitudes of  $R_i$  which can be encountered.

89. Several assumptions are involved:

a. Representative values from Table 7 apply. For convenience, they are:  $BW = 70$  kg;  $W_w = 1.6$  L/day;  $W_f = 0.02$  kg/day;  $W_p = 0.07$  kg/day;  $W_a = 0.21$  kg/day;  $W_d = 0.46$  L/day;  $BW_c = 12$  kg;  $W_{sc} = 10^{-4}$  kg/day;  $RB' = 17$  m<sup>3</sup>/day;  $C_{ss} = 10$  kg/m<sup>3</sup>;  $F_w = 0.67$ ;  $F_f = 0.076$ ; for meat consumption  $F_a = 0.5$  (pork is assumed as the sole source of meat consumed). For the fat content of a dairy cow,  $F_a = 0.3$ ; for cow's milk,  $F_a = 0.037$ .

b. Estimation equations presented in Part V are very accurate. Then, if  $K_{ij}$  and  $K_{jk}$  are two partition coefficients in a pathway equation, and  $K_{ij} = a \times K_{ow}^b$  and  $K_{jk} = c \times K_{ow}^d$ , then  $K_{ik} = K_{ij} \times K_{jk} = (a \times c) \times K_{ow}^{(b+d)}$ .

c. Equation 29 is used to estimate  $K_{oc}$ , which can be alternately written as

$$K_{oc} = 24 \times K_{ow}^{0.544} \quad (44)$$

$F_{oc}$  is assumed to be 0.02. From Equations 30 and 44,

$$K_{sw}^{-1} = 0.48 \times K_{ow}^{0.544} \quad (45)$$

Reciprocal format is convenient in view of the format of Equation 2.

d.  $K_{wf}$  is estimated from Equation 31, or

$$K_{wf}^{-1} = 1.7 \times K_{ow}^{-0.76}$$

e.  $K_{wp}$  and  $K_{sp}$  are each assumed to be equal to 50. This would represent, based on Table 11 and Equation 36, a rather adverse situation.

f. Equation 33 is used to estimate  $K_{pa}$  or  $K_{wa}$ . With pork as the meat consumed by humans,  $F_a = 0.5$  and

$$K_{pa}^{-1} \text{ or } K_{wa}^{-1} = 5.7 \times 10^3 \times K_{ow}^{-0.500}$$

g.  $K_{ad} = 1.44$ ; see paragraph 76. Then the reciprocal of the product  $K_{pa} \times K_{ad}$  is

$$(K_{pa} \times K_{ad})^{-1} = 6.6 \times 10^3 \times K_{ow}^{-0.500}$$

h. In Equation 35,  $VD_o$ , a property independent of  $K_{ow}$ , is involved. Thus,  $R_{11}$  will depend upon the value of  $VD_o$ . For demonstration purposes,  $VD_o = 10^3 \text{ mg/m}^3$ , a moderately non-volatile level.  $C_{sol}$  can be estimated from  $K_{ow}$ ; one such correlation<sup>51</sup> is

$$C_{sol} = 1.53 \times 10^4 \times K_{ow}^{-0.922} \quad (46)$$

If Equations 45 and 46 are used to evaluate  $C_{sol}$  and  $K_{sw}$ , Equation 35 becomes

$$K_{sv}^{-1} = (3.2 \times 10^4 / VD_o) \times K_{ow}^{-0.378}$$

and for  $VD_o = 10^3 \text{ mg/m}^3$ ,

$$K_{sv}^{-1} = 32 \times K_{ow}^{-0.378}$$

90. Table 13 lists  $R_i$  relations applicable to pathways presented in Part III. Note that  $R_i$  is either a function of  $K_{ow}$  or a constant. Figures 3 and 4 illustrate these functions; they are linear on the log-log scale. These figures can be used to assess  $R_i$  for a pollutant as follows:

a. Compute  $\log K_{ow}$  for the pollutant.

b. For the appropriate pathways, read  $R_i$  from Figure 3 or Figure 4.

c. Call the minimum  $R_i$  of the pathway set  $R_{1i}$ . Consider neglecting any pathway for which  $R_i / R_{1i} > 100$ . In terms of the figures,  $R_{1i}$  should be 2 log-units lower than any neglected  $R_i$ . This suggested limit is based on the expected reliability of the  $R_i$ , which is probably at best at an order of magnitude level.

Table 13

R<sub>1</sub> Relationships for Order of Magnitude Comparisons

Pathway	R <sub>1</sub> as function of K <sub>ow</sub> <sup>a</sup>	
	Water	Soil
1 (drinking water)	44	21 x K <sub>ow</sub> <sup>0.544</sup>
2 (fish consumption)	6x10 <sup>3</sup> x K <sub>ow</sub> <sup>-0.766</sup>	2.9x10 <sup>3</sup> x K <sub>ow</sub> <sup>-0.222</sup>
3 (irrigated vegetables)	20	9.6 x K <sub>ow</sub> <sup>0.544</sup>
4 (meat from animals fed irrigated feed crops)	3.8x10 <sup>4</sup> x K <sub>ow</sub> <sup>-0.500</sup>	1.8x10 <sup>4</sup> x K <sub>ow</sub> <sup>0.044</sup>
5 (meat from animals drinking water)	7.6x10 <sup>5</sup> x K <sub>ow</sub> <sup>-0.500</sup>	3.7x10 <sup>5</sup> x K <sub>ow</sub> <sup>0.044</sup>
6 (vegetables)	N/A	20
7 (meat from animals fed feed crops)	N/A	3.8x10 <sup>4</sup> x K <sub>ow</sub> <sup>-0.500</sup>
8 (dairy products from animals fed feed crops)	N/A	2.0x10 <sup>5</sup> x K <sub>ow</sub> <sup>-0.500</sup>
9 (direct soil ingestion)	N/A	1.2x10 <sup>5</sup>
10 (workers inhale dust)	N/A	1.0x10 <sup>6</sup>
11 (vapor inhalation VD <sub>0</sub> = 1,000 mg/m <sup>3</sup> )	N/A	32 x K <sub>ow</sub> <sup>-0.378</sup>

a. See paragraph 89 and Table 7 for assumptions and quantitative data.

91. Users should be aware that these figures are specific for the equations, values, and assumptions of paragraph 89. If a different set of equations and input values (particularly VD<sub>0</sub>) are used, the result may differ, but the procedure to generate the figures does not. Thus, it may be misleading to conclude too much from these figures. Three conclusions worthy of note are:

a. Dust inhalation (pathway 10) is not expected to be a pathway of great concern relative to others.

b. The pathways involved with human consumption of vegetables (pathways 3 and 6) appear to be relatively important. Admittedly, an adverse case has been used. However, this situation does suggest that methods to refine K<sub>sp</sub> and K<sub>wp</sub> estimations are needed.

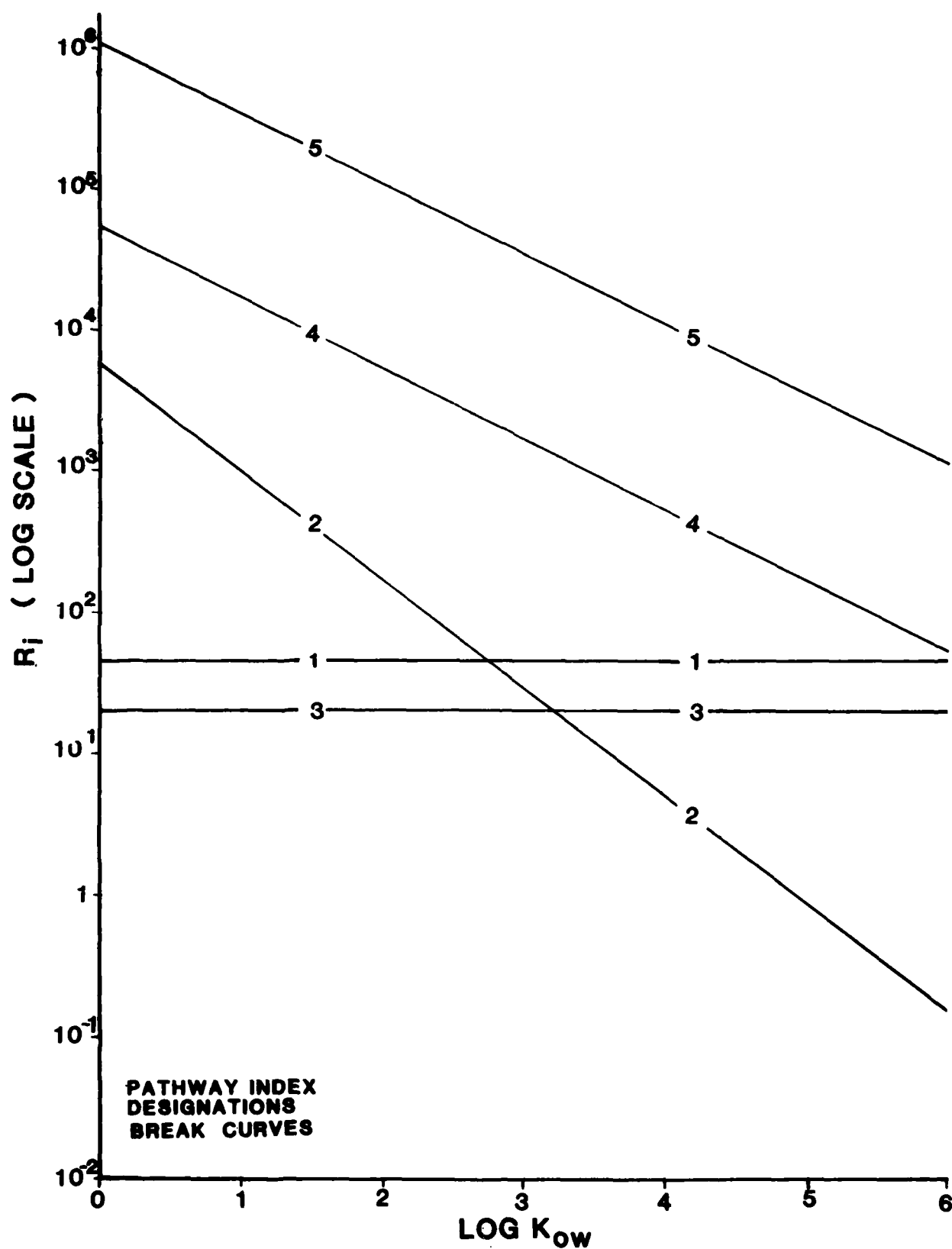


Figure 3. Relative importance of water-human pathways in determining PPLV.

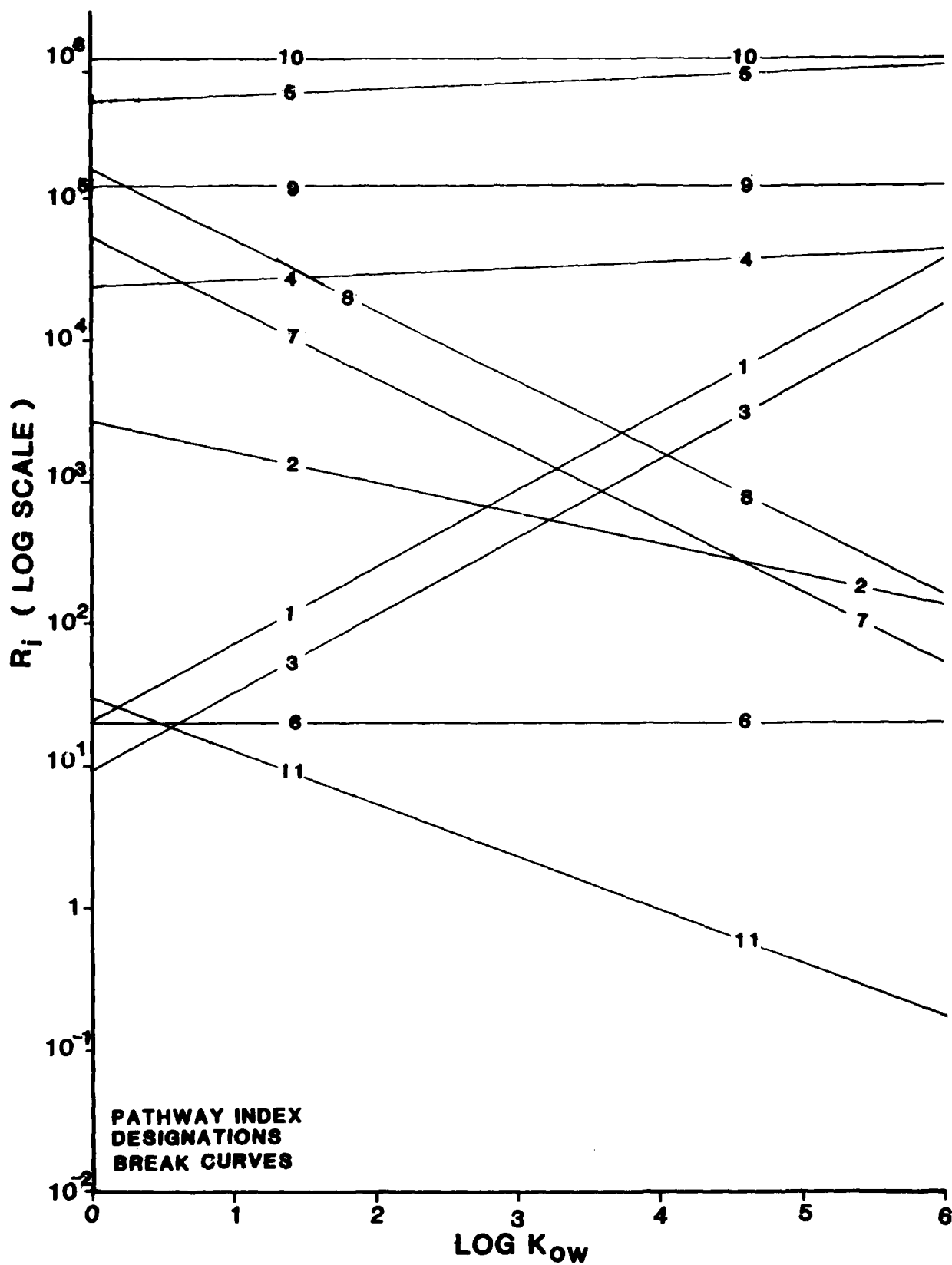


Figure 4. Relative importance of soil-human pathways in determining PPLV.

c. Relative to pathway 2, pathway 5 is not important. In other words, livestock animals apparently bioconcentrate considerably less of a pollutant from water than do fish. This is in part understandable from the intensity of contact of fish with water as compared to that of livestock and has been discussed by Kenaga.<sup>55</sup>

#### **PART VII: SEQUENTIAL STEPS OF THE PPLV APPROACH**

92. Two approaches are presented here. The first (Table 14) is a rigorous procedure which anticipates as practical the study of all aspects presented in this report. The second (Table 15) is a "fast and dirty" procedure, which may be useful when the pollutant of concern is an organic compound for which a relatively small amount of physicochemical information is available. In Table 15, one first attempts to omit pathways that are anticipated to be of minor importance in calculation of a PPLV. The procedure to omit pathways follows the suggestions presented in paragraphs 88-90. In this second approach, there is a "user's risk" that important information may be overlooked. On the other hand, situations do arise where a PPLV would be required in a short time frame, and such risk is accepted.

Table 14

Sequential Application of the PPLV Approach: The Rigorous Procedure

Step	Description	Reference
1	Define scenario(s) for land or water use	Paragraph 3
2	Define pathways and derive SPPPLV equations	Paragraph 35-45 and Appendix C, paragraphs 2,6,11-16
3	Collect relevant information on these aspects of the pollutant:  Fish toxicity (pathway 2) Organoleptic effects in water (pathways 1,2) Water solubility (pathways 1-5,11) Vapor pressure (pathway 11)	Paragraph 85 Paragraph 86 Paragraph 69 Paragraph 70
4	Determine whether $D_T$ is to be based on the premise that the pollutant is a known or potential carcinogen  If yes, select the ARL and estimate $D_T$ for the selected ARL  If no, estimate $D_T$ on the basis on avoidance of harmful effects	Paragraph 17,18  Paragraph 19, 30-33 and Appendix G  Paragraph 21-29
5	Collect data required to evaluate $IF_1$	Paragraph 10, 48-64
6	If the compartmental models presented are used, estimate the partition coefficients for evaluation of $K_1$ . Otherwise, evaluate user-derived models for required inputs other than $D_T$ .	Paragraphs 10,72-80
7	Evaluate SPPPLVs and PPLVs	Paragraphs 10,12
8	Check for the presence of "type 1" and "type 2" restrictions; adjust PPLVs as needed	Paragraph 84, Table 12



Table 15

Sequential Application of the PPLV Approach: Simplified Procedure

Step	Description	Reference
1	Define scenarios(s) for land or water use	Paragraph 3
2	Define pathways and derive SPPPLV equations	Paragraph 35-45 and Appendix C, paragraphs 2,6,11-16
3	Compute $\log K_{ow}$ or whatever predictive physicochemical property ( $C_{sol}$ , $K_{oc}$ ) is selected	Paragraphs 68,69,71
4	If pathway 11 is involved, compute $VD_o$	Paragraph 70
5	Find $R_1$ as a function of $\log K_{ow}$	Figures 3-4, Table 13
6	For each scenario, delete pathways for which $R_1 / R_{11} > 100$	Paragraph 90
7	Carry out steps 4 and 7 from Table 14	See Table 14

#### **APPENDIX A: EXTENDED REFERENCE TABLES**

1. Table A1 provides a listing of chemicals that are considered to have organoleptic effects in water and concentrations below which such effects probably would not be noted; see paragraph 86 m.t.

