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TECHNICAL REPORT 8918

THE PRELIMINARY POLLUTANT LIMIT VALUE APPROACH:

MANUAL FOR USERS

MITCHELL J. SMALL



U S ARMY BIOMEDICAL RESEARCH & DEVELOPMENT LABORATORY

Fort Detrick

Frederick, MD 21701-5010

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U S ARMY MEDICAL RESEARCH & DEVELOPMENT COMMAND

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19. ABSTRACT (Continue on reverse if necessary and identify by block number) The Preliminary Pollutant Limit Value (PPLV) Approach to developing guidance contamination levels in soil and water is an established procedure throughout the US Army. In 1984, Technical Rept 8210 was issued to provide users with a reference document as to pathway equations and efforts in the development of the Rocky Mountain Arsenal Endangerment Assessments. In the approach, unique routes for human exposure to pollutants from a common medium (soil or water) are defined. Equations are presented for 7 such routes for water and 13 such routes for soil. These routes include water consumption, fish consumption, vegetable consumption, consumption of beef or dairy, direct intake of soil, either in ordinary activities or from a dusty worksite, and inhalation of volatile contaminants from a land site. In the case of beef and dairy consumption, consideration is given to animal exposure to a contaminant which is in feed material, drinking water or soil consumed when the animals graze. <i>Exposure routes: water consumption; soil pollution; water pollution;</i>					
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Representative data or ranges of data, or data estimation procedures are provided for inputs to these equations. These data can be grouped into five categories:

- o A limiting dose (D_T) that should avoid adverse effects if the contaminant is a chronic toxicant or should cause less than a specified additional risk of cancer development within a lifetime if the contaminant is potentially carcinogenic.
- o Daily human consumption rates for foodstuffs, inhalation of air, or for unintentional exposure to soil.
- o Animal consumption factors for feed and water and intake factors for soil ingestion.
- o Site soil and climatic factors.
- o Partition coefficients which reflect the transfer of contaminants through the environment from soil or water to items which humans consume.

Case examples at Alabama Army Ammunition Plant, Rocky Mountain Arsenal, and Gratiot County, MI Landfill are discussed to demonstrate the combination of pathway equations to produce PPLVs. Procedures are presented to assess the relative importance of individual pathways, and to factor in harmful effects to other inhabitants of the environment (plants, fish, livestock) or other characteristics of contaminants (limiting physico-chemical characteristics, organoleptic effects) within the context of the PPLV analysis.

Three appendices are provided. The first presents background information as to the derivation of the PPLV, its relation to other assessment schemes, and derivation of noteworthy pathway equations. The second appendix discusses experimental toxicology and carcinogenicity bioassay testing, and how their results are interpreted as D_T values. The last appendix discusses the limits of application and accuracy of partition coefficient equations presented in the main text, and some alternate approaches.

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1.0 INTRODUCTION

The US Army owns property contaminated with chemical agents, munitions, explosives, smoke residues, or their environmental by-products. The contamination may exist in soil, surface water, or groundwater. Regardless of the property status (active, inactive, or slated for excess), these media should not have residual contamination at levels that could be harmful in current or projected land-use situations. Decisions need to be made as to whether remedial actions are required to reduce the amount or extent of contamination. In some cases, the intended property uses will be known; in other cases, several options may have to be addressed. The level of knowledge about the contaminants involved may vary in quality. Remediation decisions may be internally directed by the Army or in response to regulations of the Comprehensive Environmental Response, Compensation and Liability Act of 1980¹ (commonly called "Superfund"), as amended through 1986, or in response to regulations of the Resource Conservation and Recovery Act².

The Preliminary Pollutant Limit Value (PPLV) approach has been developed and refined at the U.S. Army Biomedical Research and Development Laboratory. It provides answers to the "How Clean is Clean?" question, which is central to determining the need for or the extent of remedial actions. As indicated in Table 1, several installation's problems have been addressed by the approach. The approach can be to determine analytical levels for investigative survey sampling requirements. The approach has been described in the open literature³⁻⁶, and more detailed procedures included in a technical report⁷. A computerized version based on that report is in the Environmental Technical Information System of the U.S. Army Construction Engineering Research Laboratory⁸.

The studies cited in Table 1 cover an 11-year period. In this time, methodological advances have refined the PPLV approach. This report is to revise the technical report⁷ to reflect these advances. This report is also intended to be the technical source for a revised computerized version. While this report should serve as a guidance document for PPLV approach applications, it should be useful for other environmental hazard assessment methods.

The PPLV approach should be kept in proper perspective; it is not intended to provide "cook-book" assessments. It incorporates reasonable treatment of toxicological data and pathways for human exposure into a computational framework whereby acceptable environmental contamination levels may be derived. Complex mathematical models are avoided when 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 other types of data inputs; some numerical inputs are well established, while others are based on

Table 1. Summary of PPLV Approach Studies Undertaken or in Progress.

Location/Reference	Situation	Problem to be Resolved
Rocky Mountain Arsenal, CO ⁹	Post was under Court order to cease contamination of of aquifer. Degraded water quality off-post.	What levels of chemicals in on-post soil will allow unrestricted use of groundwater?
Alabama Army Ammunition Plant, AL ¹⁰	Soil in portions of this old production plant contain explosive contaminants. Sections of the plant have been or are planned to be sold.	What levels of residual contaminants are allowable in soil?
Bangor Naval Submarine Base, WA ⁵	Runoff with explosives is planned for diversion to an on-base pond.	Will fish caught in the area pose a hazard if consumed?
Savanna Army Depot Activity, IL ¹¹	Explosive compounds are found in sediments of slough and in dry lagoons in Mississippi River flood plain	Can pollutant explosives contaminate fish caught in slough and endanger river as a drinking water source?
Camp Sims, DC ¹²	Riot gas may still remain in a disposal pit at a planned office building site.	Do residuals pose a hazard to construction workers or future inhabitants?
Gratoit County Landfill, MI ¹³	Polybrominated biphenyls contamination at landfill, groundwater, and nearby farms.	What levels of chemical are safe in soil and water?
Fort McClellan, AL ¹⁴	Chemical warfare decontamination by-products may remain at training sites.	What are the most likely chemicals present and what detection levels are required for soil assays?
Cornhusker Army Ammunition Plant, NE ¹⁵	Explosive compounds in soil and groundwater, which is used as a water supply for people and livestock	What residual levels of contaminants can remain in soil in otherwise cleaned-up areas?
Rocky Mountain Arsenal, CO ¹⁶	Superfund remedial investigation/feasibility study is underway at this highly contaminated site.	What are PPLV equations and data inputs for an endangerment assessment?

scanty documentation, estimation, or guesswork. Thus, the temptation to endow a PPLV with an absolute or inviolate nature should be avoided. Technically, the PPLV approach presents little that is new; as recently described¹⁷, "[it] is a conceptual framework incorporating much current environmental thinking. Any novelty to be claimed for it lies in its systematic integration of widely accepted ideas into a workable system." On the other hand,

the approach provides a useful framework in which to construct answers to environmental problems, and from which to define needs for further study.

1.1 THE PPLV APPROACH: AN OVERVIEW

For the purposes of this overview, soil is the environmental medium of concern, and contamination has occurred due to past activities. The PPLV approach primarily seeks to avoid adverse effects in exposed humans, either directly or due to consumption of foodstuffs raised or grown at the contaminated site. The approach logically consists of the following steps:

- o Determine pollutants of concern;
- o Determine land uses and pathways through which people are exposed to these pollutants;
- o Develop equations for the pathways;
- o Collect the requisite data to solve equations;
- o Compute pathway soil limits, and from these PPLVs;
- o Interpret the results in terms of the problem; and
- o Determine if other considerations constrain limits below PPLVs.

An analyst must first define the problem, which in the PPLV approach takes the format "What are the contaminants and how will people be exposed to them?" Contaminant identification should involve considerable thought. Often, a "laundry list" of parent compounds employed during active production is available. One should not unconditionally accept such a list. Certain of these, such as gases or extremely volatile liquids, can be ruled out of concern easily. Other compounds may have to be added by consideration of the environmental fate of parent compounds. When substances are elemental or ubiquitous, their extant levels need to be addressed in relation to the background levels. The prudent approach is to sample and analyze for suspected pollutants in the soil so that perceptions can be validated. In "Superfund"-related actions, this is part of the Remedial Investigation. The PPLV approach can be used to provide target analytical limit guidance.

The analyst then defines one or more land-use scenarios. These scenarios may be in terms of current or projected activities at or in the vicinity of an installation. Each scenario will have one or more pathways associated with it. The pathways describe specific routes by which man can be exposed to a soil pollutant. For example, an unused area of an installation with a fish pond may be considered as a potential recreational area. This is a land use scenario. Next, one asks the question "how will people be exposed to a soil pollutant in the scenario?" Perhaps sediment in the pond is contaminated; in that case, a soil ->

water -> fish -> human consumer pathway can be construed. Picnic and play areas may be constructed; children at these areas may ingest soil directly. Section 2.0 of this report provides case studies of scenario and pathway considerations.

A decision as to how many pathways to consider should be balanced by the realization that additional investments of time and money are incurred in the gathering of pathway information. cursory evaluations of proposed pathways can indicate that some will not be important. Evaluation procedures are discussed in Section 8.0 of this report.

For each proposed pathway, an equation must be developed to describe the relation between human intake and the pollutant level in soil. The PPLV approach first processes each pathway as the only pathway through which a contaminant in soil reaches man. The human intake of interest will depend upon some "safe" or "acceptable" dose of the contaminant. This is consistent with the so-called "reference dose" used in U. S. Environmental Protection Agency (EPA) manuals¹⁸. This dose is indicated by the symbol D_T . Methods of computing D_T based on the literature are presented in Section 3.0 of this report. The computed concentration based on D_T is called a "Single-Pathway Limit Value" or SPLV. SPLV relations have the general symbolic form:

$$SPLV_i = IF_i \times D_T / f(K_i, S_i) \quad (1)$$

where i refers to a specific pathway. IF_i is an "intake factor", that typically includes information about human weight and the rate of pollutant uptake. The term $f(K_i, S_i)$ indicates the ease of transmission of a pollutant from soil to the consumed item (if the item consumed is soil itself, this function is unity). K_i usually includes one or more partition coefficients, numbers which indicate the relative pollutant concentration in adjacent portions of a pathway. In the fish pathway discussed above, one such coefficient relates conditions in water and fish, and is commonly known as a fish bioconcentration factor. S_i involves site-specific information about soil. Section 4.0 of this report contains SPLV equations for several pathways. Section 5.0 of this report contains information on values of IF_i and S_i . Section 6.0 of this report contains information on how partition coefficients are evaluated.

As an example, Figure 1 represents a simple beef consumption pathway. Here, steers eat only contaminated pasture. This may not be the case in some areas; this is where site-specific conditions enter. However, it can be considered an "adverse case". The SPLV to be computed is called $SPLV_{s4}$, where "s4" indicates a specific soil-media pathway. If a person of body

* The term SPLV replaces the single pathway preliminary pollutant limit value used in past presentations.

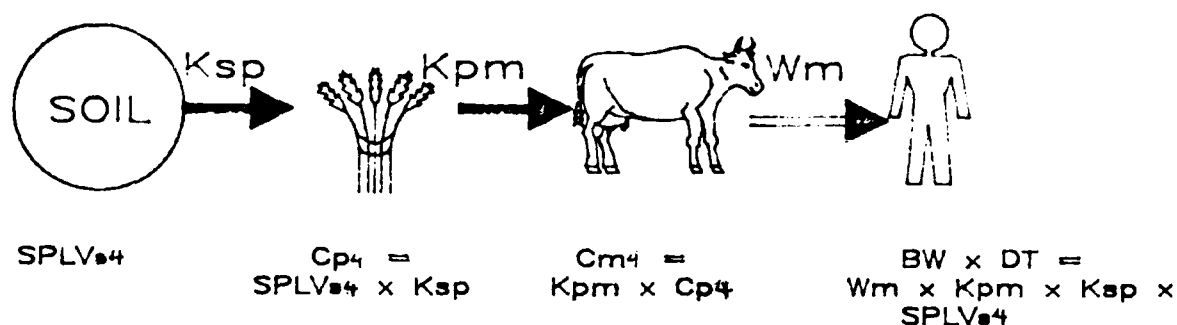


Figure 1. Model to Derive SPLV: Meat consumption, livestock raised on crops grown in contaminated soil.

weight BW eats a given daily amount of beef, Wm , and the beef provides the only source of a pollutant, a pollutant limit in beef, Cm_4 , is:

$$BW \times D_T = Wm \times Cm_4$$

Now, Cm_4 must be related to the SPLV, which involves tracing the pollutant from soil to beef. For many pollutants, a partition coefficient can be defined to relate the concentration in plant matter to that in soil. Denoting this coefficient as K_{sp} , Cp_4 , the plant concentration corresponding to the SPLV, is $K_{sp} \times SPLV_{s4}$. Moreover, a partition coefficient can be defined to indicate the concentration in meat per unit concentration in plant matter. Denoting this coefficient as K_{pm} , Cm_4 is $K_{pm} \times Cp_4$. These relations are combined and rearranged to provide an explicit equation for $SPLV_{s4}$.

$$SPLV_{s4} = (BW / Wm) \times D_T / (K_{sp} \times K_{pm}) \quad (2)$$

The correspondence of terms to those in equation 1 should be readily apparent.

The next step is to compute the PPLV for each land-use scenario "j". For the pathway equations discussed in Part 3, PPLVj has the form:

$$PPLV_j = 1 / \sum_i (SPLV_i \times T_{ij}) \quad (3)$$

T_{ij} is an element of a matrix, which relates to the i^{th} pathway in the j^{th} scenario. The matrix element is valued at unity when the i^{th} pathway is included in the j^{th} scenario; otherwise the element has a zero value. The T_{ij} matrix is a useful method of summarizing the scenarios and pathways of a PPLV analysis, and is discussed further in Section 2.0. The above relation is valid

when exposure to the pollutant is provided only by scenario pathways and $f(K_i, S_i)$ are constants. Appendix A discusses the derivation of PPLV relations and modifications that arise when these conditions are not met.

While the approach described above is geared to avoid adverse effects to humans, there is no guarantee that a PPLV will prevent adverse effects in other species of concern. Moreover, the PPLV may be a meaningless number based on the ability of a pollutant to transfer in water. These contingencies should be tested; Section 7.0 of this report discusses such assessment procedures.

1.2 REPORT ORGANIZATION

Subsequent sections 2.0 to 8.0 in this report have been mentioned in the overview. Three appendices are also included:

- o Appendix A. Mathematics of the PPLV Method and Selected Pathway Derivations.

- o Appendix B is a technical discussion of D_T estimation methods. While Section 3.0 deals with estimation techniques, this appendix provides background on how they are related to experimental procedures.

- o Appendix C is a technical discussion of partition coefficients and their documentation. While Section 6.0 deals with the equation used to estimate these coefficients, this appendix discusses a background on the equations and their restrictions.

Persons who are not acquainted with risk and health assessments should read the appendix presentations. Appendix tables, figures, and equations are preceded by their appendix identification (such as Figure C-2) to contrast them from items appearing in the main text.

After these appendices, the report concludes with a glossary of notation and acronyms, and reference citations.

2.0 LAND USE SCENARIOS AND PATHWAYS

The definition of land use scenarios and pathways is not mechanical; they will differ from site to site. Thus, decision makers should be aware of current or planned uses; clearly, local government planning agencies should be consulted. In some cases, such as the Savanna Army Depot Activity (Table 1), the use-pathway interactions are fairly simple. In cases of uncertain future land use, they are more complex. Three such cases are presented here.

2.1 ALABAMA ARMY AMMUNITION PLANT (AAAP)

This installation is situated near Childersburg, AL. During World War II, AAAP produced high explosives and propellants. Since the end of the war, the site has been idle, and is now mostly covered by forest. The Army's intent was to excess the site. Part of AAAP was purchased by a paper manufacturer, but was found to be contaminated with explosive-related chemicals and lead residuals. That parcel was leased back to the Army for remedial actions. Another parcel was planned for sale to Talladega County as a gasohol plant site. Logging was being done at other portions of the plant. A survey disclosed that 94 acres in several tracts of land scattered throughout AAAP were contaminated. Rosenblatt and Small¹⁰ sought to specify acceptable residual levels at contaminated tracts after clean-up.

Land use scenarios had to reflect current expectations (that the existing industrial and logging activities would continue) as well as possible future uses of other parts of the plant. Since no definite plans were stated, several alternate scenarios were postulated:

- o Farming, where residents raise virtually all meat they consume and grow virtually all vegetables they consume.
- o Single unit housing tracts, such as commonly found in suburban areas.
- o Apartment housing.
- o Industrial use.
- o Hunting (primarily deer).

These exposure pathways were identified:

- o Human consumption of vegetables grown in contaminated soil.
- o Meat consumption. Two pathways are involved here. The first addresses domestic animals as the meat source. The livestock are raised on plant matter (grasses or grains) grown in contaminated soil. Moreover, the animals could ingest soil directly during grazing, providing a more direct source of contamination. The second pathway addresses game animals, primarily deer. While deer

do not "graze" as do cattle, they subsist on plant matter.

- o Dairy product consumption. Similar in construction to the above livestock meat consumption pathway.
- o Soil ingestion. Primarily a problem with small children.
- o Dust inhalation. Vehicular movement and other work activities in unpaved areas could raise clouds of dust which workers would inhale.

Table 2 shows the T_{ij} matrix corresponding to the above selections.

2.2 ROCKY MOUNTAIN ARSENAL (RMA)

This 27 square-mile site is about 10 miles northeast of Denver, CO. Chemical warfare agents have been produced and disposed of by the Army from 1942 to about 1960, and pesticides have been produced by various tenant companies from 1947 to about 1975. Waste products were initially disposed into unlined pits and hastily-prepared landfills. Groundwater pollution has been a problem since the mid 1950s. In the early 1980s, a formal remedial investigation and feasibility study effort was initiated. Land contamination exists at many old industrial and dumping areas, and over 50 different organic and inorganic elemental substances are involved. The extent of clean-up has to be determined as well as cost allocation between the responsible parties. The RMA situation is the most complex and potentially could become the most expensive remediation effort for the Army, and perhaps the most expensive remediation effort in the United States.

The area around RMA is in transition from rural to suburban. West and southwest of RMA are suburban Denver communities. The southern border of RMA is adjacent to Stapleton International Airport, industrial parks, and housing tracts. On the other hand, small farms are found north of RMA, and to the east, mostly open rangeland. If RMA were converted to non-military use, parcels could be developed for housing, commercial or industrial use, or in the absence of intense development, could become farmland or open range. Moreover, existing man-made lakes at RMA would be maintained, possibly within parks. Floodplains along intermittent creeks that cross RMA could also become parkland.

The following pathways are being used for RMA analysis¹⁶:

- o Fish consumption. The fish are caught at RMA lakes; lakewater is contaminated due to contact with contaminated sediment.
- o Vegetable consumption.

Table 2. Tij Matrix - Alabama Army Ammunition Plant

Pathways	<u>Scenarios</u>				
	Farming	One-family housing	Apartment housing	Industrial	Hunting
Vegetable consumption	1	1	0	0	0
Meat consumption (domestic)	1	0	0	0	0
Meat consumption (deer)	0	0	0	0	1
Dairy product consumption	1	0	0	0	0
Soil ingestion	1	1	1	0	0
Dust inhalation	0	0	0	0	1

o Meat consumption. See discussion in Section 2.1. At RMA, rabbits, not deer, are the main game species involved.

o Dairy products consumption.

o Low-intensity direct soil intake. Includes soil ingestion, primarily by inadvertent means, intake of ambient levels of dust, and dermal adsorption of soil-containing contaminants. This is a more elaborate version of the soil ingestion pathway in Section 2.1.

o High-intensity direct soil intake. Includes soil ingestion and inhalation of dust particulates, particularly during construction activities.

o Vapor inhalation. Potential exists for persons in basements or in poorly ventilated areas in construction projects.

Table 3 shows the matrix applicable for the RMA analysis. Note that the fish consumption pathway is NOT in the matrix. If it were, surface soil clean-up objectives might be subject to tradeoff against sediment soil. Conceptually, this would make sense if the intent was to specifically protect persons who eat fish from RMA lakes and are subject to another land-use scenario. In that case, the extent of remediation of large land areas at RMA would depend upon extent of remediation of lake sediment. This is where interpretation comes into play.

Table 3. Tij Matrix - Rocky Mountain Arsenal

Pathways	<u>Scenarios</u>					
	Suburban	Rural	Commercial buildings	Industrial construction	Recreational use	Open range
Vegetables consumption	1	1	0	0	0	0
Beef consumption	0	1	0	0	0	1
Dairy product consumption	0	1	0	0	0	1
Soil intake, Civilian	1	1	1	0	1	1
Soil intake, high intensity	0	0	0	1	0	0
Vapor inhalation	1	1	1	1	0	0
Game consumption	0	1	0	0	0	1

2.3 GRATIOT COUNTY LANDFILL

This landfill is 30 miles west of Saginaw, MI. Large amounts of polybromobiphenyl compounds (PBB) had been dumped there and buried. The landfill was to be closed, capped, and restricted from other uses. PBB was present in some neighboring fields, surface water, and groundwater. A study¹³ was designed to provide guidance as to what could be potentially hazardous levels in soil and water for the purpose of monitoring, and to demonstrate the PPLV approach in a non-military setting.

Three land-use scenarios were developed based on then-current life styles: farming, residential and industrial. Pathways selected were:

- o Vegetable consumption.
- o Meat consumption from domestic animals. Similar to the situation at AAAP, PBB-contaminated plant matter or soil could be a route by which PBB was incorporated into meat. Additionally, PBB in the livestock drinking water supply was also addressed.
- o Dairy product consumption. Similar to the meat consumption situation.
- o Soil ingestion by children.

o Dust inhalation. Similar to the dust inhalation situation for AAAP.

o Water consumption by human inhabitants.

Here, target inhabitants were expected to get PBB via drinking water as well as from soil. Moreover, some of the PBB supplied from dairy and meat might be attributable to water consumed by cattle. Thus, two PPLVs were computed, one for soil and one for water. Table 4 shows two matrices, each for an independent (at least within the scope of the study) PBB-containing medium. The interpretation was that PBB contamination levels in soil and water could be traded-off to determine paired set-points for comparison against monitored data. If the monitored data exceeded the set-points, there would be cause for concern.

Table 4. Tij Matrices - Gratiot County Landfill

Pathways	Surface Soil Scenarios		
	Farming	Residential	Industrial
Vegetable consumption	1	1	0
Meat consumption	1	0	0
Dairy product consumption	1	0	0
Soil ingestion	1	1	0
Dust inhalation	0	1	0
Pathways	Water Scenarios		
	Farming	Residential	Industrial
Meat consumption	1	0	0
Dairy product consumption	1	0	0
Water consumption	1	1	0

3.0 DT ESTIMATION TECHNIQUES

DT estimation techniques involve processing information from the toxicological literature. Fortunately, summary literature references or interpretive reviews can be consulted before embarking on an in-depth source document search. They include:

- o The Registry of Toxic Effects of Chemical Substances (RTECS). The RTECS is periodically updated and provides information concerning toxicological, mutagenic, and carcinogenic studies, along with supporting citations. On-line access to the RTECS is available from National Library of Medicine or the Chemical Information System computerized data-base systems¹⁹. Since the late 1970s, the RTECS has expanded in scope as to the number of substances and information provided. The registry is rather cryptic in its presentation; new users should read its "Introduction" section. Chemicals are alphanumerically cataloged in an order that follows the chemical alphabetical name; however, the name employed in the RTECS may differ from that the analysts knows. Thus, the substance's Chemical Abstract Service number code should be known before using the RTECS; it provides a cross-reference to the RTECS number code.
- o Documentation of the Threshold Limit Values and Biological Exposure Indices (DTLV). TLVs are recommended by the American Conference of Governmental Industrial Hygienists to protect workers from permanent adverse health effects due to airborne occupational exposure. TLVs have been issued for over 600 substances. A complete edition of the DTLV was issued in 1986²⁰ which includes the numerical TLVs and the data bases from which they were derived. The DTLV is supplemented yearly to reflect changes to values, or additions or deletions of substances.
- o The Chemical Regulation Reporter, published by 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.
- o The Superfund Public Health Evaluation Manual¹⁸ (SPHEM) is issued by the EPA. It contains toxicity data that can serve as DT values for better-known or well-researched toxic waste substances. It includes information that has been supplied from other EPA studies.
- o Water Quality Criteria for the so-called "priority pollutants"²¹ were developed in response to Section 307 of the 1977 amendments to the Federal Water Pollution Control Act²². These criteria were issued in 65 separate documents, and the chemicals (or chemical groups in the case of inorganic elements) are listed in Table 5. These criteria should not be used if more recent information is available.
- o Health Advisories are issued by the Office of Drinking Water of the EPA as guidance documents for substances not subject to

drinking water standards at the time of issue. Substances for which advisories were available as of the end of 1985²³ are included in Table 5. The drinking water standards proposed should not be used directly for D_T estimation purposes, since they include provision for up to 80% intake of a pollutant from sources other than drinking water.

- o Health Effects Assessments are provided by the EPA Office of Health and Environmental Assessment as general-purpose reference studies. Chemicals for which reports were available in 1985¹⁸ are listed in Table 5.

- o The Agency for Toxic Substances and Disease Registry prepares toxicological profiles for commonly-occurring contaminants at toxic waste sites. One hundred substances were been selected for study (April 1987)²⁴; they are listed in Table 5. The Registry prioritized the scheduled issue of profiles from "1" to "4"; these priorities are shown in Table 5. As of May 1988, the profiles for "Priority 1" substances had been prepared and issued for review. In October 1988, a second group of substances was proposed for profile development.

3.1 CARCINOGEN vs. NON-CARCINOGEN CLASSIFICATION

Appendix B discusses the conceptual differences between the risk assessment of toxic substances and carcinogenic substances (more precisely, substances that are proven oncogens in man or in animals). Briefly, a toxic substance is expected to have a threshold limit below which no observable effects occur (i.e. a NOEL). A carcinogen is postulated to have no finite NOEL below which there is absolutely no risk of cancer. Since zero limits are impractical, the concept of an acceptable risk has developed, for which an acceptable dose can be determined. This concept allows assessors to handle both types of substances in the same mathematical format although the procedures used to quantify D_T differ. Thus, this classification is first addressed.

Two sources can be checked to determine if a substance should be classified as a carcinogen. Any substance listed in Exhibit C-4 of the SPHEM¹⁸ should be so considered. The RTECS¹⁹ provides summary information of studies by the National Cancer Institute (NCI), and more recently, the National Toxicology Program (NTP), and of literature reviews by the International Agency for Research on Cancer (IARC). Such information will include a "weight of evidence" notation, which qualitatively indicates the robustness of experimental studies (see Appendix B). A substance should be classified as a carcinogen if an NCI or NTP study indicates a "positive" animal result or if the IARC statement is "sufficient or limited human evidence or sufficient animal evidence".

3.2 D_T ESTIMATION PROCEDURES FOR NON-CARCINOGENS

The approaches presented here are ordered roughly in terms of preference. First, respected sources which have evaluated

Table 5. Review Documents for Toxicology of Selected Substances

Substance	Water Quality Criteria ^a	Drinking Water Advisory	Health Assessment Document	Toxicology Profile ^b
Acenaphthene	0			
Acetone			X	
Acrolein	T			3
Acrylamide		X		
Acrylonitrile	C			3
Alachlor		X		
Aldicarb		X		
Aldrin/Dieldrin	C			1
Ammonia				3
Aniline				4
Antimony	T			
Arsenic	C	X	X	1
Asbestos	C		X	
Barium		X	X	
Benzene	C	X	X	1
Benzidine	C			2
Benzoic acid				4
Beryllium	C			1
2-Butanone				4
Cadmium	T	X	X	1
Carbofuran		X		
Carbon Disulfide				4
Carbon Tetrachloride	C	X	X	2
Chlordane	C	X	X	2
Chlorinated benzenes: ^c				
Chlorobenzene	0,T	X	X	3
Dichlorobenzenes ^d		X		1(1,4-) 4(1,2-) 4(1,3-)
1,2,4-Trichlorobenzene				4
Tetrachlorobenzene	T			
Pentachlorobenzene	T			
Hexachlorobenzene	C	X	X	3
Chlorinated ethanes: ^c				
Chloroethane	N/D			2
1,1-Dichloroethane	N/D		X	3
1,2-Dichloroethane	C	X	X	2
Hexachloroethane	C			
1,1,1-Trichloroethane	C	X	X	3
1,1,2-Trichloroethane			X	2
1,1,1,2-Tetrachloroethane	N/D			
1,1,2,2-Tetrachloroethane	C		X	2
Chloroalkyl ethers: ^c				
bis-Chloromethylether	C			2
bis-(2-Chloroethyl)ether	C			2
bis-(2-Chloroisopropyl)ether	T			
Chlorinated naphthalenes	N/D			

Table 5 (continued). Review Documents for Toxicology of Selected Substances

Substance	Water Quality Criteria ^a	Drinking Water Advisory	Health Assessment Document	Toxicology Profile ^b
Chlorinated phenols: ^c				
2-Chlorophenol ^d	O			
3- and 4-Chlorophenol	O			
2,4-Dichlorophenol ^d	T,O			4
other dichlorophenols	O			
methylchlorophenols	O			
2,4,5-Trichlorophenol	O,T		X	
2,4,6-Trichlorophenol	C		X	3
2,3,4,6-Tetrachlorophenol	O,T			
Chloroform	C		X	1
p-Chloro-m-cresol				4
Chromium	T	X	X	1
Coal Tars			X	
Copper	O		X	3
Creosote			X	
Cresol			X	
Cyanide	T	X	X	1
2,4-D		X		
DDT and Metabolites	C		X	2
Dibromochloropropane		X		
3,3'-Dichlorobenzidine				2
Dichloroethylenes: ^c				
1,1-Dichloroethylene	C	X	X	2
1,2-Dichloroethylene	N/D	X	X	3
Dichloropropanes	T	X (1,2-)		2 (1,2-)
Dichloropropenes	T			
2,4-Dimethylphenol	O			4
4,6-Dinitro-2-methylphenol				4
2,4-Dinitrophenol				4
2,4-Dinitrotoluene	C			2
2,6-Dinitrotoluene				3
p-Dioxane		X		4
Dioxin (2,3,7,8-TCDD)	C ^e	X	X	1
1,2-Diphenylhydrazine	C			3
Endosulfan	T			
Endrin and endrin aldehyde	T	X		3
Epichlorohydrin		X		
Ethylbenzene	T	X	X	3
Ethylene Dibromide		X		
Ethylene Glycol		X		
Fluoranthene	T			4
Glycol Ethers			X	
Haloethers	N/D			
Halomethanes: ^c	C ^f			
Bromomethane				4
Bromodichloromethane				2

Table 5 (concluded). Review Documents for Toxicology of Selected Substances

Substance	Water Quality Criteria ^a	Drinking Water Advisory	Health Assessment Document	Toxicology Profile ^b
Benzo(b)fluoranthene				1
Benzo(k)fluoranthene				
Benzo(ghi)perylene				
Benzo(a)pyrene			X	1
Chrysene				1
Dibenzo(a)anthracene				1
Fluorene				
Ideno(1,2,3-cd)pyrene				3
Phenanthrene			X	4
Pyrene			X	
Selenium	T		X	2
Silver	T			3
Stryene		X		
Tetrachloroethylene	C	X	X	1
Thallium	T			4
Toluene	T	X	X	2
Toxaphene	C	X		3
2,4,5-TP		X		
Trichloroethylene	C	X		1
Vinyl chloride	C	X	X	1
Xylenes		X	X	3
Zinc	0		X	2

a. Summarized classifications: C - known or potential carcinogen. 0 - Organoleptic (taste or odor; see Section 7.1.4). T - Toxicant. N/D - Not sufficient data to make a determination.

b. Number indicates priority listing for report issue.

c. Several compounds discussed in one water quality report and listed immediately below.

d. Listed in category, but issued as a separate criteria report.

e. Dioxin criteria document was issued subsequent to cited notice²¹.

f. All compounds in group were considered potentially carcinogenic; compound-specific criteria were not reported.

g. Two documents listed, one for inorganic mercury, the other for alkylmercury compounds.

quantitative data should be consulted. The most useful are:

- o Exhibit C-6 in the SPHEM¹⁸ has computed values for better-known, well-researched chemicals. They may be used directly.
- o Acceptable Daily Intakes (ADIs) are recommended by the Joint FAO/WHO Expert Committee on Food Additives.* This committee, comprised of toxicological and nutritional experts, meets periodically to consider substances for recommendation or to update past recommendations. Meeting proceedings are issued in WHO Technical Reports; the toxicological data involved are included in "Toxicological Evaluation of Certain Food Additives" publications. ADI values may be used directly as D_T estimates. Unfortunately, no consolidated ADI list has been published. Thus, a user should consult the most recent WHO Technical Report and work back through earlier reports to determine if a substance has been assigned an ADI value.
- o TLVs can sometimes be used for D_T estimation purposes. First, the background information in the DTLV needs to be reviewed; a TLV can't be so used if it is based on skin or nasal irritation, offensive odors, or the prevention of suffocation. Otherwise, the following equation estimates D_T from a TLV:

$$D_T = 0.00102 \times \text{TLV} \times (\text{AA} / \text{AO}) \quad (4)$$

D_T has units of mg/kg/day when TLV is in mg/m³ of air. The term AA/AO is the ratio of the efficiency of pollutant absorption via the inhalation pathway compared to its absorption via the ingestion pathway. The constant 0.00102 includes several factors: the calendar week vs. the workweek; the volume of air inhaled per day; the body weight of a hypothetical worker; and a 100-fold "safety factor". The safety factor adjusts the TLV, which may be based on a low, but tolerable, effect level to workers, to a NOEL. The factor also accounts for the sensitivity of people of the general population (particularly the young and elderly) contrasted to a more robust work population.