Table A1

Recommended Pollutant Limits in Water Based on Organoleptic Effects

Substance	Concentration in water, mg/L
a) Priority Pollutants <sup>16</sup>	
Acenaphthene	0.020
Monochlorobenzenes	0.020
Monochlorophenols	0.0001
2,4-Dichlorophenol	0.0003
2,3-Dichlorophenol	0.00004
2,5-Dichlorophenol	0.0005
2,6-Dichlorophenol	0.0002
3,4-Dichlorophenol	0.0003
2,3,4,6-Tetrachlorophenol	0.001
2,4,5-Trichlorophenol	0.010
2,4,6-Trichlorophenol <sup>a</sup>	0.002
2-Methyl-4-chlorophenol	1.8
3-Methyl-4-chlorophenol	3.0
3-Methyl-6-chlorophenol	0.020
Copper salts	1
2,4-Dimethylphenol	0.4
Hexachlorocyclopentadiene	0.001
Nitrobenzene	0.030
Pentachlorophenol	0.030
Phenol	0.3
Zinc salts	5
b) Maximum Permissible Concentrations (USSR) <sup>60b</sup>	
Aliphatic amines, C7 to C9	0.1
Aliphatic amines, C10 to C16	0.04
Aliphatic amines, C16 (sic) to C20	0.03
2-Aminophenol	0.01
4-Aminophenol	0.05
Acetaldehyde	0.2
Acetophos	0.03
Avadex	0.03
Butyl acrylate	0.015
Butylbenzene	0.1
Butyl alcohol	1.0
Sodium vinylsiliconate	2.0
Hexachlorobutane	0.01
Hydroquinone	0.2
Dalapon	2.0
Dikotex	0.25
Dimethyldithiophosphoric acid	0.1
Dichlorovinyl dimethyl phosphate	1.0
Potassium diisopropyl dithiophosphonate	0.02
Dinitrobenzene	0.5
Dinitronaphthalene	1.0
Dinitrochlorobenzene	0.5
Dipropylamine	0.5

Substance	Concentration in water, mg/L
Cresyl dithiophosphate	0.001
Diuron	1.0
Diphenylolpropane	0.01
3,4-Dichloroaniline	0.05
2,5-Dichloroaniline	0.05
Dichlorobenzene (o- and p-)	0.002
Dichlorobutene	0.05
Dichlorohydrin	1.0
Dichlorocyclohexane	0.02
Dichloroethane	2.0
Dimethyl terephthalate	1.5
Diosbutylamine	0.07
Dicyanodiamide	10.0
Diethanolamine	0.8
Diethyl phosphorodithioic acid	0.2
Potassium diethylphosphorodithioate	0.5
Iron (II) salts	0.5
Isobutylene	0.5
Isoprene	0.005
Isopropyl phenylcarbamate	0.2
Isopropyl N-(3-chlorophenyl)carbamate	1.0
Carbide	0.03
Malathion	0.05
Kerosene	0.1
Butyl xanthate	0.001
Xylene	0.05
Maleic acid	1.0
beta-Mercaptodiethylamine	0.1
Mercaptos	0.01
Methylparathion	0.02
Methyl acrylate	0.02
Methyl dithiocarbamate	0.02
Methylnitros	0.25
Sodium methylsiliconate	2.0
Methylsystox	0.01
alpha-Methylstyrene	0.1
Monosodium salt of cyanuric acid	25.0
Monopropylamine	0.5
Monochlorohydrin	0.7
Monoethylamine	0.5
1-(p-Chlorophenyl)-3,3-dimethylurea	5.0
Sodium salt of dichlorophenoxyacetic acid	1.0
Naphthenic acids	0.3
alpha-Naphthol	0.1
p-Nitrophenylaminoethanol	0.5
p-Nitrophenylchloromethyl-carbinol	0.2
p-Nitrophenylacetylaminethanol	1.0
Nitroform	0.01
O,O-Dimethyl S-(2-ethylthioethyl) phosphorodithioate	0.001
Pentachlorobutane	0.02
Sodium pentachlorophenolate	5.0
Picric acid	0.5

Substance	Concentration in water, mg/L
Polymethylhydrosilicone	2.0
Polymethyldichlorophenyl-silicone	10.0
Polyethylhydrosilicone	10.0
Polyethyl silicone	10.0
Prometrine	3.0
Propasine	1.0
Propylbenzene	0.2
Saponin	0.2
Sevin	0.1
Carbon bisulphide	1.0
Turpentine	0.2
Styrene	0.1
Tetrahydroquinone	0.05
Tetranitromethane	0.5
Tetrachloroheptane	0.0025
Tetrachlorononane	0.003
Tetrachloropentane	0.005
Tetrachloropropane	0.01
Tetrachloroundecane	0.007
Tetrachloroethane	0.2
Thiophene	2.0
Parathion	0.003
Tributyl phosphate	0.01
Trichlorometafos-3	0.4
Triethanolamine	1.4
Phosbutyl	0.03
Phosphamide	0.03
Phthalophos	0.2
Furfural	1.0
Chloranil	0.01
Sodium chlorate	20.0
Chloronitrosocyclohexane	0.005
Chloroprene	0.1
Chlorophos	0.05
Chlorononanoic acid	0.3
Chloroundecanoic acid	0.1
Chloroheptanoic acid	0.05
Chlorocyclohexane	0.05
Chromium VI salts	0.1
Chromium III salts	0.5
Celatox	0.5
Cyanuric acid	6.0
Ethyl acrylate	0.005
Ethylbenzene	0.01
Sodium ethylsiliconate	2.0
p-Chlorophenyl p-chlorobenzenesulfonate	0.2

a. Also listed in Table 3.

b. Compounds with names other than generic or well-known form are in quotes. Consult the RTE<sup>12</sup> for generic equivalents.

## APPENDIX B: TECHNICAL DISCUSSION OF $D_T$ ESTIMATION METHODS

1. This discussion is restricted to chronic exposure situations. Short-term exposure situations have been encountered in the Fort McClellan study<sup>9</sup> and approaches are being developed to deal with them.

### STRATEGY SELECTION: CARCINOGEN OR NON-CARCINOGEN

2. The "Cancer Problem." The 1970s were a decade of almost obsessive effort to control and treat cancer. There is disagreement as to the relative importance of environmental exposure to chemicals as a cause of cancer. However, the effects of cancer are well-known and formidable. From one account,<sup>17</sup> "Cancer is the second most common cause of death in the United States. One in every four Americans will suffer from cancer sometime during his or her life. In 1981, about 400,000 Americans will die of cancer. In addition to the physical and emotional suffering caused by cancer, it is estimated that this disease may cost the Nation as much as \$30 billion each year in lost production and income, medical expenses and research costs."

3. For the purpose of carcinogenic  $D_T$  evaluation, an ARL has to be specified by the user. A given ARL specifies the expected increased incidence of cancer to an exposed individual in his lifetime if he is challenged at dose  $D_T$ . Alternately, an intake of  $D_T$  by 1 / ARL challenged persons would have an expected outcome of one additional case of cancer beyond those that would have been observed had the substance been absent from the environment. As a point of comparison, the lifetime risk of cancer for an "average" American (without adjusting for possible effects of sex, occupation, location, or smoking habits) is about 0.25.<sup>17</sup> The ARL levels that are being considered for regulatory selection appear targeted at the  $10^{-5}$  to  $10^{-7}$  range. Such risks are of the order of involuntary risks that people contend with every day. For example, the risk of death from lightning in a person's lifetime is of the order of  $5 \times 10^{-5}$ , given a yearly toll of about 175 deaths in the United States.<sup>61</sup>

### Concepts behind $D_T$ estimations.

4. The procedures involved in determining the  $D_T$  applicable to a substance differ, based on whether the substance is considered of potential or known carcinogenic hazard or not. Figure B1 is an illustration of why this is so. Dose and risk are shown in log units. Risk is in terms of lifetime exposure. Consider first some undesirable non-carcinogenic effect due to exposure to a substance. Such an effect is expected to have a finite dose threshold; below this dose, this effect will not be observed. A physiological interpretation of a threshold is that the body is able to neutralize any harmful effect of the substance without noticeable functional change. The dose-risk curve for this effect would resemble that shown in Figure B1. For practical purposes, the slope of this curve is rather steep at risk levels below approximately  $10^{-3}$ . The value of  $D_T$  sought corresponds to a dose to the left of the steep portion of the curve in the "essentially zero risk" region and is here identified as  $D_{Tn}$  to stress its non-carcinogenic basis.

\* See References section for full citation.

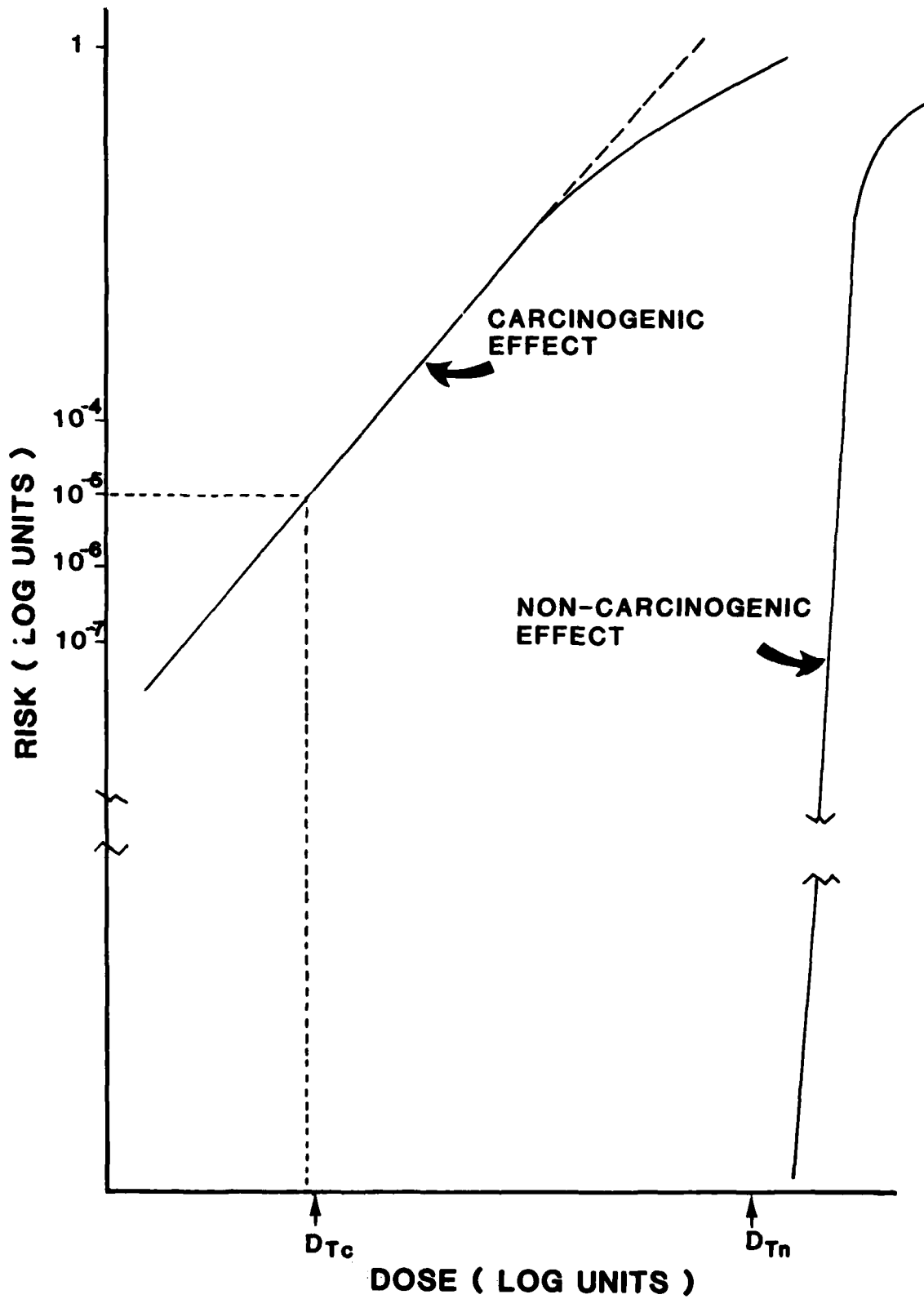


Figure B1. Dose-response characteristics of carcinogenic vs. non-carcinogenic effects for a hypothetical substance.

5. If a substance is suspected of posing a carcinogenic hazard to man (paragraph 17 m.t.), the concept of dose-risk is viewed quite differently. Figure B1 shows a simplified human carcinogenic incidence-dose curve from exposure to such a substance. This exposure is considered by the scientific community to have no threshold, i.e. the body has no special mechanism to counter cellular mutations caused by a substance. Moreover, in the risk region below about  $10^{-3}$ , the slope of the curve (on the log-log scale) is unity. In this region, a person exposed to a given dose of the substance is ten times as likely to incur cancer as one exposed to one-tenth that dose. From accepted models, the parameter  $B_H$  can be estimated; see paragraph 19. In Figure B1,  $1 / B_H$  would represent the dose for the extrapolation of the log-linear portion of the dose-response curve to  $ARL = 1$ . By this model slope characteristic,  $1 / B_H = D_T / ARL$ . Thus, any  $D_T$  estimate requires an  $ARL$ . For example, the dose corresponding to an  $ARL$  of  $10^{-5}$  is designated as  $D_{TC}$  in Figure B1.

6. For many substances, a considerable amount of toxicological information is first collected, which forms the basis for a  $D_{TN}$  estimate. However, as toxicological techniques become more refined, information is sometimes disclosed that suggests that a compound may pose a carcinogenic hazard. Usually,  $D_{TC} \ll D_{TN}$ ; see paragraph 21. This need not always be true, but extreme exceptions are not of much interest (dead people do not "catch" cancer). There are compounds for which  $D_{TC}$  and  $D_{TN}$  may be of the same magnitude; bis(2-chloroethyl)sulfide (the chemical warfare agent mustard gas) appears to be one such case.<sup>9</sup>

#### Criteria for Selection

7. Only a handful of substances are "known" carcinogens to humans. Paragraph 18b m.t. lists 17 such substances; an authoritative review<sup>62</sup> specifies (but does not list) 26 substances. With few exceptions, the hypothesis that a substance is probably carcinogenic to humans is based on results with other animal species. The mammalian bioassay test criterion of paragraph 17b m.t. is a widely-accepted basis upon which to make an extrapolation to man. The Ames Test criterion, paragraph 17c m.t., is not as well accepted in the scientific community. Its inclusion has been based on ad hoc policy decisions at USAMBRDL.<sup>4</sup> Generally, the Ames Test serves as a screen to select compounds for long-term and expensive mammalian bioassay tests. In this role, the Ames Test is subject to the pitfalls of any screening or surrogate test:

a. A substance producing a positive result with the Ames Test may not be oncogenic in animals. The probability of this has been estimated to be 13 percent.<sup>63\*</sup>

\* In the referenced study,<sup>63</sup> the authors considered 300 compounds for which studies concerning oncogenic activity in mammals and the Ames Test had been performed. A positive result in the Ames Test was declared when at least one microbiological strain/activation system had a response of greater than 0.01 reversions/nmole. The reader should realize that there was some judgment as to whether a substance was to be considered an oncogen, and subsequent studies may have changed the percentages.



b. A substance that fails to show a positive Ames Test result may be oncogenic in animals. The probability of this has been estimated to be 10 percent.<sup>63</sup>

Moreover, the mammalian bioassay is a surrogate test for human carcinogenic hazard and subject to the same pitfalls. Thus, in accepting positive Ames Test information as a sole criterion, there is some probability (in excess of 13 percent) that the involved substance will not be carcinogenic in humans. The situation has been summarized; that the Ames Test does not "in the absence of animal bioassay and epidemiology data, constitute definitive evidence as to whether a substance does (or does not) pose a carcinogenic hazard to humans. However, positive responses ... are considered suggestive evidence of a carcinogenic hazard."<sup>62</sup>

8. The Ames Test has been specifically cited because of its wide use, relatively standardized procedures, and acceptance. Other mutation tests on bacteria such as with Escherichia coli or Bacillus subtilis do exist, but their "track records" have not been established. A similar conclusion applies to tests of inhibited DNA synthesis on tissue culture cells.

#### NON-CARCINOGENIC $D_T$ ESTIMATES

9. The approaches presented in paragraphs 21-29 m.t. are based on three premises. First, recommendations arrived at by recognized public health organizations or Governmental agencies are preferable to those from other sources. The second is that less preferable approaches will require a search of the technical literature and appreciably more critical review and judgment on the part of the user. Last, users should avoid unquestioned use of published values unless they are aware of the circumstances involved in their derivation.

10. Data from which to compute  $D_T$  are seldom based on human studies. Rather, such data are derived from toxicological investigations on mammals. The results of these investigations are converted to  $D_T$  with the inclusion of a safety factor to allow for:

a. The duration of the investigation. With rodent species, which are the usual subjects for tests, 2-year studies are usually pursued only when prior evidence suggests the potential for oncogenic responses. When non-oncogenic responses are expected, 90-day studies are often performed.

b. The mammalian species involved. Regulatory requirements have tended to standardize test protocols to include two rodent species. Studies performed for purposes other than regulatory concern, in different countries, or in earlier times, have involved non-rodent mammals or just one rodent species.

c. Type of results obtained. Most ingestion studies employ several dosage levels (mg substance/kg body weight/day) as treatments including a zero level as a control. The ideal result is the second "test outcome" entry in Table 6; the other outcomes listed are less desirable. It would be a formidable task to propose safety factors for all possible outcomes

of all types of studies. In paragraph 25 m.t. and Table 6, the author has suggested factors for the more typical situations. The user has to exercise judgment in addressing other situations.

11. An inherent problem with  $D_T$  estimation techniques is whether safety factors are "too safe" or "not safe enough." If a factor is "too safe" it could lead to an unnecessarily costly decision to renovate land or a decision to over-restrict land use. On the other hand, a "not safe enough" factor defeats the whole purpose of the exercise. Several uncertainties and simplifications are associated with safety factor estimation procedures such as Table 6 and Equation 10. The distinction between "no-effects" and "effects" is sometimes subjective. Effects at a given feeding level may be rather subtle (such as a change in weight gain patterns or blood chemistry) without other observable changes. The effect may be species-specific; i.e., a metabolic response occurs that has no human parallel. Feeding studies, of necessity, are limited to a few discrete levels.  $D_T$  estimates are dependent on these levels, such that at one level no effects occur, while at the next, effects do occur. These adjacent levels may be at anywhere from 0.3 to 1.0 log intervals. In truth, an intermediate but untested feeding level could also be a no-effect level. In this respect, there is a bias to be safe-sided with outcomes "1" and "2" in Table 6.

12. Such uncertainties are compounded when several pollutants are simultaneously addressed. Consider two substances "A" and "B," with no-effect thresholds of 1 and 10, respectively. These values are actually not known,  $D_T$  estimates them. The  $D_T$  estimates should ideally meet two attributes:

a. The estimates should be unbiased. They should be reasonably close to their respective no-effect thresholds.

b. The estimates should be consistent. The ratio of  $D_T$  for substances "A" and "B" should be reasonably close to 1:10 even if the individual estimates are biased.

Unfortunately, these attributes are seldom capable of being tested. Inconsistent  $D_T$  values could lead to concern being directed towards the wrong pollutant. Stokinger and Woodward<sup>64</sup> illustrate examples of safety factor differences in comparing TLV-based extrapolations of permissible water pollutant limits to existing recommendations or standards. Calabrese<sup>65</sup> has an excellent discussion dealing with the derivation of drinking water standards and the safety factors applied.

13. The author has not included drinking water standards as bases for direct  $D_T$  estimates. The author's experience with such standards is that the substances are ubiquitous, allowances in the standards have been made for other routes of ingestion, and inconsistent safety factors have been applied to their formulation. These points are discussed in pertinent cited references.<sup>41,65</sup>

14. The Water Quality Criteria for the 129 "priority pollutants" are a new source of information and methodology. These documents represent current procedures applied by a regulatory agency, have been subject to critical scientific review, and probably will be involved in legal reviews. The values

presented in Tables 3 and 5 have been back-calculated from criteria presented in NWQCD<sup>16</sup> for two pollutant intake scenarios:

a. The intake occurs entirely as a result of the consumption of 6.5 g/day of combined fish and shellfish from contaminated water. The corresponding water criterion in mg/L is  $C_1$  and the corresponding pollutant level in fish/shellfish is  $C_{1f}$  in mg/kg.  $C_{1f}$  is related to  $C_1$  ;

$$C_{1f} = BCF \times C_1 \quad (B1)$$

where BCF is a bioconcentration factor for fish of 3 percent average lipids content; see the footnote to paragraph 74 m.t.

b. The pollutant intake occurs as a result of the consumption of fish and shellfish as above and of 2 liters of contaminated water daily. This water criterion,  $C_2$  , is related to  $C_{2f}$  by the analog of Equation B1.

15. In the first situation, the uptake of pollutant by a consuming individual, or  $U_1$  in mg/day, is

$$U_1 = 0.0065 \times BCF \times C_1 \quad (B2)$$

The corresponding equation for the second situation is

$$U_2 = 2 \times C_2 + 0.0065 \times BCF \times C_2 \quad (B3)$$

Based on the concept of water quality criteria,  $U_1 = U_2$  .  $D_T$  , the PPLV parameter, is related to  $U_1$  ;

$$D_T = U_1 / BW \quad (B4)$$

Each specific water quality criteria document includes values of BCF for addressed compounds, and if these are used, Equations B4 or B2 and B3 can be used to calculate  $D_T$  . If only values of  $C_1$  and  $C_2$  are stated, as in the NWQCD,<sup>16</sup>  $D_T$  can be computed after some substitutions. Equations B2 and B3 can be combined to express BCF in terms of  $C_1$  and  $C_2$  ,

$$BCF = 308 \times C_2 / (C_1 - C_2) \quad (B5)$$

Then Equation B6 (derived from B1, B4, and B5) provides  $D_T$  in terms of  $C_1$  and  $C_2$  .

$$D_T = 2 \times C_2 \times C_1 / [ BW \times (C_1 - C_2) ] \quad (B6)$$

16. TLVs have been compiled for more than 600 substances. Even if a TLV recommendation is not amenable to  $D_T$  computations, the documentation may provide literature citations for less preferred approaches. Moreover, the documentation serves as an important reference for organoleptic effects, or for substances whose main effect is skin irritation. The toxicological basis for a TLV varies widely from substance to substance, hence leeway in safety factor selection has been suggested in lieu of the previously suggested  $SF = 100$ .<sup>2,3</sup> Equation 9 differs from that presented in previous papers;<sup>2,3</sup> it follows the interpretation given TLV data in the summarized

water quality criteria.<sup>16</sup> The safety factor suggestions in Table 6 have been also patterned after those discussed in NWQCD.<sup>16</sup>

17. The approach in paragraph 28 m.t. is based on a report by Handy and Schindler.<sup>24</sup> They advanced procedures to estimate permissible pollutant concentrations in water and air from a LD<sub>50</sub>. Their approach involved a first-order model of a substance in humans which balances the ingested substance intake rate to the elimination rate. The elimination rate depends upon the concentration and residence time of substance in the body. As a "worst case," the body concentration should not exceed C<sub>h</sub>, a safe maximum body concentration in mg/kg body weight. The residence time, in days, is represented by the half-life  $\tau$ . The resulting balance, expressed in terms of D<sub>T</sub>, is

$$D_T = \ln 2 \times C_h / \tau \quad (B7)$$

The authors proposed that

$$C_h = 5 \times 10^{-4} \times LD_{50} \quad (B8)$$

and that  $\tau$  be evaluated as:

- a. a known value, if one was available,
- b. 30 days if  $\tau$  is not known, and the substance is not expected to be retained in the body, or
- c. 365 days if  $\tau$  is not known, but the substance is expected to be retained in the body.

Equation 11, m.t., is based upon Equations B7 and B8 and a  $\tau = 30$  days. It is unlikely that  $\tau$  would be known for a substance if the state of knowledge is such that a LD<sub>50</sub> has to be used for a D<sub>T</sub> estimate. Moreover, the 30-day value appears safe-sided based on known half-life estimates for many chemicals.

#### CARCINOGENIC D<sub>T</sub> ESTIMATES

18. Methods for computing a dose-risk correlation are highly controversial. With few exceptions, extrapolation from tests performed with laboratory rodents is the common practice. The currently accepted philosophy is to consider a statistically significant increased incidence of tumors\* in dosed animals vs. controls as suspect without regard for the morbidity or mortality associated with the tumor. Numerous models exist for such extrapolations, and each has its proponents. Predicted relationships are almost impossible to validate. Model extrapolation procedures are subject to several uncertainties; for example, the probability estimates P<sub>t</sub> and P<sub>c</sub> (paragraph 32 m.t.) may be of poor accuracy. Test results can be less than definitive and subject

\* See paragraph 33b, m.t. for the criterion applicable to the one-hit model; the NWQCD<sup>16</sup> for the multistage model.

to alternative interpretations; dimethylterephthlate results are an illustrative example.<sup>66</sup>

19. In Table 3, the  $D_T$  values for potentially carcinogenic "priority pollutants" have been back-calculated for a  $10^{-5}$  risk level. The "one-hit" model outlined in paragraph 32 m.t. was used in preliminary Water Quality Criteria presentations.<sup>34</sup> This method is fairly easy to apply without computer assistance and is used when only one dose-level datum is available. When multi-dose level data exist, the Crump multistage model is preferable and was used to compute several water quality criteria.<sup>16</sup> This model requires a computer program for execution. The reference<sup>16</sup> compared results based on each method for several compounds; results generally agreed within a factor of two. Readers are advised that the term "potency factor" with the symbol "q" is used in multistage model-derived criteria in place of  $1/B_H$ .

20. There is no acceptable method to use quantitative Ames Test data (i.e., number of reversions/mass of test compound) to estimate a  $D_T$  when paragraph 17c m.t. applies. Equation 12 has been proposed as a "first cut" procedure for this purpose. To use Equation 12,  $K_{tn}$  must be estimated. The rationale used to evaluate  $K_{tn}$  was to follow the compounds listed in Table 3 through the historical track discussed in paragraph 6. The individual Water Quality Criteria documents for these substances were reviewed for non-carcinogenic and carcinogenic information. Where a TLV recommendation was determined to be the preferable basis for estimation of  $D_{Tn}$ , the 1974 DTLV<sup>67</sup> recommendation was used. This was done to avoid TLV recommendations that were adjusted later<sup>12</sup> due to carcinogenic potential concerns. In such cases, Equation 9 was used to compute  $D_{Tn}$  from a TLV. The salient points of the review for each substance appear in Table B1. This procedure was not applied to all the compounds in Table 3; see Table B2 for a short discussion of these exceptions.

21. Based on this approach, a value of 417, the log mean of the  $K_{tn-5}$  estimates in Table B1, was selected for use in Equation 12. Then for a  $10^{-5}$  ARL, as a first approximation,  $D_{Tc} = D_{Tn} / 240$ .

#### CLOSING COMMENTS

22. The above discussion has presented, in simplified terms, the toxicological basis for methods of estimating a  $D_T$ . This discussion does not represent an in-depth review of the science. As with most generalizations, exceptions exist; if these are known a priori, adjustment should certainly be made for them. Moreover, readers are cautioned that the procedures presented reflect a mixture of science, politics, and consensus attitudes of the scientific community. The last two of these are subject to change, and it likely that they will change.

23. The outward effects of environmental substances are not simply limited to a division between "conventional" and carcinogenic considerations. Some substances are teratogens; exposure to such substances causes increased incidences of difficult pregnancies, spontaneous abortions, and congenital defects in the newborn. Such substances may not be potentially carcinogenic or even particularly toxic; nitrous oxide ( $N_2O$ ) is a classic case. A recent

presentation from a report issued by the Council on Environmental Quality<sup>94</sup> identifies several compounds that are known teratogens in humans or mammals; in several cases, the dose levels involved are of the order of those in Table 3. The status of progress in this field was described "about where cancer studies were 25 years ago."<sup>94</sup> In time, parallel procedures may be devised to identify and quantify effects of teratogens as have been devised for carcinogens.

Table B1

Basis for  $K_{tn}$  Estimates

Substance ( $K_{tn}$ )	Review of Information <sup>a</sup>
Acrylonitrile (390)	TLV of 45 mg/m <sup>3</sup> based on animal inhalation data and analogy to cyanide. <sup>67</sup> Based on SF = 1,000, $D_{Tn}$ = 4.6 <sup>-3</sup> mg/kg/day. $D_T$ / ARL estimated as 4.6 mg/kg/day from multistage model treatment of astrocytoma incidence in the nervous system of rats. Animals given acrylonitrile in drinking water. <sup>68</sup>
Aldrin/Dieldrin (330)	WHO/FAO ADI of 10 <sup>-4</sup> mg/kg/day used directly as $D_{Tn}$ . <sup>69</sup> $D_T$ / ARL estimated as 3.3x10 <sup>-2</sup> mg/kg/day from multistage model treatment of hepatocellular carcinomas incidence in female rats. Animals tested fed 0.1 to 10.0 mg/kg dieldrin in diet. High mortality at 10 mg/kg dose level. Control animal diet found to have 0.013 mg/kg dieldrin. <sup>69</sup>
Arsenic (56)	TLV of 0.5 mg/m <sup>3</sup> based on several industrial worker studies and is linked to observed urinary arsenic levels for exposed workers apparently in good health. <sup>67</sup> AA = 0.2; AO = 0.8. <sup>70</sup> Based on SF = 10, $D_{Tn}$ = 1.3x10 <sup>-3</sup> mg/kg/day. $D_T$ / ARL estimated as 7.2x10 <sup>-2</sup> mg/kg/day from analysis of skin cancer incidence in 40,421 inhabitants of region in Taiwan which has a drinking water supply with a high natural arsenic content. <sup>70</sup>
Benzene (230)	TLV of 80 mg/m <sup>3</sup> based on industrial worker studies; levels of benzene at work stations uncontrolled. <sup>67</sup> Based on SF = 100, $D_{Tn}$ = 0.082 mg/kg/day. <sup>a</sup> $D_T$ / ARL estimated as 19 mg/kg/day from epidemiology study of workers inhaling benzene, results converted to ingestion situations. <sup>71</sup>
Beryllium (5900)	TLV of 0.002 mg/m <sup>3</sup> based on Atomic Energy Commission plant limits and several retrospective industrial hygiene studies at plants supposedly in compliance. <sup>67</sup> AA = 0.6; AO = 0.2. <sup>72</sup> Based on SF = 30, $D_{Tn}$ = 2.0x10 <sup>-5</sup> mg/kg/day. $D_T$ / ARL = 0.12 mg/kg/day. Total tumors counted in male rats fed BeSO <sub>4</sub> in drinking water. One-hit model used although study did not indicate statistical significance. Another study with male rats indicated high incidence of lung reticulum cell sarcoma, although dose-response was unusual. <sup>72</sup>
Carbon tetrachloride (540)	TLV of 65 mg/m <sup>3</sup> based mainly on animal inhalation studies with some industrial observations. <sup>67</sup> Based on SF = 300, $D_{Tn}$ = 0.022 mg/kg/day. <sup>a</sup> $D_T$ / ARL estimated at 12 mg/kg/day from multistage model of liver tumors in male rats. Animals were fed by gavage 5 days/week for 78 weeks and sacrificed 10 weeks later. <sup>73</sup>
Chlordane (320)	WHO/FAO ADI of 10 <sup>-3</sup> mg/kg/day used for $D_{Tn}$ . <sup>74</sup> $D_T$ / ARL estimated as 0.32 mg/kg/day based on multistage model treatment of the incidence of liver carcinomas in female mice in an 18-month feeding study. <sup>74</sup>
Chloroform (36)	TLV of 250 mg/m <sup>3</sup> based on prevention of short-term effects, no definitive no-effect level noted. <sup>67</sup> AA = 0.6; AO = 1.0. <sup>75</sup> Based on SF = 100, $D_{Tn}$ = 0.153 mg/kg/day. $D_T$ / ARL estimated at 5.5 mg/kg/day from multistage model treatment of the incidence of hepatocellular carcinomas in female mice. Animals fed by gavage 5 days/week for 78 weeks and sacrificed 10 weeks later. <sup>75</sup>

Substance ( $K_{Tn}$ )	Review of Information <sup>a</sup>
1,2-Dichloroethane (130)	TLV of 200 mg/m <sup>3</sup> based primarily on 6-month animal inhalation tests, some industrial exposure information. <sup>67</sup> Based on SF = 100, $D_{Tn}$ = 0.204 mg/kg/day.* $D_T$ / ARL estimated at 27 mg/kg/day based on multistage model treatment of the incidence of hepatocellular carcinomas observed in male mice. Several other tumors noted in test mice and rats. <sup>76</sup>
2,4-Dinitrotoluene (640)	Dogs fed 5 mg/kg/day for 13 weeks showed no ill effects. $D_{Tn}$ estimated as $5 \times 10^{-3}$ mg/kg/day. $D_T$ / ARL estimated as 3.2 mg/kg/day based on one-hit model analysis of mammary and liver tumors (combined) in female rats. Animals fed for 24 months and sacrificed 1 month later. <sup>77</sup>
Heptachlor (6300)	TLV of 0.5 mg/m <sup>3</sup> based on analogy with closely-related compounds. <sup>67</sup> Based on SF = 1,000, $D_{Tn}$ estimated as $5.1 \times 10^{-5}$ mg/kg/day.* $D_T$ / ARL estimated as 0.32 mg/kg/day based on multistage model treatment of incidence of hepatocellular carcinomas in male mice. Mice fed for 80 weeks, sacrificed 10 weeks later. <sup>78</sup>
Hexachlorobenzene (1500)	Rat-feeding study of 15-week duration indicates a no-effect level of 0.5 mg/kg/day. <sup>79</sup> $D_{Tn}$ estimated at $5 \times 10^{-4}$ mg/kg/day. $D_T$ / ARL estimated as 0.76 mg/kg/day based on multistage model analysis of incidence of hepatomas in male Syrian Golden hamsters fed for 80 weeks. <sup>79</sup>
Hexachlorobutadiene (6500)	No effects observed on rats fed at a dose of 0.2 mg/kg/day for 22 to 24 months. <sup>80</sup> $D_{Tn}$ estimated as $2 \times 10^{-3}$ mg/kg/day. $D_T$ / ARL estimated as 13 mg/kg/day based on one-hit model analysis of the incidence of renal tubular adenomas and carcinomas in male rats in 2-year bioassay. <sup>80</sup>
Hexachlorocyclohexane (380)	Lindane 104-week feeding study on beagle dogs, no effects noted at 50 mg/kg level in diet. <sup>81</sup> Diet factors assumed as 10 kg for dog and 0.25 kg/day food intake from the RTE. <sup>12</sup> $D_{Tn}$ estimated as $2 \times 10^{-3}$ mg/kg/day. $D_T$ / ARL estimated as 0.76 mg/kg/day based on one-hit model analysis of liver tumor incidence in male mice fed 400 ppm lindane in diet for 110 weeks. <sup>81</sup>
Tetrachloroethylene (110)	TLV of 670 mg/m <sup>3</sup> based on short term (5 hours/day for 53 days) inhalation study on humans. <sup>67</sup> Based on SF = 300, $D_{Tn}$ = 0.23 mg/kg/day.* $D_T$ / ARL estimated as 25 mg/kg/day based on one-hit model analysis of the incidence of hepatocellular carcinomas in mice. Animals fed 5 days/week for 78 weeks, sacrificed at 90 weeks. <sup>82</sup>
Toxaphene (370)	Based on average value of proposed standards and recommendations, $D_{Tn}$ = $2.3 \times 10^{-3}$ mg/kg/day. <sup>83</sup> $D_T$ / ARL estimated as 0.74 mg/kg/day based on multistage model analysis of the incidence of hepatocellular adenomas and carcinomas in male mice. Animals fed for 61 weeks, sacrificed at 90 to 91 weeks. <sup>83</sup>
Vinyl chloride (72)	TLV of 770 mg/m <sup>3</sup> based on study of industrial workers over a 17-year period. Variable levels of compound at work stations. <sup>67</sup> Based on SF = 100, $D_{Tn}$ = 0.79 mg/kg/day.* $D_T$ / ARL estimated as 57 mg/kg/day based on multistage model analysis of total tumors in rats exposed to compound vapors (4 hours/day, 5 days/week for 52 weeks). Tumors counted at 135 weeks. Risk factor pharmacokinetically converted to oral basis. <sup>84</sup>

a. AA / AO = 1.0 unless otherwise specified.



Table B2

Substances Not Included in  $K_{tn}$  Estimation Process

Substance	Reference	Remarks
Benzidine	85	Carcinogenic hazard recognized in early studies.
Chloroalkyl ethers	86	Carcinogenic hazard recognized in early studies.
2,4,6-Trichlorophenol	87	Organoleptic effects at estimated ARL of $4 \times 10^{-4}$ .
Dichlorobenzidine	88	Carcinogenic hazard recognized in early studies.
1,1-Dichloroethylene	89	No no-effect levels found in early studies.
1,2-Diphenylhydrazine	90	No no-effect levels found in early studies.
Halomethanes	91	Carcinogenic $D_T$ assumed that of chloroform.
Nitrosamine compounds	92	Carcinogenic hazard recognized in early studies.
Benzo(a)pyrene and other polynuclear aromatic hydrocarbons	93	Carcinogenic hazard recognized in early studies.

## APPENDIX C: TECHNICAL DISCUSSION OF SPPPLV PATHWAYS

### EQUATIONS PRESENTED IN PART III

1. The pathway equations presented in Part III are mathematical models of inter-compartmental pollutant transfer from an environmental medium of concern to a human receptor. Within each pathway, there may be intermediate compartments, either environmental media or living receptors. A pathway need not have such compartments; pathways 1 and 9 are such situations. From Figure 1, transfer from the medium of concern to its adjacent intermediate receptor, or between adjacent intermediate compartments, involves a partition coefficient. The partition coefficients relate the concentrations of a substance in adjacent compartments. This is admittedly simplistic; these pathway models are tailored to situations where the existing information does not suffice to support a more rigorous approach. If better models can be used, the reader is encouraged to employ them.

2. The concept fundamental to these SPPPLV equation derivations is that a nominal daily quantity of pollutant,  $D_T \times BW$ , reaches man via a given pathway. The example of pathway 7 has been discussed in paragraph 10 m.t. The daily intake by an exposed human is

$$D_T \times BW = C_{a7} \times W_a \quad (C1)$$

while the pollutant level in the animal corresponding to the SPPPLV is

$$C_{a7} = C_{s7} \times K_{sp} \times K_{pa} \quad (C2)$$

Equation 3 is formed by the mutual elimination of  $C_{a7}$  from Equations C1 and C2; Equation 24 re-expresses Equation 3 in Equation 2 format. An important assumption is involved above; Equation C2 is strictly applicable for the concentration of a substance in bulk animal, Equation C1 is strictly applicable for the concentration in the meat portion consumed. Should they not be expected to be equivalent, an adjustment in the pathway equation is needed. An example is Equation 25, where  $K_{ad}$  serves to account for concentration differences between meat and dairy portions of cattle.

3. The equations for pathways 2 through 7 are strictly applicable to one specific food source, such as the potato as a vegetable or swine as livestock. They usually have been employed to cover a composite class of species, such as vegetables or meat. Quite often, partition coefficients are estimated from data available for only one species. One must assume that the values adopted are applicable to others.

4. Previous presentations of Equations 15 through 25 involved the product of estimates of daily food intake and pathway fraction of diet in place of  $W_f$ ,  $W_p$ ,  $W_a$  and  $W_d$ .<sup>1-3\*</sup> In the intervening time, literature sources for specific dietary items have been collected, allowing for more refined statements of these pathways; see Part IV, m.t. Dietary intakes are

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\* See References section for full citation.

treated as occurring daily, although the real-world situation may differ considerably.

5. Children can and do ingest soil directly; two situations are of specific interest. The first is incidental soil ingestion in the course of outdoor play where non-food dirt-covered items are mouthed. This behavior is usually outgrown by age 3.<sup>95</sup> The more serious situation is called "pica," a term used to describe the episodic ingestion of unusual amounts of non-food items. Pica has been attributed to nutritional or psychological factors, although where it is studied in detail (mainly in "inner cities"), these factors may be interrelated with the socio-economic environment.<sup>95</sup> Pica has commanded attention owing to concerns with lead uptake in young children.<sup>96</sup> Children in slum areas may eat flakes of paint with high-lead content or soil with lead from such flakes or from condensed automobile exhaust. Children with pica consume unusual amounts of paint flakes or soil and are expected to manifest more severe adverse lead effects than non-pica children. Pica appears to reach a peak incidence in 2-year old children; in some studies, almost half of the 2-year-old children observed had pica.<sup>97</sup> Studies of white children over 3 years old indicated only 3 to 4 percent with pica; for black children up to 6 years old, the incidence was still nearly 20 percent.<sup>97</sup> In the latter case, socio-economic conditions were considered most important; there appears to be no racial propensity involved. Equation 26 (pathway 9) can be used to describe either incidental soil ingestion or pica, with appropriate evaluation of  $W_{sc}$ ; see paragraph 61 m.t.

6. Other pathways can be formulated with equations similar to those presented in Part III m.t. The "venison consumption pathway" below illustrates an example. The situation proposed was that undomesticated deer shot in the hunting areas of the Alabama Army Ammunition Plant\* would supplement the meat diet of hunters' families. Each family was assumed to eat venison from one deer yearly. The venison yield from a deer was estimated at 44 kg; for a family of 4, each person would nominally consume 0.0302 kg/day. A second factor of concern was the browsing habits of deer at the property and the distribution of contaminants through the former manufacturing plant area. The assumption was made that only 10 percent of the deer's diet is derived from browse on contaminated land. One may treat the problem as if 10 percent of the venison was contaminated, i.e.,  $W_a = 3.02 \times 10^{-3}$  kg/day for this pathway. Equation 24 was expressed, with  $BW = 70$  kg, as

$$C_{s7} = 2.31 \times 10^4 \times (K_{sp} \times K_{pa})^{-1} \times D_T$$

7. Equation 27 replaces Equation C3 below, which appeared in earlier reports.<sup>1,3</sup>

$$C_{s10} = [(BW \times 10^6) / (RB \times C_{ss})] \times D_T \quad (C3)$$

where  $RB$  was a 24-hour breathing rate (18.5 m<sup>3</sup>) and  $C_{ss}$  was evaluated as 0.06 mg/m<sup>3</sup>, based on ambient particulate concentration measurements. The author believes that Equation C3 has shortcomings as a realistic pathway model:

\* All values shown here are from the Alabama Army Ammunition Plant study<sup>4</sup> and may not necessarily agree with those values presented elsewhere in this report.

a. Not all particulates are from raised soil.

b. It would be a "worst-case" assumption to expect all ambient particulate matter to be traceable to a given contaminated land area.

c. If the pollutant was initially of uniform content through the soil mass, after a period of time, the uppermost layers of the soil would become pollutant-deficient. The pollutant from these layers vaporizes to the atmosphere and is swept away by the wind. The rate of pollutant transport from lower layers is probably insufficient to maintain the initial pollutant content in upper layers. Thus, the estimated  $C_{s10}$  would be an inaccurate estimate of actual pollutant content in the soil.