In lieu of interpreted information, mammalian toxicological studies can be reviewed. These are typically retrieved by a combination of manual and computerized literature searches. In some cases, starting references may be found in the RTECS¹⁹ or the DTLV²⁰. Another useful information source is the NTP Annual Plan²⁵. Each plan summarizes work accomplished in the previous fiscal year, and plans can be reviewed to determine if toxicity tests have been accomplished with specific substances (which are indexed in the back of each plan). The International Register of Potentially Toxic Chemicals (United Nations Environmental Programme, Geneva, Switzerland) publishes a bi-yearly bulletin which summarizes ongoing international activities.

* The Food and Agricultural Organization (FAO) and the World Health Organization (WHO) are United Nations Agencies with headquarters in Rome, Italy and Geneva, Switzerland, respectively.

The preferred information is a NOEL from a chronic toxicity mammalian study (for rodents, generally two years). In such a study, the test population is divided into sub-groups, animals in each are fed the test substance at a pre-selected dose level*. A control group is included. From such a test plan, three possible outcomes can be expected; see Table 6. This table supplies an appropriate dose feeding level, FL** and a safety factor, SF, from which D_T can be calculated:

$$D_T = FL / SF$$

Next in preference is a NOEL from a sub-chronic study (for rodents, typically a 90-day study). Table 6 provides factors to determine D_T from this result. Less preferable is an lowest dose effect level (LOEL) from a chronic or sub-chronic study, the chronic study being more preferred. In this case, SF for the NOELs in Table 6 are multiplied by "severity multipliers" which range from 1 to 10. Table 7 presents these multipliers and LOELs that they characterize.

The least desirable information is from an acute toxicity test. The animals are orally administered the test substance at selected dose levels and then observed for up to 14 days for adverse effects. The test observations estimate the statistic LD₅₀, i.e., the dose in mg/kg expected to kill 50 percent of dosed animals. D_T can be estimated by equation 5, which was suggested by Layton et al²⁶.

$$D_T = 1 \times 10^{-5} \times LD_{50} \quad (5)$$

3.3 D_T ESTIMATION PROCEDURES FOR CARCINOGENS

As noted in Section 3.1, there is no unique D_T for a carcinogen. To maintain computational analogy, the following treatment is applied:

- o An assessment of a carcinogen will be at one or more "acceptable risk levels (ARLs)". These are discussed in more detail in Appendix B; computations are common for ARLs in the range of 10^{-4} to 10^{-7} .

* "Feeding" may involve integration of the test substance in drinking water or in diet rations. In some cases, force-feeding (gavage) is required.

** If FL is a dose in mg/kg-day, the term can be used directly. Sometimes, FL will be expressed as a fraction of diet (such as ppm), so information on diet intake and animal weight should be available. The RTECS¹⁹ provides approximate intake and weight data, also see Section 3.3.2.

Table 6. Safety Factors for D_T Estimation From Mammalian Feeding Tests

Type Outcome	FL	SF
At all dose feeding levels, no effects are detected.	Highest dose level (NOEL)	100 chronic 1000 subchronic
At one dose level, no effects are detected on animals, but at a higher dose feeding level, effects are detected.	Highest no effect level (NOEL)	Same as above
At all dose feeding levels, effects are detected on test animals	The lowest dose level (LOEL)	Multiply factors above by severity rating in Table 7.

o The risk of carcinogenic effects at a given dose level is reflected in a parameter called "potency" (q). Potency is in units of reciprocal dose; $1/q$ may be thought of as the extrapolated dose which corresponds to an ARL of unity (see Appendix B).

o D_T is a function of q^* and ARL :

$$D_T = ARL / q^* \quad (6)$$

Some computed q^* values can be found in Exhibit C-4 of the SPHEM¹⁸. These may be used directly in equation 6.

3.3.1 Mammalian Bioassay Data

In this study, groups of mammals (usually rats or mice) are fed a test substance at one of several dose levels.* An additional "no-dose" (control) group is also tested. These tests last one to two years. The analysis compares the incidence of specific types of tumors in dosed animals to those of control animals. If incidence increases markedly with increased dose, the compound can be called an animal carcinogen.

Two useful sources of information on bioassay studies have been found:

o National Toxicology Program/ National Cancer Institute reports. Since the mid 1970s, bioassays performed under NCI sponsorship have been published in a series of technical reports. These were identified as NCI Technical Reports until July 1980, and thereafter as NTP Technical Reports. The sequential numbering of

* Bioassay tests, although basically similar to chronic toxicity studies, are not designed to estimate a NOEL. Adverse effects (other than tumors) are not uncommon in bioassays. See Appendix B for additional information on this matter.

Table 7. Severity Multipliers for NOEL Estimates From a LOEL¹⁸

Type of Effect at lowest dose level	Severity Multiplier
Enzyme induction or other biochemical change with no pathologic changes and no change in organ weights.	1
Enzyme induction and subcellular proliferation or other changes in organelles but no other apparent effects.	2
Hyperplasia, hypertrophy or atrophy, but no change in organ weights	3
Same as above, but changes in organ weights	4
Reversible cellular changes: cloudy swelling, hydropic change or fatty changes.	5
Necrosis, or metaplasia with no apparent decrement of organ function. Any neuropathy without apparent behavioral, sensory, or physiologic changes.	6
Necrosis, atrophy, hypertrophy, or metaplasia with a detectable decrement of organ functions. Any neuropathy with a measurable change in behavioral, sensory, or physiologic activity.	7
Necrosis, atrophy, hypertrophy, or metaplasia with definitive organ dysfunction. Any neuropathy with gross changes in behavior, sensory, or motor performance. Any decrease in reproductive capacity, any evidence of fetotoxicity.	8
Pronounced pathologic changes with severe organ dysfunction. Any neuropathy with loss of behavioral or other motor control or loss of sensory ability. Reproductive dysfunction. Any teratogenic effect with maternal toxicity.	9
Death or pronounced life-shortening. Any teratogenic effect without signs of maternal toxicity.	10

reports has been continued. The RTECS¹⁹ may be consulted for back-reports. The Annual Plan of the NTP includes recently-completed studies. Report summaries are often presented in the Chemical Reporter.

o The IARC, from time to time, issues monographs summarizing carcinogenicity studies of various substances, each monograph typically dealing with a certain class of compounds. The RTECS¹⁹ often contains references to monographs of interest.

3.3.2 "One-Hit" Model Procedure

This procedure²⁷ is useful when the results from only one positive dose-response level can be compared to the control group response.

If several positive dose-response levels are available for analysis, the multistage model can be applied. The mathematics for a multistage model are rather complex, requiring at least a personal computer. On the other hand, the one-hit model computations can be done with a desk calculator and natural logarithm tables.

First, tumor incidence data according to organ site or tumor type at each dose level is collected (assistance from a toxicologist may be required). For each organ or tumor category, the lowest dose is selected for which the incidence of tumors is significantly higher than that of controls, using the Fisher exact test and a significance level < 0.05 . If required, feeding information is converted to a FL in dose units. For example, if the substance tested is reported as a certain portion of food as mg/kg feed or ppm, this can be converted to an approximate FL by the relation:

$$FL = FCR \times (\text{mg/kg in feed})$$

FCR is the ratio of feed consumed per day per unit body weight; for rats, FCR is about 0.05, for mice, 0.13²⁷. If feed intake information and animal weights are available, FCR should be computed from the data.

The following variables are enumerated:

nt = number of animals with tumors at the selected lowest dose.
 NT = number of animals in the group at the selected lowest dose.
 nc = number of animals with tumors in the control group.
 NC = number of animals in the control group.
 Le = actual maximum lifespan of animals in the group at the selected lowest dose (usually in weeks).
 AW = 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 week for rats.
 le = length of exposure to substance in test in weeks.

Then, the following intermediate variables (two estimated probabilities, an adjusted dose and an adjusted time, respectively) are computed.

$$Pt = nt / NT$$

$$Pc = nc / NC$$

$$Dadj = FL \times le / L$$

$$Tt = Le / L$$

For each tumor type or organ site, the animal risk-dose proportionality factor BA is computed by the relation

$$BA = -\ln[(1 - Pt) / (1 - Pc)] \times (Dadj \times Tt^3)^{-1}$$

From the factors computed, choose the one with maximum value (BA_{max}). q^* is estimated by the relation:

$$q^* = BA_{max} \times (70 / AW)^{(1/3)}$$

3.3.3 Estimation of D_T in the Absence of Valid Bioassay Data

This is not a rigorous procedure, but serves to provide a rough estimate of q^* . First, a D_{Tn} is computed for the substance based on toxicological considerations. Then,

$$q^* = 0.0024 / D_{Tn}$$

This relation was discussed previously in Technical Report 8210⁷.

4.0 SPLV EQUATIONS

SPLV equations for water and soil are presented in Sections 4.1 and 4.2 respectively. These have been adapted from past studies. Specific pathways will be identified by a two-character subscript. The first character refers to the medium, the second character is a number. When D_T is in units of mg/kg-day, SPLVs derived for water are in terms of mg/L and soil SPLVs are in terms of mg/kg dry soil.

With many organic substances, the partition coefficients used in these equations will have to be estimated. Section 4.3 presents equation substitutions for partition coefficients when they must be estimated in lieu of experimental data. With lesser-studied compounds, this is often the case.

With the exception of the vapor intake pathways (see Section 4.2.7), transient changes in concentration of pollutants in water or soil are not addressed. The pollutants are considered to be persistent in the environment, and not subject to chemical or biochemical transformation, or physical transfer, such as vaporization or leaching. Moreover, the "pool" of available contamination is assumed to be large enough that removal of consumed items (such as harvest of vegetables grown in contaminated soil) doesn't change pollutant levels in the time frame of interest.

4.1 SPLV EQUATIONS FOR WATER PATHWAYS

4.1.1 Contaminated Water Consumption

This is the simplest of the equations:

$$SPLV_{wl} = (BW / Ww) \times D_T \quad (7)$$

where

BW = Body weight of a human in kg. For adults, a 70 kg value is often used (see Section 5.1.1.).

Ww = Daily intake of water, L/day. For adults, this is about 1.6 L/day.

D_T = Reference dose in mg/day per kg of body weight (mg/kg/day).

4.1.2. Contaminated Fish Consumption

Equation 8 applies when the primary source of pollutant exposure to the fish is expected to be from dissolved pollutant in water, as opposed to polluted sediment (bottom feeders) or through accumulation in their food chain. Appendix C suggests that this is so for substances with an octanol-water partition coefficient less than about 10,000 (see Section 6.1.1). Fish uptake from water is characterized by the bioconcentration factor BCF.

$$SPLV_{w2} = (BW / W_f) \times D_T / BCF \quad (8)$$

where

W_f = Averaged daily intake of contaminated fish by a human receptor. A default value of 0.0065 kg/day is suggested (see Section 5.1.2).

BCF = Bioconcentration factor relating the mg/kg of a substance in fish tissue to the mg/L of a substance in the surrounding water (see Section 6.2).

4.1.3 Contaminated Vegetable Consumption

Equation 9 applies to situations where contaminated hydroponic or irrigation water is used to water crops. Moreover, the uptake of pollutant by plants is fast enough that the partitioning of pollutant to soil as a means of reducing contaminant levels in water can be ignored.

$$SPLV_{w3} = (BW / W_v) \times D_T / K_{wv} \quad (9)$$

where

W_v = Averaged daily intake of contaminated vegetables by a human receptor in kg (dry weight)/day (see Section 5.1.4 for a range of values).

K_{wv} = Partition coefficient relating the mg/kg of a substance in dry weight vegetable matter to the mg/L of the substance in water used to grow the plants (see Section 6.3).

4.1.4 Contaminated Meat Consumption

Two equations are presented here, each to account for different combined exposure routes to cattle. Equation 10 expresses the situation where contaminated drinking water is the main route of exposure for the target animal. Equation 11 is for the case where, in addition to use as a drinking water supply, contaminated water is used to irrigate pasture crops. In the latter case, the assumptions stated in Section 4.1.3 for vegetables apply.

$$SPLV_{w4} = (BW / W_m) \times D_T / (K_{pm} \times U_{wm} / U_{pm}) \quad (10)$$

$$SPLV_{w4} = (BW / W_m) \times D_T / (K_{pm} \times [U_{wm} / U_{pm} + K_{wp}]) \quad (11)$$

where

W_m = Averaged daily intake of contaminated meat by a human receptor in kg/day. A default value of 0.1 kg/day is suggested (see Section 5.1.5)

K_{pm} = Partition coefficient relating the mg/kg of a substance in beef to the mg/kg (dry weight) of the substance in feed (pasture) consumed by beef cattle (see Section 4.3).

U_{wm} = Daily intake of water by cattle, L/day. A default value of 15.3 L/day intake is suggested (see

Section 5.2.2).

Upm = Daily intake of feed (dry weight basis) by cattle, kg/day. A default value of 6.6 kg/day is suggested (see Section 5.2.1).

Kwp = Partition coefficient relating the mg/kg of a substance in dry weight feed (pasture) to the mg/L of the substance in water used to grow the pasture (see Section 4.3).

If these equations were derived as discussed in Section 1.1, a water to cattle partition coefficient would be expected. It is more convenient to use the plant to meat partition coefficient Kpm. These equations assume that the source of contaminant (water or plant) is unimportant; the absorption of from either source is the same.

4.1.5 Contaminated Milk Consumption

The two equations presented here parallel those presented above for beef cattle; however, a plant to milk partition coefficient, Kpd is used.

$$SPLV_{w5} = (BW / Wd) \times D_T / (Kpd \times Uwd / Upd) \quad (12)$$

$$SPLV_{w5} = (BW / Wd) \times D_T / (Kpd \times [Uwd / Upd + Kwp]) \quad (13)$$

where

Wd = Averaged daily intake of contaminated milk by a human receptor in kg/day. A default value of 0.3 kg/day is suggested (see Section 5.1.6)

Kpd = Partition coefficient relating the mg/L of a substance in milk to the mg/kg (dry weight) of the substance in feed (pasture) consumed by dairy cattle (see Section 4.3).

Uwm = Daily intake of water by cattle, L/day. A default value of 78 L/day intake is suggested (see Section 5.2.4).

Upm = Daily intake of feed (dry weight basis) by cattle, kg/day. A default value of 16.6 kg/day is suggested (see Section 5.2.3).

4.2 SPLV EQUATIONS FOR SOIL PATHWAYS

The equations presented in Sections 4.2.1 through 4.2.5 are analogs of those in Section 4.1. The major difference is inclusion of a term for partitioning of a pollutant between soil and water, called Kd' :

$$Kd' = Kd + \theta / \rho \quad (14)$$

where

K_d = Partition coefficient indicating the concentrations of a substance in soil (mg/kg) and water (mg/L) when the soil and water phases attain equilibrium (see Section 4.3).

θ = Fractional volume of soil filled with water (see Section 5.3.1).

ρ = Bulk density of dry soil, kg/L (see Section 5.3.1).

Undisturbed soil is a matrix of solid particulates; the gaps or pores between these can contain water or air. The term θ / ρ accounts for pollutant contained in "soil-pore water". K_d' is then an adjusted K_d for use in SPLV equations, where the pollutant concentration is on a dry soil basis. Previously, $1 / K_d'$ was referred to as K_{sw} . However, K_d is widely-used, and has been incorporated into the PPLV nomenclature.

The other sub-sections deal with direct contact with soil (ingestion, skin contact, or inhalation of particulates) or of inhalation of vapors emanating from soil.

4.2.1 Contaminated Water Consumption

In equation 15, the term $f(S1)$ indicates a "dilution" effect which would be peculiar to each situation. For example, a portion of lake-bed sediment may be contaminated, in that case the ratio of contaminated area to total lake-bed area would be $f(S1)$. If water drained from a contaminated soil surface area, $f(S1)$ would represent the ratio of contaminated area to entire watershed area of the body of water computed at the point of contaminated drainage outfall. The maximum value of $f(S1)$ is unity, indicating no dilution, which might be approached with a slow-moving spring or a spring-fed pond.

$$SPLV_{S1} = (BW / Ww) \times D_T \times K_d' / f(S1) \quad (15)$$

4.2.2 Contaminated Fish Consumption

Equation 16 represents a situation where a body of water with fish becomes contaminated due to contact with pollutant in sediment. As in the case above, $f(S2)$ accounts for possible dilution effects.

$$SPLV_{S2} = (BW / Wf) \times D_T \times K_d' / (BCF \times f(S2)) \quad (16)$$

4.2.3 Contaminated Vegetable Consumption

In this case, the soil is initially contaminated. The soil-pore water becomes contaminated, as a limiting case, the distribution of pollutant between soil and soil-pore water is indicated by K_d' . This water is transferred to plants, and is the only source of contamination to the plant. Then,

$$SPLV_{S3} = (BW / Wv) \times D_T \times Kd' / Kwv \quad (17)$$

4.2.4 Contaminated Meat Consumption

Three equations are presented here. Equation 18 applies to pasture grown in contaminated soil as the exposure route to meat animals. The other equations include the effect of concurrent consumption of soil by grazing cows (equation 19), and for contaminated water intake, such as from a spring or artificial storage pond on contaminated land (equation 20). For brevity, $IS4 = (BW / Wm) \times D_T / Kpm$.

$$SPLV_{S4} = IS4 / (Kwp / Kd') \quad (18)$$

$$SPLV_{S4} = IS4 / (Kwp / Kd' + Usm / Upm) \quad (19)$$

$$SPLV_{S4} = IS4 / (Kwp / Kd1' + Usm / Upm + Uwm / [Upm \times Kd2']) \quad (20)$$

where

Usm = Soil ingested by beef animal, kg/day. A default value of 0.35 kg/day is suggested (see Section 5.2.5)

In equation 20, two Kd' parameters appear. $Kd1'$ refers to surface soil and $Kd2'$ refers to soil which contaminates the water source. Based on the composition of the soils involved, and the particulars of the situation, they may differ.

4.2.5 Contaminated Milk Consumption

Equations analogous to equations 18, 19 and 20 are used. For brevity, $IS5 = (BW / Wd) \times D_T / Kpd$.

$$SPLV_{S5} = IS5 / (Kwp / Kd') \quad (21)$$

$$SPLV_{S5} = IS5 / (Kwp / Kd' + Usd / Upd) \quad (22)$$

$$SPLV_{S5} = IS5 / (Kwp / Kd1' + Usd / Upd + Uwd / [Upd \times Kd2']) \quad (23)$$

where

Usd = Daily ingestion of soil by dairy cow, kg/day. A default value of 0.87 kg/day is suggested (see Section 5.2.5)

4.2.6 Direct Soil Intake

Two pathway equations are presented here. Equation 24 involves exposure to "normal" levels of soil through direct ingestion, dermal absorption, and particulate inhalation.

$$SPLV_{S6} = (BW / Ws6) \times D_T \quad (24)$$

$Ws6$ is an "averaged" soil intake in kg/day, which accounts for an age-varying exposure regime. A default value of 7.4×10^{-5} kg/day

is developed for Ws6 in Section 5.1.8. In contrast, equation 25 describes a pathway which involves work activities when high levels of dust can be anticipated, such as from construction, dirt moving, or logging activities (the first use of this equation was for AAAP)¹⁰. The people at risk are expected to be adults.

$$SPLV_{S7} = (BW / Wsa7) \times D_T \quad (25)$$

Wsa7 is an adjusted soil intake in kg/day which accounts for airborne concentrations, breathing rate, and working conditions. A default value of 1.8×10^{-4} kg/day is developed for Wsa7 in Section 5.1.9.

4.2.7 Volatile Pollutant Inhalation

This pathway involves the inhalation of pollutant; the pollutant enters the air via volatilization from soil. Two specific situations have been studied. The first, represented by equation 26, relates to inhalation in an enclosed space such as a basement or sub-surface construction site.

$$SPLV_{S8} = (BW / Rb) \times D_T \times VAR / (Favn \times TAC) \quad (26)$$

where

Rb = Volume/day of contaminated air inhaled. A default value of 1.5 m^3 is suggested (see Section 5.1.7).

VAR = Ratio of room volume to area in contact with contaminated soil, meters. A default value of 1.34 m is suggested (see Section 5.3.3).

TAC = Time for one air change in a basement or enclosure, days. A default value of 0.083 days is suggested (see Section 5.3.3.)

Favn represents the time-averaged normalized flux of diffusing pollutant from soil, based on an initial condition of 1 mg pollutant/kg soil. Favn has units of $\text{mg/m}^2\text{-day}$ per mg/kg soil, or $\text{kg soil/m}^2\text{-day}$. A simple expression for Favn is presented in the next section. Generally, such expressions will require inputs concerning soil density and porosity, the contaminant K_d , aqueous solubility and vapor pressure.

Equation 27 relates to inhalation in open areas at a contamination site.

$$SPLV_{S8} = (BW / Rb) \times D_T \times (VW \times MH) / (LS \times Favn) \quad (27)$$

where

LS = A representative length dimension of a contaminated site in meters, and is discussed in Section 5.3.4.

VW = A representative wind speed at a contaminated site in m/day, and is discussed in Section 5.3.4.

MH = The mixing height of a contaminated air layer in meters, and is discussed in Section 5.3.4. This is assumed to be the upper limit of appreciable contamination.

Favn has the same meaning as above, but the soil characteristics involved with a surface soil may differ from those at lower levels (see Section 5.3.1). Rb is the air volume consumed daily by exposed persons at the model site. In this case, a 17 m³/day default value is suggested (see Section 5.1.7).

Equation 27 applies to for target individuals within a contaminated area; for affected people elsewhere, an expression involving air transport, mixing, and relative location with respect to prevailing winds would be involved. Such exposure should be considerably less than that represented in equation 27, thus, off-site relations are not developed further.

Equations 26 and 27 may be considered special cases of the relation:

$$SPLV_{S8} = (BW / Rb) \times D_T \times f(S8) / Favn$$

where f(S8) indicates the mg/m³ in air per mg/m²-day flux. Generally, f(S8) would be obtained from a dispersion model equation. Moreover, models more complex than shown in Section 4.2.8 for Favn can be employed for diffusion situations when sufficient information can be provided as input.

4.2.8 Simple Vapor Diffusion Relation

The relations given below provide a conservative predictor of the vapor emanating from a contaminated soil mass due to pollutant diffusion in soil-pore air. Details of the derivation and assumptions involved are in Appendix A.

$$Favn = (2 / [T1 - To]) \times (T1 \times \Phi(T1) - To \times \Phi(To)) \quad (28)$$

where

To = Starting time of an evaluation, in days.

T1 = Ending time of an evaluation, in days.

$\Phi(To)$ = Flux at time To, mg/m²-day per mg/kg in soil.

$\Phi(T1)$ = Flux at time T1, mg/m²-day per mg/kg in soil.

To and T1 are related to some initial zero time at which diffusion is assumed to begin. To is not necessarily zero time; when it is, the term To x $\Phi(To)$ drops out of equation 28. At any arbitrary time T, $\Phi(T)$ is given by:

$$\Phi(T) = (10^3 \times Kh / Kd') \times (Das \times [\epsilon + \Theta / Kh + \rho \times Kd' / Kh])^{0.5} / (\pi \times T)^{0.5} \quad (29)$$

where K_h is the Henry's Law constant in dimensionless units. This constant is the rate of increase of vapor density of a pollutant per unit increase in the pollutant concentration in solution when the liquid and vapor phases are in equilibrium under isothermal conditions. Its evaluation is discussed in Section 6.6. D_{as} is the molecular diffusivity of pollutant in soil-pore air. It has units of m^2/day and is related to the molecular diffusivity D_a :

$$D_{as} = D_a \times \epsilon^{10/3} / (\theta + \epsilon)^2 \quad (30)$$

where

D_a = Molecular diffusivity of the pollutant in air, in m^2/day . This term is discussed further in Section 6.7.

ϵ = Fraction of soil occupied by air, unitless; see Section 5.3.1.

4.3 ALTERNATE FORMS OF VARIABLES

If a contaminant (particularly an organic compound) does not to react with water or with other components of soil, and is expected to reversibly sorb on the organic carbon portion of the soil matrix (SOC), K_d can be estimated in term of K_{oc} :

$$K_d = f_{oc} \times K_{oc} \quad (31)$$

where

K_{oc} = Partition coefficient relating the mg/kg of pollutant adsorbed on organic carbon in soil to the mg/L of pollutant in water in equilibrium with the soil. Methods to estimate K_{oc} are presented in Section 6.5.

f_{oc} = Fraction of soil mass that is organic carbon; see Section 5.3.2.

Correlations have been proposed for a partition coefficient K_{pat} , which relates the pollutant level in adipose (fatty) tissue to that in feed (see Section 6.2.4). As a first approximation,

$$K_{pm} = K_{pat} \times f_m \quad (32)$$

and

$$K_{pd} = K_{pat} \times f_d \quad (33)$$

In these equations, f_m represents the fraction of adipose tissue in meat and f_d represents the fat content in milk. A default value of 0.2 is suggested for f_m and 0.04 for f_d ; see Section 5.3.6.

For convenience, all partition coefficients to plants (vegetables and pasture) have been expressed as K_{wv} or K_{wp} . However, information may be available in terms of corresponding

concentrations of pollutant in soil and incorporated into edible plant matter. From this information, a partition coefficient either for pasture (K_{sp} in mg pollutant per kg dry plant matter per mg pollutant per kg in soil) or for a vegetable (K_{sv} in the same units). In that case, with the assumptions above, K_{wp} can be determined from K_{sp} (or K_{wv} from K_{sv}):

$$K_{wp} = K_{sp} \times K_d' \quad (34)$$

In the absence of available information, the following may be assumed:

$$K_{wp} = K_{wv}$$

and

$$K_{sp} = K_{sv}$$

One or more of the above relations may be inserted in equations 9 to 23 to provide somewhat different versions of those equations. For example, equation 2 in the overview can be developed from substituting equation 34 in equation 18. Clearly, many variants can be generated with adaptation of one or more of equations discussed in this section.

5.0 NON-SPECIFIC CHEMICAL DATA INPUTS DOCUMENTATION

This section discusses the valuation of non-chemical specific pathway equation variables. Section 5.1 deals with variables which are associated with human exposure, such as consumption values and body weights. Section 5.2 deals mainly with cattle consumption data, as they are intermediates in the meat and milk intake pathways to the human consumer. Section 5.3 involves site-specific and miscellaneous parameters.

5.1 HUMAN EXPOSURE AND INTAKE-RELATED VARIABLES

Most human dietary information presented here has been taken from United States Department of Agriculture (USDA) sources, and is in terms of "per-capita" consumption. This is basically the ratio of foodstuffs available in the United States each year divided by the civilian population. Although such a measure includes all age groups, it should approximate adult intake. The USDA information is expressed either as direct intake based on interview data, on a retail-weight equivalent basis, or on a farm-weight equivalent basis. Information from the first two bases is used here. The author does not imply that the USDA is the only supplier of useful information, or that their information is more valid than that from other sources. Users should be aware, in any case, of qualifications to referenced data.

As in the previous report⁷, default or representative values for variables are presented along with a discussion of how they are developed. One may wish to consider special situations, and if so, different values may be justified. For example, section 5.1.2 indicates that water intake is about 1.6 to 2 L/day. If a problem involved an extremely hot region, as much as 10 L/day might be realistic. Otherwise, the author recommends the use of representative values. Many of the partition coefficient estimates to be discussed in Section 6 are, at best, accurate to an order of magnitude. Generally, D_T values are biased to be safe-sided. Thus, while extensive efforts to fine-tune or provide "worst-case" intakes may be satisfying, it may not be worth the time investment and can lead to overly restrictive PPLVs, with unmerited emphasis on the "worst-case" pathway.

Reference information sources of specific interest include: Scientific Tables²⁸, issued periodically by Geigy Pharmaceuticals, which have extensive information on human physiology and biochemistry; The Report of the Task Group on Reference Man²⁹, prepared for the International Commission on Radiological Protection, which has specific recommendations for typical values for a wide range of anatomical and physiological attributes of man as well as supporting commentary and sources; and "Composition of Foods"³⁰, the first in a group of publications called "Agriculture Handbook No. 8", which is used here to provide for moisture content data for vegetables and fat content data for meats. More specialized approaches are presented in the "Methods for Assessing Exposure to Chemical Substances"³¹ issued by the EPA's Office of

Toxic Substances.

5.1.1 Body Weight (BW)

In the SPHEM¹⁸, and for most other regulatory purposes, a 70 kg weight is considered representative of an adult. The 10 kg child is used to represent a sensitive group for short-term exposure evaluations¹⁸. Table 8 is a summary table of children's weights at different ages, as well as the central 80% range of weights at a given age. Weight distributions are well-researched; pediatricians often have graphical representations of age-weight relations along with percentile ranges.