The scenario applicable in Equation 27 circumvents these problems by dealing with dust raised during labor-related activities. The SPPPLV provided by Equation 27 is about 1/63 that of Equation C3, with all non- $D_T$  terms evaluated from Table 7. In this respect, the scenario portrayed in Equation 27 is more severe than that of Equation C3.

8. Pathway 11 was first encountered in the Camp Sims study,<sup>8</sup> where an excavation scenario was addressed. The term  $C_{s11} \times K_{sv}$  represents a vapor density ( $VD$ , in  $mg/m^3$ ); Equation 28 is an inhalation analog of Equation C1. As noted in Appendix D, paragraph 2,  $VD$  is an equilibrium vapor density that would exist in air entrained in soil pores. Whether  $VD$  can be attained in a large enough air volume to influence human activities is uncertain. The assumption that it is attained represents an adverse-case situation.

9. Equation 27 should be used with caution; it is possible to compute a SPPPLV in excess of  $1 \times 10^6$  mg/kg, which describes a "soil" which is pure pollutant. With the representative values from Table 12 substituted into Equation 27, this SPPPLV would occur when  $D_T > 1$  mg/kg/day. Two interpretations can be drawn: if other pathways are co-considered, pathway 10 is unimportant; alternatively, if pathway 10 is the only pathway involved in a scenario, no clean-up is required. An analogous case can be developed with Equation 28, since there is no prior certainty that  $BW \times D_T$  is at least equal to  $RB' \times VD_0$ . Moreover,  $C_{s11} \times K_{sv}$  cannot exceed  $VD_0$ . If  $BW \times D_T > RB' \times VD_0$ , this inequality applies for any vapor density less than  $VD_0$ . With representative data for  $BW$  and  $RB'$ , pathway 11 fails to provide a realistic SPPPLV if, in specified units,  $VD_0 < 4 \times D_T$ . The interpretations stated above also apply here.

#### SPECIAL PATHWAY DERIVATIONS

10. The pathways presented have been derived by the process described in paragraph 2. Somewhat more sophisticated problems have been encountered and are here discussed. The key to each pathway's formulation involves addressing the uptake situation of the item that is consumed by man.

##### Soil Ingestion by Livestock

11. Grazing animals ingest soil along with plant matter. Such soil may provide the animal with a significant amount of pollutant as compared to the

amount derived from plant matter. A quantitative comparison of the pollutant intake by a grazing animal from these two sources was formulated in the Alabama Army Ammunition Plant study.<sup>4</sup>

12. The cow is considered the animal of interest and the pathway 7 situation is first considered. A representative dairy cow on pasture ingests about 16.5 kg/day of dry plant matter and 0.72 kg/day of included soil.<sup>4</sup> For pathway 7,

$$U_{c7} = 16.5 \times C_{p7}$$

where  $U_{c7}$  is the uptake of the pollutant by the animal when  $C_{p7}$  is the pollutant level in consumed plant matter corresponding to the SPPPLV  $C_{s7}$ . Then,

$$U_{c7} = 16.5 \times C_{s7} \times K_{sp}$$

This equation is solved for  $C_{s7}$ ,  $C_{s7} = U_{c7} / (K_{sp} \times 16.5)$ , and then used in conjunction with Equation 24 to yield

$$U_{c7} = 16.5 \times BW \times D_T / (W_a \times K_{pa}) \quad (C4)$$

$U_{c7}$  is now expressed in terms of  $D_T$ . For a pathway where only soil provides the pollutant to livestock cattle, arbitrarily called pathway "x",

$$U_{cx} = 0.72 \times C_{sx} \quad (C5)$$

$C_{sx}$  denotes the soil SPPPLV for this pathway. From the pathway concept, Equations C4 and C5 can be set equal to each other, from which  $C_{sx}$  can be evaluated,

$$C_{sx} = (16.5/0.72) \times (BW/W_a) \times (K_{pa})^{-1} \times D_T$$

By use of Equation 24,  $C_{sx}$  can be expressed in terms of  $C_{s7}$ ,

$$C_{sx} = C_{s7} \times (23 \times K_{sp})$$

13. The comparable pollutant contribution from direct soil ingestion by pathway "x" would be of importance only when  $K_{sp} < 1$ . From information in Table 11, this is often not the usual situation; neglecting pathway "x" here should be a reasonable simplification. However, for situations dealing with animals other than cattle or poor quality pastures, this comparison should be reconsidered. The above treatment should prove helpful in that case.

#### Bottom-Feeding Fish

14. The Savanna Army Depot Activity, IL, has approximately 223 hectares of waterways from which fish are caught for human consumption.<sup>6</sup> Several varieties of fish caught (carp, catfish) are bottom-feeding fish. About 10 hectares of these waterway floor areas are postulated to be covered with burnt munitions residues. There was concern that humans could ingest hazardous amounts of munitions-related substances as a result of eating these fish. SPPPLVs for specific components of these residues were sought.

15. The model invoked to formulate a pathway (here called "y") included several assumptions:

a. As a worst-case situation, the consumed fish has a pollutant content  $C_{fy}$ , such that

$$W_f \times C_{fy} = BW \times D_T \quad (C6)$$

b.  $C_{fy}$  is maintained in the fish by an equilibrium between the fish's rate of uptake from sediment and the fish's rate of clearance of pollutant to water. This is not unlike the Handy and Schindler model for humans (Appendix B, paragraph 17).

c. Diet derived from sediment has the same pollutant concentration as the sediment. The uptake of pollutant in fish,  $U_{fy}$ , in mg/kg/day (fish weight basis) is related to  $C_{sy}$ , the desired SPPPLV.

$$U_{fy} = 0.06 \times 0.0405 \times C_{sy} = 2.43 \times 10^{-3} \times C_{sy} \quad (C7)$$

where 0.06 is the fraction of fish weight that is consumed daily (a 1 kg fish eats 60 g of food daily) and 0.0405 represents the fraction of waterway floor area covered with residue.\* The loss of pollutant by clearance is a first-order process dependent upon  $C_{fy}$ .

$$\text{Loss} = U_{fy} = k_2 \times C_{fy} \quad (C8)$$

Here,  $k_2$  is the clearance rate constant for this process, which can be estimated from the octanol-water partition coefficient;<sup>6</sup>

$$k_2 = \text{antilog} ( 1.47 - 0.414 \times \log K_{ow} )$$

Equations C6, C7, and C8 can be combined to eliminate  $C_{fy}$  and to express  $C_{sy}$  in terms of  $D_T$ . For  $BW = 70$  kg and  $W_f = 0.01$  kg/day,

$$C_{sy} = 2.6 \times 10^6 \times k_2 \times D_T$$

16. For the munitions products considered,  $C_{sy}$  values were found to be in excess of 100 mg/kg, well in excess of any measured levels of any residue component in sediment. Thus, it was suggested that fishing could continue without added restrictions.

\* Numerical data used here taken from the case study.<sup>6</sup>

## APPENDIX D: TECHNICAL DISCUSSION OF PARTITION COEFFICIENTS

### THE MODEL SOIL-WATER-AIR SYSTEM

1. To this point, the state of a pollutant in soil has not been of particular concern.  $C_{sol}$ ,  $VD_o$ , and  $K_{oc}$  describe the equilibrium concentration of a substance in and between different phases. The dissolved pollutant in water or the vaporized pollutant in air are fairly easy to comprehend; the pollutant in soil state is not. Figure D1 illustrates the system that is assumed to apply. The soil particles (two are shown) contain a matrix of mineral matter and SOC. The pollutant is physically sorbed on SOC, but is not associated with mineral matter to any extent. Thus, if the concentration of pollutant in soil is  $C_s$ , its concentration in SOC is  $(C_s / F_{oc})$ .\* The soil particles also contain water, which can be adsorbed from air, supplied from rainfall, or drawn from groundwater by capillary action. Whatever the source, this water supposedly coats all surfaces of the soil particle. A soil moisture content of 3 percent is sufficient to correspond to a condition where particles are covered with a monomolecular layer of water.<sup>98\*\*</sup> Unless soil has been subjected to a protracted dry spell, a 3 percent or higher moisture content can be readily maintained.  $K_{oc}$  can be interpreted as the analog in the SOC-water system to  $K_{ow}$  in the octanol-water system. However, the concentration of pollutant in water is limited by  $C_{sol}$ . Thus, if the equilibrium soil concentration of a pollutant exceeds  $C_{sol} \times K_{sw}$ , the concept of  $K_{sw}$  as a proportionality factor is no longer valid; see Figure D2.

2. The system in Figure D1 also contains air in void spaces or pores between the soil particles. At equilibrium, the density of pollutant vapor in these pores would be defined as  $C_s \times K_{sv}$ . Equation 35 allows  $K_{sv}$  to be computed; this equation incorporates two assumptions. The first assumption is that sorbed pollutant on SOC will not exert a vapor pressure in the absence of a monomolecular layer of water on soil. Based on studies of dieldrin, lindane, DDT, and DDT-related compounds reviewed by Spencer et al.,<sup>98</sup> this situation has been experimentally observed. The second assumption is that at equilibrium, the partitioning of pollutant between the water layer on soil and air in pores is characterized by Henry's Law. Then,

$$C_w / VD = C_{sol} / VD_o \quad (D1)$$

In Figure D2, the relation between  $C_w$  and  $C_s$  is shown as the linear function with slope  $K_{sw}$ ,  $0 < C_s < (C_{sol} \times K_{sw})$ . With the Henry's Law assumption above, the relation between  $VD$  and  $C_s$  is also linear in the same  $C_s$  range. As noted previously, if  $C_s > C_{sol} \times K_{sw}$ ,  $VD = VD_o$ , and  $K_{sv}$  is not a valid partition coefficient.

\* If  $K_{sw}$  has been measured, the suppositions regarding SOC need not apply.

\*\* See References section for full citation.

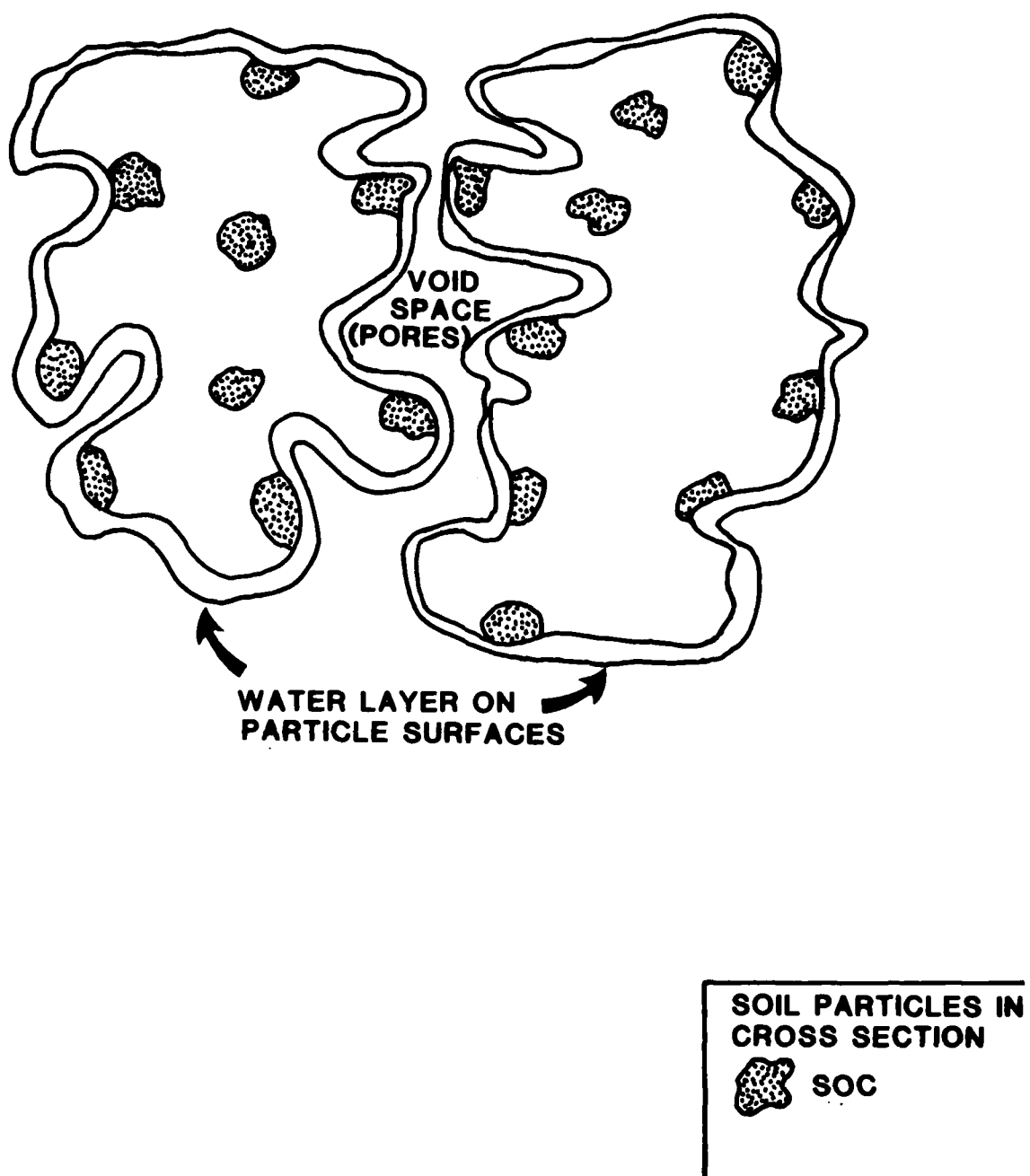


Figure D1. Physical representation of the soil-water-air system.



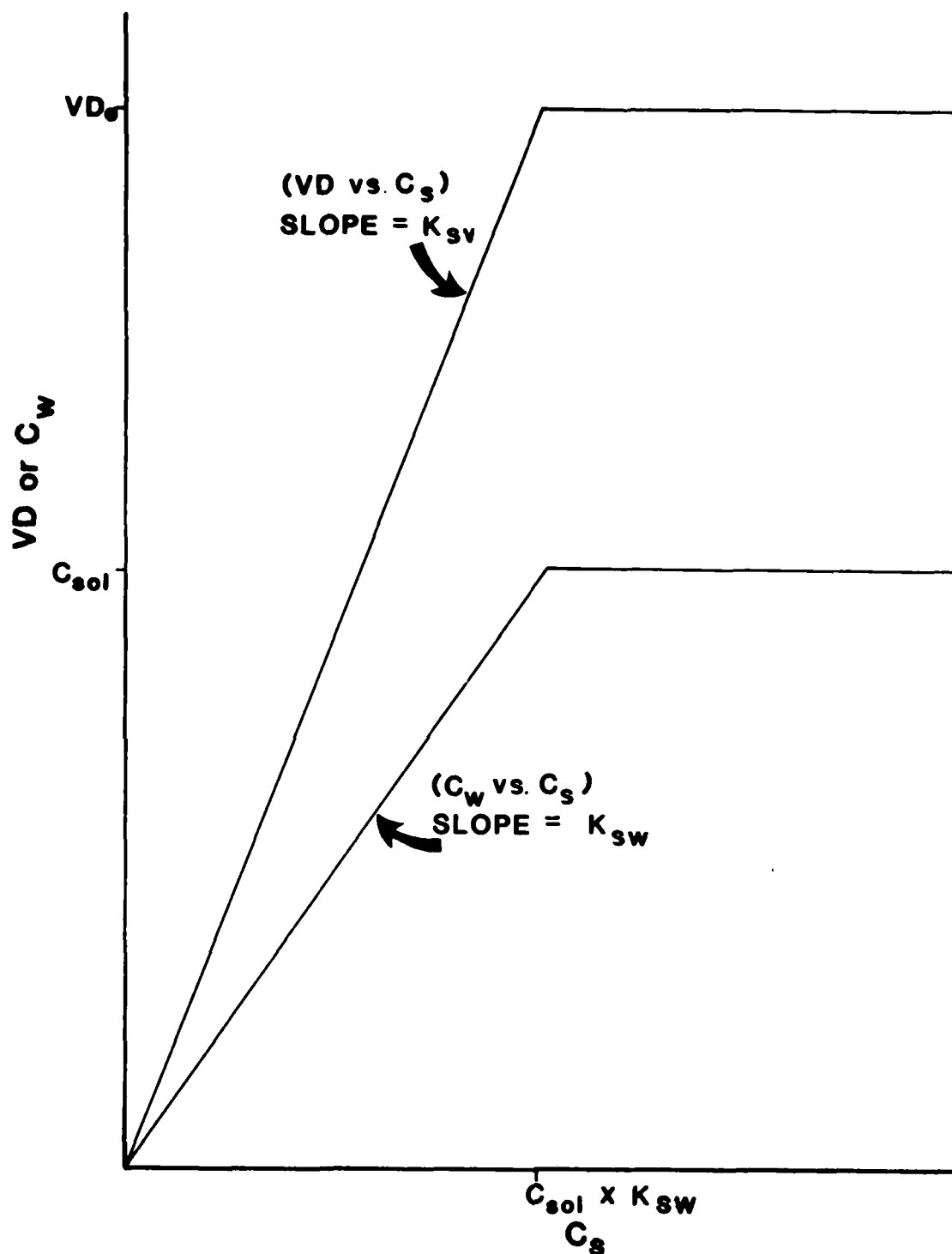


Figure D2. Relationship of partition coefficients for a pollutant in model soil-water-air system.

3. The model presented above probably does not accurately describe the behavior of highly water-soluble pollutants. As a general rule, such pollutants are polar, and their interaction with soil mineral matter may overshadow their interaction with SOC as characterized by  $K_{sw}$ . Moreover, for such pollutants, Equation D1 is usually not valid. For dilute solutions ( $< 0.1$  molar),

$$\frac{d(C_w)}{d VD} = \text{Constant}$$

but the constant is not necessarily  $C_{sol} / VD_0$ . Unfortunately, Henry's Law data for such pollutants is not extensive. Finally, since  $K_{sw}$  is approximately proportional to  $(C_{sol})^{0.5}$  (see paragraphs 71-72 m.t.), the soil-water equilibrium is adverse to soil retention; the pollutant is likely to be leached.

#### ESTIMATION EQUATIONS

4. The procedures presented in Part III are restricted to organic substances. Most of the equations presented are in the form

$$(\text{Estimate}) = \text{antilog} [a_1 + a_2 \times \log (\text{Predictor})] \quad (\text{D2})$$

The theory is developed to the point where equations of the form of D2 are expected, but not to the extent that the constants  $a_1$  and  $a_2$  can be quantified. These constants have been determined usually from correlations of paired predictor-estimate data for a group of organic compounds. As an example, Table D1 presents the compounds whose characteristics were used to generate Equations 33 and 34. Statistical summary parameters presented along with such relations may be misleading. A frequently reported parameter is the correlation coefficient. For equations derived as described here, this coefficient indicates the "fit" based only on the compounds used in formulating each equation. The coefficient cannot be used to estimate the accuracy of an estimate for a compound selected "at random." These equations are biased by the selection of compounds involved in their formulation; typical selections are often dominated by pesticides, herbicides, polychlorobiphenyl mixtures, and their precursors. Different sets of compounds can lead to markedly different relations. This is well illustrated by Figure 4-2 in CPEM.<sup>51</sup>

5. The accuracy that can be expected from equations of the form of Equation D2 is relatively poor. For example, in Figure 5-1 of CPEM,<sup>51</sup> data from 74 compounds (as dots) are graphically presented relative to Equation 31. Fifty-five of these predicted BCF values were within  $\pm$  one-half log unit of their experimentally determined values. Accuracy of this level is understandable. Organic compounds can adsorb or absorb on the mineral portion of soil. SOC, fish lipids, and animal fats contain organic compounds other than octanol. Different soils have different organic constituents represented as SOC. Animals can metabolize pollutants that would, if the model were strictly followed, only partition between compartments. Despite these drawbacks, such estimation techniques are to date the best devised. One will probably never be able to predict exactly what happens in a specific environment. Experimental observations are always preferable to predictions and the

Table D1

Chemical and Animal Data Base for Equations 33  
and 34<sup>a</sup>

Chemical <sup>b</sup>	Animal
Aldrin	Cattle/Swine
Chlordane	Cattle/Swine
DDT	Cattle/Swine
Dieldrin	Cattle/Swine
Endrin	Cattle/Swine
Heptachlor	Cattle/Swine
Methoxychlor	Cattle/Swine
Lindane	Cattle
6-Chloropicolinic acid	Cattle
Clopidol	Cattle
Chlorpyrifos	Cattle
Chlorpyrifos-methyl	Cattle
Cyhexatin	Cattle
2,4-D	Cattle
Dalapon	Cattle
3,6-Dichloropicolinic acid	Cattle
Picloram (K salt)	Cattle
Ronnel	Cattle
Silvex	Cattle
2,4,5-T	Cattle
TCDD	Cattle
Triclopyr	Cattle
3,5,6-Trichloropyridinol	Cattle

a. From Kenaga.<sup>55</sup>

b. See RTE<sup>12</sup> for generic names.

experiment perceived to best approximate the environment is preferred to others. Without experiments, the preferable estimation equation is derived from data on compounds closely related to the compound of concern or is based on a large variety of compounds.

#### PPLV PARTITION COEFFICIENTS

6. In the initial development of the approach,<sup>99</sup> the partition coefficients were simply definitions. For example, if pollutant was transferred from water to fish, the corresponding concentrations  $C_f$  and  $C_w$  were defined to be related by

$$C_f = C_w \times K_{wf}$$

Procedures to estimate the partition coefficients were left to the resourcefulness of the user. Most of the equations presented with the format of Equation D2 have been recently developed. As indicated in paragraph 67 m.t., the equations are derived for a restricted set of circumstances. As with most model situations, these circumstances may not be fully applicable to the expected environmental situation. Often, the user is faced with the choice of using these equations with this knowledge or not being able to compute SPPPLV.

7. The estimation equations presented for partition coefficients in paragraphs 72-77 are based on the assumption that equilibrium is attained between the media/organisms involved. This assumption should be valid if the expected exposure time in the environment exceeds that involved in the experimental studies from which the equations are drawn. Soil adsorption test procedures generally involve contact times of about 48 hours.<sup>54</sup> Groundwater moves relatively slowly, with flows of the order of 1 m/day. Thus, for most practical situations, groundwater should equilibrate with soil. Recommended BCF measurement procedures involve up to 28 days exposure of fish to test water.<sup>54</sup> Fish exposure to polluted water in the environment is generally for a longer period of time. Similarly, the studies employed by Kenaga<sup>55</sup> to devise Equations 33 and 34 involved a controlled diet regimen for 28 days, in which time pollutant levels in test animals reached asymptotic levels. If animals are raised in an area until their utilization (either to be slaughtered for meat or to be dairy animals), their residence time in the area is usually in excess of 28 days.

8. Scenarios may arise where equilibrium may not be expected to be attained, such as stream flow through a pollutant-contaminated area. The contact time between soil and water may be considerably shorter than 48 hours. In such case, the incorrect assumption of equilibrium will be a safe-sided error; the computed SPPPLV would be lower than one which would be computed on the basis of a non-steady state transfer model.

9. BCF (and  $K_{wf}$ ) used in Equations 13 and 14 assumes that the uptake of pollutants from water is through external membrane surfaces (gills).<sup>51</sup> In the real world, pollutants may be included in water-borne organisms that the fish consumes, or for the case of bottom feeders or scavengers, in sediment. Ingestion of such organisms can lead to a biomagnification effect. One treatment for scavengers and bottom feeders was presented in Appendix C, paragraph 15, and may be useful in modeling a pathway to account for biomagnification.

10. A partition coefficient may not specifically relate to an actual process. For example,  $K_{sp}$  nominally represents partitioning of a pollutant between soil and plant matter. As noted in Appendix E, the actual transfer may involve soil-water transport into the plants' circulatory system via the roots or absorption of vaporized pollutant into the plants' leaves. Unlike fish or livestock animals, plants do not have fat or lipid components that might provide a basis for expecting organic-water partitioning to occur. The information available is usually in the form of concurrent concentration of a pollutant in soil or water and in grown plant matter. From this measurement set, a nominal  $K_{sp}$  or  $K_{wp}$  is determined.

11. Equations 5 and 7 include the common factor  $R_1$ . In Equation 5,  $R_1$  is evaluated at a SPPPLV; in Equation 7,  $R_1$  is calculated at a PPLV. It follows that the  $K_1$  (if any) involved in  $R_1$  should not be soil or water concentration-dependent. The author suspects that this will generally not be the case, although as noted in paragraph 6, the evaluator rarely has a better approach. For example, paragraph 73 m.t. discusses the relation of  $K_{sw}$  with  $n_f$ , the Freundlich isotherm exponent. Should  $n_f \neq 1$ , the linearity assumption incorporated into Figure D2 becomes invalid ( $K_{oc}$  is not soil-concentration independent). If  $K_1$  is a function of  $C_s$  or  $C_w$ , the PPLV computation by Equation 4 is not valid. However, a trial and error approach is suggested.\*

a. Determine a "trial PPLV" from Equation 4 after computing component SPPPLVs.

b. Compute component  $D_{T1}$  from Equation 7 and a "comparison  $D_T$ " from Equation 6.

c. If the "comparison  $D_T$ "  $> D_T$ , assume a lower PPLV than the "trial PPLV" and repeat step b. If the "comparison  $D_T$ "  $< D_T$ , assume a higher PPLV than the "trial PPLV" and repeat step b.

d. The iterative execution of steps b and c can be repeated until the "comparison  $D_T$ " equals  $D_T$ . For practical purposes, the process can be terminated when the "comparison  $D_T$ " is reasonably close (say within 5 percent) of  $D_T$ .

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\* Equations 6 and 7 comprise a less restrictive method for determining a PPLV than Equation 4. Equation 4 requires  $K_1$  to be a constant; Equations 6 and 7 probably only require  $K_1$  to be a well-behaved function of  $C_s$  or  $C_w$ . The opportunity to try this approach in a practical application has not arisen.

## APPENDIX E: PLANT POLLUTANT UPTAKE FROM SOIL - AN INITIAL ASSESSMENT

by W. Dickinson Burrows, Ph.D.\*

### SEARCH STRATEGY

1. Through contacts with known experts in the United States Department of Agriculture research community, the author found that the latest and only review of uptake of organic chemicals by plants was published in 1974.<sup>100\*\*</sup> With this review at hand, a machine search was initiated to retrieve data on uptake, translocation, and metabolism of organic chemicals by plants, with emphasis on material published after 1970. Not suprisingly, nearly all citations recovered concerned commercial biocides (insecticides, herbicides, fungicides). Of roughly 1,000 references returned, only those articles were retrieved that appeared to offer quantitative data on root uptake of chemicals by plants important in the food chain or that promised to provide an insight analysis of the mechanism of uptake.

### ELEMENTS OF PLANT PHYSIOLOGY

2. Uptake of chemicals has been shown to occur through the roots, leaves, and developing shoots of plants. Although absorption through submerged portions only is of primary concern in this report, it should be noted that significant uptake of some chemicals (notably DDT)<sup>\*\*\*</sup> can occur through the leaves by reason of volatilization from the soil.<sup>100</sup> There are two principal transport systems in plants; the xylem, through which water flows, and the phloem, through which food substances pass. As will be discussed further, chemicals taken up by the plant are most readily transported in the xylem, but they can also appear in the phloem. Chemicals are commonly stored in the roots and leaves and occasionally in reproductive structures such as seeds, pomes, and tubers. One should note that the mechanics of plant metabolism and nutrient transport differ greatly from that of mammals or fish. Therefore, one should not anticipate significant bioconcentration of stable lipophilic materials such as the chlorinated pesticides and PCBs.

3. The metabolic capability of plants, as with animals, shows high specific variability, which is in part the basis for herbicide action. Although plants lack the obvious metabolic structures of animals such as the liver and kidney, they are still able to perform many complex metabolic transformations, including conjugation.<sup>101</sup> As will be discussed later, there is evidence that some plants are able to derive elemental nutrients (nitrogen,

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\*\* See References section for full citation.

\*\*\* The biocides discussed here are frequently referred to by their trade names as contrasted to their generic names. Moreover, commercial products seldom contain the generic chemical in purified form. Thus, in this appendix, trade names will be used. The RTE<sup>12</sup> can be used to determine the generic equivalent. Unusual or ambiguous names will be identified.

phosphorus, sulfur) through degradation of complex and presumably xenobiotic compounds.

#### SOIL ADSORPTION

4. For the purpose of worst-case analysis, it has been assumed that soil adsorption of organic compounds does not compete with plant uptake; a comprehensive theory will have to include considerations of soil structure and composition. Although no special effort was made during the course of this study to derive principles for soil adsorption of organic chemicals, certain rules can be postulated:

a. The availability of neutral organic compounds is inversely dependent on the organic content of the soil.<sup>100</sup>

b. The availability of charged organic compounds such as diquat and paraquat is inversely dependent on the ion exchange capacity of the soil.<sup>102,103</sup>

c. The availability of organic compounds is dependent on the water content of the soil.<sup>104</sup>

The effect of adsorption can be very significant. For example, adsorption of 2,4-dichlorophenoxyacetic acid on humic acid (as measured by the Freundlich isotherm) is ten times as great as on illite, 100 times as great as on montmorillonite, and 100 times as great as on sand.<sup>102</sup> Such order of magnitude differences generally far exceeded differences between plant species for uptake of chemicals reviewed.

#### DATA PRESENTATION

5. With few exceptions, plant uptake data are available only for organic chemicals intentionally applied to crops or soil. Thus, agricultural chemicals (chlorocarbons, triazines, phosphonates, carbamates, etc.) are fairly well covered, but there are almost no data for industrial organic compounds that may have entered soil from a chemical dump or through contaminated irrigation water.

6. The plant uptake data recovered represent both field and laboratory greenhouse studies. Worst-case plant:soil concentration ratios or plant bioconcentration factors (PBF) derived from data compiled by Nash<sup>100</sup> for a variety of field and garden crops exposed to insecticides and fungicides are presented in Table E1. These data are arbitrarily divided according to crop types in order to emphasize the relative risks engendered through different paths of consumption. Thus, leafy vegetables eaten by humans are tabulated under "leaf," while leafy plants more commonly eaten by domestic animals are listed under "forage." The sugar beet, used for both root and forage, is listed under both categories. A distinction is made between peanuts and other seeds because peanuts grow underground and may concentrate contaminants directly rather than through circulation within the plant. There are a number of considerations that limit the reliability of computed PBF values to the nearest order of magnitude. These are:

a. In many cases, field soil concentrations have been calculated from application rates (i.e. pound/acre) based on the premise that applied pesticides uniformly penetrate the first 6 inches of soil and no deeper. Evaporation, washout, and biochemical transformations are neglected.

b. In many cases, radiolabeled chemicals have been applied to the soil, and only specific radioactivity has been measured. Thus, no distinction can be made between the chemical applied and soil or plant metabolites which retain the label.

c. Some chemicals, such as aldrin/dieldrin and lindane/BHC, are applied and analyzed as mixtures, making it impractical to sort out each individual PBF.

d. Distribution of the chemical is non-uniform. Thus, lower leaves may have higher concentrations than upper leaves, and roots show higher concentrations in the outer layers. For example, the peelings of a carrot often are more contaminated than the interior portions.

e. Where similar experiments have been performed by different investigators, there is considerable scatter in derived values of PBF, although agreement is generally within  $\pm 50$  percent for the same soil type and different chemical concentrations.

f. There appears to be no consistent policy on reporting concentrations in terms of wet or dry weight, either among different investigators or by the same investigator with respect to different plant parts. Unless otherwise indicated, PBF values reported herein are presumed to be based on fresh weights.

7. Some more recent studies are summarized in Table E2 (plants in pesticide-treated soil), Table E3 (from phytotoxicity studies of chlorophenyl methyl sulfur-compounds) and Table E4 (hydroponic conditions). Values of PBF listed therein are by no means equilibrium constants; rather they represent the weight ratio of the chemical (and in most cases, metabolites thereof) in the plant or plant part to the chemical in the soil or nutrient solution at the time the sample was taken.

#### DATA INTERPRETATION

##### Effect of Solubility

8. From a limited review of the literature, it appears that a chemical contacting the roots of a plant may penetrate the outer epidermis and proceed no further, or it may penetrate to the xylem and be transported to the stem and leaves. Highly insoluble materials, such as high molecular weight chlorinated hydrocarbons, do not appear to progress much beyond the roots (except in rapidly growing seedlings), and where they are detected in the lower leaves of a plant, the exposure is suspected to be due to vaporization of the chemical directly from the soil or to splashing by rain.<sup>100</sup> This may or may not be an important distinction depending on the extent to which introduction of chemicals from contaminated soil and groundwater resembles introduction through direct application of pesticides. On the other hand, there are lipid barriers



Table E1

Worst-Case Plant Bioconcentration Factors (Wet Weight Basis)  
for Selected Insecticides and Fungicides<sup>100</sup>

Plant Part	Plant	Soil	PBF
(a) Mixture of Aldrin and Dieldrin			
Root	Carrot	Sandy loam	8.2
Seed	Peanut	Not given	5
	Soybean	Sandy loam	0.1
Fruit	Pumpkin	Clayey loam	0.08
Leaf	Kale	Silty loam	0.3
Forage	Alfalfa	Silty loam	0.3
(b) Endrin			
Root	Carrot	Sandy loam	0.5
Seed	Soybean	Sandy loam	0.2
Forage	Bromegrass	Clay	1.5
(c) Heptachlor			
Root	Carrot	Silty loam	0.8
Seed	Peanut	Not given	1
	Wheat	Not given	0.1
Fruit	Pumpkin	Not given	0.04
Leaf	Lettuce	Silty loam	0.05
Forage	Bromegrass	Clayey loam	3.2
(d) Chlordane			
Root	Carrot	Very sandy loam	0.5
Seed	Soybean	Not given	0.005
Fruit	Cucumber	Silty loam	0.008
(e) Toxaphene			
Root	Radish	Sandy loam	0.3
Seed	Cotton	Not given	0.002
(f) Lindane/BHC			
Root	Potato	Sandy loam	1.6
Seed	Soybean	Sandy loam	0.06
Forage	Corn	Hydroponic	2

Plant Part	Plant	Soil	PBF
(g) Technical Grade DDT			
Root	Carrot	Sandy loam	1.5
Seed	Peanut	Not given	0.2
	Soybean	Not given	0.07
Leaf	Rape	Not given	0.1
Forage	Corn	Sandy loam	0.5
(h) Ethylene bromide			
Root	Sugarbeet	Sandy loam	1.4
Forage	Sugarbeet	Sandy loam	0.9
(i) Diazinon			
Forage	Rice	Clay	0.2
(j) Disulfoton			
Leaf	Spinach	Not given	0.3
Forage	Pea vines	Sandy loam	0.4
(k) Phorate			
Leaf	Spinach	Not given	0.5
(l) Chlorphenvinphos			
Root	Carrot	Not given	2.6
(m) Aldicarb			
Seed	Cotton	Not given	4.5
Forage	Cotton	Not given	34

Table E2

Plant Bioconcentration Factors (Wet Weight Basis) Summarized From Selected  
Studies of Pesticides and Related Chemicals Applied to Soils

Chemical	Plant	Soil	PBF for Analyzed Plant Part			Notes	Reference
			Tops	Root	Seed		
Arochlor 1254	Soybean	Sand	0.007			a	105
	Pescue	Sand	0.09			a	105
Nitrosodipropylamine	Soybean	Silty loam	<0.03	0.3	Nil	b	106
Nitrosopendimethalin	Soybean	Silty loam	0.14	0.8	Nil	c	106
Atrazine	Sudan grass	Sandy loam	200			d,e,f	107
	Sorgham	Sandy loam	170			d,e,f	107
	Corn	Sandy loam	38			d,f	107
Ethoprop	Onion	Sand	0.09			a	108
	Carrot	Sand	0.06			a	108
	Radish	Sand	0.04			a	108
	Eggplant	Sand	0.006			a,g	108
Hydroxyatrazine	Oat	Sandy loam	0.25	0.5		h,i	109
Ethofumesate	Sugarbeet	Clayey loam	13	1.6		a	110
Ethylenebis (dithiocarbamate)	Soybean	Sandy loam	220			f,j,k	111
Ethylenethiourea	Soybean	Sandy loam	200			f,k	111
Carbofuran	Corn	Silty loam	1			1	112
BPMC <sup>m</sup>	Rice	Alluvial	2	2		n	113
IBP <sup>o</sup>	Rice	Alluvial	0.7	0.7		p	113
DIMP <sup>q</sup>	Sugar beet	Sandy loam	3.3	0.6		a,d	114
	Carrot	Sandy loam	3.5	0.7		a,d	114
	Bean	Sandy loam	6.0	4.1		a,d	114
	Wheat	Sandy loam	5.3	1.1		a,d	114
	Alfalfa	Sandy loam	1.2	0.3		a,d	114

- a. Metabolism not reported.  
b. Metabolism reported rapid in soil.  
c. 29% metabolized in 110 days.  
d. Based on total 14-C count.  
e. Significant growth inhibition noted at 0.5 ppm chemical in soil.  
f. PBF based on dry weight of plant.  
g. Fruit PBF reported.  
h. Shoots PBF reported.  
i. 100% of chemical conjugated in plant.  
j. Based on assay of manganese salt.  
k. Converted to ethyleneurea.  
l. > 90% metabolized in silage.  
m. O-sec-butylphenyl ester of methylcarbamic acid.  
n. Observed to disappear rapidly after first day.  
o. S-benzyl-0,0-diisopropyl ester of phosphorothioic acid.  
p. Observed to disappear moderately after first day.  
q. Diisopropyl ester of methylphosphonic acid.

Table E3

Plant Bioconcentration Factors (Dry Weight Basis) for Chlorophenyl Methyl  
Sulfur-Compounds in Prepared Soils<sup>115</sup>

Plant/soil	Conc. Level <sup>a</sup>	Plant Bioconcentration Factor for Cited Compound and Plant Portion					
		Sulfide		Sulfoxide		Sulfone	
		Tops	Roots	Tops	Roots	Tops	Roots
Alfalfa/ sandy loam	L	53	11	64	14	50	11
	M	154	16	231	23	135	14
	H	63 <sup>b</sup>	0 <sup>b</sup>	27 <sup>b</sup>	-- <sup>b,c</sup>	33 <sup>b</sup>	-- <sup>b,c</sup>
Corn/ sandy loam	L	25	11	31	10	38	12
	M	67	11	63	12	70	12
	H	94	20 <sup>b</sup>	115	25 <sup>b</sup>	144 <sup>b</sup>	24 <sup>b</sup>
Fescue/ sandy loam	L	120	9	94	8	108	6
	M	168	7	197	8	137	6
	H	229 <sup>b</sup>	9 <sup>b</sup>	135 <sup>b</sup>	12 <sup>b</sup>	153 <sup>b</sup>	11 <sup>b</sup>
Sugar beets/ sandy loam	L	185	18	215	20	232	17
	M	212	20	216	11	194	18
	H	175 <sup>b</sup>	4 <sup>b</sup>	-- <sup>b,c</sup>	-- <sup>b,c</sup>	104 <sup>b</sup>	-- <sup>b,c</sup>
Wheat/ sandy loam	L	92	29	79	25	93	42
	M	180	35	135	18	124	20
	H	102	16	94 <sup>b</sup>	15 <sup>b</sup>	89 <sup>b</sup>	11 <sup>b</sup>
Wheat/ loam	L	101	24	91	26	88	25
	M	208	24	220	22	208	24
	H	182 <sup>b</sup>	18 <sup>b</sup>	166 <sup>b</sup>	19 <sup>b</sup>	172 <sup>b</sup>	19 <sup>b</sup>

a. Initial soil concentrations for sulfide are expressed in terms of ranges:

L = 0.31 - 0.42 µg/g, M = 2.82 - 4.07 µg/g, and H = 10.5 - 18.2 µg/g.