5.1.2 Water Intake (Ww)

This refers to the intake of water per se, as opposed to the intake of water included in milk or foods. Several studies have been reviewed by the National Academy of Sciences³² which indicate the average intake is 1.6 L/day for an adult. For criteria-setting and drinking water regulations of the EPA¹⁸, a 2 L/day value is employed for an adult and 1 L/day for a child of 10 kg weight*. For long-term exposure situations, the water intake for an adult woman averages about 1.2 L/day, and for a 10-year old child, it averages about 1.0 L/day²⁹.

5.1.3 Consumption of Fish (Wf)

Nutritional literature often discusses the "meat, fish and poultry" category as a composite group. This is in recognition of the interconvertability of these foodstuffs in the diet. As a point of reference here and in later sections, Table 9 presents "model" diets that have been cited for different age groups as well as per-capita consumption levels estimated from USDA data.

The fish intake component of the per-capita diet above is 0.018 kg/day, which is in close agreement with the 18.7 g/day value reported by Cordle, et al.³⁸. The main problem which arises in determining a Wf (as well as other dietary constituents) is accounting for the source of fish and segment of the population involved. The EPA determination of mercury water quality criteria included³⁷ an in-depth review of fish consumption information and surveys. For the nation as a whole, marine waters provided about two-thirds of fish requirements; thus the 6.5 g/day used in water quality criteria²¹ represented fish from fresh and estuarine waters. This value is recommended as a "default value".

* Specifically, EPA employs the model 10 kg child and 1 L/day water intake in the short-term exposure evaluations of drinking water advisories. For a short-term situation, such as summer conditions, 10 kg children may drink as much as 1 L/day water. This may be contrasted to the long-term situation, which indicates that the average intake by a 10-year old child is 1 L/day of water. This illustrates the importance of stipulating conditions.

Table 8. Weight of Humans at Selected Ages²⁸

Age	Weight of males, kg		Weight of females, kg	
	Mean	80% Range	Mean	80% Range
1 year	10.0	8.9 - 11.5	9.8	8.4 - 11.2
2 years	12.6	11.2 - 14.5	12.3	10.7 - 14.4
5 years	19.4	16.6 - 22.5	18.8	16.4 - 21.9
10 years	32.6	27.7 - 40.8	31.9	25.9 - 40.7
18 years	63.0	54.4 - 76.7	54.4	47.0 - 65.5

Table 9. Food Items and Daily Dietary Intakes at Selected Ages

Food Group	Dietary Intake, kg/day		
	2-Year Child ³³	18-Year Old Male ³⁴	Per capita 1981 ³⁵
Dairy products	0.560	0.704	0.674
Meat, fish, poultry	0.136	0.262	0.324
Grains and cereals	0.150	0.424	0.185
Potatoes	0.037	0.177	0.108
Other vegetables ^a	0.088	0.240	0.283
Fruits ^b	0.145	0.222	0.196

a. Other vegetables include leafy, legumes, root, and tomatoes.

b. Fruits includes juices, but excludes such items as melons, strawberries, watermelons, which are in the "other vegetable" group.

EBASCO, 1987¹⁶ used fish catch statistics at Colorado Lakes to estimate a W_f for anglers at RMA freshwater lakes (see Section 2.2). They estimated that intake by anglers could range from 1.6 to 41.6 g/day, with a most likely estimate of 13.3 g/day. When compared to survey results (Table 10), this range and estimate would suggest that the anglers' total intake of fish is similar to that of the general population, but that they consume their own catch as a substitute for marine fish.

5.1.4 Consumption of Vegetables (W_v)

Other than on a per-capita basis, W_v is difficult to define, given the large number of specific vegetables in the diet and personal preferences. Moreover, vegetables are ingredients in many processed foodstuffs, such as tomato in catsup or pizza sauce or potatoes in potato chips. Here, vegetable intake is in terms of readily-recognizable items. W_v is in terms of a dry-weight intake; the conversion from fresh to dry-weight is first addressed. Table 11 shows the conversion based on 1981 retail-weight per-capita consumption information for the more

Table 10. Average and 95th Percentile of Fish Consumption by Sex and Age, 1973-1974 Data³⁷.

Age, years	Male Consumption, g/day		Female consumption, g/day	
	Average	95th Percentile	Average	95th Percentile
0-9	6.3	17.3	6.1	15.8
10-19	11.2	29.1	9.0	25.0
20-29	16.1	43.7	13.4	34.5
30-39	17.0	45.6	14.9	41.8
40-49	18.2	47.7	16.7	49.6
50-59	22.8	57.5	19.5	50.1
60-69	24.4	61.1	19.0	46.3
70 and over	15.8	41.7	10.7	31.7

popular vegetables. In some cases, I chose to exclude vegetable items which I thought would be unlikely to be prepared from home-grown produce, such as potato chips and shoestring potatoes. Otherwise, consumption was based on fresh, canned, and frozen item data. From this information, dry-weight intake of non-potato vegetables is about 9.8 percent the fresh-weight intake (14.09 g/day and 144.5 g/day respectively) and for potato-type vegetables, the dry-weight intake is about 21 percent of the fresh-weight intake.

Next, total non-potato vegetable intake is addressed, wherein vegetables less intensely consumed than those listed in Table 11³⁵ are also included. The per-capita value computed from USDA data³⁵ is 158.7 lb/year, or 197 g/day. Thus, on a dry-weight basis, per-capita consumption of non-potato vegetables is 19.3 g/day. On a dry-weight basis, the consumption of potato-type vegetables is about 17.7 g/day (see Table 11).

Next, the distinction between outside sources and garden sources of vegetables is discussed. Yost and Miles³⁸ estimated the average percent of annual consumption which is home-produced for three categories of homes: homes in urban and suburban areas, homes in rural areas not on farms, homes on farms in rural areas. Table 12 is a summary of their findings (data were also presented for seasonal percentages) for homes in each category. Yost and Miles³⁸ adjusted these percentages for the percentage of households in each category with gardens (43, 41, and 84 percent respectively; see Table 13). They assumed only persons in households with gardens consumed home-grown vegetables. They derived the "percent home-grown" items shown in Table 13, which when multiplied by the daily consumption of vegetables and non-potatoes (19.3 and 17.7 g/day dry weight respectively), provides the values in the two right-hand columns of Table 13. These consumption values are recommended for use as a function of generic locale.

Table 11. Data Base for Vegetable Fresh Weight to Dry-Weight Conversions.

Item	Consumption, lb/year ^a			Intake g/day	Dry Weight percent ^b	Dry Weight intake, g/day
	Fresh	Canned	Frozen			
Tomato	11.3	7.0 ^c	NL ^d	22.7	6.5	1.48
Beans ^e	1.3	5.6	1.6	10.6	6.6	0.69
Lettuce	23.8	NL	NL	29.5	5.5	1.62
Cabbage	7.6	1.2 ^f	NL	10.9	7.6	0.83
Celery	6.5	NL	NL	8.1	4.9	0.39
Carrots	6.3	0.4	1.0	9.6	11.8	1.13
Corn ^g	6.9	5.1	2.1	17.5	27.3	4.77
Onions	9.2	NL	0.7	12.3	11.9	1.46
Melons ^h	18.8	NL	NL	23.3	7.4	1.72
Subtotal, non-potato vegetables				144.5	9.8 ⁱ	14.09
Potatoes ^j	46.3	1.1	18.2	81.5	20.2	16.46
Sweet potato	2.6	0.9	NL	4.3	29.4	1.26
Subtotal, all potatoes				85.8	20.7 ⁱ	17.72
Total, all vegetables				230.3	13.8 ⁱ	31.81

a. Reference 35, 1981 Data

b. Reference 30

c. Excludes soups, pastes, sauce, catsup, juice use of tomato.

d. Not listed in consumption category.

e. Includes green beans and lima beans.

f. As sauerkraut

g. As the vegetable, as contrasted to corn meal, oil, or cereals.

h. Watermelon dry-weight used; item comprises about 60% of melons.

i. Back-calculated from dry and fresh weight intakes.

j. Chips, shoestring or dehydrated potatoes not included in total.

Table 12. Estimated Home-Supplied Percent of Food Groups³⁸

Food Group	All	Urban	Rural	
			Non-farm	Farm
Milk, cream, cheese	4.00	nil	3.99	39.94
Fats and oils	1.89	nil	1.63	15.18
Flour and cereal	0.43	nil	0.82	1.56
Meat	5.25	0.78	6.14	44.16
Poultry and fish	7.38	2.85	11.90	34.26
Eggs	7.51	0.62	9.14	47.93
Sugar and sweets	3.31	1.61	4.95	8.99
Potatoes and sweet potatoes	9.30	1.21	14.62	44.83
Fresh vegetables	21.20	7.55	35.65	70.03
Fresh fruit	8.11	3.24	13.20	31.29
Fruit and vegetable juices	1.92	0.68	4.13	11.04
Dried fruits and vegetables	4.44	2.63	6.90	16.67

5.1.5 Consumption of Beef (Wm)

In-depth information about specific animal source meat intake similar to that given above for fish and vegetables has not been found; thus, only 1983 retail-weight basis per-capita information from Bunch³⁵ is presented here. Beef intake is 78.7 lb/year or 0.098 kg/day; pork intake is 62.2 lb/year or 0.077 kg/day. On a per-capita basis, intake of veal and lamb are relatively minor (less than 2 lb/year). For calculation purposes, an intake of 0.1 kg/day is recommended.

5.1.6 Consumption of Milk (Wd)

Milk has become a raw ingredient in a multitude of modern food processing products. Thus, while figures are available for dairy products (see Table 9), I expected that they would overestimate the intake of persons from their own resources. My reasoning was that they would purchase high-fat products such as butter, cheese or ice cream, and that the milk from which such products were derived was not contaminated. A value of 0.3 L/day for adults is recommended, based on the 1983 per-capita intake of whole milk (fat content about 4%) and other beverage milk (Table 9, Bunch³⁵). If a more adverse case is desired, the per-capita intake cited in Table 9 may be used. For young children, the 0.56 L/day intake cited in Table 9 should be used; it is assumed their intake is primarily milk.

5.1.7 Inhalation Rates

For equation 27 (Section 4.2.6), the worker's daily air intake at an industrial site is required to estimate the variable W_{sa7} (see Section 5.1.9). A recommended value for this intake is 17 m³. Inhalation rates have been reported in two reference documents^{28,29} for qualitative classifications of work. This value is a compromise between the highest volume for "light work" (14.9 m³; "light work" includes office, laboratory, and most hospital work) and the lowest volume for "heavy work" (20.6 m³; "heavy work" includes commercial fishing, mining, or foundry work, and postal delivery on foot)²⁹.

If other situations need evaluation, a 9.6 m³ volume is recommended for 8 hours of non-occupational waking activity, and a 3.6 m³ volume for 8 hours of rest²⁴. Data for women and children may be obtained from references^{23,24}. As a rough rule of thumb for children, the daily intake of air in m³ equals the age. In the situation described in equation 26, R_b represents daily air volume inhalation in a basement area. A value of 1.5 m³/day is suggested for use. This value is based on a hourly respiration rate of 1.2 m³ in the basement (from above for non-occupational activity) and 1.2 hour/day basement residence time; this time was assumed by Moeller and Fujimoto³⁹.

Table 13. Calculation of Home-Grown Vegetable Intakes at Generic Locales³⁸

Locale	Homes With Gardens, Percent	Home-Grown Vegetables, Percent	Home-Grown Potatoes, Percent	Intake of Non-potato Vegetables g/day, dry weight	Intake of Potatoes
Urban and Suburban	43	11	3	2.1	0.5
Rural non-farm	41	58	36	11	6.4 ^a
Farm	84	66	53	13	9.4

a. For example, Table 12 indicates that 14.62 percent of the intake of potato-type vegetables at non-farm households is from gardens. Table 13 states that 41 percent of such households have gardens. Then, households with gardens are expected to provide $14.62\% / 0.41$ or 36 percent of their potato and sweet potato needs from their gardens. From Table 11, the total needs are 17.7 g; 36 percent of this is 6.4 g.

5.1.8 Incidental Soil Ingestion, "Normal Conditions" (Ws6)

This parameter is valued to reflect a time-varying amount of intake for the lifetime of a target individual. The derivation can be adapted for shorter-term exposure, and starts with a point-in-time relation between total acceptable intake of a pollutant and its level in soil. For example, at age i ,

$$SPLV_{S6} = BW_i \times D_T / W_{Si} \quad (35)$$

W_{Si} is the daily intake of soil, which can vary with age, as does BW_i . Since the pollutant is assumed refractory in soil, $SPLV_{S6}$ should be a constant. A value of $SPLV_{S6}$ can be derived by time-averaging BW_i / W_{Si} over a "model" lifetime (25600 days).

$$SPLV_{S6} = D_T \times (1 / 25600) \int_0^{25600} (BW_i / W_{Si}) dT \quad (36)$$

BW_i , at least in terms of mean values for the population, is a well-known function of time. Considerable research has been done to attempt to quantify W_{Si} . The approach taken by Hawley⁴⁰ is presented, wherein ingestion, dermal adsorption and inhalation are involved. His approach has the attractive feature that it provides estimates of intake based on a life-style rationale. Hawley developed three age-specific scenarios: for a 2-1/2 year old child, a 6-year old child, and an adult (19-70 years of age). Each scenario includes many factors, as typified by oral ingestion of soil by the 2-1/2 year old child. Four components are involved: intake of 250 mg/day of "outdoors dirt" five days per week in the May to October half-year; 50 mg/day of "indoor dirt"

(of which 80% is estimated to be from outside) during this time frame; no intake of "outdoors dirt" in the November to April half-year; and 100 mg/day intake of "indoor" dirt in this half-year. A summary of averaged daily intake factors for these three age scenarios by intake route appears in Table 14.

Hawley⁴⁰ used the following approach for other times:

- o At time=0 (birth), $W_{si} = 0$.
- o Soil intake increases linearly to 2-1/2 years of age, when it reaches 160 mg/day.
- o Soil intake decreases linearly to age 6, when it reaches 30 mg/day.
- o Soil intake increases linearly to age 18, when it reaches 66 mg/day, at which level it remains through age 70.

The integral in equation 36 can be approximated by a series summed yearly; input values used are in Table 15. Weight and soil intake values are computed for the half-year at one-year intervals from birth to adulthood at age 18. The summation of BW_i / W_{si} , factoring out the adult weight, and division by the lifetime*, gives a recommended W_{s6} of 7.4×10^{-5} kg/day.

In terms of lifetime exposure, the relative contribution from childhood to Hawley's model is muted in effect, since 52 years exposure to 66 mg/day is factored in. On the other hand, the relative intensity of exposure at 2.5 years of age is about twelve times the time-averaged value.** Thus, when this pathway is involved, pollutant toxicological data should be evaluated to account for a situation where an adverse effect might occur with less-than-lifetime exposure to a dose 12 times higher than D_T .

Hawley's approach does not account for unusual pica behavior. Pica describes two patterns of behavior⁴¹. The first is a sampling of non-food items via ingestion, which is common among preschool children. The peak in soil intake at age two and one-half is a consequence of this. The second is an uncommon condition, characterized by a craving for and habitual ingestion of nonfood items. This condition has been associated with dietary disorders, malnutrition, or neurobehavioral disorders. The daily intake of soil by such persons has been estimated to be as much as 5000 mg/day⁴¹.

* The summation on a yearly basis is valid as long as the division is by a yearly lifetime and intake is on a per-day basis.

** This can be understood by realizing that the 2-3 year old child is about one-fifth the weight of an adult but that the child's dirt intake is more than twice that of an adult.

Table 14. Model Intakes of Soil Estimated by Hawley⁴⁰

Route	2.5-Year Old Intake, g/day	6-Year Old Intake, g/day	Adult Intake, g/day
Oral ingestion	150	23.4	60
Dermal absorption	7.5	5.9	5.1
Inhaled particulates	0.2	0.2	0.9
Total intake, mg/day	160	30	66

Table 15. Values of Soil Intake and Weight Used to Compute Ws6

Age interval, years	Wsi, mg/day	BWi ^a , kg	BWi/Wsi, kg / (kg/day)
0 - 1	32	7.4	2.31x10 ⁵
1 - 2	96	11.3	1.18x "
2 - 3	160	13.2	0.82x "
3 - 4	123	15.4	1.25x "
4 - 5	86	17.4	2.02x "
5 - 6	48	20.3	4.23x "
6 - 7	31.5	22.6	7.17x "
7 - 8	34.5	25.5	7.39x "
8 - 9	37.5	28.2	7.52x "
9 - 10	40.5	30.9	7.63x "
10 - 11	43.5	33.8	7.77x "
11 - 12	46.5	37.2	8.00x "
12 - 13	49.5	41.3	8.34x "
13 - 14	52.5	46.2	8.80x "
14 - 15	55.5	51.0	9.19x "
15 - 16	58.5	54.5	9.32x "
16 - 17	61.5	59.0	9.59x "
17 - 18	64.5	63.3	9.81x "
18 - 70	66	70	10.6 x "

a. Weights shown represent an average between mean male and female weights at the mid-point of each age range. Weight data from reference 28.

5.1.9 Incidental Soil Ingestion, "Working-Site Conditions" (Wsa7)

This parameter incorporates intakes from inhalation, absorption, and ingestion of raised dust during outdoor work such as logging, excavation, or construction. Since the target population involves adult workers, time-averaging dust intakes is not involved. However, the quantification of dust intakes is less certain than in the case above.

There have been studies concerning the dust levels attained in the process of dumping soil (Sutter⁴²), and those in the vicinity of tanks, armored personnel carriers or other vehicles (Nicholson and Cardinale⁴³; Pinnick et al.⁴⁴). Dust concentrations of the order of 40-1000 mg/m³ have been measured; as points of reference, the

particulate levels associated with "clear" air are about $10 \mu\text{g}/\text{m}^3$ and dust storm particulate levels are of about $20 \text{ mg}/\text{m}^3$.

The above studies involved well-dried or arid soils, which may not always be the case in an outdoors work situation. Even if such levels were attained, it is doubtful whether they could be maintained for an extended period of time. If they were, work operations could be severely restricted due to poor visibility. Further, prolonged exposure to dust concentrations in excess of $10 \text{ mg}/\text{m}^3$ is not recommended¹⁹. For model purposes, a dust concentration of $10 \text{ mg}/\text{m}^3$ is suggested. From Section 5.1.7, an adult male worker is estimated to inhale 17 m^3 of air during eight hours of work; in an 8-hour work-day, 170 mg of dust is inhaled. As a conservative assumption, all this dust reaches the lungs. Pinnick et al.⁴⁴ observed that the major component of dust raised from passing vehicles comprised particulates in excess of $10 \mu\text{m}$; particulates of that size are usually retained in the nose and do not to penetrate further⁴⁵.

A second route of intake is by ingestion. Hawley⁴⁰ discusses different scenarios where inadvertent soil ingestion occurs, and derives soil intake estimates which range from 110 to $480 \text{ mg}/\text{day}$. These are "soft" numbers, since many factors can be involved, such as smoking dust-covered cigarettes (in one scenario, seven such cigarettes are smoked during a work-day), lip-smacking to remove adhering soil, and eating food with dust-covered hands. A intake of $230 \text{ mg}/\text{day}$ is suggested, the geometric mean of the endpoints of the above range.

A third route of intake is by skin absorption. In the scenario in which $480 \text{ mg}/\text{day}$ intake via ingestion was estimated, Hawley⁴⁰ estimated dermal intake to be $38 \text{ mg}/\text{day}$. Given the higher magnitude of the other intakes, and the tenuous basis for them, the skin absorption route is not included in further calculations.

Based on inhalation and ingestion intakes, workers could be exposed to the equivalent of $400 \text{ mg}/\text{day}$ of dust. However, workers do not spend every day at work. Factoring in a nominal 5-day work week, holidays, vacations, and sick time, work would be restricted to perhaps two-thirds of calendar days. A further adjustment may be taken for inclement weather, which may either suspend work or wet soil sufficiently to suppress dust raising. In the previous report⁷, the fraction of precipitation-free days to calendar days was suggested for this adjustment. In the Washington, D.C. area, this factor would be about 0.67; the potential for dusty conditions would occur two-thirds of the time. In that area, "dusty work-days" would involve about 44 percent of calendar days. On this basis, the calendar-day equivalent intake would be $176 \text{ mg}/\text{day}$, 44 percent of $400 \text{ mg}/\text{day}$. Then, in consistent units with BW and D_T , $Wsa7$ is $1.8 \times 10^{-4} \text{ kg}/\text{day}$.

5.2 CATTLE INTAKE AND FAT CONTENT FACTORS

Here, cattle are addressed as a source of meat and milk to the human diet. In this respect, there are differences between dairy and beef cows. The dairy cow is an adult animal, where a plateau of weight and food intake is expected. Its diet is geared to the express purpose of providing milk. The beef cow is a growing animal, usually slaughtered before it matures. Its weight gain patterns can be controlled.

There have been many studies with penned cattle fed known amounts of contaminated rations for the purpose of determining pollutant uptake; some of which are reviewed below. However, the intake of pasture in the open is not controllable. One can observe the progress of the animal (either in terms of milk output for a dairy cow or weight gain for a steer) to determine if pasture alone is adequate. If pasture is not adequate, supplemental feed may be provided to attain production objectives.

I have assumed that pasture consumption rates by cattle in the open will be similar to those observed for confined cattle. In the open, cows need additional energy to walk and graze as contrasted to animals in experimental situations. Thus, on a given day, cows in the open may well consume more pasture than their penned counterparts. There are factors which offset this additional intake. In colder climates, livestock may have to be fed completely with rations during periods of deep snow cover or low wind-chill. In warm, well-pastured areas, the energy expenditure should be low.

Feed requirements are in terms of air-dry weight, where the moisture content is about 10 percent of total feed weight. This is the moisture content in most hays, and one of the bases upon which ration tradeoffs are based. The FCR, initially used in Section 3.3.2, here indicates the liters of water or kg of feed (air-dry weight basis) consumed daily per kg of cattle weight.

5.2.1 Plant Consumption by Steers (Upm)

Baxter et al.⁴⁶ studied the uptake of heavy metals and persistent pesticides in cattle tissues when the animals were fed a dry sludge-amended diet. As part of this study, 5-month-old Hereford steers were fed either a sludge-free diet (controls) or a diet with 12 percent sludge content for 270 days. Eight animals were in each group. The control animals were estimated to consume 12808 kg of feed, which averaged over the number of animals and days indicates a nominal 5.9 kg/day intake. Animal weight were measured at the start, after 90 and 180 days, and at the end of the feeding study, and averaged 224, 323, 358, and 446 kg respectively. Based on the nominal average intake and the time-average animal weight (335 kg), FCR was 17.5 g/kg-day. Animals gained an average of 0.81 kg/day in this study.

Wilson et al.⁴⁷ fed steers on diets which included: apple waste, (91 percent dry weight); haylage, a hay-silage mix (54.2 percent dry weight); hay (89.6 percent dry weight); and a concentrate (assumed 90 percent dry weight). Animals were feed on selected mixtures of these ingredients for about 5-1/2 months. Seven Herefords fed a haylage and concentrate mixture were found to consume an average of 10.6 kg/day; during the test the animals average weight went from 333 to 456 kg. Based on the time-average weight of these animals, FCR was 27 g/kg-day. A group of 7 Angus cows fed hay and concentrate were found to consume an average of 9.28 kg/day; during the test, the animals average weight increased from 253 to 402 kg. As explained above, FCR was 28 g/kg-day. A group of 6 Holsteins fed an apple waste-haylage-concentrate diet consumed an average of 10.2 kg/day. Their average weights increased from 358 to 487 kg, which on a time-average weight basis, corresponded to a FCR of 24 g/kg-day.

Albritton⁴⁸ reported FCRs of 23-30 g/kg-day, based on specific diets and weight of animal. Juergenson⁴⁹ presented model recommended feed diets to provide different levels of weight gain. For a 0.75 kg/day gain objective, diets for 150, 200, 300, and 400 kg animals corresponded to FCRs of 22, 27, 27, and 25 g/kg-day, respectively.

These studies suggest that FCRs for growing steers would fall in a range of 17.5 to 30 g/kg-day. The daily intake value sought is a time-averaged intake:

$$(T_s - T_w)^{-1} \times \int_{T_w}^{T_s} FCR \times AW(T) \, dT$$

where T_s is the time at slaughter, T_w is the time at weaning, and $AW(T)$ is animal weight at any time within the lifetime period. For evaluation purposes, the following lifetime scenario is used, which is considered a reasonable model for a beef steer raised on pasture:

- o The animal is born on March 1.
- o The animal is weaned on August 1 at a weight of 180 kg. Feed consumption to this point is nil.
- o The animal pastures through November 30, at which time it weights 240 kg. During this period, FCR is 25 g/kg-day. The animal gains weight at a constant rate (about 0.5 kg/day).
- o During December-February, the animal does not gain weight. The FCR drops to 17 g/kg-day (approximately a maintenance level).
- o From March 1 of the next year to November 30, when it is slaughtered, the animal gains weight at a constant rate to a final level of 400 kg. The FCR is 25 g/kg-day in this time period.

The above model data can be used in an approximation to the integral as the sum of products, each based on a period of growth or maintenance (starting from the weaning date):

$$\begin{aligned} & (1/487 \text{ days}) \times [(122 \text{ days} \times 25 \text{ g/kg-day} \times 210 \text{ kg}) + \dots \\ & (90 \text{ days} \times 17 \text{ g/kg-day} \times 240 \text{ kg}) + \dots \\ & (275 \text{ days} \times 25 \text{ g/kg-day} \times 320 \text{ kg})] \times 1 \text{ kg}/1000 \text{ g} = 6.6 \text{ kg/day.} \end{aligned}$$

There may be species-related or regional differences, and for these, local agriculture experts can be consulted.

5.2.2 Water Consumption by Steers (Uwm)

There are no firm figures on water intake; generally steers are given water ad libitum. Albritton⁴⁸ reports nutritional requirements for mature female 500 kg cows as 0.06 L/kg-day or 30 L/day and a mature 800 kg male of 0.047 L/kg-day or 37.6 L/day. For evaluation purposes, a 0.055 L/kg-day value is used, and when substituted in the above summation expression in place of FCRs, the computed value is 15.3 L/day.

5.2.3 Plant Consumption by Dairy Cows (Upd)

Fries et al.⁵⁰ studied the dynamics of polychlorobiphenyl (PCB) transfer to milk and animal fat in the cow. Cows were fed a PCB-dosed diet for 60 days. Based on initial weight of animals and average diet, FCRs ranged from 26.5 to 33.7 g/kg-day. Link et al.⁵¹ fed dairy cows pesticide-dosed feed in a study of fat uptake and toxic effects. Feeding was carried out for 12-16 weeks. Based on average weight of animals and average diet, FCRs ranged from 29 to 35 g/kg-day. Higher FCR levels in dairy cows than in steers can be expected, since a portion of the feed is converted to milk.

Rather than deriving Upd as was done for Upm, the process is simplified by assuming a constant animal weight. A dairy cow can produce milk for several years; thus the relative contribution of pasture intake during its non-productive years to its overall intake is small. Based on the two studies above, a maturation weight of 520 kg appears reasonable*, as does a FCR of 32 g/kg-day. This yields a Upd of 16.6 kg/day.

5.2.4 Water Consumption by Dairy Cows (Uwd)

As is the situation with steers, dairy cows are given water ad libitum, and there is not much information on water uptake. Albritton⁴⁸ reports that mature dairy cows in lactation should have 150 mL/kg of water. For a 520 kg animal, this corresponds to 78 L/day.

* Cows in the Fries et al. study⁵⁰ weighed 495 to 587 kg, those of Link et al.⁵¹, 448 to 519 kg.

5.2.5 Soil Ingestion by Grazing Cattle (Usm and Upd)

Healy⁵², Baxter et al.⁴⁶, and Thorton and Abrahams⁵³ have reported studies of soil uptake by grazing cattle. The experimental procedures involve titanium assays in soil and in deposited fecal matter from these cows. Titanium does not transfer from soil to plant matter⁴⁶, thus the titanium detected in fecal matter is from soil. Reported values are not exact, since the digestibility of graze and the intake of food enter into calculations, and these have to be estimated.

Healy's work was done in New Zealand with dairy cows⁵². An average daily soil intake of 0.72 kg/day was estimated. Within the animal involved in a given feeding pattern, the range of intakes was somewhat over a factor of two. Baxter et al. studied fecal matter of beef cows grazing at Lowry Air Force Base, CO, and estimated their soil intake to be 8 percent of diet⁴⁶. Thorton and Abrahams studied farms in mining and smelting areas of the United Kingdom⁵³. They noted high soil intake levels in cows during periods of sparse pasture (from 2.7 to 18 percent of diet in early Spring) which decreased to less than 1 percent of diet in late Spring when pasture was more plentiful, and then increased to about 3.2 percent of diet in August.

For default purposes, a soil content of 5 percent of diet appears a reasonable estimate. Thus, for dairy cows, where Upd is estimated at 16.6 kg/day, about 0.87 kg/day of soil would be consumed (since Upd is the pasture component of such a diet, the computation is $16.6 \times [5/95]$). For steers, Usm is 0.35 kg/day.

5.2.6 Fat Content of Meat and Milk (fm and fd)

Representative values of fat content in beef on a "total edible, trimmed to retail level and raw" basis ranged from 25.1 percent for choice meat to 15.8 percent for standard meat³⁰. A 0.2 value for fm is taken as a compromise value, although one might expect that animals raised on pasture would tend to be leaner than those raised, in part, under feed-lot conditions. On the other hand, cooking removes relatively more moisture than fat from meat; the fat fraction in cooked beef is higher than in raw beef.

For milk, a fd of 0.04 is suggested³⁰. Standards for whole milk range between 3.5 and 3.7 percent fat³⁰. In work by Fries et al.⁵⁰, the milk of specific Holstein cows ranged from 3.4 to 4.3 percent fat. Inter-breed differences also exist, so when possible, local breeds should be assessed. As an example, Davis⁵⁴ cites these species-specific representative fat contents:

Ayshire	4.0 percent
Brown Swiss	4.0 percent
Guernsey	4.9 percent
Holstein	3.6 percent
Jersey	5.4 percent

5.3 SOIL, HOME, AND CLIMATIC FACTORS

5.3.1 Soil Density and Voids (ρ , θ , and ϵ)

The mineral components of soil have densities from 2.3 to 5.2 kg/L⁵⁵ and voidless soils usually have densities of about 2.6 - 2.8 kg/L. However, dried, undisturbed topsoils usually have densities which range from 1 to 2 kg/L. An appreciable fraction of such soils is voids space, which is partially filled with air or water. Depending upon the pathway involved, θ (the void fraction with water) or ϵ (the void fraction with air) is needed. The information given here is of necessity general; the US Geological Survey or State offices can be contacted for information about specific areas.

Pathways 1 and 2 : Bulk density will depend upon the type sediment or soil involved. Yeh⁵⁶ reports representative values for sand (1.18 - 1.58 kg/L), silt (1.29 - 1.8 kg/L), and clay (1.4 - 2.2 kg/L). Since sediments are under water, θ should be in the approximate range 0.4 to 0.6¹⁶.

Pathways 3, 4, and 5 : In these pathways, surface soil conditions are involved. As a rule, pores will partially filled with water. In this case, the field capacity is suggested as an upper limit on θ . Field capacity is roughly the moisture level in a soil 1 to 3 days after the soil has been thoroughly soaked⁵⁷. Generally, field capacity values range from 10 to 25 percent. As a lower limit, 4 percent is reasonable; capillary action would prevent extreme moisture depletion except in periods of drought. A representative value of θ would depend upon climate; in a rainy area, a value near the field capacity might be selected, in a dry area, a value near 5 percent might be appropriate. In equations 25 and 28, two different soil conditions may apply; see the above paragraph for θ values in water-logged sediment.

Pathway 8 : In a basement problem, soil from the surface to several meters deep is often excavated, mixed, and then placed around the basement. Sub-soil is expected to be more dense than is surface soil; based on information from EBASCO¹⁶, the density increase is about 20 percent. Assuming that soils from all strata have the same density on a voidless basis, sub-soil will be less porous than topsoil. Field capacity is recommended for θ in this situation; adjustments should be made for very wet or dry areas. The value of ϵ is the difference between the total void fraction and θ .

5.3.2 Organic Carbon Fraction of Soil (foc)

The foc can vary greatly between soils; in topsoils, from less than 0.01 to, in unusual cases, in excess of 0.1. In past work, a default value of 0.02 has been used¹⁰. Thus, when possible, information on the specific soil in an area should be obtained, or foc assays performed. Some published information reports the soil organic matter fraction; the foc would be about half this

fraction⁵⁸ (although a conversion of foc = 0.58 x soil organic matter is cited as a rule of thumb⁵⁹, experimental results indicate that conversion factor is less). The foc often decreases with depth in soil, which should be taken into account where subsoil is involved in the transfer process. For example, Table 16 shows organic matter levels as a function of depth for selected Colorado soil profiles.

5.3.3 Basement Dimensional Factors (VAR and TAC)

VAR is based on the volume and area of a basement. Since basement geometries differ, VAR will be judgmental, although from a practical view, it cannot vary over an extreme of values. For a representative value, a basement was assumed to have a 140m³ volume (7 m x 10 m x 2 m high), and half the area on the sides was covered by soil. The soil-covered area (half of four sides and the floor) is 104 m². The ratio 140/104 equals 1.35.

Air exchange rates for single family detached houses are generally between 0.5 and 1.5 air changes/hour⁶⁰. The air exchange rate for basements should be on the low side of this range since they are usually most poorly ventilated part of a house, and homes built today are more air-tight than in the past. An a 0.5 air change/hour rate corresponds to a 0.083 day/air change TAC .

5.3.4 On-Site Size and Dispersion Factors (LS, VW, and MH)

The site characteristics will be unique in each situation. LS is a characteristic length downwind dimension. This will have to be determined for each site. The most conservative situation is when the worker is at the downwind edge of a contaminated area. For a square-shaped site, LS is the square root of the area. For other shaped sites, other formulae could be applied, but unless the site has an unusual shape, LS as computed above can will suffice.

VW estimates can be developed from meteorological data. The National Climatic Center in Asheville, NC has detailed information available for 250 major stations. For these stations, seasonal information is available concerning frequency of occurrence of the six Pasquill air stability categories**, and for each category, the median windspeed. Information should be obtained for day and night. Discard nighttime data and, based on locale, winter data. For the rest, compute an average windspeed:

$$\text{Average windspeed} = \Sigma (p(F) \times VF) / \Sigma p(F)$$

where p(F) is the frequency of a given seasonal stability and VF is the corresponding windspeed. This averaged value is converted to a m/day basis. A default value for VW of 2 m/sec (173,000 m/day) has been suggested⁶².

** The six Pasquill categories describe conditions from "A" (rapid rising of air during calm, sunlit afternoons) to "F" (inversions during calm evenings).

Table 16. Organic Matter in Selected Colorado Soils^a

Soil	Topsoil	Lower soil layers ^b				
Ascalon sandy loam	1.5 (0-4)	1.3 (4-7)	1.2 (7-14)	1.1 (14-18)	0.6 (18-25)	0.2 (25-60)
Heldt clay	1.2 (0-5)	0.9 (5-14)	0.8 (14-22)	0.6 (22-32)	0.3 (32-40)	0.3 (40-60)
Weld loam	2.2 (0-4)	2.0 (5-10)	1.7 (10-15)	1.3 (15-19)	0.6 (19-28)	0.1 (28-60)
Platner loam	1.3 (0-5)	1.2 (5-14)	1.1 (14-18)	0.8 (18-23)	0.5 (23-36)	0.1 (36-60)
Truckton sandy loam	1.5 (0-4)	1.6 (4-8)	1.0 (8-21)	0.3 (21-28)	0.3 (28-54)	0.1 (>54)
Valentine sand	0.4 (0-3)	0.3 (3-10)	0.1 (10-24)	0.1 (24-60)		

a. Source, reference 61. The first number in each entry is the percent organic matter. The numbers in brackets is the location of a specific sub-layer of soil in inches below the soil surface.

b. The researchers classified soil according to horizon; thus the extent of specific sub-layers differs between soils.

MH estimation methods are not well-developed. Shultz et al.⁶² suggest a 2 m default value for receptors at the edge of a site to 200 m downwind of the edge, but acknowledges that the value is probably conservative. I suggest a MH of 20 m since most work is usually performed in the daytime when considerable vertical mixing can occur.

5.3.5 Flux Evaluation Times (To and Tl)

In the case of inhalation in basements, To should exceed zero, since there is usually a time interval between the time soil is placed around a poured basement and building occupancy. In Rocky Mountain Arsenal assessments¹⁶, To was assumed to be 60 days. For lifetime occupancy, Tl can be taken as 25,600 days (70 years). In the case of vapor emissions from the surface of a contaminated site, the specific scenario will dictate the times. If ground is not undisturbed (such as future use of a site as a playground), To may be greater than zero, since time will have elapsed between clean-up activities and first scenario use, while Tl may be as long as 70 years. If ground is continually disturbed, such as during hypothetical post-remediation construction activities, To may be zero, and Tl as low as one day.

6.0 PARTITION COEFFICIENTS AND RELATED PROPERTIES OF COMPOUNDS.

Experimental partition coefficient measurements mainly are restricted to well-known and widely-used pesticides or important organic solvents. Thus, equations for estimating these coefficients from other physical or chemical properties have been developed. They are not perfect by any means, as explained in Appendix C. Most are correlations of existing data for a select group of compounds. The most valid estimation equation should be based upon compounds similar to the pollutant being considered. In lieu of equations specific to certain types of compounds, "general use" equations are presented here. Lyman et al.⁵⁹ provides other equations, and their book will be cited frequently in this section.

Estimation methods presented are generally restricted to organic compounds which are expected (or in lieu of available information, can be assumed) to be:

- o chemically inert in the environment (see Section 4.0);
- o in soil, primarily physically adsorbed on SOC (see Section 4.3);
- o in fish, primarily stored in lipids; and
- o in terrestrial animals, stored in adipose tissue or in the fatty portion of milk (see Section 4.3).

First, relevant physical or chemical properties are discussed. In some cases, even these may have to be estimated, and estimation procedures for them are discussed.

6.1 PHYSICAL AND CHEMICAL PROPERTIES

6.1.1 Kow

The octanol-water partition coefficient, Kow is the ratio of the concentration of a substance in n-octanol to that in water. Kow, is a key property from which to estimate other coefficients. Value of Kow range from less than 1 to in excess of 10^6 , so the base 10 logarithm, Log Kow, is often reported. Kow can be measured directly in accord with the definition above, or can be measured by chromatographic techniques⁶³. Hansch and Leo⁶⁴ have developed the "Fragment Constant" method to estimating Log Kow based on molecular structure. It can be estimated from analogous measurements with a different non-polar organic solvent and water; Lyman, et. al.⁵⁹ present equations for this purpose.

6.1.2 Aqueous Solubility Limit

This is the concentration of a dissolved substance in water that can be attained at equilibrium with the substance in its "normal

state". Sources useful for solubility data include standard chemical handbooks, notably the handbook by Yerschuere⁶⁵, and for specific compounds, the DTLV²⁰, or the SPHEM¹⁸. Aqueous solubility can be estimated from Log Kow⁹; several proposed equations are presented in Lyman, et al.⁵⁹. This factor is represented in equations by SW when units of mg/L are involved; when mole/L units are involved, the term SWm is used. SW is a temperature-specific property. In this report, a 25 °C temperature is assumed. Environmental problems for some locales may merit a different temperature; however, methods to extrapolate solubilities from one temperature to another are not general.

6.2 BIOCONCENTRATION FACTOR (BCF)

BCF is the ratio of pollutant concentration in fish to that in the water in which the fish resides. The BCF does not take into account biomagnification effects, where pollutant is supplied from the food chain, components of which can contain the pollutant at a much higher concentration than does the ambient water. BCFs have been experimentally obtained for many pesticides and widely-used organic solvents. Equations have been proposed to predict BCF from either Log Kow or SW⁵⁹. Several such relations are presented in Lyman et al.⁵⁹. A generally applicable equation from which to estimate BCF from Log Kow is :

$$BCF = 10^{(0.76 \text{ Log Kow} - 0.23)} \quad (37)$$

This equation was developed for the EPA by Veith and co-workers, and used to estimate BCF for water quality criteria⁶⁶ calculations when credible experimental data was not available. It was developed for freshwater fish with a lipids content of about 0.076. Other such relations often don't specify a lipids level. An applicable equation in which SW is the predictor is:

$$BCF = 10^{(3.002 - 0.444 \text{ Log SW})} \quad (38)$$

This relation is from Davies and Dobbs⁶⁷; here converted to a mg/L basis.

6.3 SOIL - WATER PARTITION COEFFICIENTS (Kd)

Soil adsorption isotherms are the usual experimental means to measure Kd (or estimate Koc allowing adjustment for foc). The Freundlich isotherm often fits experimental data satisfactorily:

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

Cse and Cwe are the corresponding soil and water concentrations of a substance when equilibrium is attained. The constants Kf and nf are experimentally determined. If nf = 1, Kf = Kd. If nf doesn't equal unity, Kd will be a function of Cs. In that case, although Kd can be experimentally determined, the computation of a PPLV from equation 3 may not be valid. Chapter

4 in Lyman et al.⁵⁹ discusses the relative impact of divergence of n_f from unity.

In lieu of experimental data, K_{oc} can be estimated from $\log K_{ow}$ or SW . Lyman and Loreti⁶⁸ have suggested the following relations:

$$K_{oc} = 10^{(0.806 \log K_{ow} + 0.473)} \quad (39)$$

$$K_{oc} = 10^{(-0.602 \log SW_m + 0.656)}$$

6.4 PLANT - ANIMAL ADIPOSE TISSUE PARTITION COEFFICIENTS (K_{pat})

Three papers have advanced prediction equations: Kenaga⁶⁹, Garten and Trebalka⁷⁰, and Travis and Arms⁷¹. The author favors the equations presented in Garten and Trebalka⁷⁰ (converted here from $\mu g/L$ to mg/L):

$$K_{pat} = 10^{(-1.633 - 0.608 \log SW)}$$

$$K_{pat} = 10^{(-3.935 + 0.511 \log K_{ow})} \quad (40)$$

6.5 WATER - PLANT PARTITION COEFFICIENTS (K_{wv} , K_{wp})

Procedures to estimate these coefficients are not well developed. Briggs, as reported in Calamari et al.⁷² has proposed a stem concentration factor (SCF) for plant matter on a wet-weight basis:

$$SCF = 0.784 \times (0.82 + 10^{E1}) \times 10^{E2} \quad (41)$$

where

$$E1 = 0.95 \log K_{ow} - 2.05$$

$$E2 = -0.178 \times (\log K_{ow} - 1.78)^2$$

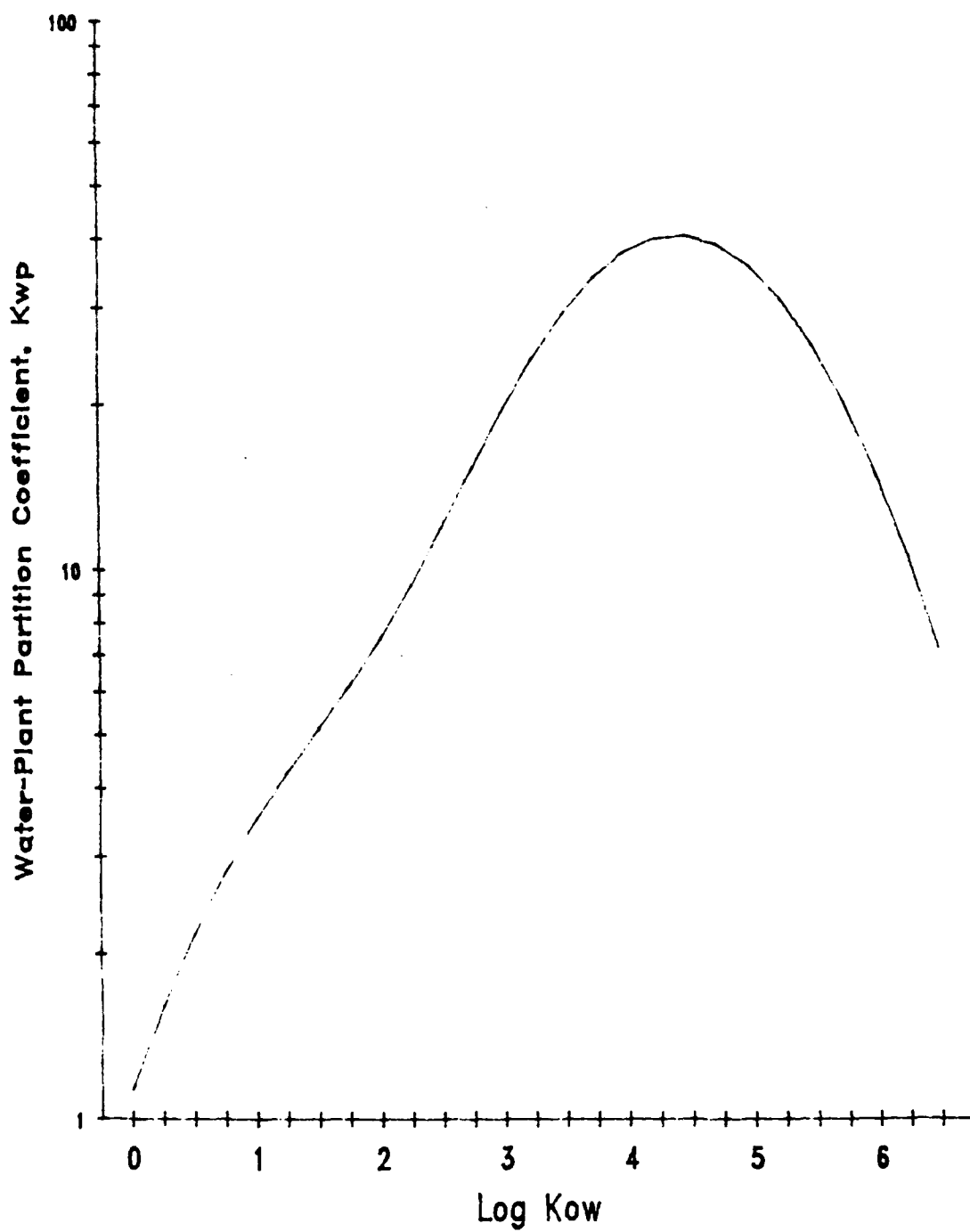
Davidson⁷³ demonstrated fair agreement of SCF with experimental results from studies measuring uptake of several pesticides. I recommend that a coefficient of 5 be used in lieu of 0.784 to adjust to a dry-weight basis, and that this equation be used for both K_{wp} and K_{wv} . The recommended equation is shown as a function of $\log K_{ow}$ in Figure 2.

6.6 HENRY'S LAW CONSTANT (K_h)

This constant reflects the near-ideal behavior of very dilute aqueous solutions. When mass equilibrium is established between air and an aqueous solution of a volatile substance, the ratio of the substance's unsaturated vapor pressure to its concentration in solution will be nearly constant and not a function of the solution concentration. This behavior, particularly for relatively insoluble compounds, is maintained to the limits of aqueous solubility. Therefore, the constant is taken as the ratio of saturation vapor pressure (VP) to SW .

In equation 29, K_h is in dimensionless terms, the ratio of molar density in air to molar density in water (at corresponding

Figure 2. Proposed K_{wp} vs Log K_{ow} Relation



saturation limits). Thus, conversions from other commonly-used units can be readily accomplished with the knowledge that the millimolar density of a gas at 1 atmosphere (760 mm Hg, 14.7 psia, or 1.013×10^5 Pa) and 25 °C is 41 millimoles/L. For example, if a hypothetical substance has a molecular weight of 250, VP is 0.01 mm Hg, and SW is 350 mg/L, the conversion is:

$$(0.01 / 760) \times 41 / (350 / 250) = 3.84 \times 10^{-4}$$

The aqueous solubility has been covered in Section 6.1.2; here, discussion is limited to the determining VP. The documents listed in Section 6.1.2 have either VP information at 25° (the default temperature of interest) or information from which it can be estimated. Liley and Gambrill⁷⁴ list the temperatures at which selected vapor pressures occur for industrially important substances.

Lyman et al.⁵⁹ contain numerous methods to extrapolate from a measured VP at a given temperature to a different temperature. The state of the substance at 25 °C (assumed temperature of concern) and the state of the substance involved at the baseline datum conditions should be known. Sometimes, the substance is solid at 25 °C, while the datum is the boiling point (liquid substance). In such as case, two extrapolations will be needed. The first is from the baseline datum to a hypothetical supercooled liquid state at 25 °C; the second is from the supercooled liquid to the solid state. If the supercooled liquid saturation vapor pressure is VP_l , the corresponding solid state pressure, VP_s can be estimated from equation 14-10 in Lyman et al.⁵⁹, written here for 25 °C.

$$VP_s / VP_l = \exp (-6.81 \times [tm/298.2 - 1])$$

where tm is the substance melting point in °K. McKay (reported in Layton, et al.⁷⁵) presents an estimation equation for VP_s which requires the boiling and melting points, tb and tm (both in °K):

$$\begin{aligned} \ln VP_s &= (\text{in atmospheres}) \\ &-(4.4 + \ln tb) \times (1.803 [tb / 298.2 - 1] - 0.803 \ln (tb / 298.2)) \\ &-6.81 (tm / 298.2 - 1) \end{aligned}$$

The first term on the right estimates VP_l ; the term on the next line converts to VP_s . A rough estimate of the boiling point for organic substances is

$$tb = 1.713 \, tm$$

Lyman et al.⁵⁹ presents procedures to estimate the melting point and boiling point temperatures from molecular structure and atomic constituents. With experimental boiling point data as a starting point, extrapolation methods can be of low accuracy; for extrapolations below 10^{-3} mm Hg, accuracy is of the order of a factor of two. With these points estimated, even poorer accuracy

should be expected.

6.7 MOLECULAR DIFFUSIVITY IN AIR (Da)

Lyman et al.⁵⁹ present methods to estimate Da . These are applicable to many types of organic compounds, but do exclude groups for which information has not been developed, such as nitro-aromatics. As a default estimate, the following relation may be used (result in m²/day):

$$Da = 8 / [\text{molecular weight}]^{0.5}$$

7.0 CONSTRAINT ANALYSIS

The PPLV approach determines a medium contamination limit based on either avoiding or minimizing adverse human health effects. For each pollutant, such effects are embodied in the parameter D_T , from which SPLVs are computed via equation 1, and PPLVs are computed via equation 3.

This should not complete the analysis. Pathways can involve several biota species between the contaminated medium and a target human. These species may suffer adverse effects if the PPLV is a cleanup target level, and an assessment should consider this contingency. If there is an impact, a "type 1" constraint is said to exist; factors other than the PPLV may dictate the target medium limit.

As an example, equation 20 (which deals with consumption of meat from cattle fed and watered on contaminated land) involves plants and cattle as biota that can be affected by soil contamination. If the PPLV exceeds a phytotoxic effects limit, the PPLV would be suspect; if the PPLV were the pollutant concentration in soil, plant growth in that soil would not occur. Moreover, cattle would ingest I_m mg/day of contaminant, where

$$I_m = \text{PPLV} \times (U_{pm} \times K_{wp} / K_{d1'} + U_{wm} / K_{d2'} + U_{sm}) \quad (42)$$

If cattle were adversely affected by this intake, the soil limit might have to be set below the PPLV to a value commensurate with the protection of cattle.

A different limitation on PPLV applicability is due to contaminant physical constraints, particularly solubility and vapor pressure. The possibility exists that saturation solubility and vapor pressure conditions can be attained in soil-pore water at a soil content lower than the PPLV. If this happens, the intake $BW \times D_T$ nominally related to the PPLV will not be attained. This situation is called a "type 2" constraint, and, based on the pathway selections for a scenario, can lead to a revised soil limit higher than the PPLV.

Table 17 identifies possible constraints for pathways. This section presents guidance on how these constraints can be identified, and procedures to contrast the PPLV to limits related to them.

7.1 "TYPE 1" CONSTRAINTS

7.1.1 Aquatic Life Concerns

Until about 15 years ago, aquatic toxicity studies addressed survival of fish in contaminated water. The time frame of these studies was usually less than two weeks. A typical measure of pollutant toxicity was the 96LC_{50} , the concentration at which 50% mortality occurs to a fish population after 96 hours of exposure.

Table 17. Possible Constraints in PPLV Pathways Analysis

Pathway and Section	Type 1 Constraint	Type 2 Constraint
<u>Water-Based Pathways</u>		
1 (4.1.1)	Organoleptic property	Solubility
2 (4.1.2)	Aquatic life concerns, fish taste	" "
3 (4.1.3)	Phytotoxicity	" "
4 (4.1.4)	Cattle toxicity, phytotoxicity.	" "
5 (4.1.5)	Same as above	" "
<u>Soil-Based Pathways</u>		
1 (4.2.1)	Organoleptic property	Solubility
2 (4.2.2)	Aquatic life concerns, fish taste	" "
3 (4.2.3)	Phytotoxicity	" "
4 (4.2.4)	Cattle toxicity, phytotoxicity	" "
5 (4.2.5)	Same as above	" "
6 (4.2.6)	N/A	
7 (4.2.6)	N/A	
8 (4.2.7)	N/A	Solubility or Vapor Pressure

A safety factor was used with the 96LC50 to estimate a "NOEL" for lifetime exposure of fish to a water contaminant. Since then, more sophisticated approaches to testing have been developed for at least three reasons: (1) use of a "rule-of-thumb" safety factor did not consistently lead to a low enough "NOEL"; (2) 96LC50 estimates differed considerably between fish species; and (3) tested fish species, while at the apex of an aquatic food chain, often were not the most sensitive species in that chain. Thus, aquatic toxicologists have developed a series of studies upon model food-web species of an aquatic community from which a "freshwater chronic value" can be developed.

However, such values have been developed for relatively few substances. Generally, they include some compounds listed as "Priority Pollutants" for which aquatic life-based water quality criteria have been developed (see Table 5) and pesticides. For many compounds, 96LC50 estimates remains the extent of available information, and for them, the 96LC50 / 100 for the most sensitive freshwater fish species can be used as type 1 constraint limit.

Readily-found sources of information for 96LC50 include the water quality criteria documents from 1980 (for many substances, insufficient information existed from which to determine a chronic lifetime value). Every June, the Journal of the Water Pollution Control Federation has a literature summary issue, in which

aquatic toxic effects have been included as a separate chapter. Earlier compilations, such as by McKee and Wolf⁷⁶, should be used with caution due to a lack of standard protocols at that time.

If water is the medium of interest, the PPLV should be less than type 1 constraint parameter (the freshwater chronic value or the 96LC50 / 100). If the PPLV is for sediment, a water concentration based on the PPLV is computed. For example, equation 15 describes a soil to water to fish route of intake. The water concentration corresponding to the soil PPLV is

$$\text{PPLV} \times K_d' / f(S1)$$

If this concentration exceeds the constraint parameter, a type 1 constraint exists.

7.1.2 Phytotoxicity

Most phytotoxicity information is limited to compounds used as herbicides or weed-killers. In experimental studies, a test compound is added to either a hydroponic solution or soil test plot, and the chemical concentration in either medium* is related to an effect on plant growth, yield, or emergence. In some cases, a no-effect threshold limit is not found; in any case, the lowest effect concentration should be divided by a safety factor (at least 10 is suggested) to account for sensitive species. A soil threshold limit based on aqueous media concentration can be estimated by the product aqueous concentration $\times K_d$. If the limit is less than the PPLV, a type 1 constraint exists.

7.1.3 Animal Toxicity

Generally, reports dealing with toxic effects of chemicals to domestic animal (livestock or fowl) are based on incidents rather than planned experiments. Thus, such data are usually restricted to herbicides, weed-killers, and pesticides. If a soil or water concentration can be estimated, it should be reduced by a safety factor of from 10 to 100, based on the reported severity of effect, to determine a constraint concentration. If that constraint concentration is less than the PPLV, it indicates a possible "type 1" constraint situation.

Otherwise, mammalian toxicity data discussed in Section 3 can be used with safety factors determine a NOEL dose for cattle. The factors presented in Table 6 are probably overly conservative for cattle, and can be decreased to about 10 for a NOEL from a chronic study and perhaps to 10 to 100 for a NOEL from a sub-chronic

* Some care is required in interpreting soil application rates. Some chemicals are applied to the soil surface and mixed into topsoil. In the absence of a specific data, soil of 1.4 kg/L bulk density and a 15 cm mixing depth may be assumed. The surface application of 1 kg/ha (or 2.47 acres) corresponds to an approximate topsoil concentration of 0.47 mg/kg.

study. It is stressed that these cattle factors are only recommendations. The dose so derived may be multiplied by a representative animal weight (such as 250 kg for steers or 520 kg for dairy cow) to compute a limiting intake. Next, I_m is computed based on the PPLV and corresponding plant and water levels (when appropriate). For example, in equation 42, the plant concentration is $PPLV \times K_{wp} / K_{d1}$; the water concentration is $PPLV / K_{d2}$. If I_m exceeds the limiting intake, a type 1 constraint is indicated.

This approach is best restricted to domestic animals, who are controlled as to where and what they consume. With game animals, there are many confounding factors (changes in food supply with season, the effects of weather, disease and predators on yield, etc.), which makes type 1 assessments extremely difficult.

7.1.4 Organoleptic Limits

Many chemicals (particularly phenols and chlorophenols) impart an unpleasant taste, smell or unusual color to water at relatively low concentrations. As a result, people are unable or reluctant to consume the water, even though there are no toxic effects caused by its consumption. If the concentration at which this occurs is less than the water PPLV, a type 1 constraint is indicated.

Table A1 in the previous report⁷ listed organoleptic limits for "Priority Pollutants" (as designated by the Clean Water Act²²)⁷ and for compounds considered by the Ministry of Health of the USSR⁷⁷. In 1973, the American Society for Testing and Materials compiled threshold concentrations⁷⁸ for many substances⁷⁸. Another useful source is McKee and Wolf⁷⁶.

There is much subjective judgment involved with determining these limits. In early studies, the test procedures were not standardized, and may have led to biases (the most common being that a sampler knows that a sample is tainted, and is more likely to respond positively). There is a difference between a substance being "detected" (i.e.: tainted water tastes different than a control sample) and being "recognized" (i.e.: a specific taste is consistently identified in a water sample). A complicating factor

* There are problems of extrapolation, such as the differences in weight (the order of 300 kg for cattle vs. 0.3 kg for rats and 0.03 kg for mice), and of digestion mechanisms; cattle have a ruminal digestive system. There are two arguments for a less stringent safety factor. First, the indicators of an effect above a NOEL are often very subtle (such as blood chemistry component changes) and of unknown significance. At higher dose levels, weight loss, a common LOEL response, is of economic concern, and not acceptable. Thus, the baseline dose from which extrapolations is made is probably higher than the NOEL. Second, cattle are raised for production over a portion of a lifetime. Thus, the need for lifetime protection is less important.

is that natural or chlorinated water often a distinct taste; tests with a distilled water substrate may not accurately mirror the impact of the substance in a water supply. For purposes of setting a organoleptic limit with only taste detection data, a detection concentration should be tripled.

7.1.5 Other Effects

While fish taste can be an adverse effect due to water contamination, data relating the "threshold" of such an effect to aqueous concentration are much less common than for water taste. For many chemicals, there is a considerable amount of data for odor thresholds (either detectable or recognizable) in air. However, models to relate a level in air to water can be quite complex. For odors from compounds in soil, a first approximation is a treatment based on equation 27. In this case, the averaged air concentration, C_{av} , is:

$$C_{av} = PPLV \times LS \times F_{avn} / (VW \times MH)$$

C_{av} can be compared to threshold odor levels to determine if a constant may exist.

7.2 TYPE 2 CONSTRAINTS

A type 2 constraint occurs if the human receptor cannot obtain the intake $BW \times D_T$ in a scenario at the PPLV due to physical properties of a compound. The narrative first shows how to identify such pathways, and then how to adjust a PPLV. The adjusted value will be higher.

7.2.1 Identification of Type 2 Constraints.

If water is the medium of interest, a type 2 constraint will exist when the PPLV exceeds a pollutant's aqueous solubility. However, the PPLV cannot be adjusted since all pathways are intake-constrained.

With soil as the medium of interest, the impact of solubility is more complex. Figure 3 indicates the impact of the solubility limit in vapor-diffusion pathways. The pollutant concentration in soil-pore water, C_{we} , and that in soil-pore air, C_{ae} , are shown as functions of the pollutant concentration in soil, C_{se} . Equilibrium is assumed to exist between the three media. The relation of C_{we} to C_{se} is given by the curve ABC. Below point B, the relation between C_{we} and C_{ae} is characterized by the partition coefficient K_d . Above point B, the curve is expected to flatten out since the point at which $C_{we} = SW$ corresponds to a soil concentration at which the SOC sorption capacity in soil would be attained (point C). The soil concentration at this point need not be B'. Since point B may be difficult to determine, the point B' is taken as the approximate limit of the applicability of K_d .