Initial soil concentrations for the other compounds were:

L = 0.5 µg/g, M = 5.0 µg/g, and H = 25 µg/g.

b. Significant growth inhibition observed.

c. Plant died before experiment was completed.

TABLE E4

Plant Bioconcentration Factors for Pesticides and Related Chemicals  
From Hydroponic Culture Studies

Chemical	Plant/part	PBF	Remarks	Reference
Linuron	Soybean/root	9	a,b,c	116
	Soybean/top	8	d	117
	Soybean/root	6	e	117
	Crabgrass/top	6	d	117
	Crabgrass/root	6	d	117
Chlorpropham	Soybean/root	12	a,b,c	116
EPTC	Soybean/root	6	a,b,c,f	116
Amiben	Soybean/root	3.4	a,b,c	116
Atrazine	Soybean/root	3.6	a,b,c	116
	Barley/ts	0.75	b,c,g	118
	Barley/root	1.85	b,c	118
Hydroxyatrazine	Barley/ts	0.75	b,c,g,h	119
	Barley/ts	0.56	b,c,g,i	119
	Barley/root	2.17	b,c	118
Simazine	Barley/ts	0.90	b,c,g	118
	Barley/root	4.54	b,c	118
Atraton	Barley/ts	0.78	b,c,g,h	119
	Barley/ts	0.47	b,c,g,i	119
	Barley/root	1.28	b,c	118
Ethirimol	Barley/ts	0.09	b,c,g,h	119
	Barley/ts	0.18	b,c,g,i	119
	Barley/root	0.66	b,c	118
Diuron	Barley/ts	0.81	b,c,g	118
	Barley/root	3.10	b,c	118
2,4-D	Barley/ts	0.14	b,c,g,h	119
	Barley/ts	3.12	b,c,g,i	119
	Barley/root	8.07	b,c,g,h	119
	Barley/root	88.4	b,c,g,i	119
Pyrazon	Chenopodium/root	1.8	b,c	120
	Chenopodium/plant	0.4	j	120
	Sugarbeet/root	1.2	b,k	120
	Sugarbeet/plant	0.2	l	120
Dichlobenil	Bean/root	3.1(3.2)	m	121
	Bean/stem	2 (2.3)	m	121
	Bean/leaf	0.2(0.4)	m	121
Trichloroacetic acid	Wheat/root	1.8-4.4	n	122
	Wheat/shoot	0.7-1.6	n	122
	Wheat/plant	1 -2	n	122
	Oat/root	1 -1.6	n	122
	Oat/shoot	0.6-1	n	122
	Oat/plant	0.7-1.3	n	122
Nitrosodipropylamine	Soybean/root,shoot	2.5	o	123
Carboxin	Bean/plant	21	p	124
Oxycarboxin	Bean/plant	18	q	124
Diphenamid	Wheat/root	0.9	r	125
	Wheat/shoot	2	r	125
	Tomato/root	1	r	125
	Tomato/shoot	3	r	125

Chemical	Plant/part	PBF	Remarks	Reference
Chloroneb	Bean/root	1.5	s	126
	Bean/leaves	0.6	s	126
Thiobendazole	Pepper/leaf margin	20	t	127
	Pepper/stem	3.4	t	127
	Pepper/root	1.4	t	127
MBC	Pepper/leaf margin	24	u,v	127
	Pepper/stem	1.4	u,v	127
	Pepper/root	0.8	u,v	127
	Onion/root	0.8	b,c	128
4,4'-Diaminodiphenyl sulfone	Broadbean/ts	0.4	g	129
Sulphanilamide	Broadbean/ts	0.2	g	129
Sulphadiazine	Broadbean/ts	0.15	g	129
Sulphacetamide	Broadbean/ts	0.1	g	129
Sulphathiazole	Broadbean/ts	0.02	g	129
Griseofulvin	Broadbean/ts	0.1	g	129
Lead-EDTA chelate	Wheat/ts	0.01	g	129
DIMP	Radish/leaf	5-10	b,c,x	114
	Radish/root	1- 2	b,c,x	114
	Bean/leaf	2- 5	b,c,x	114
	Bean/fruit	0.5	b,c,x	114
	Bean/stem	0.5-1	b,c,x	114
	Bean/root	0.5	b,c,x	114
	Tomato/fruit	1.7	b,c,x	114
	Tomato/leaf	4	b,c,x	114
	Tomato/root	7	b,c,x	114
	Tomato/stem	0.7	b,c,x	114

- a. Excised root.
- b. Metabolism not reported.
- c. 14-C measured.
- d. 10-20% conversion in 1 week to demethylated linuron and dichloroaniline.
- e. No metabolism measured.
- f. S-ethyl ester of dipropylthiocarbamic acid.
- g. ts = transpiration stream
- h. Solution at pH 6.5.
- i. Solution at pH 4.
- j. Approximately 1% per hour metabolized.
- k. Tritium measured.
- l. Approximately 10% per hour metabolized.
- m. Gives indicated levels of 3- and/or 4- hydroxy derivatives and conjugates thereof in 5 days.
- n. Minor metabolism noted after 4 days, range presented, PBF inversely dependent on concentration of chemical in solution.
- o. Rapid metabolism to 99%.
- p. Oxidized to sulfoxide, hydrolyzed to aniline in roots(70% in 7 days).
- q. Hydrolyzed to aniline in roots, not leaves.
- r. Over 5 days, both plants demonstrate moderate to substantial metabolism to didemethyl diphenamid, as well as a glucose conjugate.
- s. Demethylated to phenol, which is converted to glycoside.
- t. Metabolites not identified.
- u. Methyl-2-benzimidazole carbamate.
- v. Metabolized in part to 2-aminobenzimidazole in leaves.
- x. Diisopropyl ester of methylphosphonic acid.

that must be passed by a chemical penetrating the xylem, so that a chemical must possess fat solubility in some degree to reach the transpiration stream. The PBF for 2,4-dichlorophenoxyacetic acid in the transpiration stream of barley increased at pH 4 compared to pH 6.5;<sup>119</sup> this was attributed to increased lipid solubility at the lower pH.

#### Effects of Metabolism

9. The transpiration stream is in more or less direct equilibrium with surrounding soil (or nutrient medium), and the concentration of pollutant in the stream is generally equal to or less than that in soil (or nutrient medium)<sup>118,119</sup> Chemicals in the transpiration stream may concentrate in the leaves, particularly in the leaf margins, and quite high values of PBF may be observed there. Much recent work (including most of that reported in Tables E2, E3, and E4) has used radiolabeled compounds, and in most cases no effort has been made to establish the degree of transformation. Where large PBF values are observed (based on total radioactivity), extensive biotransformation may be involved. Some metabolism may serve to provide a nutrient source for the plant, as when sulfur and/or nitrogen are removed from a chemical;<sup>111</sup> in other cases, transformation may serve to solubilize or otherwise mobilize the chemical, as when chloroneb is converted first to a free phenol and then to the glycoside in the bean plant.<sup>126</sup> Biotransformation of some systemic fungicides may be a detoxification mechanism, not by the host plant but by the infecting fungus. Rapid metabolism is not necessarily accompanied by a high PBF; nitrosodipropylamine is rapidly metabolized by soybean from soil<sup>106</sup> or nutrient solution,<sup>123</sup> but PBF values are not large (of course, it is possible that metabolism to carbon dioxide may be rapid). From a practical standpoint, metabolism cannot be systematically related to the hazard associated with chemical uptake, since metabolites may be more or less toxic to consumers than the parent chemical. Understandably, no provision for the conversion to metabolites can be proposed.

#### Effects of Phytotoxicity

10. There is no consistent relation between PBF and phytotoxicity, as is apparent from Table E3. For a given plant species, the bioconcentration of the compound in this table at a non-phytotoxic level (level "L") is approximately equal. However, as the soil content of these compounds increases to level "H," bioconcentration factors change differently for different plants. For example, alfalfa, sugarbeet, and wheat exhibit lower PBF, while for corn and fescue, PBF values increase. This latter behavior may be surprising, but it may be due to a smaller plant size rather than a larger mass of chemical assimilated.

## APPENDIX F: TREATMENT OF A UBIQUITOUS SUBSTANCE BY THE PPLV METHOD

### INTRODUCTION

1. The Alabama Army Ammunition Plant (AAAP) produced high explosives and propellants during World War II. In August 1945, munitions production ceased.<sup>4\*</sup> In 1975, this industrial property was declared excess by the U.S. Army.<sup>4</sup> Since then some parcels of land have been sold; other parcels are proposed for sale. Several areas within the tract have high soil-lead content; assays as high as 3,000 ppm have been reported.<sup>4</sup> The land areas of concern (about 94 contaminated acres) are a small fraction of AAAP property (5,168 total acres).<sup>4</sup> Moreover, metallic lead has been observed in some areas.<sup>4</sup> The lead was probably introduced by 2 modes of action: burning of scrap or off-grade propellants containing lead salts and burial of lead-lined vessels used as temporary storage containers for nitroglycerin. Elemental lead is slowly converted by environmental processes to salts.

2. A study was requested on the property from the perspective of rendering the land safe for several possible land uses. Two of the considered use scenarios are discussed here:

a. Subsistence farming involves raising the bulk of a family's dietary needs of vegetables, dairy products, and meat. The livestock (dairy and meat animals) derive their sustenance from crops grown on the land.

b. Residential housing involves plots of land for single family housing units. The plots are large enough for a family to obtain the bulk of its vegetable needs through home garden cultivation.

3. Several simplifications were made concerning these scenarios:

a. Only beef is used as a source meat and substitutes for poultry or fish.

b. Cattle are raised on pasture.

c. The background lead level in soil in the AAAP area is 30 µg/kg.

d. Any foods not derived from lead-contaminated soil may be presumed as being derived from soil with the background lead level.

e. Pica behavior is not of concern.

4. The literature on lead pollution is rather extensive. This literature suggested that procedures different from those discussed in the main text were in order. Specifically,

a. The uptake of lead in plants is not highly dependent on the lead content of soil.<sup>95</sup> Thus, a "type 2" restriction was to be anticipated.

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\* See References section for full citation.



b. Children are a high-risk group with respect to lead intake.<sup>41,95-97</sup> Thus, the target human would have different representative food intakes than presented in Part IV m.t. Fortunately, reasonably reliable data were available for the lead content in component food groups of a child's diet.<sup>43,97</sup>

c. Lead is an ubiquitous substance. Hence, those foodstuffs that are not locally produced and usually not specifically addressed in pathways had to be reckoned with, since they also contribute lead to the diet.

d. Lead transfer from soil or plant matter to the cow does not obey the partition-coefficient model implied in equations in Part III.

#### PATHWAYS

5. The pathways identified for the two scenarios are illustrated in Figure F1. Pathways 6, 7, 8, and 9 correspond with the numbering sequence in Part III. Two other pathways numbered "x" and "z" account for the uptake of lead in soil that a cow consumes during grazing activities, part of which becomes incorporated into meat and dairy products. In the subsistence scenario, pathways 6, 7, and 8 are subject to a "type 2" restriction; see paragraph 4a. Since lead is ubiquitous, other ingested foods and water contribute some lead to the human diet. These are identified as being derived from "elsewhere." The "residential housing" scenario is somewhat simpler. Two pathways are identified; pathway 6 is subject to a "type 2" restriction. In this scenario, meat and dairy products are included in foodstuffs that provide lead from "elsewhere."

#### General Strategy

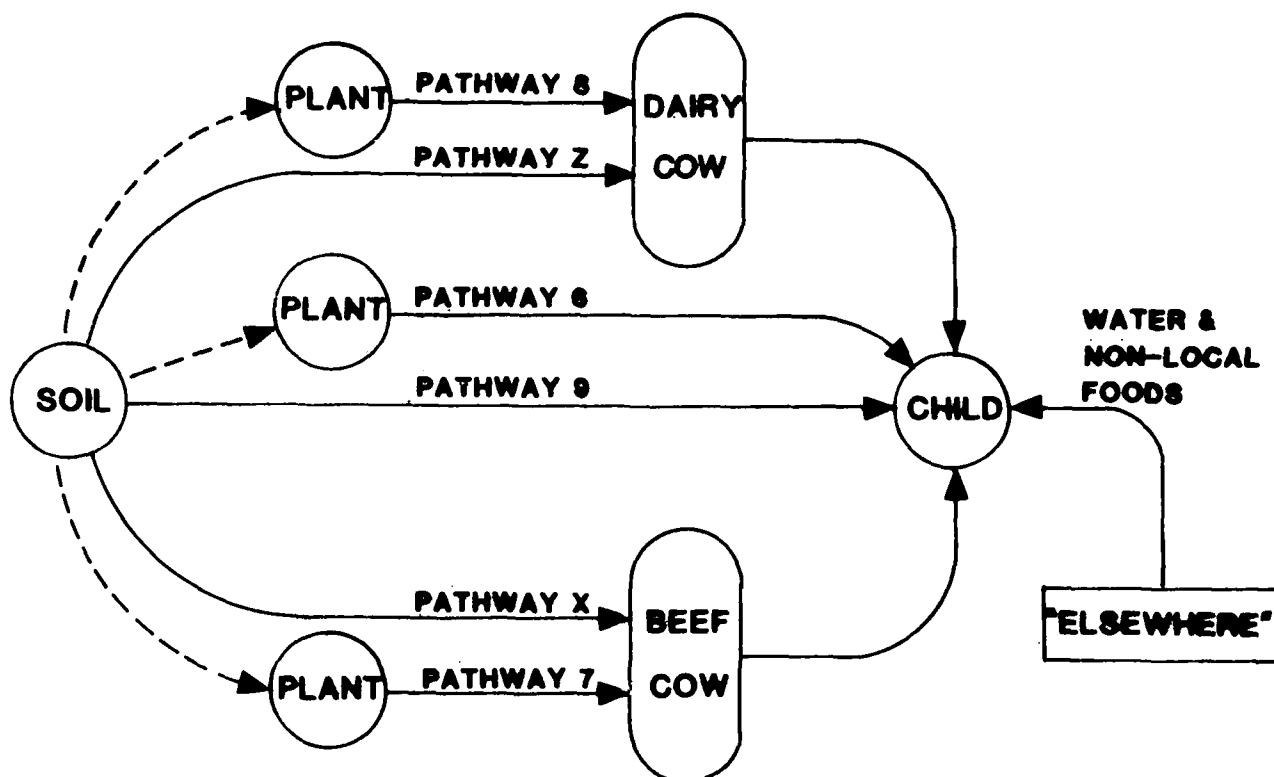
6. The PPLVs were computed from SPPPLVs for pathways 9, x, and z for the subsistence scenario and pathway 9 for the residential scenario.  $D_T$  was twice-adjusted, once for lead intake from "elsewhere" and once for lead intake via restricted pathways. In the format of Equation 43,

$$D_{Tr} = D_T - D_{Te} - D_{Tl} \quad (F1)$$

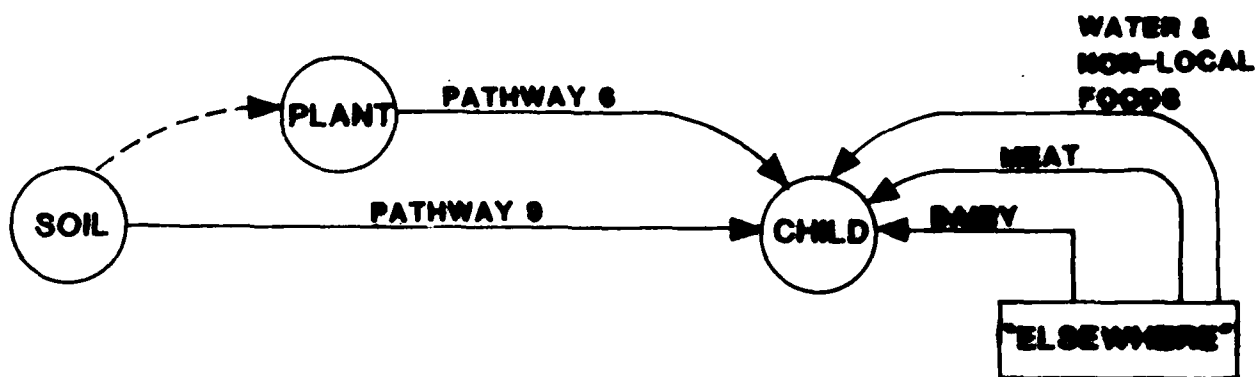
$D_T$ ,  $D_{Tr}$ , and  $D_{Tl}$  are defined as in the main text except for a unit difference (see below), and  $D_{Te}$  represents lead from "elsewhere." After accounting for  $D_{Te}$ , pathways with a common end-item consumed by a target child were treated together. In this way, the restricted pathway contribution to  $D_{Tl}$  and the equation from which a SPPPLV is computed were found.

#### VALUATION OF $D_T$ AND $D_{Te}$

7. Here,  $D_T$  will be used to indicate lead intake in  $\mu\text{g/day}$  rather than dose in  $\text{mg/kg/day}$ . This was a matter of convenience as well as in keeping with the format of reported information. An ingestion intake limit of 150  $\mu\text{g Pb/day}$  for the 2-year old child was recommended by Mahaffey.<sup>130</sup> An intake limit of 600  $\mu\text{g Pb/day}$  was suggested for adults.<sup>131</sup> A 2-year-old child consumes roughly 50 percent the mass of an adult diet, although the relative proportions of specific food groups, particularly dairy, differ. Based upon relative diet mass intake, a 300  $\mu\text{g Pb/day}$  intake level might be expected.



(a) SUBSISTENCE FARMING



(b) RESIDENTIAL HOUSING

Note: Dashed line segments indicate  
"Type 2" restrictions

Figure F1. Lead ingestion pathways for Alabama Army Ammunition  
Plant scenarios.

AD-A150 767

THE PRELIMINARY POLLUTANT LIMIT VALUE APPROACH:  
PROCEDURES AND DATA BASE(U) ARMY MEDICAL BIOENGINEERING  
RESEARCH AND DEVELOPMENT LAB FORT. M J SMALL JUN 84  
USAMBRDL-TR-8210

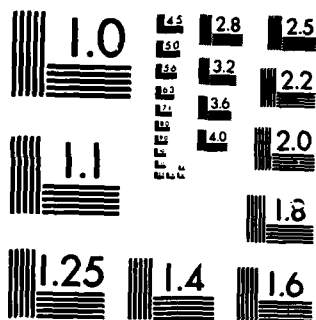
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MICROCOPY RESOLUTION TEST CHART  
NATIONAL BUREAU OF STANDARDS-1963-A

Mahaffey's more restrictive recommendation recognized the higher absorptive capacity of children for lead. The 150  $\mu\text{g}$  Pb/day value was used as the lead  $D_T$ , applicable to a model 2-year-old child of 12 kg weight.