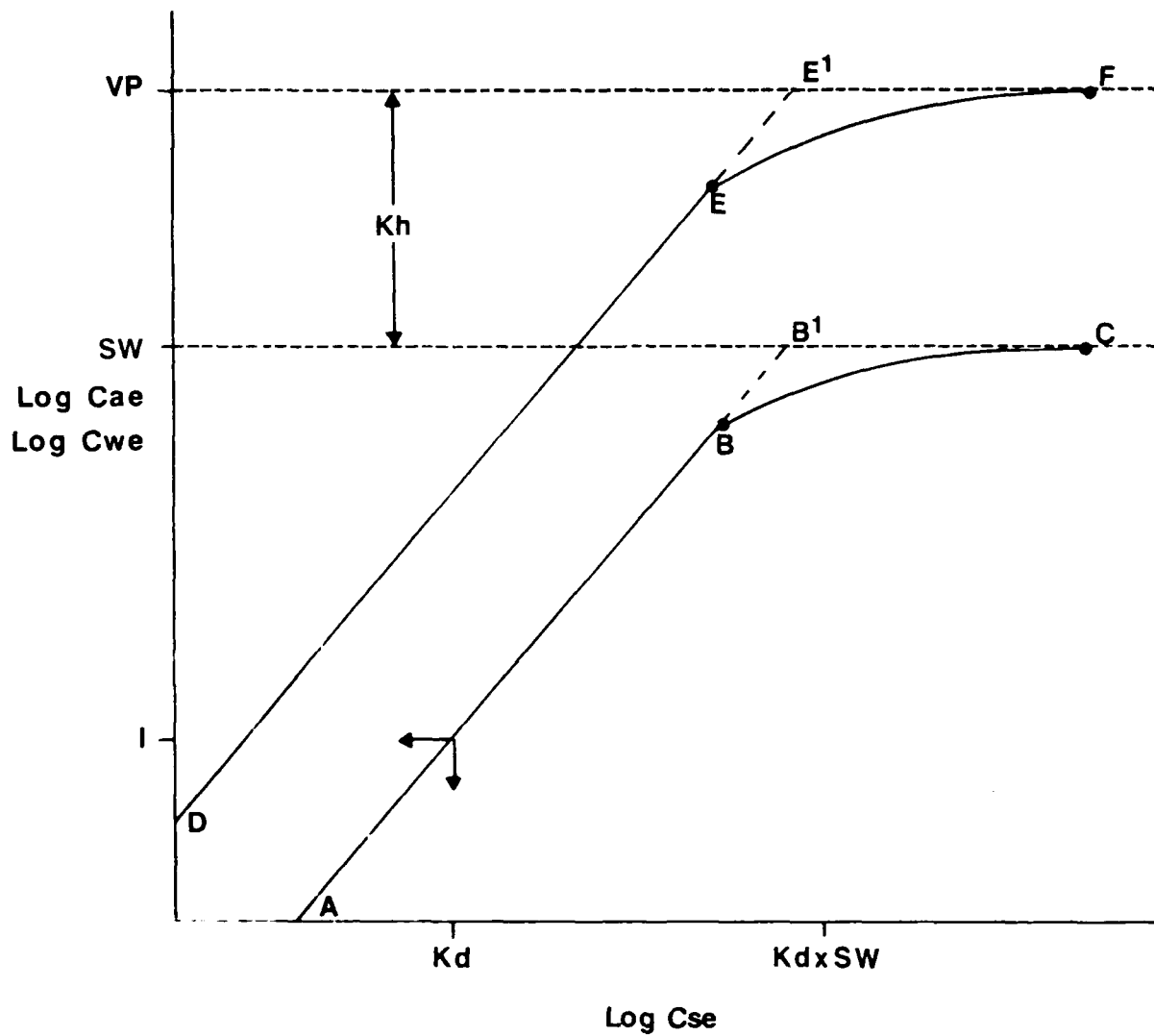


Figure 3. Relations Between Pollutant Concentrations in Soil, Soil-Pore Water, and Soil-Pore Air at Equilibrium

The curve DEF indicates the relation between C_{ae} and C_{se} . This curve is offset from ABC by the ratio VP / SW , the Henry's Law constant. At point B', the values of C_{ae} and C_{se} are VP and SW respectively.

At a soil concentration in excess of B', the soil-pore water concentration does not exceed SW ; the soil-pore air concentration does not exceed VP . At a soil concentration in excess of B', the amount of exposure via pathways in which these media are intermediates will be capped. With such pathways, if the soil PPLV exceeds $K_d \times SW$, a type 2 constraint situation is indicated.

7.2.2 Adjusted Soil Limits With Type 2 Constraints

In this section, using the PPLV as the starting point, a soil limit is computed where the maximum intake to an exposed human is $BW \times D_T$. The procedure is to: (1) identify the pathways subject to the constraint; (2) convert the SPLV equation set to intake format; (3) replace the constrained intakes by their limits in constrained equations; and (4) compute the relaxed limit with constrained intakes.

These steps are best illustrated by example. Table 18 provides the tests in terms of equations presented in Section 4. Suppose that equations 16, 19 and 24 are the SPLV equation set, and that a type 2 constraint exists in equation 19 (the water concentration predicted from $PPLV \times K_d$ exceeds SW). The intake equations corresponding to SPLV equations are formed by substituting PPLV for the SPLV, and by replacing the product $BW \times D_T$ by an intake term. Since the PPLV is less than any SPLV, any intake term will be less than $BW \times D_T$. However, the sum of all intakes will be the product $BW \times D_T$. Identifying each intake by equation number, these equations are:

$$I_{16} = PPLV \times BCF \times f(S_2) \times W_f / K_{d2}' \quad (43)$$

$$I_{19} = K_{pm} \times W_m \times [PPLV \times K_{wp} / K_{d1}' + PPLV \times U_{sm} / U_{pm}] \quad (44)$$

$$I_{24} = PPLV \times W_{s6} \quad (45)$$

The sum of intakes is

$$I_{max} = I_{16} + I_{19} + I_{24} = BW \times D_T$$

The constraint applies to only the first term of equation 44, since the second term describes livestock pollutant intake via soil ingestion. In equation 44, $PPLV / K_{d1}'$ is replaced by SW ; by the model of pollutant transfer, the plant concentration of pollutant cannot exceed $SW \times K_{wp}$. The result is

$$I_{19}' = K_{pm} \times W_m \times [SW \times K_{wp} + PPLV \times U_{sm} / U_{pm}] \quad (46)$$

Table 18. Identification Tests for Type 2 Constraints

Equation	Test
15	$PPLV \times f(S1) / Kd' > SW$
16	$PPLV \times f(S2) / Kd' > SW$
17	$PPLV / Kd' > SW$
18,19	" "
20	$PPLV / Kd1' > SW$ or $PPLV / Kd2' > SW$
21-23	Same as for equations 18-20, respectively.
29	$PPLV / Kd' > SW$

The sum $I_{16} + I_{19}' + I_{24}$ is less than I_{max} . A soil limit PLV2 will restore this sum to I_{max} . When PLV2 is substituted for the PPLV in equations 43, 45 and 46, the sum becomes:

$$I_{16}'' = PLV2 \times BCF \times f(S2) \times Wf / Kd'$$

$$I_{19}'' = Kpm \times Wm \times SW \times Kpd + PLV2 \times Kpm \times Wm \times Usm/Upm$$

$$I_{24}'' = PLV2 \times Ws6$$

$$I_{max} = I_{16}'' + I_{19}'' + I_{24}''$$

I_j'' notation indicates that PLV2 is substituted. Then,

$$PLV2 = (I_{max} - R_{C2} \times SW) / R_{sum}$$

where

$$R_{C2} = Kpm \times Wm \times Kwp$$

$$R_{sum} = BCF \times f(S2) \times Wf/Kd' + Kpm \times Wm \times Usm/Upm + Ws6$$

This approach can be generalized. The term R_{C2} is the sum of terms which multiply SW due to the constraint. The term R_{sum} is the sum of terms which multiply $PLV2$.

Three matters should be addressed in a Type 2 constraint analysis. First, not every intake set can be solved for $PLV2$. One may find that every pathway is constrained; in that case, $R_{sum} = 0$. The implication is that human health effects may not be a valid limiting criterion. Second, the process above may have to be reiterated. In the example above, the $PLV2$ could cause a Type 2 constraint in the fish pathway; the water concentration predicted by $PLV2 \times f(S2) / Kd'$ could exceed SW . Lastly, while the $PPLV$ may not cause a Type 1 constraint to be "triggered", the larger $PLV2$ may introduce a Type 1 constraint restriction.

8.0 APPLICATIONS AND SCREENING TECHNIQUES

Table 1 illustrated past PPLV applications. This section discusses them in concept and presents techniques to indicate the relative importance of pathways. These techniques are useful when little data exists about a compound, or when answers are needed in a short time frame. The techniques allow the decision-maker to focus his efforts.

8.1 EVALUATION OF EXISTING SITUATION

In broadest terms, the PPLV relates a soil or water pollutant level to a value of D_T in terms of a selected group of pathways. Thus, a PPLV serves as a "go - no go" indicator that an area (or body of water) poses a problem. If actual pollutant levels are below the PPLV, the area is "safe" for the scenario. Thus, the PPLV can be used to indicate if a site poses a problem. In terms of "Superfund" actions, this is an endangerment assessment.

This procedure can be extended to a situation where several contaminants exist at a site. Call the concentrations of these substances $CP_1, \dots, CP_n$, where the numerical index indicates a different contaminant. Then the PPLVs for each substance, $PPLV_1, \dots, PPLV_n$ can be used to determine a hazard index (HI)

$$HI = \sum_i CP_i / PPLV_i \quad (47)$$

If $HI < 1$, the site can be considered "safe". Equation 47 is done separately for non-carcinogens and carcinogens. Strictly, only those non-carcinogens which are expected to cause similar effects should be so evaluated for a HI. If the analyst is not clear about this, all non-carcinogens should be included in the summation.

Similarly, only those carcinogens which are expected to cause a similar cancer should be included in a summation. If the analyst is not clear, all carcinogens should be placed in the summation. The PPLVs for all carcinogens should be based on a common ARL. If $HI > 1$, the product $HI \times ARL$ indicates the risk level for the mixture.

Equation 47 is strictly valid when effects from different substances are additive. This assumption is often made because information to the contrary* is rarely available. An $HI > 1$ does not immediately mean that a hazardous situation exists. PPLVs are based on safe-sided D_T values. It is difficult to quantify the extent of safesiding involved; this is discussed further in Appendix C. Thus, in a "Superfund" situation, an $HI > 1$ would indicate the need to consider (but not necessarily undertake) remedial actions.

* Call the actual HI from several compounds HI_{act} , and that from equation 47: HI_{47} . Synergism occurs if $HI_{act} > HI_{47}$ and antagonism occurs if $HI_{act} < HI_{47}$.

8.2 EVALUATION OF TREATMENT OPTIONS AND ANALYTICAL NEEDS

Remedial actions are options which should reduce a HI to 1. With more than one compound involved, a "tradeoff" situation can occur, as shown in Figure 4. Here, a two-compound contamination situation is shown, and $PPLV_{C1}$ and $PPLV_{C2}$ are shown. For any combination of pollutant concentrations outside of the triangle $PPLV_{C1}$ - origin - $PPLV_{C2}$, HI exceeds 1. Point "Q1" is one such combination. A remedial action can be considered one means of reaching the triangular area for which $HI < 1$. In Figure 4, several actions are represented as dotted lines from the point Q1 to the above triangle.* Clearly, different paths to reach this area exist; in concept, the feasibility study seeks to determine the least costly method to reduce HI to unity.

The PPLV approach application to determine analytical levels in a single substance case is straightforward; the PPLV should be capable of accurate detection. The multiple substance case is more complex. From Figure 4, if a PPLV can't be measured in the medium of concern, a determination that $HI = 1$ cannot be made.

8.3 PPLV ANALYSIS FOR SUBSTANCES WITH DIFFERENT D_T FOR THE ORAL AND INHALATION MODE

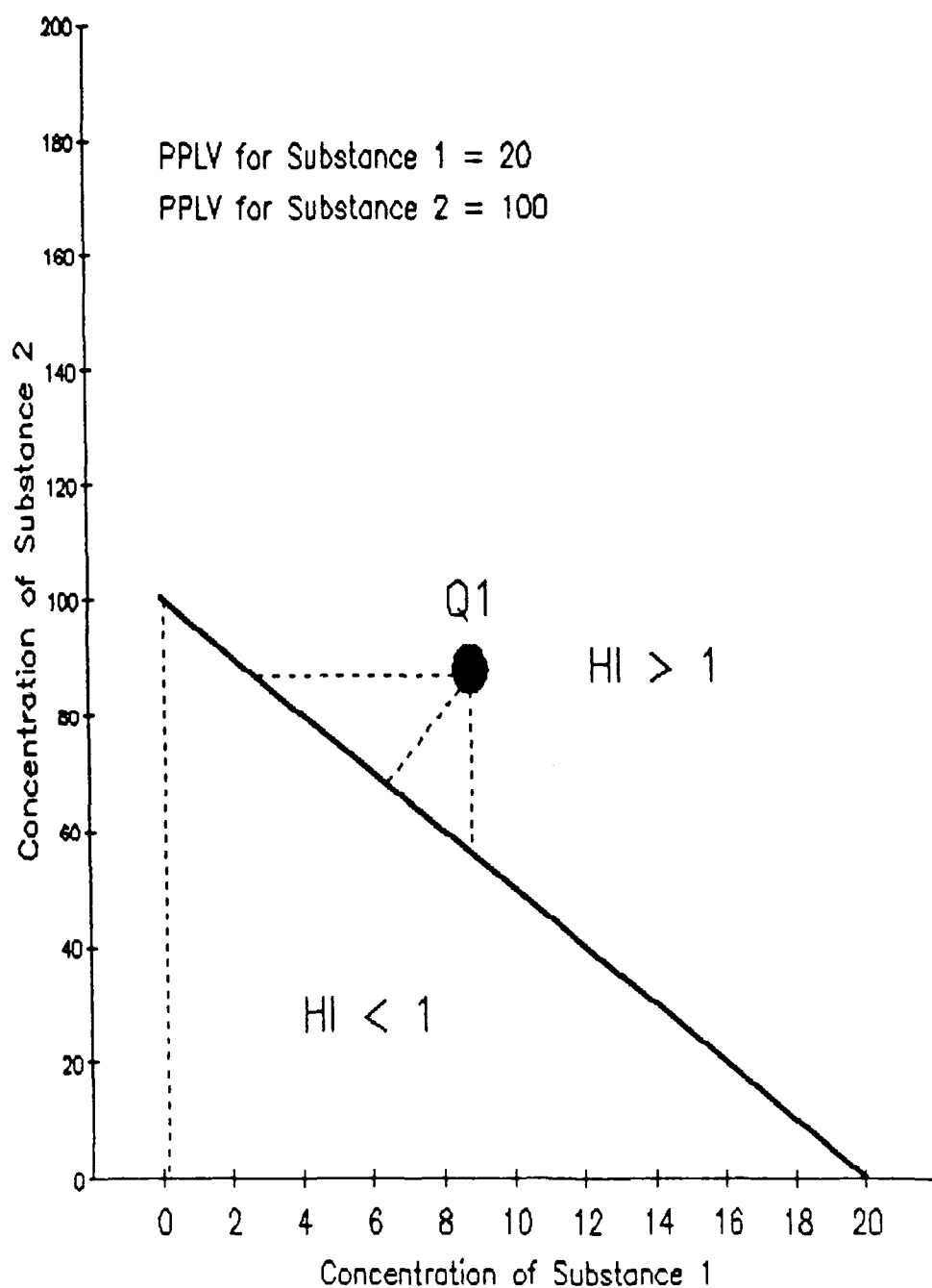
Equation 4 illustrates a situation where the response to a given mass of pollutant via ingestion may differ from that via inhalation. In that case, the efficiency of delivery to the bloodstream by the respiratory system as contrasted to delivery by the digestive system is involved. For some substances, the difference is substantial, and the D_T will be route-specific. Other substances have different adverse effects when inhaled as opposed to when they are ingested, and the D_T by these different modes of entry will differ. An unusual case of this is the chromium VI salts^{**}. When fumes of such salts are inhaled, they can cause tumors²³. However, ingested salts, although quite toxic, have not been observed to cause tumors.

In the PPLV analysis, the substance can be replaced by two "pseudo-substances", one which is only inhaled, the other which is only ingested. The D_T values for each "substance" is

* With three substances, the analogous figure would be three dimensional. The lines between the PPLVs define a plane below which $HI < 1$. In place of a right triangular area in which $HI < 1$, the analog is a right pyramid whose corners are the 3 PPLVs and the origin. With more substances, the planes becomes hyperplanes. Other than the differences in the geometric interpretation of the $HI < 1$ boundary, the above discussion applies to more than two substances.

** For ubiquitous anions, the valence state can have a pronounced effect on D_T . For example, in small amounts, Chromium III is an essential nutrient.

Figure 4. Hazard Index as a Function of PPLV:
Two Substance Case



determined. Next, the pathways are allocated to the ingested or the "inhaled" substance. In the case of soil pathways 6 and 7, this involves a pro rata process. Section 5.1.8 indicates that the inhaled and dermal portion probably comprises one-eleventh of adult intake, thus the inhaled W_{s6} will be about eleven times the value computed for all processes (the dermal route is assumed to be characterized by the same D_T as the inhalation route). The information in Section 5.1.9 suggested that workday inhalation intake of particulates was 170 mg/day; workday ingestion of particulates was 230 mg/day. Then, the inhalation $W_{sa7} = 400 \times W_{sa7} / 170$ for both processes.

Next, a PPLV for the inhaled substance and a PPLV for the ingested substance are computed. From these, a composite PPLV is computed:

$$PPLV = 1 / (1/"inhaled PPLV" + 1/"ingested PPLV")$$

8.4 PATHWAY SCREENING TECHNIQUES

From the discussion in Section 1.1, if IF_i , K_i , and S_i are not functions of concentration, the symbolic SPLV relation, equation 1, can be written as

$$SPLV_i = r_i \times D_T \quad (48)$$

The r_i can be thought of $SPLV_i$ when $D_T = 1$. Since each such equation relates to a common value of D_T , the r_i can be examined to assess the relative importance of SPLVs. From equation 3, the PPLV for scenario "j" is:

$$PPLV_j = 1 / \sum_i (SPLV_i \times T_{ij}) = D_T / \sum_i (r_i \times T_{ij})$$

The $SPLV_i$ with minimum r_i has the most influence on the value of $PPLV_j$, and should, within reason, be the most accurately determined SPLV.

Here, the equations presented in Section 4 are cast in the format of equation 48. The information presented in Section 5 provides values for non-chemical specific variables, while the equations in Section 6 based on $\log K_{ow}$ as a predictor are used to estimate partition coefficients. For convenience, the numerical information is presented in Table 19. Estimation equations from Section 6 are in Table 20, but have been converted to a K_{ow} power-law basis. For purposes of brevity, the equation for K_{wp} is not included in the table; Figure 2 shows the K_{wp} estimated from $\log K_{ow}$. Moreover, $K_{wp} = K_{wv}$ where applicable. Table 21 presents the resulting expressions for the r_i . These functions are shown graphically: Figure 5 shows the water pathways discussed in Sections 4.1.1 to 4.1.5; Figure 6 shows the soil pathways discussed in Sections 4.2.1 through 4.2.3 and 4.2.6; and Figure 7 shows the soil pathways discussed in Sections 4.2.4 and the basement pathway of Section 4.2.7.

Table 19. Variable Data Used in SPLV Equations to Estimate r_i .

Variable	Equations	Value
BW	7-13, 15-27	70 kg
Ww	7, 15	1.6 L/day
Wf	8, 16	0.0065 kg/day ^a
Wv	9, 17	0.017 kg/day ^a
Wm	10, 11, 18-20	0.1 kg/day
fm	32	0.2
Uwm	10, 11, 18-20	15.3 L/day
Upm	10, 11, 18-20	6.6 kg/day
Wd	12, 13, 21-23	0.3 L/day
fd	33	0.04
Uwd	12, 13, 21-23	78 L/day
Upd	12, 13, 21-23	16.6 kg/day
foc	31	0.01 surface 0.10 sediment 0.003 sub-surface
θ	14, 29, 30	0.10 surface 0.40 sediment 0.20 sub-surface
ρ	14, 29	1.4 kg/L surface 1.4 kg/L sediment 1.6 kg/L sub-surface
f(S1)	15	1
f(S2)	16	1
Usm	19, 20	0.35 kg/day
Usd	22, 23	0.87 kg/day
Ws6	24	7.4×10^{-5} kg/day
Wsa7	25	1.8×10^{-4} kg/day
e	29, 30	0.2
Da	30	$0.48 \text{ m}^2/\text{day}$
Rb	26	$1.5 \text{ m}^3/\text{day}$
VAR	26	1.34
TAC	26	0.083 days
Tl	28	25600 days
To	28	60 days

a. Sum of potato and non-potato dry-weights for rural non-farm situation (Table 13)

The reader is cautioned that the relations shown and conclusions drawn depend upon the pathway equations, the numerical inputs in Table 19, and presume that the partition coefficient equations are correct.

Figure 5 indicates that drinking water is a very important pathway, exceeded in importance only by fish intake when Log Kow exceeds 3.5. Vegetable intake could be an important pathway; the minimum r_i is 101 when Log Kow = 4.5. However, the assumption that $K_{wv} = K_{wp}$ is expected to be conservative; a higher r_i for the vegetable intake is likely. The added effect of plant consumption to the meat pathway SPLV is evident by the

Table 20. Partition Coefficient Estimation Equations Used in Table 21.

Variable	Equation in text	Expression
BCF	37	$0.59 Kow^{0.76}$
Kwv	41 (coefficient of 5)	See Figure 2.
Kpm	32, 40	$2.3 \times 10^{-5} Kow^{0.511}$
Kpd	32, 40	$4.6 \times 10^{-6} Kow^{0.511}$
Koc	39	$2.97 Kow^{0.806}$
Kd'	15, 16	$0.286 + 0.297 Kow^{0.806}$
Kd'	17-19, 21, 22	$0.071 + 0.0297 Kow^{0.806}$
Kd1'	20, 23	See Kd' for eqtn. 17-19
Kd2'	20, 23	See Kd' for eqtn. 15, 16
Kd'	29	$0.143 + 0.00891 Kow^{0.806}$

curve for "Meat/W+P" vs. that for "Meat/Water". The inclusion of plant intake reduces the SPLV as much as a factor of 20 around a Log Kow of 4.5, where Kwp is a maximum (see Figure 2). The ri curves for the dairy products pathways were excluded for purposes of clarity. From the equations in Table 21, the dairy product ri values would be about 30 percent higher than those shown for beef.

Due to the term θ / ρ in equation 14, and the non-linear dependence of Kwp on Log Kow in Figure 2, the soil SPLV equations are more complicated than their water counterparts. For purposes of brevity, the Kd' have been specified in Table 20, and the Kwp and Kd' terms are used directly in Table 21 rather than their closed forms. From Figure 6, the water pathway is most important when $\text{Log Kow} < 2.5$, then the vegetable pathways may be the most important pathway until $\text{Log Kow} > 4$. Above Log Kow of about 1, the ri of the water pathway increases almost linearly with Log Kow. The relation of the fish pathway ri to Log Kow is relatively insensitive, since the exponent of Log Kow in the Kd' and BCF equations nearly cancel each other out, and for $Kow > 10$, the term $5420 \times Kow^{0.046}$ dominates. The two direct dirt pathways (6 for incidental intake and 7 for dusty work conditions) do not depend upon Kow.

Table 21. Expressions for r_i

Pathway	Text Equation	r_i Expression
<u>Water Pathways</u>		
Water consumption	7	44
Fish consumption	8	$18300 K_{ow}^{-0.76}$
Vegetable consumption	9	$4100 / K_{wp}$
Meat consumption	10	$1.3 \times 10^7 K_{ow}^{-0.489}$
Meat consumption	11	$3.04 \times 10^7 K_{ow}^{-0.489} / (2.32 + K_{wp})$
Dairy consumption	12	$1.08 \times 10^7 K_{ow}^{-0.489}$
Dairy consumption	13	$5.07 \times 10^7 K_{ow}^{-0.489} / (4.7 + K_{wp})$
<u>Soil pathways</u>		
Water consumption	15	$12.6 + 13.1 K_{ow}^{0.806}$
Fish consumption	16	$5420 K_{ow}^{0.046} + 5220 K_{ow}^{-0.76}$
Vegetable consumption	17	$(122 K_{ow}^{0.806} + 294) / K_{wp}$
Meat consumption	18	$K_{wp}^{-1} \times$ $(2.15 \times 10^6 K_{ow}^{-0.489} + 9.03 \times 10^5 K_{ow}^{0.317})$ $(3.04 \times 10^7 K_{ow}^{-0.489} / (K_{wp} / K_{d'}))$
Meat consumption	19	$(3.04 \times 10^7 K_{ow}^{-0.489}) /$ $(K_{wp} / K_{d'} + 0.053)$
Meat consumption	20	$(3.04 \times 10^7 \times K_{ow}^{-0.489}) /$ $(K_{wp} / K_{d1'} + 0.053 + 15.3 / [6.6 + K_{d2'}])$
Dairy consumption	21	$5.07 \times 10^7 K_{ow}^{-0.489} / (K_{wp} / K_{d'})$
Dairy consumption	22	$(5.07 \times 10^7 K_{ow}^{-0.489}) /$ $(K_{wp} / K_{d'} + 0.053)$
Dairy consumption	23	$(5.07 \times 10^7 K_{ow}^{-0.489}) /$ $(K_{wp} / K_{d1'} + 0.053 + 78 / [16.6 + K_{d2'}])$
Incidental soil intake	24	9.5×10^5
Work-related soil intake	25	3.9×10^5
Basement vapor diffusion	26, 28-30	$941 / \text{constant}; \text{constant} =$ $(K_h / K_{d'}) \times (0.2 + 0.2 / K_h + 1.4 K_{d'} / K_h)^{0.5}$

Figure 5. r_l vs Log K_{ow} for Selected Water Pathways

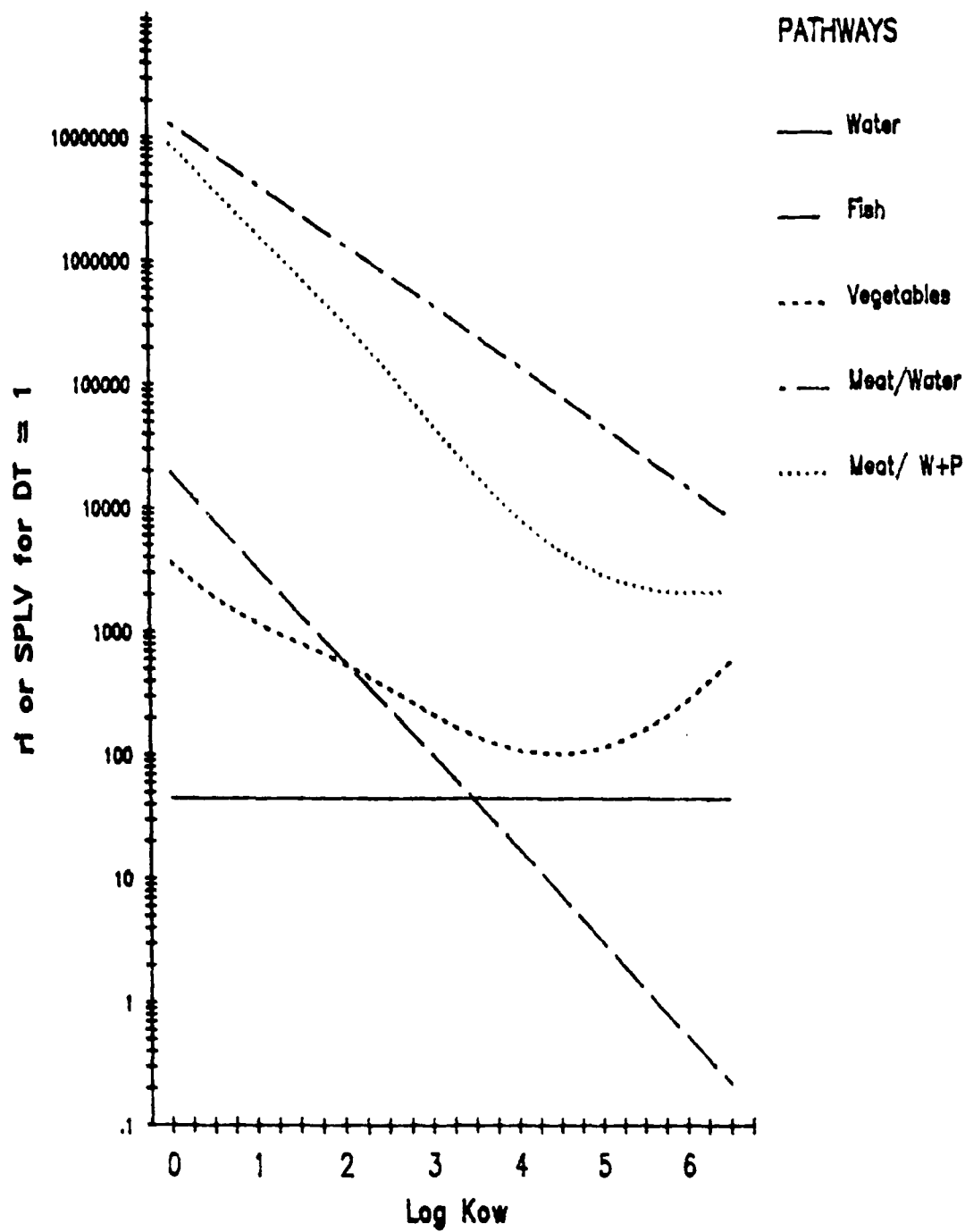


Figure 6. r_1 vs Log K_{ow} for Selected Soil Pathways

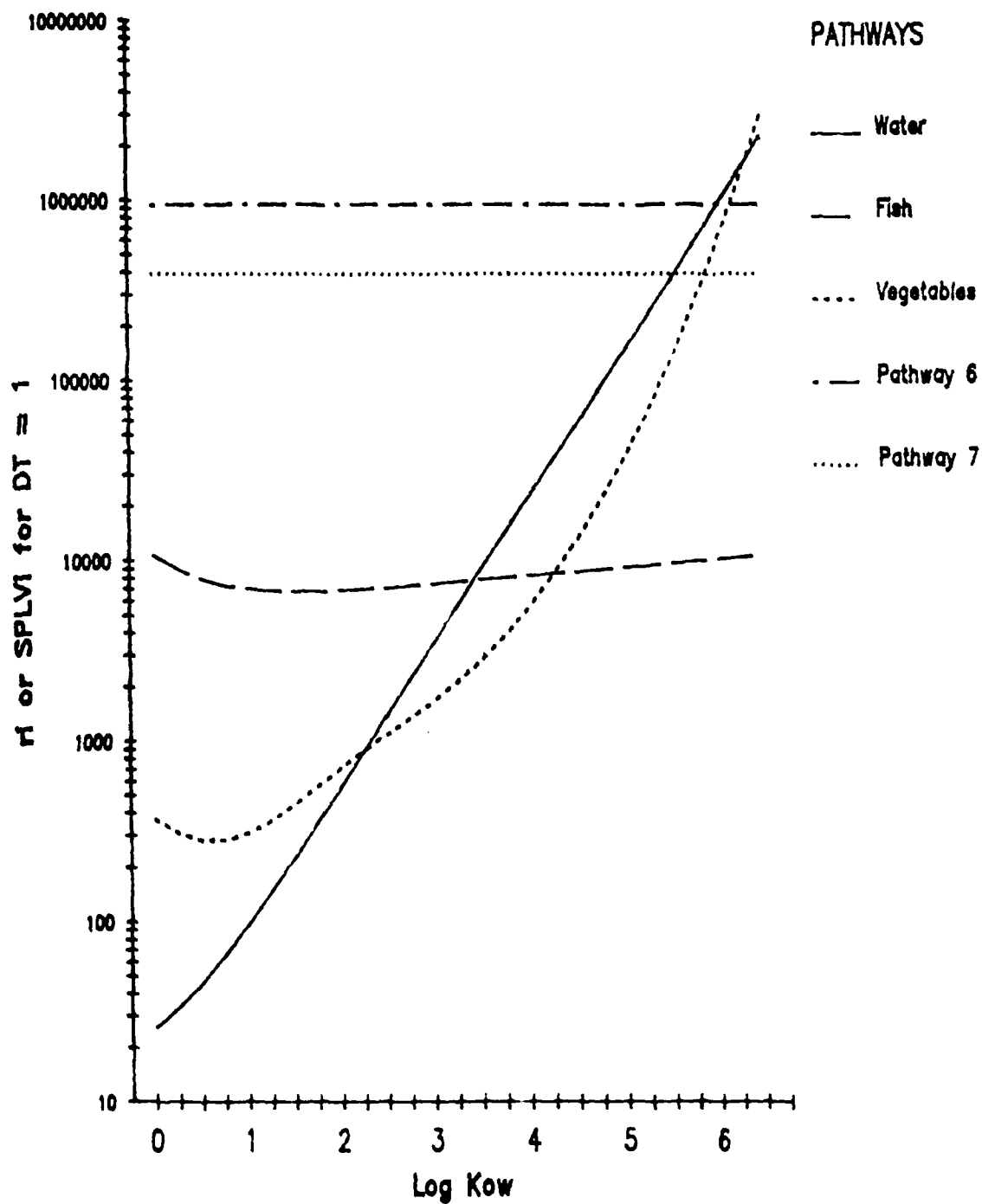


Figure 7. r_1 vs Log K_{ow} for Beef Intake and Vapor Diffusion Pathways

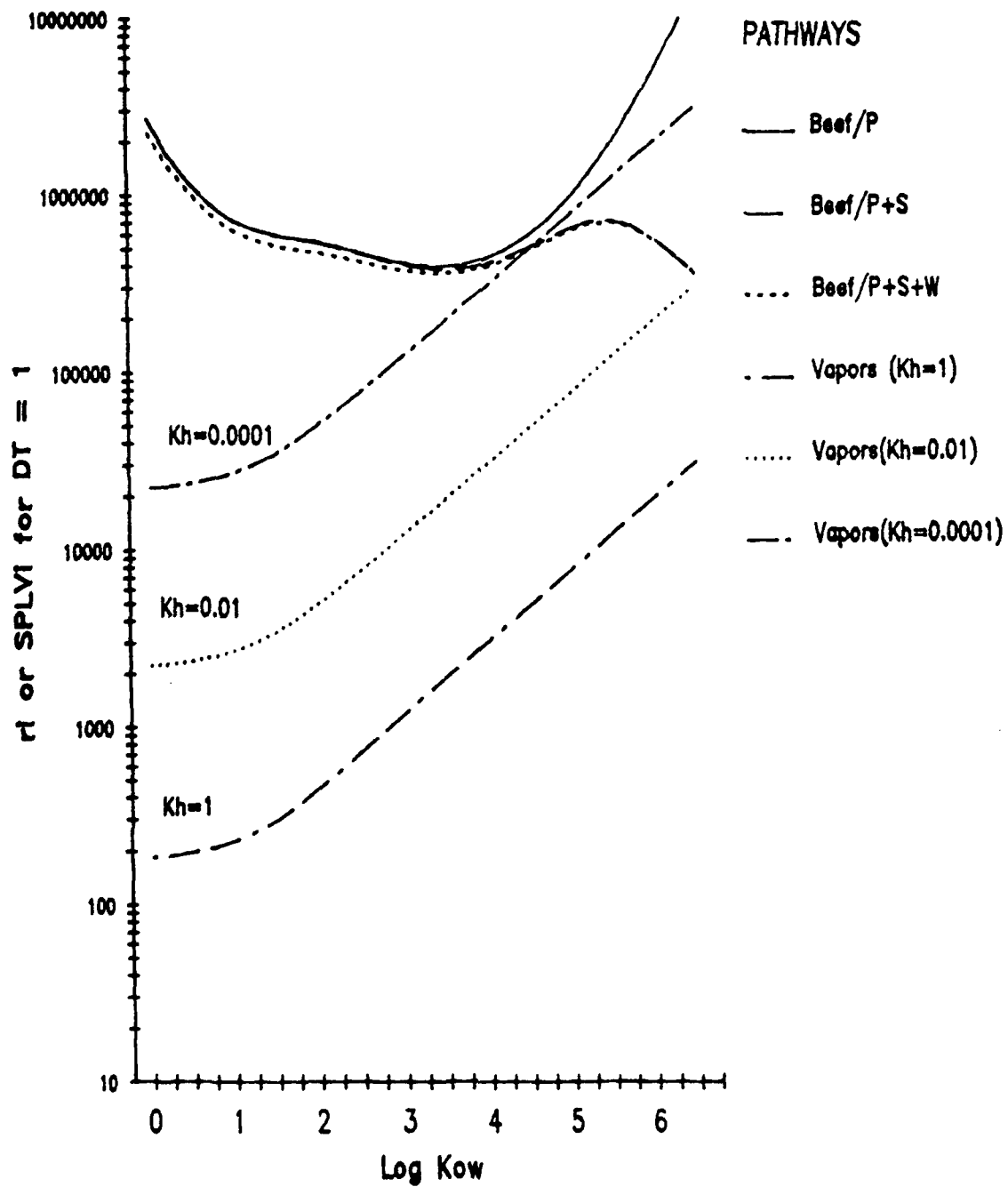


Figure 7 shows the r_i corresponding to the three beef pathways from equations 18, 19 and 20. The curve for equation 18 (Beef/P) shows that in the $\log K_{ow}$ range 0.17 to 4 , the term $2.15 \times 10^6 K_{ow}^{-0.489} + 9.03 \times 10^5 K_{ow}^{0.317}$ increases more slowly than does K_{wp} , and r_i decreases. As K_{wp} goes through a maximum and then decreases, the r_i then increases sharply with increasing $\log K_{ow}$. Equation 18 is shown in two forms; the first better explains the behavior with $\log K_{ow}$, the second form better illustrates the impact of additional pollutant sources to livestock. The contribution of soil ingestion to r_i is relatively unimportant until $\log K_{ow}$ exceeds 4. When $\log K_{ow}$ exceeds 5.0, soil ingestion becomes the dominant source of pollutant to the cow. The decrease in r_i due to inclusion of water intake by livestock is relatively small. Dairy results have the same trend; as in the case with water SPLVs, the value are offset about 30% above those of the beef pathways.

Figure 7 also shows r_i for three values of K_h . A $K_h = 1$ would typically be indicative of a very volatile substance, typical persistent soil pollutants have K_h that are much less than 1. The flat portion indicates the area where the term θ / ρ dominates the contribution to K_d' . For K_h less than 0.0001, other curves can be constructed readily. At such levels,

$$r_i \propto (K_h)^{0.5}$$

or for every 100-fold decrease in K_h , the r_i would increase by tenfold.

APPENDIX A. MATHEMATICS OF THE PPLV METHOD AND SELECTED PATHWAY DERIVATIONS.

A.1 THE GENERAL PROBLEM

Basically, environmental risk assessments involve a set of equations relating human intake of a pollutant by one or more pathways from a polluted medium or media where the total intake is constrained. The single medium problem is addressed here; for convenience, soil is chosen. The assessment equations are:

$$\begin{aligned} A_1 \times C_s &= I_1 \\ \dot{A}_i \times \dot{C}_s &= \dot{I}_i \\ \dot{A}_n \times \dot{C}_s &= \dot{I}_n \end{aligned} \tag{A-1}$$

$$\Sigma I_i = I_{\max} \tag{A-2}$$

$I_{\max}$, the specified constraint, is known and is based upon some limiting level of intake considered "safe" (this was discussed in Section 3.0). If the A_i are not functions of C_s , equations A-1 describe a set of linear equations whose solution, subject to the constraint of equation A-2, is:

$$C_s = I_{\max} / \Sigma A_i \tag{A-3}$$

This approach is been proposed for hazardous waste site cleanup guidance⁷⁹.

In the PPLV approach, a SPLV is determined for each path as the sole means by which a human target is exposed to pollutant to generate a series of equations in the form:

$$SPLV_i = r_i \times D_T \tag{A-4}$$

This is equation 48 from the main text. A constant term, BW , can be removed from r_i , and $I_{\max}$ can be equated to the product $BW \times D_T$. Define the PPLV as

$$PPLV = 1 / \Sigma (1 / SPLV_i)^{-1}$$

When the relations above for the $SPLV_i$ are inserted:

$$PPLV = I_{\max} / \Sigma (1 / [r_i / BW]) \tag{A-5}$$

Comparison to equation A-3 indicates that the PPLV equals C_s when $r_i / BW = A_i$. The major difference in the PPLV approach to that above is that media concentrations are computed in pathway equations rather than pollutant intakes.

A.2 r_i AS A FUNCTION OF CONCENTRATION OR TIME

From Section A.1, equations A-4 and A-5 provide a meaningful PPLV

when r_i is not a function of medium concentration and $I_{max} = BW \times D_T$. Graphically, Figure A-1 illustrates a two-pathway situation where two relations corresponding to equation A-4 are shown. Each pathway corresponds to a dimension; for n pathways, one has an " n "-space. The SPLVs are identified as SPLV₁ and SPLV₂ on the C₁ and C₂ axes respectively. The PPLV corresponds to the intersection of the line $C_1 = C_2$ with a line drawn between the SPLVs (for more pathways, the line between SPLVs becomes a plane or a hyperplane). This line also represents a surface dividing what would be considered all combinations of "safe" intakes from those which are, at best, less "safe" or of some concern. This is analogous to the situation discussed in Section 8.1 with multiple pollutants.

If the r_i are functions of C_i , the surface is not linear. This case is shown on Figure A-1 as the dashed curve connecting SPLV₁ with SPLV₂. However, as long as the pathways relate to the same medium, the intersection of the line $C_1 = C_2$ (and in higher dimensions, $C_1 = \dots = C_n$) with this surface satisfies equations A-1 and A-2*. This solution, called PPLV_a in Figure A-1, is not necessarily equal to the PPLV.

This figure also helps illustrate what happens if the pathways are not based on one medium. For example, suppose in Figure A-1 that C₁ was for surface soil but C₂ for sediment. To the extent that these soils are independent, a PPLV can be determined, but it may have no practical significance. However, if tradeoffs between limits in different media are tenable, as was proposed in the Gratiot County Landfill study¹², the line SPLV₁ - SPLV₂ indicates the locus of these tradeoffs.

The derivation of W_{s6} in Section 5.1.8 can be applied to other pathways when the ratio of body weight to intake of a consumable (including dirt or air) is not constant over a lifetime. As noted there, the SPLV from a time-averaged equation such as equation 36 must be viewed carefully so that short-term adverse health effects are not overlooked. Often, the maximum value of W_i / BW_i occurs in childhood. As a result, a child can be exposed to relatively higher levels of a substance than an adult. As noted in Section 5.1.8, a time-averaged result tends to underplay this, since the model 70-year lifetime includes 52 years of adult life.

For toxic pollutants (as opposed to potentially carcinogenic pollutants), when soil intake, dairy products intake or vapor inhalation are pathways of interest, an alternate analysis should be considered for a child, where D_T would refer to safe dose to avoid an adverse effect during a shorter-than-lifetime exposure period. The soil intake situation has been discussed in Section 5.1.8. The level of milk consumption of the two-year old child could exceed that of an adult by a factor of two (see Section 5.1.6), while the child weight is about one-sixth that of an adult

* Mathematically, the r_i should be continuous, singled-valued functions of C_i .

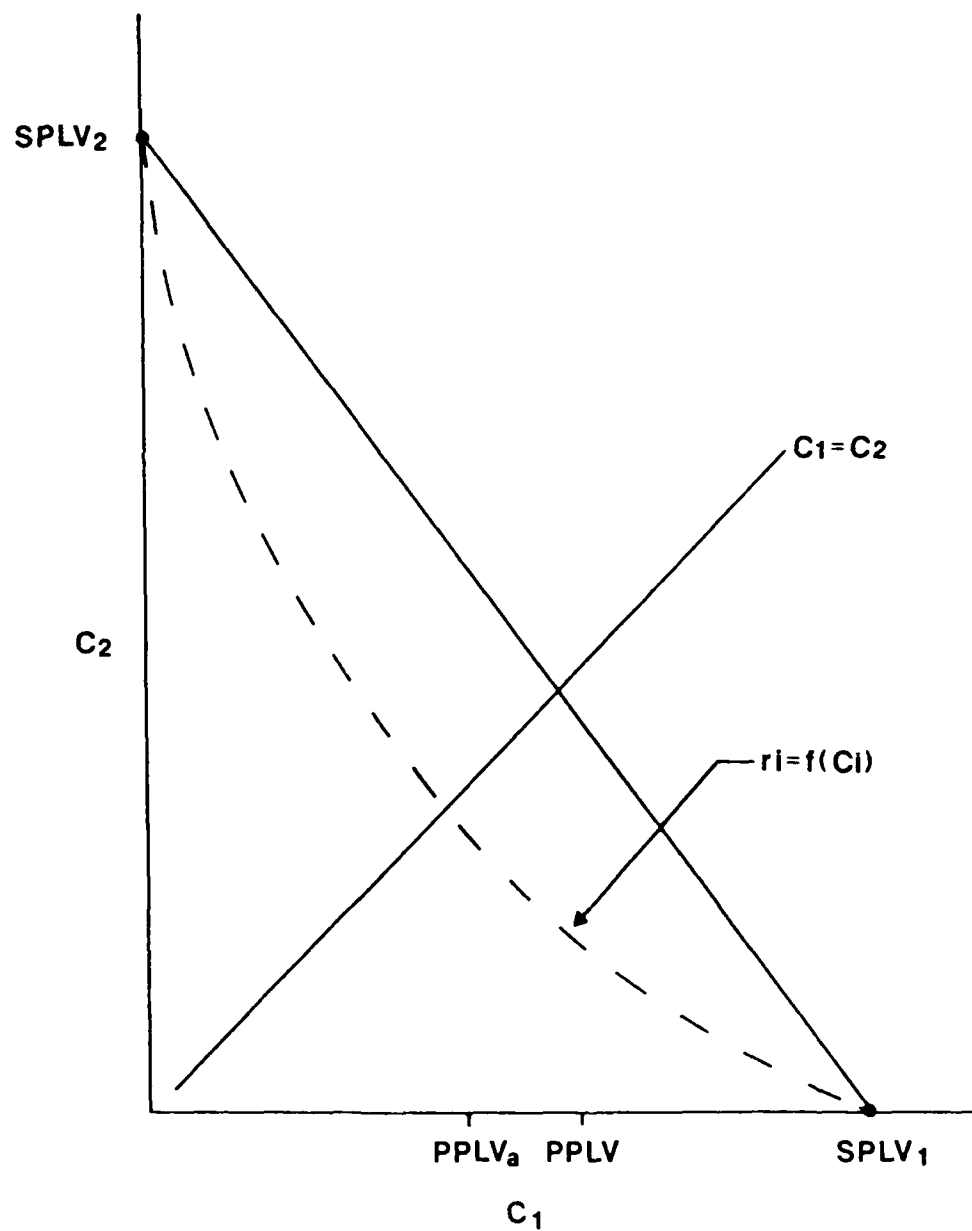


Figure A-1. Relation of the PPLV to its Component SPLVs

(see Table 8). Thus, for a two-year old child, the term BW / Wd could approach twelve times that of an adult, much the same situation as discussed above.

Equation 28, which expresses F_{avn} in terms of two time-point fluxes, is also a time-averaged approach. The model and derivation will be discussed in Section A.5. For the present, note that equation 29 has the form

$$\Phi(T) = \text{Constant} / T^{0.5}$$

Inserting this expression in equation 28,

$$F_{avn} = (2 / [T_1 - T_0]) \times \text{Constant} \times [T_1^{0.5} - T_0^{0.5}] \quad (\text{A-6})$$

Since F_{avn} is a time averaged flux, a time T_2 exists when

$$F_{avn} = \Phi(T_2) \quad (\text{A-7})$$

Equation A-6 and A-7 can be combined to eliminate F_{avn} . For $T_1 = 25600$ days and $T_0 = 60$ days,

$$T_2 = [(25600 - 60) / (2 \times (25600^{0.5} - 60^{0.5}))]^2 = 7000 \text{ days.}$$

From the square root dependency, the flux at 60 days is about 11 times higher than F_{avn} . Thus, careful consideration of what D_T represents in equation 28 is also in order.

A.3 BEEF AND DAIRY PRODUCT PATHWAYS

Sections 4.1.4, 4.1.5, 4.2.4, and 4.2.5 described situations where either beef or dairy cattle are exposed to contaminants by multiple routes. These section's equations can be derived as is shown here for equation 11 of section 4.1.4. From the situation described by equation 10, the intake of pollutant by a cow would be the product $SPLV_{w4a} \times U_{wm}$. The "a" is added to the subscript to delineate it from the concentration from equation 11, $SPLV_{w4b}$, which is to be expressed in terms of C_{w4a} . With contaminant from both water and plants, the intake would be

$$U_{wm} \times SPLV_{w4b} + U_{pm} \times C_{p4b}$$

C_{p4b} is the contaminant level in plants corresponding to $SPLV_{w4b}$, and is related to it via K_{wp} . Thus, this intake can be restated as

$$U_{wm} \times SPLV_{w4b} + U_{pm} \times K_{wp} \times SPLV_{w4b}.$$

The animal's internal treatment of a contaminant from water or plants (and in other sections, soil) is assumed not to depend upon the medium in which it is obtained. Then, one can equate animal intakes from equations 10 and 11 to obtain equation A-8.

$$SPLV_{w4b} = SPLV_{w4a} / [1 + K_{wp} \times U_{pm} / U_{wm}] \quad (\text{A-8})$$

Substituting equation 10 in equation A-8 yields equation 11, q.e.d.

A.4 CONSTRAINTS

Figure A-1 illustrated the relation of the PPLV to its component SPLVs in the two-dimensional case. Here, the two types of constraints are viewed in the same manner in Figure A-2. As in Figure A-1, the SPLV are shown on each axis, and the PPLV is the intersection of the line $C_1 = C_2$ to the line connecting the SPLVs. A type 1 constraint is indicated by the vertical line C_{1c} , positioned such that $C_{1c} < \text{PPLV}$. Depending upon the level of importance associated with the constraint, its impact could be to revise the basis upon which a limit is determined, and to cause a lower limit than the PPLV to be determined.

Figure A-3 illustrates the type 2 constraint. The constraint is shown to apply to pathway 2 at a concentration C_{2c} , which is less than PPLV (otherwise it would not be a constraint). The procedure discussed in Section 7.2.2 is illustrated by the following construction. Determine the point (SPLV2 - C_{2c}) on the pathway 2 axis. Since the SPLV₂ is proportional to D_T , the segment between this point and SPLV₂ accounts for the pathway maximum attainable intake. From this point, draw a line parallel to the line between SPLV₂ and SPLV₁. This line is the locus of all values of C_1 and C_2 providing the remaining intake. The adjusted limit is the intersection of this line with the C_1 axis. The adjustment of intake for the constraint corresponds to reducing the problem space by one dimension, and in this case, to a one-dimension problem.

With more than two pathways, the procedure can be more complicated. If just one pathway is subject to a Type 2 constraint, the above procedure can be applied with allowance for the additional dimensions. In the three pathway analog, a plane passing through (SPLV₂ - C_{2c}) would be constructed parallel to the plane SPLV₁ - SPLV₂ - SPLV₃. The intersections of the constructed plane with the C_1 and C_3 axes defines two adjusted SPLVs; from these, an adjusted limit can be determined as shown in Figure A-1. If more than one pathway is subject to a Type 2 constraint, the procedure can be repeated until a problem space consisting of only unconstrained pathways occurs, and the adjusted limit is determined from the adjusted SPLVs.

A.5 VAPOR INHALATION PATHWAYS

Spencer, et al.⁸⁰ reviewed the volatilization of substances (particularly pesticides) from soil. Salient points were:

- o When soil is dry, substances adsorbed on SOC do not volatilize. In a closed system, if the soil is wetted in excess of a certain water content level, the vapor pressure in soil-pore air attains the saturation vapor pressure. This level appears to correspond with the water content required to cover soil particulates with a

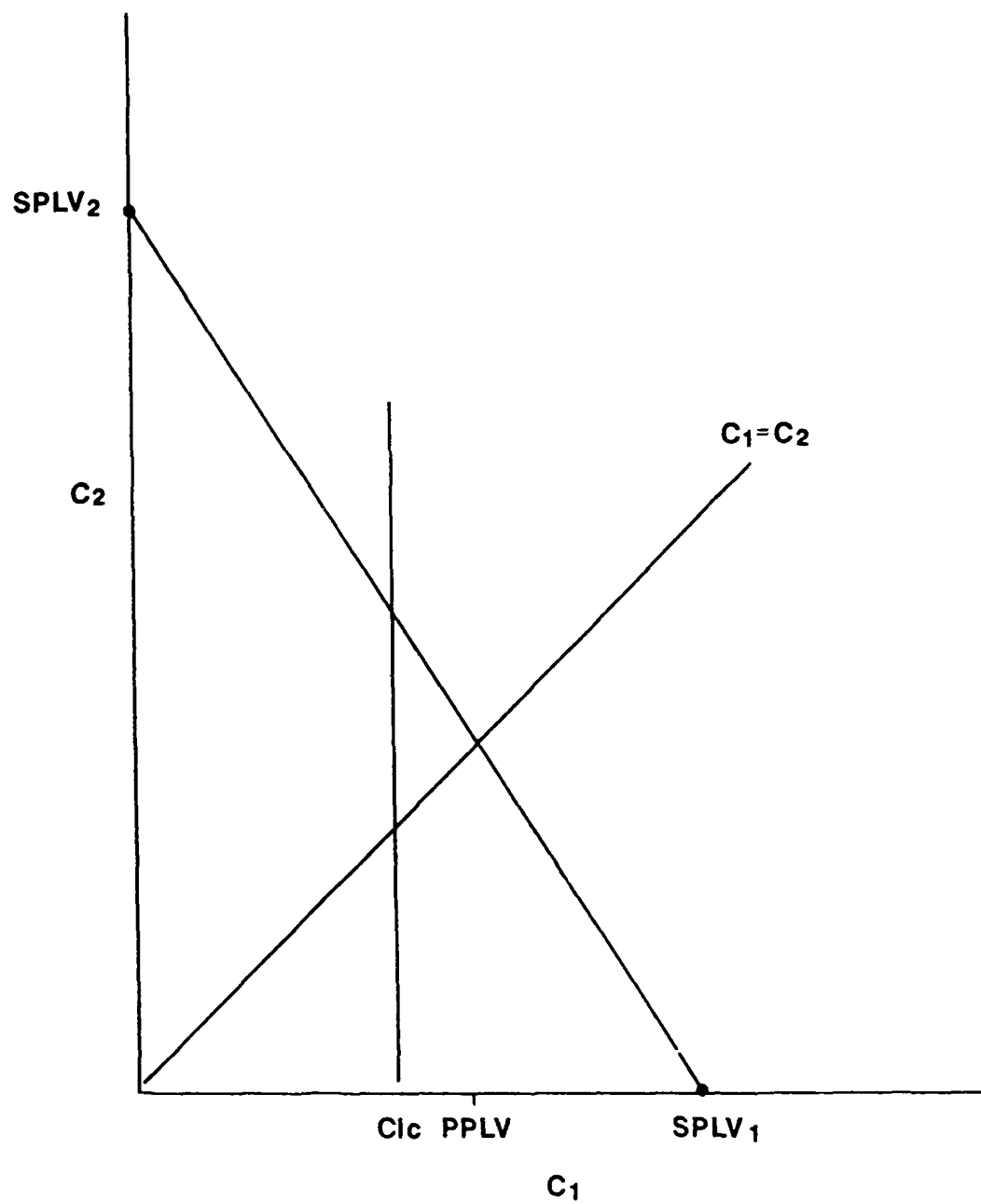


Figure A-2. The Type 1 Constraint

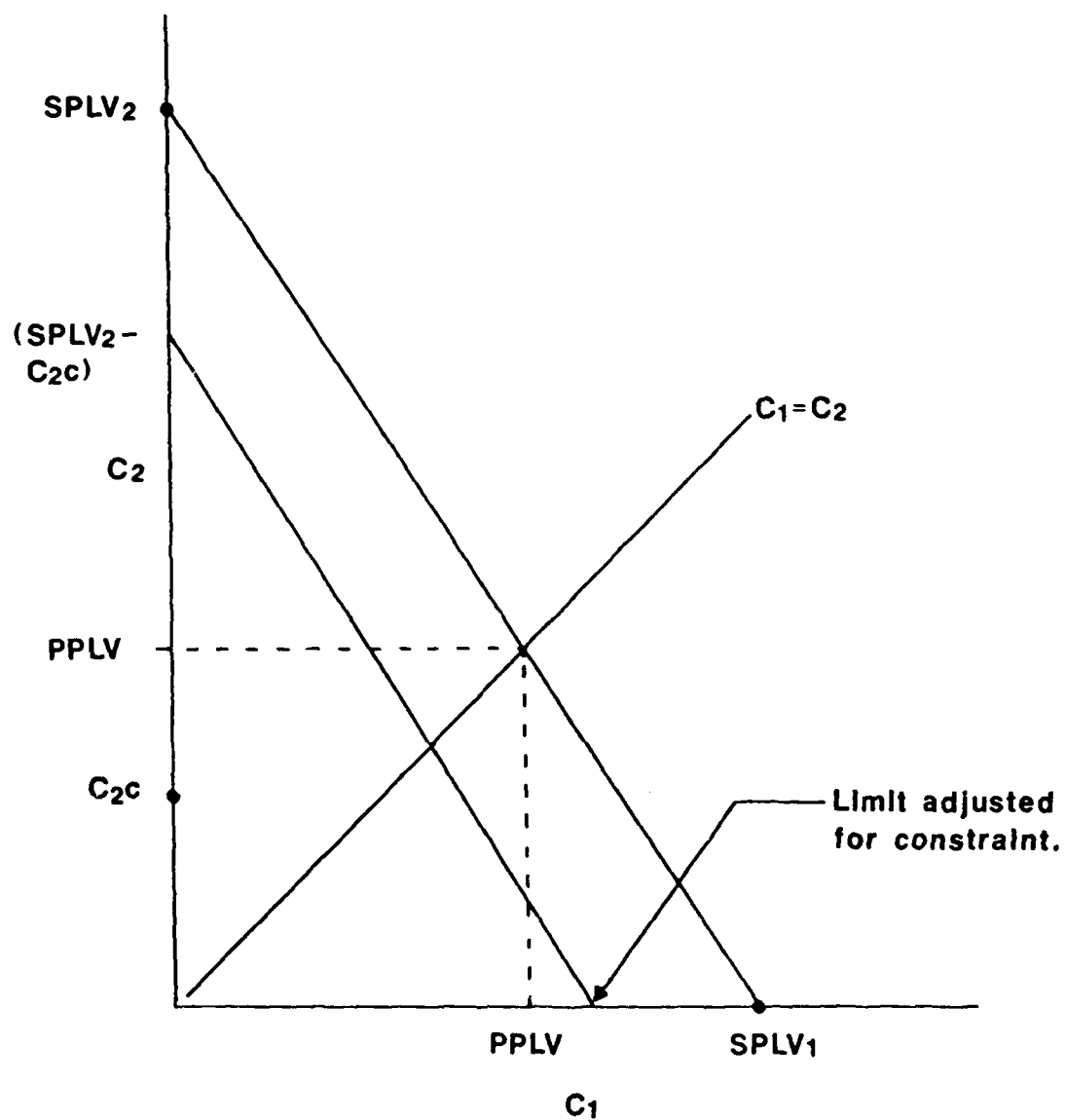


Figure A-3. The Type 2 Constraint: Two Pathways, One Constrained

one-molecule thick water layer; in terms of θ , this level is about 3 percent for surface soils.

- o If soil is sufficiently wet, the vapor density over the soil (in a closed system) will relate to the soil content as shown in Figure 3 of the main text.

- o In an open system, the surface of an initially uniformly contaminated soil mass in contact with air will be rapidly depleted of contaminant. A concentration gradient will develop across which contaminant can diffuse in soil-pore air to the soil surface.

- o If water is drawn to the soil surface, such as by solar heating, soluble contaminants can be transported to the surface to volatilize. This has been called the "wick effect"⁸⁰.

Lyman et al.⁶² have suggested that appreciable contaminant may diffuse in the liquid phase in soil even in the absence of bulk mass transport of liquid. A rough comparison of the relative importance of liquid and vapor diffusion can be made. For a given contaminant, the diffusion coefficient in water is about 10^{-4} times less than the coefficient in air. However, the mass of contaminant in soil-water per volume of bulk soil may be considerably more than in soil-pore air. Above K_h of 10^{-4} , vapor diffusion will be the predominant diffusion mode; below that level, diffusion in water will predominate. From the above discussion, it may be advisable to perform the vapor diffusion calculations for $K_h = 10^{-4}$ if $K_h < 10^{-4}$.

The treatment below concerns vapor diffusion only. While the other mechanisms will be operative, and perhaps predominate over vapor diffusion in removing contaminant from bulk soil, the information required to model all processes is formidable.

A plot of soil of infinite extent (edge effects can be neglected) is contaminated with a volatile pollutant. The basic equation to be solved is

$$\partial^2 C / \partial X^2 = D \partial C / \partial T$$

where C is the concentration of pollutant in bulk undisturbed soil (all phases), X is the depth dimension (increasing with depth), and T is time. Once the concentration profile is defined in terms of X and T , the flux from the surface is:

$$\text{flux}(T) = D \left(\partial C / \partial T \right)_{X=0} \quad (A-9)$$

Farmer and Letey⁸¹ reviewed different solutions to this equations based on different boundary conditions and their "real-world" approximations. The least cumbersome solution was for the following conditions:

- o The contamination is of infinite depth

- o The soil volume is initially uniformly contaminated with the pollutant.

- o Immediately after the start of diffusion, the surface concentration drops to zero.

The solution was found to be conservative compared to others, in that at a given time, the flux predicted by the solution was higher than for other boundary conditions.

Hwang⁸² solved the equation dealing directly with the soil-pore air concentration. In his treatment, the effective diffusivity, Dei , is expressed as the product $Da \times \epsilon^{1/3}$. The equation was

$$a \partial^2 C_{ae} / \partial X^2 = \partial C_a / \partial T$$

where

$$a = (\epsilon Dei) / (\epsilon + \rho Kd' / Kh)$$

and C_{ae} was related to C_{se}

$$C_{ae} = (Kh / Kd') \times C_{se}$$

If the initial concentration of pollutant in soil is unity, the corresponding concentration gradient is:

$$C_{se} = 1 \times (Kh / Kd') \operatorname{erf} (X / [4 a T])$$

The corresponding the flux generated by a unit concentration pollutant in soil is, based on Equation A-9:

$$\Phi(T) = \epsilon \times Dei \times (Kh / Kd') / [\pi a T]^{0.5} \quad (A-10)$$

Other than for rearrangement, equation 29 differs from equation A-10 in three respects:

- o A 1000 factor is included because of conversions from L to m^3 and kg to mg.