8. Table F1 lists representative data for the daily diet of a 2-year-old child. The foods were presumed to be "table foods" as contrasted to bottled baby foods. Also included in the table are estimates of the lead content of such foods. The lead content estimates are subject to some uncertainty; see the notes in the table. One major reason for this is the accuracy and sensitivity of assay methods. Food samples often assay as "trace or undetectable;" computations that treat such qualitative results as zeros are probably underestimates. This problem is well discussed elsewhere.<sup>43,95</sup>

TABLE F1

Food Items and Their Estimated Lead Content for the Model Diet of a Two-Year Old Child

Food Item	Daily Intake, $\text{kg}^a$	Pb Content, $\mu\text{g}/\text{kg}^a$	Daily Pb Intake, $\mu\text{g}/\text{day}$
Dairy products <sup>b</sup>	0.560	50 <sup>c</sup>	28.0
Meat, fish, and poultry <sup>b</sup>	0.136	71	9.7
Grains and cereals	0.150	67	10.0
Potatoes <sup>b</sup>	0.037	48	1.8
"Other vegetables" <sup>b</sup>	0.088	200 <sup>d</sup>	17.6
Fruits	0.145	72	10.4
Oils, fats, and shortening	0.021	57	1.2
Sugar and adjuncts	0.037	56	2.1
Beverages(includes water)	0.387	21	8.1

- a. Unless otherwise specified, daily intake is from Table 8 of Kolybe et al.;<sup>43</sup> Pb content from Table 6.<sup>43</sup>
- b. Assumed derived from farming at AAAP in subsistence farming scenario.
- c. Kolybe et al.<sup>43</sup> indicates that the lead content in dairy products can range from "trace" to 90  $\mu\text{g}/\text{kg}$ , based on assumed values for "trace" assays. A 47 ppb value was reported<sup>43</sup> as an average value for raw milk, which is in line with a national average of 49 ppb reported in Lynch et al.<sup>133</sup> The 50  $\mu\text{g}/\text{kg}$  value is rounded up from these latter data.
- d. Based on average of Table 6<sup>43</sup> estimates for garden fruits and leafy, legume and root vegetables.

9. From the data in Table F1, 31.8  $\mu\text{g Pb/day}$  was estimated to be consumed in foods and water not concerned with either scenario. Moreover, the 19.4  $\mu\text{g Pb}$  associated with "other vegetables" and potatoes can be used as the intake of a target child via the restricted pathway 6. For the residential housing scenario, the 28.0  $\mu\text{g Pb}$  in dairy foods and 9.7  $\mu\text{g}$  in meat can be used to compute the lead intake of these foodstuffs from beverages and non-local foods. Thus,  $D_{Te}$  was evaluated for both pathways; 31.8  $\mu\text{g Pb/day}$  for subsistence farming and 69.5  $\mu\text{g Pb/day}$  for residential housing. Equation F1 can be restated with data from this sub-section. For the subsistence scenario,

$$D_{Tr} = 150 - (D_{Tl})_{7,8} - 19.4 - 31.8 = 98.8 - (D_{Tl})_{7,8} \quad (F2)$$

where the "7,8" subscript indicates that these pathways are involved in the determination of  $D_{Tl}$ . For the residential scenario,

$$D_{Tr} = 150 - 28.0 - 9.7 - 19.4 - 31.8 = 61.1 \mu\text{g Pb/day} \quad (F3)$$

#### LEAD IN PLANT MATTER

10. A 1980 National Academy of Sciences report<sup>95</sup> summarized many plant studies; in general, the lead content in plants appears dominated by uptake processes from the air rather than from the soil. As a specific example, Chaney et al.,<sup>132</sup> have studied the lead content of collard greens grown in gardens in the Baltimore area. A correlation between lead in leaves (dry-weight basis) and the lead in garden soil was

$$C_p = 6.26 + 3.2 \times 10^{-4} \times C_s \quad (F4)$$

As an example of the lack of sensitivity of  $C_p$  to  $C_s$ , when  $C_s = 1,000$  mg/kg, Equation F4 predicts  $C_p = 6.58$  mg/kg. Collard greens are about 86 percent water.<sup>40</sup> Thus, a  $C_p$  of the order of 6.3 mg/kg content translates to about 900  $\mu\text{g/kg}$  on a wet-weight basis. This is high when compared to data for vegetable matter in Table F1, but not extremely so. Dry-weight basis for plants is commonly employed in the dairy and livestock industry for equating animal feed requirements from alternative sources. For model purposes, the lead content in plant matter used as livestock feed was set at 5 mg Pb/kg, dry weight basis.<sup>4</sup>

#### PATHWAY EQUATION EVALUATIONS

##### Dairy Products

11. The procedure started with the relation

$$D_{Tr} + (D_{Tl})_8 = W_d \times C_{dz} \quad (F5)$$

where  $W_d$  is the daily intake of dairy products for a 2-year-old child.  $C_d$  had to be expressed in terms of lead in the cattle diet, which involves plant matter (of lead content 5 mg/kg) and included soil. The simplest such expression was

$$C_d = A \times U_c \quad (F6)$$

where  $U_c$  is the daily intake of lead by the cow in  $\mu\text{g/day}$  and  $A$  is a constant to be evaluated. Lynch et al.,<sup>133</sup> have shown that there is a correspondence between  $C_d$  and  $U_c$ . Specifically, a pair of lactating cows were fed a dose of  $11 \text{ mg Pb}(\text{CO}_3)_2 / \text{kg body weight /day}$  for 14 days. At the end of 14 days, the lead content in their milk averaged 1,520 ppb vs. 43.6 ppb in milk of control cows. In the subsistence farming scenario, the lead would come from soil and plants. The lead intake via plants is assumed to be relatively insensitive to  $C_s$ ; the lead intake via soil is directly related to  $C_s$ . Thus, Equation F5 can be expanded to

$$C_d = A (C_p \times U_{cp} + C_s \times U_{cs}) \quad (\text{F7})$$

where  $U_{cp}$  and  $U_{cs}$  denote the  $\text{kg/day}$  of dry plant matter and dry soil ingested by a dairy cow. The term  $(C_p \times U_{cp})$  in Equation F7 corresponds to pathway 8; the term  $(C_s \times U_{cs})$  corresponds to pathway z. Estimates of  $U_{cp}$  and  $U_{cs}$  of 16.5  $\text{kg/day}$  and 0.72  $\text{kg/day}$  were employed.<sup>4\*</sup> Equation F7 then can be written

$$C_d = A (82.5 + 0.72 \times C_s) \quad (\text{F8})$$

12. The constant  $A$  was estimated by assuming that Equation F8 predicts  $C_d = 50 \text{ } \mu\text{g Pb/kg}$  (see Table F1) for  $C_s = 30 \text{ mg Pb/kg}$ , the background lead content in AAAP soil. Then  $A = 0.48$ , and

$$C_d = 39.6 + 0.346 \times C_s \quad (\text{F9})$$

It should be cautioned that Equation F7 is an unproved model and that the constant  $A$  was estimated with somewhat contrived data. Plant, milk, and soil data in the AAAP area should form a more reliable basis and should be sought before a decision concerning farming is made. From the SPPPLV concept, when  $C_s = C_{sz}$ ,  $C_d = C_{dz}$ . Equation F5, with substitution from Equation F9 and  $W_d = 0.56 \text{ kg/day}$ , becomes

$$D_{Tr} + (D_{Tl})_8 = 22.0 + 0.194 \times C_{sz}$$

The 22  $\mu\text{g Pb/day}$  component represents lead intake which is derived from plant matter ingested by the dairy cow. The other component,  $0.194 \times C_{sz}$ , represents the lead intake which is derived from soil ingested by the dairy cow. Thus,

$$(D_{Tl})_8 = 22.0 \quad (\text{F10})$$

$$D_{Tr} = 0.194 \times C_{sz} \quad (\text{F11})$$

Equation F11 was the SPPPLV relation used for pathway z.

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\* Numerical data used here and in subsequent paragraphs are taken from the AAAP study.<sup>4</sup>

## Meat

13. A more complex approach was employed for the SPPPLV of pathway "x." Like other heavy metals, lead accumulates in animals, and is preferentially retained in specific organs of animals. Since livestock cattle are usually slaughtered at a pre-determined age, the lead content in meat can be expected to depend upon animal age. With representative values of factors which express the relative accumulation of lead and the retention of lead in specific organs, the lead content in meat can be quantitatively estimated.

14. The analog to Equation F5 is

$$D_{Tr} + (D_{Tl})_7 = W_m \times C_{ax} \quad (F12)$$

where  $C_{ax}$  is the lead concentration in meat (in  $\mu\text{g/kg}$ ) corresponding to  $C_{ax}$ . For calculation purposes, livestock would be raised for 2 years, of which 530 days would be spent in the field consuming pasture at an uptake rate of  $U_c$  (from paragraph 11, 16.5 kg/day of dry plant matter and 0.72 kg/day of soil). The retained lead was estimated to be 1.5 percent of that ingested. The accumulated lead in the slaughtered animal,  $L_a$  in  $\mu\text{g Pb}$ , is

$$L_a = 0.015 \times 530 \times U_c \times 1000 = 7950 \times U_c \quad (F13)$$

15. "Meat" was considered to comprise 70 percent muscle and 30 percent fat. Lead was preferentially retained in the liver, kidney, and bones of the cow; no lead was expected to be retained in body fat. Muscle was assumed to have the lead content of other portions of the animal not specified above. A hypothetical livestock animal was estimated to include 88 kg weight of liver, kidneys, and bones and 318 kg of other non-fat matter. Liver, kidneys, and bone were estimated to have 75 times the concentration of non-fat matter portions of the cow. A mass balance incorporating this degree of lead-preference indicates that

$$L_a = 75 \times 88 \times C_{am} + 318 \times C_{am} = 6918 \times C_{am} \quad (F14)$$

where  $C_{am}$  represents the lead content in "other non-fat matter" and has units of  $\mu\text{g Pb/kg}$ .

16. Equation F13 and F14 can be combined to eliminate  $L_a$ :

$$C_{am} = 1.15 \times U_c \quad (F15)$$

Since meat was assumed to be 70 percent muscle,  $C_{am}$  can be replaced in Equation F15 by  $C_a$ ;

$$C_a = 0.805 \times U_c \quad (F16)$$

$U_c$  can be expressed in terms of its plant and soil components; see paragraph 11. Inserting these in Equation F16, the analog of Equation F9 results;

$$C_a = 66.4 + 0.58 \times C_s \quad (F17)$$

Equation F17 can be inserted in Equation F12 and solved for  $C_a = C_{ax}$ . By the argument presented in paragraph 12,



$$(D_{T2})_7 = 9.0 \quad (F18)$$

$$D_{Tr} = 0.079 \times C_{sx} \quad (F19)$$

Equation F19 was the SPPPLV relation used for pathway x.

#### Soil Ingestion

17. The SPPPLV equation for pathway 9 was easily derived

$$D_{Tr} = 0.1 \times C_{s9} \quad (F20)$$

#### PPLV EVALUATION

##### Residential Scenario

18. Figure F2 reproduces the situation shown in Figure F1 with the requisite information needed to compute PPLVs. Equations F3 and F20 were combined to evaluate the required PPLV directly.

$$61.1 = 0.1 \times C_s$$

or the PPLV = 611 mg Pb/kg.

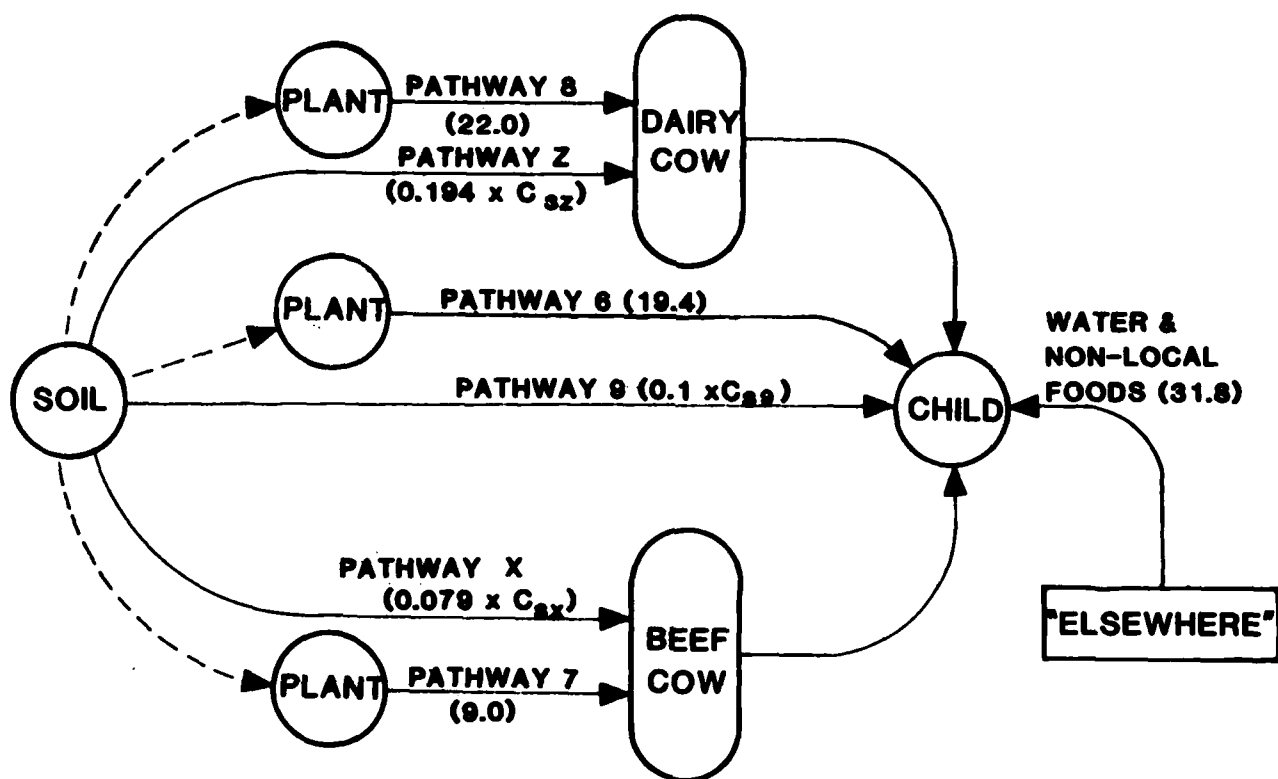
##### Subsistence Farming

19. Equations F2, F10, and F18 provided the needed data to evaluate  $D_{Tr}$ ;  $98.8 - 22 - 9.0 = 67.8 \mu\text{g Pb/day}$ . The SPPPLVs for pathways 9, x, and z (Equations F20, F19, and F11) were respectively, 678, 858, and 349 mg/kg. The PPLV was thus computed as 182 mg/kg.

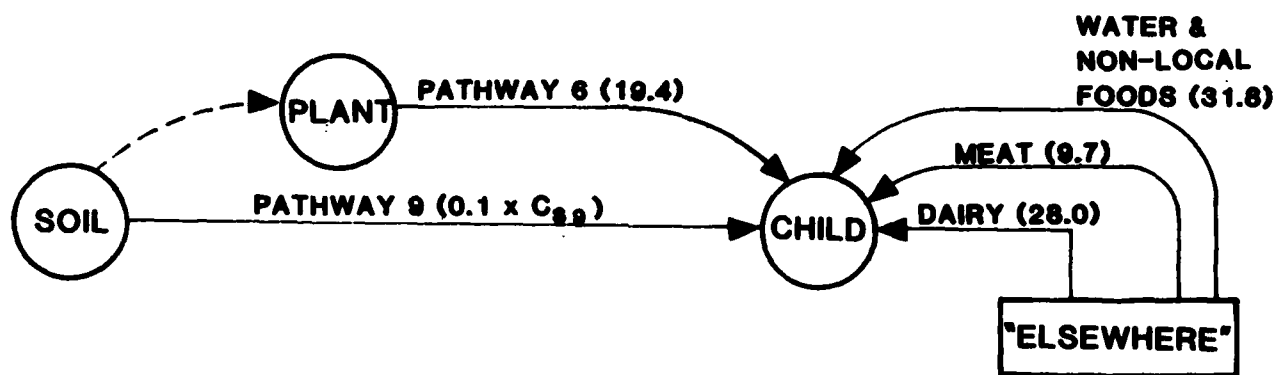
#### COMMENTS

20. The specific approach used for lead in paragraph 6 should be useful for other ubiquitous substances provided that sufficient information is available to evaluate dietary components. The  $D_T$  used here was 150  $\mu\text{g Pb/day}$ ; previously 125  $\mu\text{g Pb/day}$  was used.<sup>4</sup> The author believes, in retrospect, that the arguments advanced for the lower  $D_T$  were not that compelling. Since there are considerable deductions from  $D_T$  (Equation F1), the 25  $\mu\text{g Pb/day}$  difference caused a considerable change in results. For example, the residential pathway PPLV was 611 mg Pb/kg here, 338 mg Pb/kg previously.<sup>4</sup>

21. The approach used to model lead intake in an animal, paragraphs 13-16, is the most complex discussed in the report; again, the background information is available for its application. As an alternative treatment, one could follow the procedure used for the dairy pathways. In this treatment, the meat analog equation to Equation F8 is solved subject to  $C_a = 70 \mu\text{g/kg}$  when  $C_s = 30 \text{ mg/kg}$  (see Table F1). The resulting SPPPLV for pathway "x" is 1030 mg/kg, and the resulting subsistence scenario SPPPLV is 192 mg/kg. The agreement between alternative approaches is rather good.



(a) SUBSISTENCE FARMING



(b) RESIDENTIAL HOUSING

Note: Values in braces are in  $\mu\text{g Pb/day}$

Figure F2. Evaluation of lead ingestion pathways for Alabama Army Ammunition Plant scenarios.

## APPENDIX G: POPULATION FACTORS FOR SCENARIOS

1. This appendix presents methods to estimate the population densities (persons/land area) that could be involved in scenarios. A decision to pursue a land-renovation option involves a cost to the Army that is ultimately financed by the general public. Some benefit should be derived from this decision; ideally some ratio of benefit to cost should be optimized. One variable in an optimization analysis would be the population that is expected to benefit. The second use of population factors is in a decision to set an ARL (paragraph 19 m.t.) for a pollutant. The lower the risk for a given pollutant situation, the higher the cost to achieve that risk level. As a qualitative observation, the ARL for a small population that derives benefit from a specific land renovation option should be higher than that for a large population. The population potentially involved is then a factor in deciding the risk level.

2. The population densities derived may be considered of "ball-park" accuracy. One never knows the actual population density of a scenario situation until the scenario becomes a reality. There are many factors that could be considered in these estimates, and the user will have to exercise best judgment in dealing with them.

### HOUSING SCENARIOS

3. Scenarios wherein land areas are converted to subdivisions have been previously addressed.<sup>4\*</sup> If the area in question is subject to county or city zoning, the appropriate zoning board can be consulted to provide information. In the absence of this, housing unit density data in Table G1 can be used for estimation purposes. A single family housing unit may be assumed to be occupied by four persons. Apartments are perhaps more likely to be inhabited by groups such as newly-weds, retirees, or cohabiting single adults. In this case, perhaps two or three people per housing unit is more appropriate. The range of densities for each description reflects the availability of land in different locales and contemporary styles of housing development design. The data in Table G1 account for adjacent open areas and roadways but not for non-residential land areas such as shopping areas or schools.

### FARMING SCENARIOS

4. Three estimates relating to specific pathways are discussed here. The first is the use of land to provide vegetables for human consumption (pathway 6). The second is the use of land to provide crops for domesticated animals that in turn provide meat for the human diet (pathway 7). The last is the use of land to provide crops for cows that provide dairy products (milk) for the human diet (pathway 8).

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\* See References section for full citation.

Table G1

Typical Residential Density Levels

Description	Units/Ha <sup>a</sup>
Single family, detached, one floor	2.5 - 9.4
Single family, duplex or townhouse, one floor	4.9 - 9.6
Single family, detached, two floors	4.9 - 9.9
Single family, duplex or townhouse, two floors	9.1 - 11.9
Walk-up, two-story garden apartment	9.6 - 12.4
Three-story walk-up garden apartment	12.1 - 14.8
Four-story walk-up garden apartment	13.6 - 16.1
Apartments with elevator service:	
6-story	14.6 - 17.0
8-story	15.3 - 17.8
10-story	16.1 - 18.5
18-story	20.3 - 20.8

a. Values are taken from HUD Training Manual "Land Use Intensity Range for Various Building Types".<sup>134</sup> Values in document are in units/acre author has converted them to units/ha.

**Vegetables**

5. Table G2 presents representative yield data for selected vegetables from AGST.<sup>37</sup> This reference also has data on a state-by-state basis. Local county extension agents can provide more specific information. Also presented in Table G2 are the per capita vegetable consumption data of Table 8, expressed here on an annual basis. The population that can derive its yearly diet of a specific vegetable from a given land area is:

$$\text{People/ha} = (\text{Yield/ha}) / (\text{Consumption/person yearly})$$

These values are also presented in Table G2. A composite population density based on land providing all these foodstuffs can be computed on the basis of these people/ha estimates with adjustment to a vegetable consumption rate of 0.459 kg/day (paragraph 59 m.t.). The density computed is 153 persons/ha.

Table G2

Representative Vegetable Yield Data and Population Supported per Hectare at  
Per Capita Consumption Rates

Vegetable	Yield kg/ha	Per Capita Consumption, kg/year	Persons/ha	Table in AGST, <sup>38</sup> Year, <sup>a</sup> and Notes
Cabbage	26,900	4.74	5,700	213, 1970
Carrots	29,400	4.02	7,400	217, 1970
Celery	59,600	3.65	16,000	221, 1970 <sup>b</sup>
Corn	3,600	7.30	490	35, 1970
Cucumbers	11,700	5.11	2,270	226, 1971
Lettuce	24,700	10.6	2,340	234, 1970, escarole not included
Onions	35,600	4.02	8,900	237, 1973
Snap beans	4,900	4.02	1,220	206, 1972 <sup>c</sup>
Tomatoes	16,500	8.03	2,050	257, 1970
White potato	28,700	53.3	540	242, 1970

a. Lowest yield of the 1970-1973 period cited; author has converted data to kg/ha.

b. 20 kg/bushel useful weight assumed.

c. Values in table given for fresh and processed beans; average used here.

#### Livestock for Slaughter

6. Only cattle and swine are addressed, since they are the two mainstays of the average American meat diet. For simplicity, a limited number of alternative livestock production scenarios are presented. Factors that need to be defined in the determination of population density in terms of human meat consumption needs include: selection of feed for the animal, yield of feed from the land, consumption of feed by livestock, age and weight of a slaughtered animal, the amount of useful meat from a slaughtered animal, and the consumption of meat by human beings. These factors are highly interrelated.

7. The simplest case is pasture-fed cattle. A beef cow can be raised on 1 acre (0.405 ha) of well-managed, well-watered pasture.<sup>135</sup> This approximates an "ideal situation;" 2 acres (0.81 ha) or more of uncultivated pasture may be required per animal in an area with sufficient rain, while cattle-raising on range pasture (common in the Upper Plains or Inter-mountain West) can involve 10 acres (4.05 ha)/animal.<sup>135</sup> A pasture-fed animal takes about 21 months to reach a 900-pound (408 kg) weight.<sup>135</sup> Taking into account seasonal factors (21 months time includes at least one winter during which stored plant feed supplements may be required), and allowing for less-than ideal conditions, 1 hectare should be a representative area to feed one cow, which is available for slaughter at the end of 2 years.

8. A 408 kg animal provides about a 55 percent meat yield (excluding the organic cuts) or about 224 kg of meat.<sup>135</sup> The representative per-capita meat consumption of 0.21 kg/day corresponds to 77 kg/year. The computation of population supported in terms of land use is:

$(112 \text{ kg meat per year per ha}) / (77 \text{ kg/year per person}) \text{ or}$

1.46 persons/ha. This does not take into account the maintenance of a breeder herd if the animals are bred at the same area. Since cows usually breed 1 animal per birth with a 285 day gestation period, the presence of breeders could considerably reduce the density computed.

9. A second case is that of cattle raised on a prepared plant feed diet, or "feedlot conditions." Such cattle can attain a weight of 1,000 pounds (454 kg) in 12 months.<sup>136</sup> The feed is a combination of grain, hay, and/or silage. The quantity of feed is a function of animal age and weight. An estimation of the total feed requirements throughout the animal's lifetime is the daily ration at time of slaughter applied over a 6-month period. The ration factor overestimates true consumption, but the time factor underestimates true lifetime. One such ration is 20 pounds (9.07 kg) of corn and 10 pounds (4.54 kg) of hay daily,<sup>135</sup> which would translate to a lifetime feed requirement of 1,655 kg of corn and 829 kg of hay for an animal.

10. "Corn" referred to above is considered a dry feed such as shelled corn or ground corn-cobs. An adjustment is needed between husked fresh corn and dry feed to account for different water content levels. Based on conversions in AGST,<sup>37</sup> 2.5 kg of husked fresh corn produces 1 kg of feed corn. Based on 1970 data, the average corn yield in the United States was 72.4 bushels/acre<sup>37</sup> or 5,670 kg/ha. In terms of dry corn feed, this is about 2,270 kg/ha. Yields for dry hay are also available in AGST;<sup>37</sup> a yield of 2.06 tons/acre (4,620 kg/ha) is used in computations. Thus, the feed needs for one animal requires use of about 0.91 ha of land.

11. A 454-kg animal provides about 250 kg meat on a 55 percent yield basis. Given a per-capita meat consumption of 77 kg/year, the population density for this case is

$(250 \text{ kg meat per year/ } 0.91 \text{ ha}) / (77 \text{ kg/year per person}) \text{ or}$

3.6 persons/ha. Again, this does not include land requirements for a breeder herd.

12. The final case addressed is swine production. Input data relative to swine production are:

a. A pig can be raised to slaughter at 220 pounds (100 kg) in 5 months.<sup>137</sup> The slaughtered animal will provide about 84 pounds (38 kg) of useful meat.<sup>49\*</sup>

b. Based on weight-gain information by Baker and Juergenson,<sup>137</sup> swine raised as above, in their lifetime, consume three times their weight at slaughter in feed. This corresponds to 300 kg feed per animal. If shell corn (a common pig feed) provides the bulk of this diet, 0.13 ha of land are required per animal.

These values are scaled to a 1-year basis. The meat yield from 12/5 or 2.4 animals is 91.2 kg/year. The corn consumed by 2.4 pigs requires 0.32 hectares of land. Thus, one hectare of land provides 285 kg/year of meat. The estimated population density is

$$(285 \text{ kg meat per year per ha}) / (77 \text{ kg/year per person}) \text{ or}$$

3.7 person per ha. Pigs have multiple birth litters (eight or more is not uncommon) and a gestation period of about 4 months. Thus, land needs for breeder sows and boars is less important than for cows and bulls.

#### Dairy Farming

13. The approach to dairy-based population density estimates is somewhat different from those above because a dairy cow is a mature animal with a multi-year lifetime. A mature dairy cow that has been well-raised should weigh at least 1,000 pounds (454 kg) and, depending upon breed, usually in excess of 1,500 pounds (680 kg).<sup>138</sup> For computations a 1,320 pound (600 kg) animal is considered. Dietary needs of a dairy cow are about 25 g of dry weight feed per kg body weight<sup>38</sup> or for this model situation, 15 kg/day. As was the case with beef cattle, dairy cattle can be raised on several different diets. For discussion, the 2:1 corn to hay diet employed previously will be used. The weights of feeds are 10 kg corn and 5 kg hay per day or, on an annual basis, 3,650 kg corn and 1,825 kg hay. From the yield values used before, one dairy cow requires the produce from 2.0 ha of land.\*\* Milk yields depend upon breed; a representative yield from a relatively productive animal is 11,000 pounds/year (5,000 kg/year).<sup>136</sup> From paragraph 60, m.t. the annual representative consumption rate is 168 kg. The population density is then computed at

\* "Useful meat" refers to hams, roasts, butts, chops, sausage, and cuts other than bacon or lard. The author believes these selected cuts best represent the meat yield from a hog in terms of substitution of pork cuts for cattle cuts. For reference, the hypothetical meat yield from the hog is 135 pounds (61.2 kg) of which 20 pounds (9.1 kg) is bacon and 31 pounds (14.0 kg) is lard.<sup>49</sup>

\*\* Dairy cattle may be raised on pasture. There are several problems involved with this that cannot be easily accounted for.<sup>36</sup>

$$(5,000 \text{ kg milk}/2.0 \text{ ha}) / (168 \text{ kg/person}) = 14.9 \text{ persons/ha.}$$

Estimators may wish to account for other aspects of dairy cow farming. For example, in the first 3 years of a dairy cow's life, no milk production occurs. The useful life of a dairy cow for milk production is about 3 to 7 years. On the other hand, spent milk cows can be slaughtered for meat while calves can be slaughtered to produce veal meat. These factors tend to counterbalance each other.



## APPENDIX H: NOTATION

1. Unconventional symbols and acronyms used in this report are defined in this Appendix. Due to the length of the listing, the footnotes appear here:

\* See References for full citation.

\*\* Unless otherwise specified, see variable "i" for pathway numbering system. For example,  $C_{a7}$  would be the pollutant content in an animal corresponding to the SPPPLV for pathway 7 (meat from animals fed crops raised in contaminated soil).

$a_1, a_2$	Constants in Equation D2
A	Proportionality constant between lead content in dairy and in soil, $\mu\text{g/L}$ per $\text{mg/kg}$
AA	Efficiency of absorption of pollutant to bloodstream via respiratory system
AO	Efficiency of absorption of pollutant to bloodstream via gastrointestinal system
ADI	Acceptable Daily Intake, $\text{mg/kg/day}$
AH8	Agriculture Handbook Number 8 <sup>40*</sup>
AAAP	Alabama Army Ammunition Plant
AGST	Agricultural statistics <sup>37*</sup>
ARL	Acceptable risk level
B	Proportionality constant between lead content in meat and soil, $\mu\text{g/kg}$ per $\text{mg/kg}$
$B_A$	Risk-dose proportionality factor for a specific tumor
$B_{A\text{max}}$	Maximum value of $B_A$ for a set of tumors
$B_H$	Human risk-dose proportionality factor
BW	Adult human body weight, kg
$BW_C$	Child body weight, kg
BCF	Pollutant bioconcentration factor in fish, $\text{mg/kg fish per mg/L water}$
BDB	Biology Data Book <sup>36*</sup>
$C_1$	Water Quality Criteria based on ingestion of fish, $\text{mg/L}$

$C_2$	Water Quality Criteria based on ingestion of fish and water, mg/L
$C_a$	Pollutant concentration in livestock or dairy-producing animal, mg/kg ( $\mu\text{g/Kg}$ in Appendix F)
$C_{ai}$	$C_a$ corresponding to SPPPLV for pathway i,** mg/kg ( $\mu\text{g/L}$ in Appendix F)
$C_{am}$	Lead content in livestock animal muscle, $\mu\text{g/kg}$
$C_{ax}$	$C_a$ corresponding to SPPPLV for pathway x, $\mu\text{g/L}$ (Appendix F)
$C_d$	Pollutant concentration in dairy product, mg/L ( $\mu\text{g/L}$ in Appendix F)
$C_{dz}$	$C_d$ corresponding to SPPPLV for pathway z, $\mu\text{g/L}$ (Appendix F)
$C_f$	Pollutant concentration in fish, mg/kg
$C_{fd}$	Pollutant concentration in food diet for mammalian bioassay, mg/kg
$C_{ff}$	$C_f$ corresponding to a PPLV, mg/kg
$C_{1f}, C_{2f}$	Pollutant concentration in fish corresponding to $C_1$ and $C_2$ in water, respectively, mg/kg
$C_{fy}$	$C_f$ corresponding to SPPPLV for pathway y, mg/kg
$C_h$	Pollutant concentration in human body, mg/kg
$C_{il}$	Pollutant concentration in matter consumed by human in pathway i** subject to "type 2" restriction, mg/kg or mg/L.
$C_p$	Pollutant concentration in plant matter, usually dry weight, mg/kg
$C_{pf}$	$C_p$ corresponding to a PPLV, mg/kg
$C_{pi}$	$C_p$ corresponding to a SPPPLV for pathway i, mg/kg
$C_s$	Pollutant concentration in soil, mg/kg
$C_{se}$	$C_s$ in equilibrium with $C_{we}$ in isotherm study, mg/kg
$C_{sf}$	Soil PPLV, mg/kg
$C_{si}$	Soil SPPPLV for pathway i, mg/kg**
$C_{ss}$	Dust concentration in air, $\text{mg/m}^3$
$C_w$	Pollutant concentration in water, mg/L
$C_{we}$	$C_w$ in equilibrium with $C_{se}$ in isotherm study, mg/L
$C_{wf}$	Water PPLV, mg/L

$C_{wi}$	Water SPPPLV for pathway i, mg/kg**
$C_{wt}$	Pollutant concentration in water toxic to fish, mg/L
$C_{sol}$	Pollutant solubility limit in water, mg/L
CAS	Chemical Abstracts Service
CPEM	Chemical Property Estimation Methods <sup>51*</sup>
D	Lifetime adjusted dose, mg/kg/day
$D_T$	Pollutant acceptable daily human dose, mg/kg/day ( $\mu$ g/day in Appendix F)
$D_{Tc}$	$D_T$ based on carcinogenic considerations, mg/kg/day
$D_{Te}$	$D_T$ from nonpathway related sources, $\mu$ g/day
$D_{Ti}$	Portion of $D_T$ provided by pathway i** for PPLV
$D_{Tl}$	Dose provided by pathways subject to "type 2" restrictions, mg/kg/day ( $\mu$ g/day in Appendix F)
$D_{Tn}$	$D_T$ based on toxicological considerations, mg/kg/day
$D_{Tr}$	$D_T$ reduced for "type 2" restrictions and nonpathway-related intake, mg/kg/day ( $\mu$ g/day in Appendix F)
DE	Equivalent daily dose in bioassay test, mg/kg/day
DTLV	Documentation of the Threshold Limit Values <sup>13*</sup>
EPA	Environmental Protection Agency
F	Diet consumed daily as a fraction of body weight
$F_a$	Fraction of fat in livestock or dairy
$F_f$	Fraction of lipids in fish
$F_w$	Fraction of year during which dust can occur
$F_{oc}$	Fraction of organic carbon in soil
FL	Selected feeding dose level for $D_T$ estimate by Equation 10, mg/kg/day
FAO	Food and Agricultural Organization, United Nations
H	Henry's Law Constant $m^3$ air/L water

i	Pathway index with specific assignments of:
	<ul style="list-style-type: none"> <li>1 Drinking water</li> <li>2 Eating fish</li> <li>3 Eating vegetables irrigated with contaminated water</li> <li>4 Eating meat from animals fed irrigated crops</li> <li>5 Eating meat from animals who drink irrigation water</li> <li>6 Eating vegetables raised in contaminated soil</li> <li>7 Eating meat fed crops raised in contaminated soil</li> <li>8 Eating dairy products from animals fed crops raised in contaminated soil</li> <li>9 Ingestion of s</li> <li>10 Inhalation of dust</li> <li>11 Inhalation of vapors</li> <li>x Similar to 7, except that pollutant is in soil ingested by animal</li> <li>y Eating fish who feed on organisms in sediment</li> <li>z Similar to 8, except that pollutant is in soil ingested by animal</li> </ul>
IF <sub>i</sub>	Intake factor for pathway i,** units vary
k <sub>2</sub>	Clearance rate constant for pollutant from fish to clean water, day <sup>-1</sup>
k <sub>f</sub>	Freundlich isotherm coefficient
K <sub>i</sub>	Overall pollutant partition coefficient for pathway i,** units vary
K <sub>ad</sub>	Pollutant partition coefficient between butterfat and animal adipose tissue, mg/L per mg/kg
K <sub>ij</sub> , K <sub>jk</sub>	Nonspecified pollutant partition coefficients
K <sub>oc</sub>	Organic carbon in soil-water partition coefficient, mg/kg in soil organic carbon per mg/L in water
K <sub>ow</sub>	Octanol-water partition coefficient, mg/L in octanol per mg/L in water
K <sub>pa</sub>	Pollutant partition coefficient between plant matter and animal, mg/kg in animal per mg/kg in plant
K <sub>sp</sub>	Pollutant partition coefficient between soil and plant matter, mg/kg in plant per mg/kg in soil
K <sub>sv</sub>	Pollutant partition coefficient between soil and vapor in soil-pores, mg/m <sup>3</sup> in air per mg/kg in soil
K <sub>sw</sub>	Pollutant partition coefficient between soil and water, mg/L in water per mg/kg in soil
K <sub>tn</sub>	Proportionality factor relating D <sub>Tc</sub> to D <sub>Tn</sub>

$K_{wa}$	Pollutant partition coefficient between water and animal, mg/kg in animal per mg/L in water
$K_{wf}$	Pollutant partition coefficient between water and fish, mg/kg in fish per mg/L in water
$K_{wp}$	Pollutant partition coefficient between water and plant matter, mg/kg in plant per mg/L in water
$K_{wv}$	Pollutant partition coefficient between water and air, mg/m <sup>3</sup> air per mg/l water
$l_e$	Length of time of dosing of animals in bioassay test, weeks
$L$	Expected lifespan of animals in bioassay test, weeks
$L_a$	Accumulated lead content in livestock animal, $\mu$ g
$L_e$	Actual lifespan of animals at a specific dose level in bioassay test, weeks
96-LC50	Estimated pollutant concentration in water lethal to 50 percent of a fish species after 96 hours of exposure, mg/L
LD50	Estimated one-time pollutant dose lethal to 50 percent of a mammalian species, mg/kg
m.t.	Main text
MW	Molecular weight, g/g-mole
$n_c$	Number of animals with a specific tumor in bioassay test control group
$n_f$	Freundlich isotherm reciprocal exponent
$n_t$	Number of animals with a specific tumor at specific dose in bioassay test
NC	Number of animals in control group in bioassay test
NT	Number of animals given specific dose in bioassay test
NTP	National Toxicology Program
NWQCD	Notice of Water Quality Criteria Documents <sup>16*</sup>
$P_c$	Observed tumor incidence probability in bioassay control group
$P_o$	Vapor pressure, mm Hg
$P_t$	Observed tumor incidence probability at selected dose of bioassay test

PBF	Plant bioconcentration factor of pollutant, mg/kg in plant per mg/kg in soil
PPLV	Preliminary Pollutant Limit Value, mg/kg soil or mg/L water
$R_i$	Proportionality factor between SPPPLV and $D_T$ for pathway i,** units vary
$R_{1i}$	Lowest $R_i$ for a set of pathways used to compute a PPLV
RB	Inhaled volume of air daily, $m^3$
RB'	Inhaled volume of air in 8 hours by workers, $m^3$
RTE	Registry of Toxic Effects <sup>12*</sup>
RTRM	Report on the Task Group on Reference Man <sup>39*</sup>
SF	Safety factor in Equation 9 or Equation 10
SOC	Soil organic carbon content, g/g
STAB	Scientific tables <sup>35*</sup>
SVNM	Standard Values in Nutrition and Metabolism <sup>38*</sup>
SNARL	Suggested No-Adverse Response Level
SPPPLV	Single pathway PPLV, mg/kg soil or mg/L water
T	Temperature, °K or °C
$T_t$	Test time to lifetime ratio in bioassay test
TLV	Threshold Limit Value, mg/ $m^3$
$U_1$	Human intake of pollutant from fish corresponding to $C_1$ , mg/day
$U_2$	Human intake of pollutant from fish and drinking water, mg/day
$U_c$	Uptake of lead by cow in plant and soil, $\mu g/day$
$U_{c7}$	Uptake of pollutant by cow in plant matter corresponding to $C_{s7}$ , mg/day
$U_{cp}$	Uptake of lead by cow from plant matter, $\mu g/day$
$U_{cs}$	Uptake of lead by cow from ingested soil, $\mu g/day$
$U_{cx}$	Uptake of pollutant by cow from ingested soil corresponding to $C_{sx}$ , mg/day
$U_{fy}$	Uptake of pollutant by fish from sediment, mg/day

USAMBRDL	US Army Medical Bioengineering Research and Development Laboratory
VD	Vapor density corresponding to $C_w < C_{sol}$ in equilibrium with $C_s$ , mg/m <sup>3</sup>
VD <sub>0</sub>	Saturation vapor density, mg/m <sup>3</sup>
w	Average animal weight in bioassay test at specific dose, kg
W <sub>a</sub>	Human consumption of meat, kg/day
W <sub>d</sub>	Human consumption of dairy, L/day
W <sub>f</sub>	Human consumption of fish, kg/day
W <sub>i</sub>	Human consumption of matter in pathway i, kg/day**
W <sub>p</sub>	Human consumption of vegetables, kg/day
W <sub>sc</sub>	Child ingestion of soil, kg/day
W <sub>w</sub>	Human consumption of drinking water, L/day
WHO	World Health Organization, United Nations
T	Half-life of substance retention in body, days

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