- o When $Da \times \epsilon^{4/3}$ is substituted in equation A-10, the term $Da \times \epsilon^{4/3}$ appears. Equation 29 uses the term in equation 30 instead. Equation 30, ascribed to Millington and Quirk⁸³, reduces to $Da \times \epsilon^{4/3}$ for a dry soil. Dry soil conditions, an implicit assumption of Hwang's approach, is unnecessarily conservative since diffusion from soil of a substance sorbed on the soil's SOC would not occur.

- o The term θ / Kh is included to account for pollutant in soil-pore water.

F_{avn} , the time-averaged flux from a soil with initial unit contamination, is:

$$F_{avn} = (T_1 - T_0)^{-1} \times \int_{T_0}^{T_1} \Phi(T) dT$$

The integration is done by parts. Equation 29 is in the form

$$\Phi(T) = K / T^{1/2}$$

which, integrated from zero to finite positive time T , yields

$$\int_0^T \Phi(T) dT = 2 K \times T^{1/2} = 2 \times T \times \Phi(T) \quad (A-11)$$

The integration from time T_0 to T_1 can be done in two parts:

$$F_{avn} = (T_1 - T_0)^{-1} \times \left[\int_0^{T_1} \Phi(T) dT - \int_0^{T_0} \Phi(T) dT \right]$$

Each integral is evaluated via equation A-11. Insertion of the appropriate limits leads to equation 28.

APPENDIX B. D_T ESTIMATION METHODS: A TECHNICAL DISCUSSION

B.1 TOXICITY-BASED D_T METHODS

While D_T is a human-related parameter, it is rarely based on human studies. Rather, it is derived from animal study results. Here, an overview is presented of how animal studies are conducted and how the results are converted to a D_T . The studies described involve the oral route of intake. Historically, there was no driving central requirement for consistent experimental protocols. Economics and Federal regulations have altered this. Thus, much of the discussion is based on the Environmental Protection Agency's "Health Effects Testing Guidelines"⁸⁴ developed for the Toxic Substances Control Act. The guidelines are not intended to be "toxicological cookbooks". A considerable amount of professional judgment has to be applied, which can't be readily described in narrative.

Toxicological testing has its roots in pharmacology. Drugs were observed to be non-effective at low doses, effective at a higher doses, and toxic at even higher doses.* The dose-response relationship reflects this observation. While most environmental pollutants are not "drugs" in the pharmacological sense, the test protocols seek to quantify this relationship.

In a sequence of extensive toxicity testing, the acute toxicity test provides a starting point for longer-term tests. Historically, this test has often been an end in itself, to provide a "first cut" estimate of toxicity in acute exposure situations. The rat is a favorite test animal, due to its relatively large size, short lifespan, established breeding history, and ease of handling. Other species used include mice, dogs, rabbits, and guinea pigs. The acute toxicity test usually involves less than 50 animals per species. The animals are assigned to different dose level groups. Each animal is dosed once with the substance (usually on a mg substance/kg body weight basis). The animals are observed for gross observable effects for 14 days. At the end of 14 days, the mortality rate (number of deaths per number of dosed animals) in each sub-group is determined. All test animals are anatomically examined.

Statistical procedures determine the LD_{50} , the dose estimated to cause 50% fatalities in the animal species population. This statistic has many drawbacks, and testing for the sole purpose of its determination has been discouraged⁸⁴. However, it is often the only toxicological datum available for many substances. This has lead to attempts to use the LD_{50} as an estimator for other test outcomes, such as the chronic NOEL. Equation 5 is a recent example of such an effort.

* This is strictly true for xenobiotic substances. Some ubiquitous substances (such as the trace nutrient metals) have an effect-concentration relation which includes a region where their presence is required to avoid adverse effects.

The next test procedure is a range-finding test, which involves daily doses applied over a short time period, often 14 days. Surprisingly, this test is not included in guidelines. It involves several levels of dosing to animal groups (usually one strain of rat and of dog). While doses would be less than the one-day LD₅₀, the dose selections is judgmental. In this case, a no-dose or control group is included. The dose is applied daily for 14 days, after which the animals are observed for another 7 days prior to sacrifice. Again, gross behavioral observations are made, weight is watched, and animals may be examined anatomically. Different measures of toxicity can be formed; a common measure is the LD₁₀. Observational experience is that the LD₁₀/2 is a predictor of the high dose in the next test in the sequence, the sub-chronic oral toxicity test.

As stated in the guidelines⁸⁰, the sub-chronic oral toxicity test study "...has been designed to permit the determination of the no-observed-effect level and toxic effects associated with continuous or repeated exposure to a test substance...The test is not capable of determining those effects which have a long latency period for development [such as carcinogenicity]...It will provide information on target organisms, the possibilities of accumulation, and can be of use in selecting dose levels for chronic studies and for establishing safety criteria for human exposure." The procedure, in general terms, is similar to that used in the 14-day test procedure. Usually, one does not strive to have mortalities, and a typical dose pattern is the 14-day LD₁₀/2 (high dose), the LD₁₀/4 (intermediate dose), the LD₁₀/8 (low dose), and the control (no dose). The observations are generally more detailed than in the 14-day test, and include hematology and clinical biochemistry, as well as more intensive necropsy and histopathology.

Finally, a chronic oral toxicity study may be undertaken to estimate the doses considered to be no-effect/effect levels where responses are expected after a long latency period or are expected to be occur only after cumulative exposure. The exposure period may last one year or longer. Procedures and objectives are similar to those described for the sub-chronic test.

Ideally, the sub-chronic or chronic toxicity tests indicate one dose level which would considered a "no-effect" dose level and a higher dose level at which some effect would be observed. This is the second outcome mentioned in Table 6, main text. Interpreting test results takes considerable judgment. The distinction between "effect" and "no-effect" can be rather subtle, such as a statistically-detectable change in weight gain patterns or a blood chemical parameter. The biological significance of statistically detected differences will vary for different parameters. Effect may be species-specific, such as a

alteration of a metabolic chemical that the human system does not produce.

B.2 SAFETY FACTORS

The literature sometimes refers to these as "uncertainty factors". They are numbers which divide a dose level derived from animal tests to extrapolate to human conditions. If the dose level is a NOEL, the extrapolated human counterpart is commonly called an "acceptable daily intake". A safety factor as defined will exceed 1. Each factor is the product of component factors. The most commonly cited component factors have been presented in EPA guidance¹⁸. A factor of 10 is applied for inter-species conversion, a factor of 10 is applied for intra-human sensitivity considerations, and when necessary, a factor of 10 is applied for conversion from a sub-chronic test conclusion to a chronic NOEL estimate. A fourth factor, between 1 and 10 (see Table 7, main text) is included should toxicity test results fail to identify a dose low enough to be a NOEL.

Layton et al.²⁶ and Dourson and Stara⁸⁵ have reviewed "case study" determination of safety factors. The first review²⁶ analyzed four previous studies in which sub-chronic and chronic tests results were compared. In these studies, the mean ratio
sub-chronic NOEL : chronic NOEL
was about two, and a safety factor of 10 (see the above paragraph) was found to be conservative (i.e.: a smaller factor would have⁸⁵ sufficed) in 95 percent of the observations. Dourson and Stara⁸⁵ looked at this factor and several others. They derived the ratio of LD₅₀ : LD_{0.13} for 490 determinations of acute toxicity. The latter term represented the dose required to cause marginally more mortality than would be noted with a non-exposed group of animals. Thus, the ratio approximated the safety factor allowing for sensitivity. In this case study, the ratio exceeded 5.5 in about 14 percent of the observations. With respect to animal-human species adjustment, the information is specific for specific classes of compounds, and the ten-fold adjustment is closer to the mean than are the other factors cited above. Dourson and Stara⁸⁵ discuss the problem of compounding multiplied conservative factors, and provide some examples.

Regulators are prone to be conservative, particularly when the mandate for regulation involves "adequate margins of safety", or similar terminology. Given the slim probability that sufficient data are available about a substance from which to select lower safety factors, EPA's values are best followed.

B.3 STRATEGY SELECTION: CARCINOGEN OR NON-CARCINOGEN?

The impact of cancer is well-known and formidable. One authoritative account states⁸⁶ "Cancer is the second most common cause of death in the United States. One in every four Americans will suffer from cancer sometime during their lifetime; one in every five will die from cancer...In addition to the physical and

emotional suffering caused by cancer, this disease may cost the Nation as much as \$39 billion each year in lost production and income, medical expenses, and research resources."

Due to this concern, efforts are under way to reduce the exposure to cancer-causing agents. Many xenobiotic substances in the environment were identified as being potentially carcinogenic to humans,⁸⁷ and collectively, were cited as the source of most cancers. While it is debatable that this is so*, they have become highly regulated by Federal and State governments.

From the PPLV viewpoint, the differentiation between carcinogens and non-carcinogens is reflected in the DT estimation procedures for each. However, while it can be argued that almost any substance is toxic at some level of intake, the same cannot be said about carcinogenicity. Yet, the political atmosphere is that substances are suspected to be potentially carcinogenic until the experimental evidence shows otherwise. Thus, a review of the criteria by which a substance is judged to be potentially carcinogenic is merited. These criteria are not "black and white"; the decision-maker will have to decide the amount of "gray" to include.

B.3.1 Assessment of Carcinogenic Evidence

The evidence that a substance is a carcinogen can be of widely-differing quality. Thus, several classifications statements of evidence have been developed to qualitatively assess the available information. Three concepts are first clarified.

1. An accepted definition of a neoplasm or tumor is an autonomous new growth of tissues in an organism, which is uncoordinated with that of natural tissue, and persists⁸⁸ after cessation of the stimuli which evoked its development. In many cases, the specific stimulus is not known. Neoplasms may be benign; such neoplasms do not increase in size, and apparently cause no harm. Cancer is considered the malignant expansion of neoplasms through the body.

2. The term cause is used in a strict sense. While it is facile to conclude that compound "A" causes cancer when a group of people are exposed to it and many of them develop cancer, a more objective approach is to validate that:

- o There was no identified bias which could explain the association (such as an unusually large number of cigarette smokers in the group).

* Radon may be the substance in the ambient environment which is the largest single cause of cancer. It is a radioactive element in gaseous form rather than a man-made substance. The belated effort of EPA to deal with its emissions does not speak well for the EPA's ability to discern major problems from minor problems.

- o The possibility of confounding (non-obvious causes) had been considered and ruled out. This is typical of well-designed studies.

- o The possibility of chance occurrence was unlikely.

3. Sources of evidence. Ideally, causal carcinogenicity should be based on human tests. Realistically, human evidence is based on unexpected situations. For example:

- o Tars from wood smoke were found to cause testicular cancer when it was noted that of most victims were chimney sweepers;

- o Sulfur mustard was identified as a human carcinogen due to the high incidence of cancers in Japanese chemical warfare workers and exposed World War I soldiers¹⁴;

- o Vinyl chloride was identified as a human carcinogen because production workers developed a very rare liver cancer after occupational exposure;

- o Arsenic was implicated as an oral human carcinogen because of the high incidence of skin cancers in persons living in an area of Taiwan where the drinking water had high arsenic levels.

In lieu of human evidence, mammalian surrogates are involved in experiments, a situation similar to toxicants. The practice of using animal test results as evidence has gained scientific acceptance, although there is considerable controversy concerning the design, conduct, analysis, and interpretation of test results⁸⁹.

B.3.1.1 IARC Statements of Evidence

The IARC has studied and assessed the literature for over 500 compounds. Their evidence assessment scheme has undergone several changes; the most recent one is described in Table B-1. This scheme separates human results from animal results, and rates evidence as sufficient, limited or inadequate for each.

B.3.1.2 NTP Statements of Evidence

The NTP has devised the scheme presented in Table B-2 to describe results of animal bioassays, particularly those of male and female mice and rats. While not a comprehensive scheme, it deserves mention; the NTP controls and manages much of the testing being funded by the U.S. Government, and these results often determine standards or criteria.

B.3.1.3 EPA Statements of Evidence

Unlike the above organizations, the EPA is involved with regulatory activities. A need was perceived to mesh qualitative

Table B-1. IARC Statements of Evidence of Carcinogenicity⁹⁰

Human Studies

Sufficient evidence - causal relationship

Limited evidence - A causal relationship is credible, but alternative explanations, such as chance, bias or confounding could not adequately be excluded.

Inadequate evidence - (1) There were few pertinent data, or (2) the available studies, while showing evidence of association, did not exclude chance, bias or confounding, or (3) studies were available which did not show evidence of carcinogenicity.

Animal studies

Sufficient evidence - there is an increased incidence of malignant tumors: (1) in multiple species or strains; or (2) in multiple experiments (preferably with different routes of administration or using different dose levels); or (3) to an usual degree with regard to incidence, site of type of tumor, or age at onset. Additional evidence may be provided by data on dose-response effects, as well as information from short-term tests or on chemical structure.

Limited evidence - the data suggest a carcinogenic effect but are limited because: (1) the studies involve a single species, strain, or experiment; or (2) the experiments are restricted by inadequate dosage levels, inadequate duration of exposure to the agent, inadequate period of follow-up, poor survival, too few animals, or inadequate reporting; or (3) the neoplasms produced often occur spontaneously and, in the past, have been difficult to classify as malignant by histological criteria alone (e.g., lung and liver tumors in mice).

Inadequate evidence - because of major qualitative or quantitative limitations, the studies cannot be interpreted as showing either the presence or absence of a carcinogenic effect; or that within the limits of the tests used, the chemical is not carcinogenic. The number of negative studies is small, since, in general, studies that show no effect are less likely to be published than those suggesting carcinogenicity.

statements as to human and animal test results into a classification scheme, which is shown in Table B-3. is indicates the devised scheme.

While any scheme has its supporters and detractors, the EPA scheme is most appropriate, particularly when a contamination situation subject to their regulations is involved. In their scheme, a compound whose evidence can be classified in the "E" group could be dismissed from suspicion. Group "D" evidence is essentially null evidence; nothing definitive can be said because

Table B-2. NTP Categories of Carcinogenic Evidence⁸⁹

Studies are presumed to have been performed on male and female rats and male and female mice. These categories may apply to one or more species, genders, or genders within species.

CLEAR EVIDENCE OF CARCINOGENICITY ... studies that are interpreted as showing a chemically related increase of malignant neoplasms, studies that exhibit a substantially increased incidence of benign neoplasms, or studies that exhibit an increased incidence of a combination of malignant and benign neoplasms where each increases with dose.

SOME EVIDENCE OF CARCINOGENICITY .. studies that are interpreted as showing a chemically related increased incidence of benign neoplasms, studies that exhibit marginal increases in neoplasms of several organs/tissues, or studies that exhibit a slight increase in uncommon malignant or benign neoplasms.

EQUIVOCAL EVIDENCE OF CARCINOGENICITY ... studies that are interpreted as showing a chemically related marginal increase of neoplasms.

NO EVIDENCE OF CARCINOGENICITY ... studies that are interpreted as showing no chemically related increases in malignant or benign neoplasms.

INADEQUATE STUDY OF CARCINOGENICITY demonstrates that because of major qualitative or quantitative limitations, the studies cannot be interpreted as valid for showing either the presence or absence of a carcinogenic effect.

the substance hasn't been studied. The difference between the "B2" and "C" categories has become controversial. The drinking water standard for a substance with "B2" category evidence is usually more stringent than if the evidence was in the "C" category²³. Moreover, hazardous air pollution regulation decisions may hinge upon the selection of category²². Generally, a substance whose evidence is in group "A" or "B" should be treated as a carcinogen. This scheme is currently in the process of formal review.

B.3.1.4 In Vitro Tests

The animal bioassay test (see section B.4.2) is an "in vivo" test. The test, including preliminaries, may cost about \$500,000 per substance. From the economic viewpoint, bioassays are not undertaken frivolously. Since the 1970, a number of "in vitro" tests have been developed to measure the ability of a substance to

* The "rule-of-thumb" policy is to regulate substances with "B2" evidence at an ARL of 10^{-6} , and to regulate substances with "C" evidence at a level of human NOEL / 10 .

Table B-3. EPA Weight of Evidence Categories for Potential Carcinogens.⁹¹

GROUP AND STATEMENT	LEVEL OF EVIDENCE
A - Human carcinogen	Sufficient* evidence from epidemiology studies.
B - Probable human carcinogen	(B1) At least limited* evidence of carcinogenicity to humans (B2) Usually a combination of sufficient evidence in animals and inadequate evidence in humans.
C - Possible human carcinogen	Limited evidence of carcinogenicity in animals in the absence of human data.
D - Not classified	Inadequate animal evidence of carcinogenicity.
E - No evidence of carcinogenicity in humans.	No evidence of carcinogenicity in at least two adequate animal tests in different species or in both epidemiology and animal studies.

* See IARC Statement (Table B-1) for meaning of "sufficient" and "limited".

alter the function or genetic structure of one-cell organisms or cellular culture from higher organisms. The best known of these is the "Ames Test", which uses Salmonella typhimurium mutant strains that cannot synthesize histidine. In the basic test, a histidine-free medium is plated with mutant cells. Theoretically, no cells should survive in the medium. However, in a control situation (no substance in the medium), some cells mutate to the natural state, synthesize histidine, and form colonies. If the number of colonies increases markedly with increased concentration of the test substance in plate mediums, the substance is a mutagen. Such substances are often animal carcinogens as well.

These tests are relatively inexpensive and fast to perform compared to bioassays. A long range goal is to use these tests as a "battery", the results of which could be used to qualitatively predict the outcome of a bioassay. Tennant et al.⁹³ indicate that current tests have yet to meet this goal.

B.4. CARCINOGENIC PARAMETERS

B.4.1 Acceptable Risk Levels

Toxic chemicals are expected to behave like "drugs"; some threshold exists below which their intake would have no effect. D_T is an estimate of a level lower than this threshold. A threshold is postulated to exist since the human body has some mechanism to counter or minimize the impact of a low chemical dose. Then, at D_T , there is "no risk" of an effect. With carcinogens, the situation is viewed differently. The body has no special mechanism to counter cellular mutations that a carcinogen may create. Based on radiation as a model, there is no threshold

to a carcinogenic dose. Such a model could be interpreted to mean that a carcinogenic substance should be totally removed from a soil or water mass to avoid cancer risk. While this is a laudable goal, it is impractical to implement. Thus, the acceptable risk level has been conceived. The level expresses the added risk that cancer will occur to an individual at age 70 given a constant dosage of a substance from birth.

Quantitative risk levels have been the source of extensive commentary⁹⁴. There are two broad categories of risk: voluntary risk and involuntary risks. Voluntary risks are accepted by people as part of their life style because there is a benefit derived from the risk. For example, the risk of death in an automobile accident is about 0.014 (5×10^{-4} deaths/year x 70 years divided by a population of 2.5×10^8), yet few people stop driving or riding in automobiles because of this risk. Involuntary risks are placed upon people without their consent or direct benefit, such as airborne radiation releases from a nuclear power plant. People (and society) seem willing to accept higher levels of voluntary risk than of involuntary risk. Acceptable involuntary risks appear to be of the order of 10^{-4} to 10^{-7} , and this range is often involved in regulatory agency considerations*.

B.4.2 Bioassays

Since cancer is considered to develop over an extended period of time with low-level exposure to a carcinogen, the bioassay test is designed to be a near-lifetime study. Procedures have become fairly standardized⁸⁹. Fischer 344 rats and B6F3C1 mice are recommended as test subjects in lieu of extenuating factors. Usually, 200 animals are tested at each dose level, 50 of each species and sex. The doses used are typically selected from results of a sub-chronic assay, particularly a "maximum tolerated dose" (MTD), defined as "the highest dose of the test agent given during the chronic study that can be predicted not to alter the animal's normal longevity from effects other than carcinogenicity."⁸⁹ Toxic effects can be expected at the MTD. A typical dose selection regime is the MTD, MTD / 2, MTD / 4, and a control (compare with the sub-chronic toxicity test doses based on the 14-day LD₁₀). Animals sacrificed at selected time intervals in the study are assayed for tumors, as are any animals that die during the exposure period. The tumors and types are enumerated for all studied animals. The tests are conducted for the lifetime of the test animals, which is about two years for mice and rats.

The bioassay provides information on two matters: first, whether there is increased incidence of tumors with increased dose, and secondly, the tumor counts involved (from which potency is

* For example, in the New York State Water Classifications and Quality Standards⁹⁵, "...the 95 percent lower confidence limit on the dose corresponding to an excess lifetime cancer risk of one in one million shall be the basis of the standard [for oncogens]"

determined). The first matter involves the probability of a chance outcome. One assesses whether the incidence of tumors in dosed animals differs from those in the control group. This assessment is done for each tumor type. For this reason, the incidence of tumors in dosed animals should exceed 10 percent.⁹⁶ Otherwise, the statistical tests are not likely to indicate a significant dose-response curve if in fact one does exist.

If there is an increase of any type of tumor with increased dose (see Table B-2), the potency can be determined. Since the information involves incidences of the order of 0.1, while results are desired for incidences of the order of 10^{-4} to 10^{-7} , mathematical models are employed. The model of choice, in lieu of evidence to suggest another model, is the multistage model developed by Crump⁹⁷. Basically, this model fits the incidence-dose data to a polynomial, which when extrapolated to incidence levels below about 0.01, becomes a log-linear relation of dose to incidence with a slope of 1. This is shown in Figure B-1. The model also determines a confidence band about this relation. The 95 percent confidence bands are also linear; when the lower band (with respect to dose) is extrapolated to unity incidence, it defines the dose $1/q$. The reciprocal of this dose is the animal potency estimate.

The final step is to compute the human potency, as described in Section 3.3.2. By virtue of the log-linear extrapolation, an acceptable dose is related to an acceptable risk level by equation 6.

B.5 CLOSING COMMENTS

In simplified terms, this Appendix has presented the bases by which D_T is estimated for toxic substances and carcinogens. The presentation has not been intended as an in-depth review of toxicology or oncology. As with most generalizations, exceptions exist. Moreover, the procedures presented reflect a position which is a mixture of science, politics, and the consensus attitudes of the scientific community. They all are subject to change, and thus the procedures are likely to change.

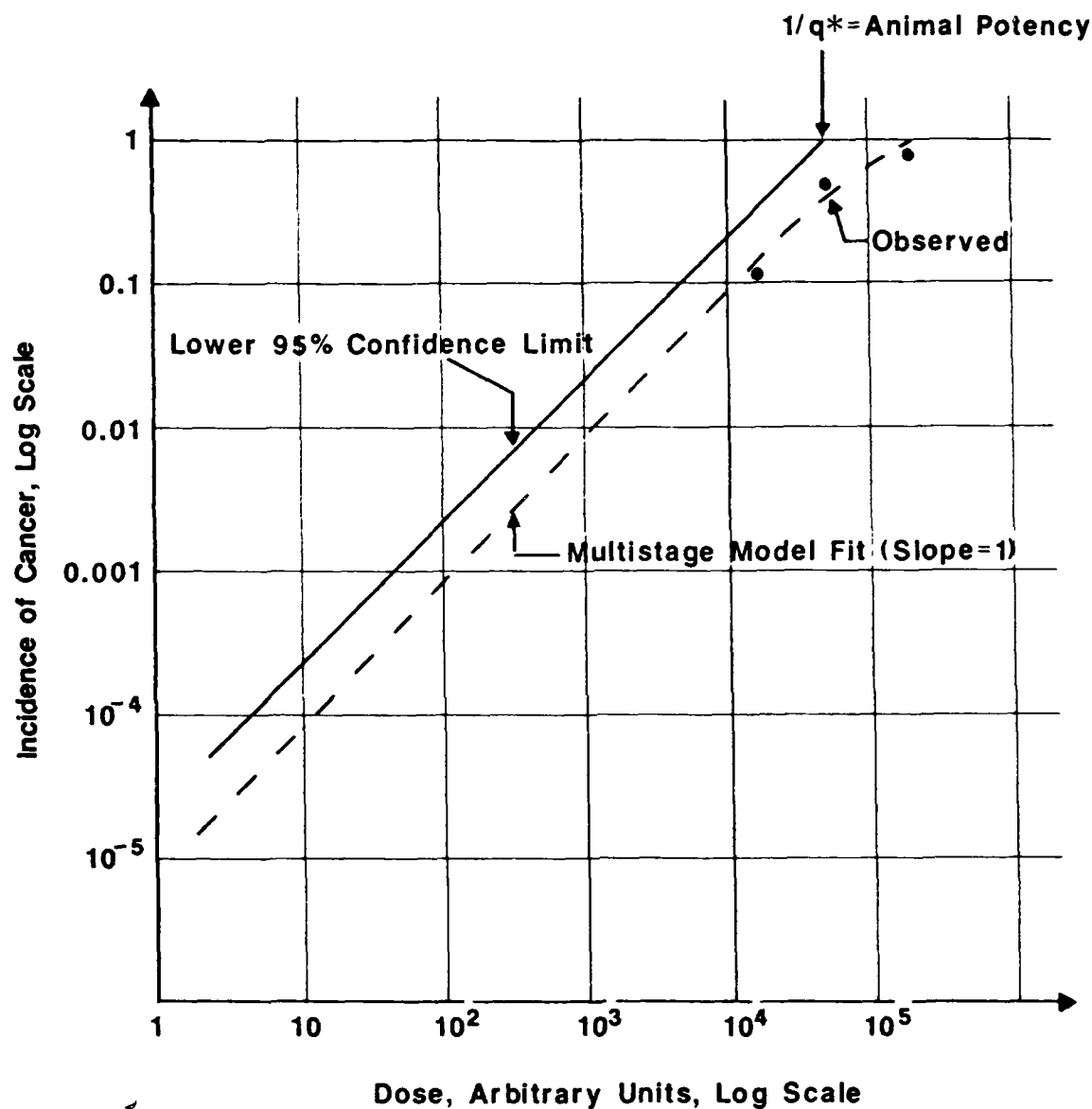


Figure B-1. Graphical Representation of the Extrapolation of Tumor Incidence Data to Determine q^*

APPENDIX C. PARTITION COEFFICIENTS

In early PPLV approach⁹ presentations, 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 related by:

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

where K_{wf} was a partition coefficient between water and fish. Procedures to estimate the partition coefficients were left to the resourcefulness of the user. Within the last 15 years, many equations have been developed for partition coefficients along the lines of those presented in Section 6. As seen below, they are at best "first approximations" to be used in lieu of experimental information. Often, the user has only the choice of with using the equations with the knowledge of their limited accuracy or not being able to compute SPLVs.

C.1 ACCURACY OF PARTITION COEFFICIENT EQUATIONS

The equations presented in Section 6, main text, are restricted to organic compounds. The equations are in the form

$$Y = 10^{(c_1 + c_2 \log X)}$$

where c_1 and c_2 are constants, Y is to be estimated and X is the known predictor parameter. This format is easier to program in computers than the form shown in most literature

$$\log Y = c_1 + c_2 \log X$$

The theory is developed to the point where equations in this form can be expected, but not to the extent that the constants can be theoretically determined. The constants for a given equation are usually determined from a paired X - Y data set based on selected compounds.

There can be marked disagreement between correlations published for the same factor. Isnard and Lambert¹⁰ reviewed 13 equations relating BCF to K_{ow} . In these equations, c_1 ranged from -1.82 to 0.188. Thus, at $\log K_{ow} = 0$, a difference of up to 100-fold could occur just from choice of equation. There are several reasons for this. First, each equation often address a limited subset of the universe of substances, and these subsets are often dominated by a certain class of chemicals. Another source of inaccuracy is caused by the uncertainty of low solubility or of high $\log K_{ow}$ measurements. These measurements tend to be the extreme members of a data set used in a correlation. If a least-sum-of-squares regression treatment is used, these measurements can disproportionately impact the results. Some authors have employed "apple and orange"-type data bases, with some predictors being estimated rather than measured or being measured by older experimental procedures.

To minimize such effects in a BCF - Log Kow equation, Davies and Dobbs⁶⁷ selected test case substances according to these criteria:

- o all data were experimental
- o steady state had appeared to be reached
- o the BCF were based on flow-through studies
- o the BCF was determined for freshwater fish
- o fish were acclimated to test conditions
- o the level of test substance was not known to be toxic to fish.
- o BCF values obtained immediately after spawning were disregarded.
- o test substance concentration was based on sampling and analysis.
- o Kow was determined by either the shake-flask or sealed-centrifuge tube method
- o water solubility data were obtained by a method which excluded contributions from suspended particulates.

The potential sources of "error" could be quite numerous. Even with such safeguards, the accuracy of a BCF estimate that can be expected from a given equation is probably not much better than order of magnitude. As an example, Isnard and Lambert⁹⁸ graphically displayed the 107-compound data set (all experimental data) upon which their equation

$$BCF = 10^{(0.80 \times \text{Log Kow} - 0.52)} \quad (C-1)$$

is based. Only 48 data sets indicated that the computed BCF was within the range of 1/3.16 to 3.16 times the experimental BCF (plus or minus one-half order of magnitude). For 21 compounds, the computed BCF was at least one order of magnitude different than the experimental result. It should be kept in mind that BCF estimation equations are probably more accurate than those for other partition coefficients that will be discussed here.

Statistical summary parameters presented along with such equations can be misleading. One frequently reported is the regression coefficient (often called "r²"). It describes the "fit" or "scatter" of the data to the derived equation. To the extent that such compounds were not selected "at random", it may not describe the fit of other compounds. When possible, predictions should be based on equations derived for compounds similar to the ones in consideration.

C.2 TEST CONDITIONS VS. "REAL WORLD" CONDITIONS

The estimation equations are based on experiments where equilibrium or pseudo-equilibrium is attained between the two components of the partition coefficient. EPA guideline experimental procedures^{63,99} include recommended times for tests. The time frame of tests from which coefficients are developed should be shorter than the time frame in the real world. The decision-maker should assess the extent to which experimental conditions reflect the environmental situation.

For example, BCF test procedures can take (after an acclimation period) from several hours to up to 28 days.⁹⁹ In a situation where fish are in a relatively closed water system, such as a pond, the BCF should approximate actual conditions. If fish can leave a contaminated region of water (such as a stratified lake with contaminated sediment where the fish generally stay in the epilimnion), the BCF may overestimate the actual fish contamination levels. On the other hand, the BCF may underestimate a pollutant level in the body of a bottom-feeder fish (see Section C.3). Empirical studies of K_{pat} described in Saha¹⁰⁰ have extended from 30 to 112 days. Thus, K_{pat} should be a useful value when animals are raised on a food source for an extended period. However, livestock are often sent to a feedlot before slaughter. If the feedlot feed is not contaminated, pollutant will be removed from the animal, and K_{pat} should overestimate the contamination level in meat.

C.3 BCF RELATIONS

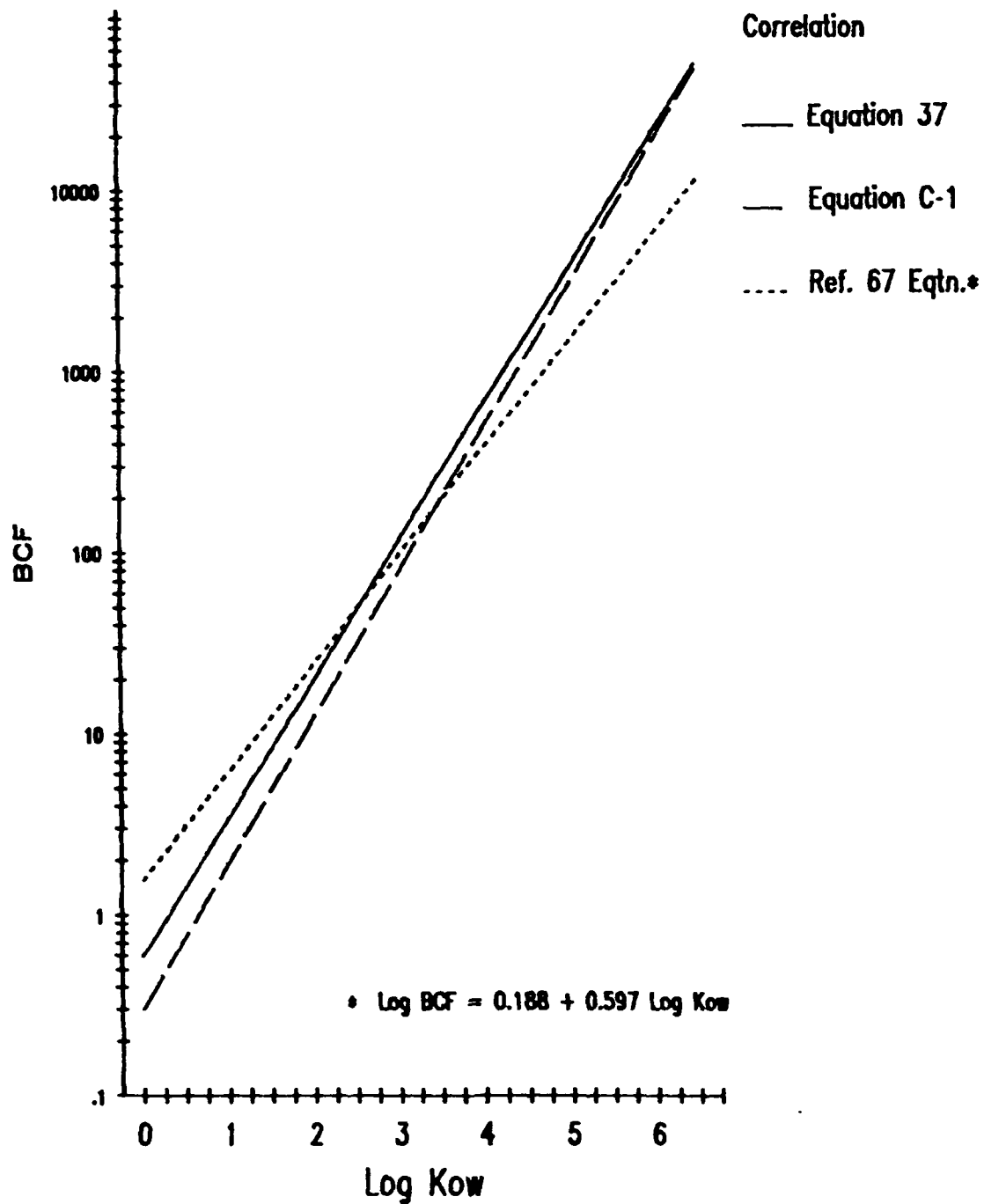
As a general use correlation based on Log K_{ow}, equation 37, the relation derived by Veith⁶⁶ is used. Although it is 10 years⁶⁷ old, more recent equations⁹⁸ such as proposed by Davies and Dobbs⁶⁷ or by Isnard and Lambert⁹⁸ do not provide markedly different estimates when Log K_{ow} > 1 (relatively few BCF have been measured for substances of lower K_{ow}). These relations are shown in Figure C-1. Equation 38⁶⁷ where SW is the predictor, was suggested by Davies and Dobbs⁶⁷, and agrees⁹⁸ closely with a more recent correlation of Isnard and Lambert.

The accuracy of BCF relations has been commented on above. There are some fish-unique sources of error that can contribute to this. The BCF is based on a balance between intake and removal in a fish. If fish have different rates of metabolism for compounds of similar SW or Log K_{ow}, the BCFs observed will be different. Analysts have used different portions of fish sample for BCF evaluation; in some cases, whole fish samples are used, in others, muscle samples. As mentioned in Section 6.2, equation 37 is specific to 7.6 percent lipids content; other equations don't specify a lipids level. Perhaps more accurate correlations could be obtained if BCF were expressed on a per unit lipids content basis.

The BCF relationships do not account for external sources of pollutant in the environment, such as food consumed by bottom-feeder fish. This situation was discussed by Rosenblatt¹¹, and a SPLV relation was derived for consumed fish that were exposed to a pollutant only by ingestion of sediment. Here, a combined relation, involving water and sediment sources, is proposed.

The intake of pollutant from water is first addressed. At equilibrium, the intake and removal of a contaminant balance. The fish processes water at a rate of U_{wf} kg/kg fish-day, and removal is assumed to follow first-order kinetics. The mass balance of contaminant is:

Figure C-1. BCF Correlations Based on Log Kow



$$U_{wf} \times C_w - k_2 (C_f - C_w) = 0 \quad (C-2)$$

C_f is the pollutant level in fish. The removal rate constant is $k_2 \text{ day}^{-1}$. A proposed predictor equation for k_2 was reported by Rosenblatt¹¹

$$k_2 = 10^{(1.47 - 0.414 \text{ Log } K_{ow})} \quad (C-3)$$

BCF is defined as the fraction C_f / C_w ; and from equation C-2,

$$BCF = (U_{wf} / k_2) + 1 \quad (C-4)$$

Now, the effect of sediment is addressed. The bottom-feeder has an intake of sediment U_{sf} ; the sediment contamination level is C_{sed} . At equilibrium, an equation similar to C-2 should apply:

$$U_{sf} \times C_{sed} + U_{wf} \times C_w - k_2 (C_f - C_w) = 0 \quad (C-5)$$

Here, C_{sed} is assumed related to C_w by an biosorption-water partition coefficient (K_B) proposed by Baughman and Paris, and reported in Spanggord, et al.¹⁰:

$$K_B = 10^{(-0.361 + 0.907 \text{ Log } K_{ow})} \quad (C-6)$$

Equation C-5 can be rewritten as

$$(U_{sf} \times K_B + U_{wf} + k_2) / k_2 = C_f / C_w \quad (C-7)$$

C_f / C_w in equation C-7 is called as BCF_a to delineate it from the BCF in equation C-4. These two terms are to be compared. They can be substituted in equation C-7 to obtain

$$BCF_a / BCF = 1 + (U_{sf} \times K_B) / (k_2 \times BCF)$$

U_{sf} has been estimated at 0.06. When this estimate, equation C-3 (for k_2), equation C-6 (for K_B), and equation 37 (for BCF) are substituted in the above equation, and terms are rearranged, the ratio becomes:

$$BCF_a / BCF = 1 + 0.0015 \times K_{ow}^{0.561}$$

This equation indicates that below $\text{Log } K_{ow}$ of about 4, relatively little of a fish's pollutant burden comes from food. However, at $\text{Log } K_{ow}$ of 6, about four-fifths of the burden would come from food. Thus, highly lipid substances in sediment may accumulate in fish tissue to a higher extent than would be predicted a water-based BCF correlation.

C.4 Koc RELATIONS

Lyman and Loreti⁶⁸ have done an extensive review of the Koc estimation literature. They note that Koc measurements are often confounded. Organic compounds, particularly polar

compounds, can adsorb on the mineral portion of soil. The organic matter of a given soil, while grossly classed as SOC, is comprised of several different compounds, each of which adsorbs organics differently. As an extreme case, Carter and Suffet¹⁰² obtained Koc estimates for dichloro-diphenyl-trichloroethane (DDT) that ranged from less than 10,000 to 525,000 depending upon the specific soil fulvic or humic acid comprising the SOC. Other substances may ionize, the ionized entity behaving much differently from the base compound. There is an experimental "solids concentration" effect apparently caused by non-settled soil particulates remaining in the water phase after a Kd test, and the pollutant content therein being counted in the post-test water concentration analysis.⁶⁸ In such tests, Kd values decrease with an increasing ratio of soil to water.

Lyman and Loreti suggested an improved equation based on 52 chemicals:

$$K_{oc} = 10^{(0.779 \text{ Log } K_{ow} + 0.460)} \quad (C-8)$$

which excluded compound measurements likely to include the solids concentration effect. However, the surviving data-base was heavily weighted to aromatic compounds. Without excluding compounds, they developed the relation

$$K_{oc} = 10^{(0.806 \text{ Log } K_{ow} + 0.473)} \quad (C-9)$$

based on 76 chemicals, which agrees closely with equation C-8, and is the equation 39 in the main text. They also presented equations based compounds that were either aromatic or non-aromatic. While there was a difference in the relations: for aromatics:

$$K_{oc} = 10^{(0.881 \text{ Log } K_{ow} + 0.214)} \quad (C-10)$$

and for non-aromatics:

$$K_{oc} = 10^{(0.533 \text{ Log } K_{ow} + 1.151)} \quad (C-11)$$

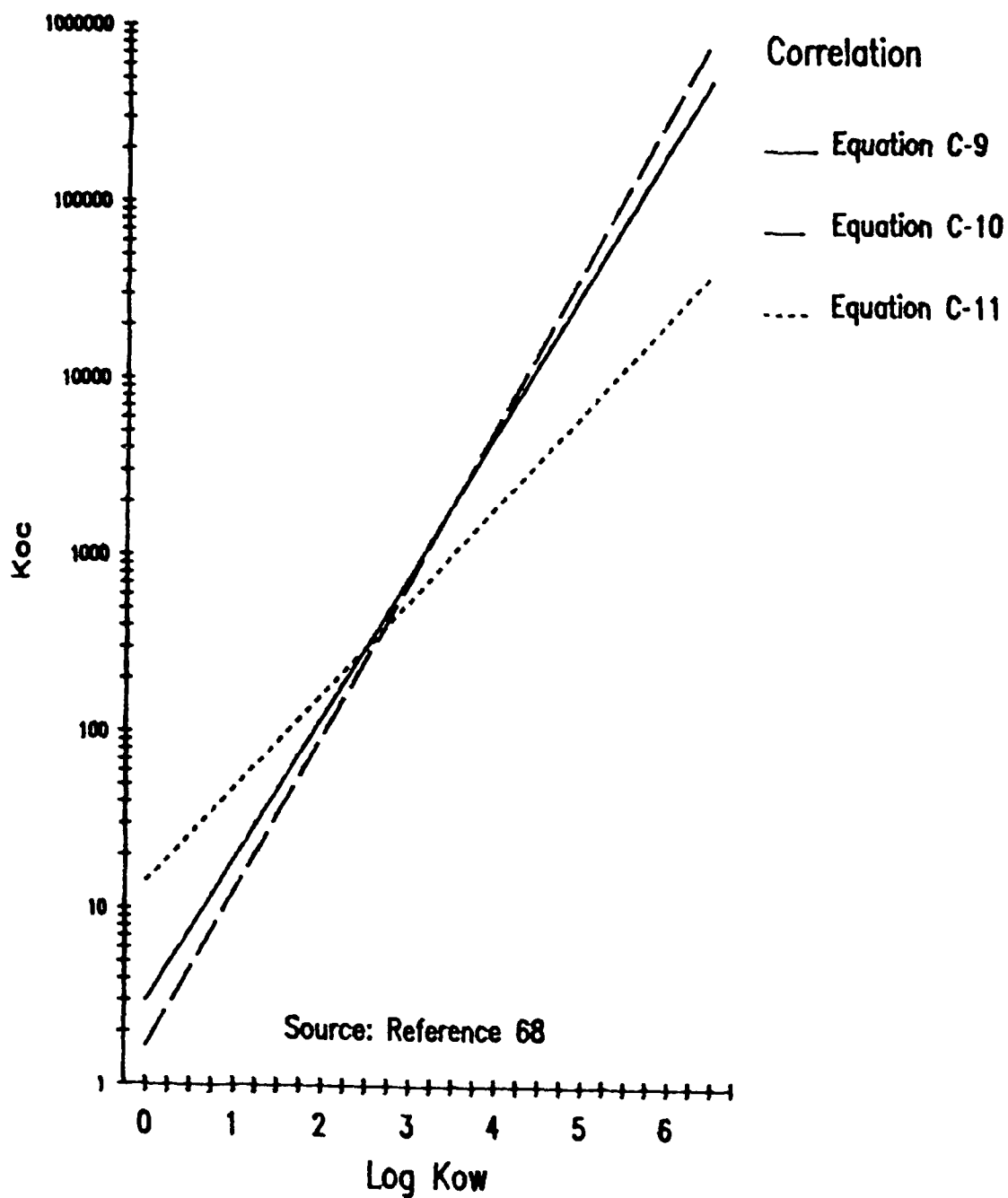
they did not check the statistical differences between them. Figure C-2 shows equations C-9, C-10, and C-11.

A similar approach was taken for equations based on aqueous solubility, and again, the equation with all chemicals is used in the main text. Karickhoff, as reported by Lyman and Loreti⁶⁸ has suggested that a factor be included in Koc - solubility equations for substances with melting points above 25 °C. This factor accounts for the energy to convert these substances to the subcooled liquid state. However, the evidence to support use of a specific quantitative factor is not well-established.

C.5 PLANT TO MEAT OR MILK PARTITION COEFFICIENTS

In the 1950s and 1960s, pesticides were found in the meat and milk

Figure C-2. Koc Correlations Based on Log Kow from Lyman and Loreti



of cows fed pesticide-contaminated feed¹⁰⁰. Kenaga seems to be the first⁶⁹ to suggest a BCF - type relation for terrestrial animals. He presented equations to predict an adipose tissue concentration factor, called BF, from Kow, SW, or BCF. Garten and Trabalka⁷⁰ were critical of the experimental data base of Kenaga's work, which included a large amount of unpublished results, and they studied the literature for information concerning bioaccumulation in ruminants, other mammals, or poultry. Their relations for ruminant animals appear in Section 6.4; equations for other species were suggested in their paper. One feature of note was a high correlation between rodent bioaccumulation and of other animals. Thus, a bioaccumulation study in rodents might be useful to predict uptake in beef and milk, despite the markedly different digestive systems of rodents and cows.

Travis and Arms⁷¹ have suggested a biotransfer factor, defined as contaminant concentration in meat or milk per mg/day contaminant intake. For beef, the factor (Bb) is:

$$Bb = 10^{(-7.6 + \text{Log Kow})} \quad (\text{C-12})$$

This is a constrained regression where the exponent of Kow was forced to unity (the unconstrained exponent was 1.033). A Kpat can be approximated based on 25 percent fat content in meat and 8 kg/day food intake (values suggested by Travis and Arms):

$$\text{Kpat} \approx 10^{(-6.1 + \text{Log Kow})} \quad (\text{C-13})$$

This equation and Garten and Trabalka's relation (equation 40) appear in Figure C-3. The divergence between them is somewhat surprising in that Travis and Arms used Kenaga⁶⁹ as the reference for about one-third of their data set compounds and equation 40 is in very close agreement with Kenaga's equation:

$$\text{Kpat} = 10^{(-3.456 + 0.500 \text{ Log Kow})} \quad (\text{C-14})$$

This equation is also shown in Figure C-3.

The biotransfer factor for milk (Bm) was:

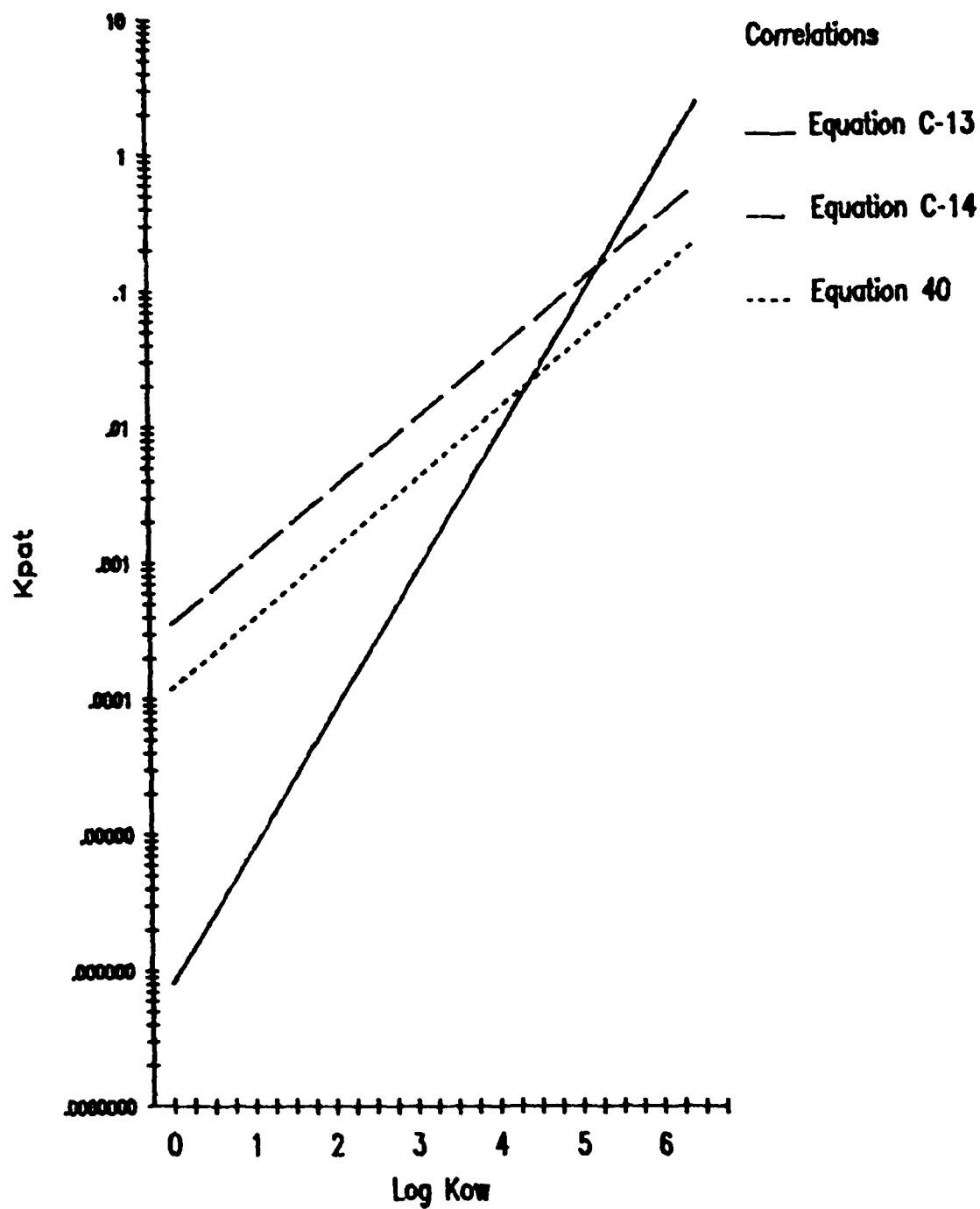
$$Bm = 10^{(-8.1 + \text{Log Kow})}$$

On a fresh weight basis, the biotransfer factor for meat is about 3.2 times that of milk. However, when expressed on a unit fat basis (milk has about an 3.68 percent fat content)⁷¹, the factor for milk is about 2.2 times that of meat. This suggests that use of a milk-based partition coefficient to predict a meat-based coefficient and vice versa should be avoided unless more accurate procedures are not available.

C.6 Kwp AND Kwv

Appendix E of the previous report⁷ detailed the complexities of

Figure C-3. Kpat Correlations Based on Log Kow



pollution transfer to plants. The flowering plants (which include most vegetables and pasture material) do not "eat" in the sense that animals eat. Rather, food or food precursors are drawn into the plants via roots. Additionally, plants "breathe" in the sense that gases (CO_2 , O_2) are transferred into and out of leaf stomata, and volatile pollutants can enter the leaves by this route. Dry surface soil can be transported in air as dust and then deposited onto leaf surfaces, or can be splashed onto leaf surfaces by rain. Pollutant in this soil can deposit on the leaves.

The metabolism of xenobiotics by plants is poorly understood, and probably varies between species. Moreover, the rate and reactions of metabolism change as the plants sprout, grow, flower, and are harvested (for some vegetables, harvest occurs before flowering). In some cases, the harvested plant has stopped growing and has been dried (such as hay). Some pollutants tend to concentrate in specific parts of the plant, and this partitioning is yet to be correlated to compound structure. In some studies, root uptake is studied, the results of which are of dubious applicability to the instant exposure situation.

Briggs et al.¹⁰³ have done considerable work with the uptake of O-methylcarbamoyloximes and substituted phenylureas in barley plants. From these studies, equation 54 has been developed. The first term in the equation,

$$0.784 \times 10^{([\text{Log Kow} - 1.78]^2 / 2.44)}$$

is based on studies of the relative concentration of a test compound in the root and the xylem stream in the barley stem. Apparently, polar compounds ($\text{Log Kow} < 1.78$) are not highly sorbed on lipids in the root, and do not transfer well to the xylem. Less polar compounds ($\text{Log Kow} > 1.78$), while sorbed on lipids in the roots, are restricted in membrane transfer; this may be more of a molecular weight effect than a Log Kow effect (for a homologous series of compounds, Log Kow and molecular weight correlate). The second term,

$$10^{(0.95 \text{ Log Kow} - 2.05) - 0.82}$$

accounts for the concentration of chemicals in the stem relative to that of the xylem lignin.

It should be cautioned that the studies were limited to 10-day old barley plants grown in hydroponic solution, and the test period for given study was 1 or 2 days. Thus, one might suspect that the equation is probably most representative of grassy-type pastures. The equation may overestimate what occurs with other plant matter. For example, Travis and Arms present a correlation for a vegetative bioconcentration factor B_v , which would be called K_{sp} in PPLV terminology:

$$B_v = 10^{(1.558 - 0.578 \text{ Log Kow})} \quad (\text{C-15})$$

This cannot be compared directly to equation 41, main text. However, an approximate K_{wp} relation can be constructed for a specific f_{oc} content in soil presuming that equation 39 correctly predicts K_{oc} . Then

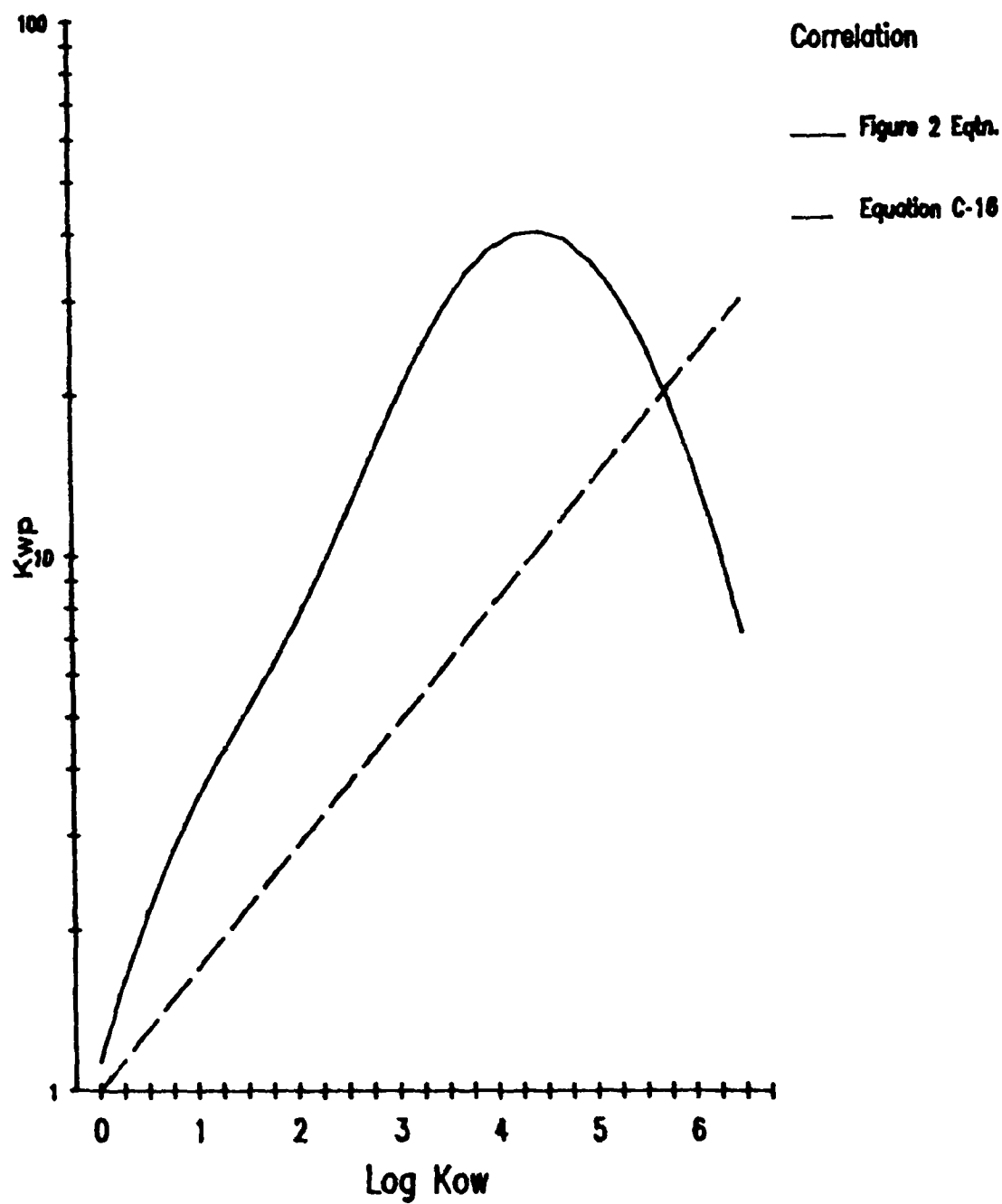
$$K_{wp} \approx B_v \times f_{oc} \times K_{oc} = f_{oc} \times 10^{(2.031 + 0.228 \text{ Log } K_{ow})}$$

For an $f_{oc} = 0.01$, this relation becomes approximately

$$K_{wp} \approx 10^{0.228 \text{ Log } K_{ow}} \quad (C-16)$$

Equation C-16 and equation 41 (the 0.784 has been replaced by 5, to convert to a dry-weight basis) are both shown in Figure C-4. In equation C-16, a maximum does not occur, and for most of the $\text{Log } K_{ow}$ range, equation 41 provides the higher K_{wp} . It is heartening to see predictions which are within two orders of magnitude, given the diverse nature of the background data for the studies.

Figure C-4. Comparison of K_{wp} from Figure 2 and Equation C-16 ($f_{oc} = 0.01$)



GLOSSARY

Symbols and acronyms which appear in more than one subsection of the main text or in a subsection and an Appendix are defined here. Footnotes relevant to them are presented immediately below.

* See "References" for full citation.

** Plant matter (i.e.: pasture) weight is assumed to be on an air-dried basis. Vegetable weight is assumed to be on a totally-dry basis.

AAAP	Alabama Army Ammunition Plant
ARL	Acceptable risk level (additional risk of developing cancer within a lifetime due to the presence of a contaminant in the environment.
AW	Animal weight, kg.
BW	Human body weight, kg. When not subscripted, for an adult; if subscripted, the subscript denotes a cited age.
BCF	Bioconcentration factor between pollutant concentration in fish (mg/kg) and in water (mg/L).
C	Concentration of pollutant in bulk soil (all phases). C _{ci} refers to the pollutant level in unspecified media for a multi-pollutant situation.
Ca	Concentration of pollutant in air, mg/m ³ . C _{ae} refers to soil-pore air in equilibrium with other components of the soil system. C _{av} refers to a time-average concentration in air due to vaporization of pollutant from a site.
Cp	Concentration in plant, mg/kg. Subscript indicates that C _p corresponds to the prevailing SPLV for the subscripted pathway.
Cs	Concentration of pollutant in soil, mg/kg. C _{se} refers to soil concentration in equilibrium with other components of the soil system.
Cw	Concentration of pollutant in water, mg/L. C _{we} refers to soil-pore water in equilibrium with other components of the soil system.
Da	Molecular diffusivity of pollutant in air, m ² /day.
Das	Molecular diffusivity of pollutant in soil-pore air, m ² /day.
D _T	Reference dose for computing SPLVs, mg/kg-day.
DTLV	Documentation of the Threshold Limit Values and Biological Exposure Indices*.
EPA	U.S. Environmental Protection Agency
Favn	Time averaged flux generated (mg/m ² -day) from soil with an initial 1 mg/kg contamination level.

PCR	Food consumption ratio, mg food/kg body weight-day.
fd	Fat content in milk.
FL	Feeding dose level, mg/kg-day.
fm	Fat content in meat.
foc	Fraction of organic carbon in soil.
f(S1)	Fraction of soil area involved in contamination of drinking water source.
f(S2)	Fraction of soil area involved in contamination of water body with a fish population of concern.
HI	Hazard Index
I	Intake of pollutant, mg/day. Numerical subscripts indicate specific pathways. Im indicates intake by steer. I _{max} is the maximum acceptable intake for humans.
IARC	International Agency for Research on Cancer.
IFi	Generic intake factor term in a SPLV equation.
Kd	Partition coefficient between pollutant in soil (mg/kg) and pollutant in water (mg/L) at equilibrium.
Kd'	Kd adjusted for pollutant contained in soil-pore water, $Kd + \theta / \rho$. Subscript "1" indicates a surface-soil, subscript "2" indicates a contaminant-laden soil involved in contamination of a body of water.
Kh	Henry's Law constant, usually VP / SW_m in dimensionless units.
Ki	Generic partition coefficient term in a SPLV equation.
Koc	Partition coefficient between pollutant in soil organic carbon (mg/kg) and pollutant in water (mg/L) at equilibrium.
Kow	Octanol-water partition coefficient.
Kpat	Partition coefficient: mg/kg pollutant in adipose tissue of animal per mg/kg pollutant in diet**.
Kpd	Partition coefficient: mg/L pollutant in milk per mg/kg pollutant in diet**.
Kpm	Partition coefficient: mg/kg pollutant in meat per mg/kg pollutant in diet**.
Ksp	Partition coefficient: mg/kg pollutant in plant matter** per mg/kg in soil.
Kwp	Partition coefficient: mg/kg pollutant in plant matter** per mg/L in water.
Kwv	Partition coefficient: mg/kg pollutant in edible portion of vegetable**.
LD _m	Estimated one-time dose required to cause "m" percent mortality in a species population, mg/kg.
LOEL	Lowest applied dose level in an animal feeding test at which an effect is observed, mg/kg-day.
LS	Length dimension for a contaminated site, m.
MH	Height for contaminant mixing into air passing over a contaminated site, m.
NCI	National Cancer Institute.

NOEL Highest applied dose level in an animal feeding test at which no effect is observed, mg/kg-day.

NTP National Toxicology Plan.

PBB Polybrominated biphenyls.

PPLV Preliminary Pollutant Limit Value, mg/kg in soil; mg/L in water. PPLV_{ci} refers to a specific pollutant in a multi-pollutant system (one scenario). PPLV_j refers to a specific scenario (one pollutant).

q* Carcinogenic potency, kg-day/mg.

Rb Air volume respired during exposure period, m³/day.

ri Proportionality constant between D_T and an SPLV.

RMA Rocky Mountain Arsenal.

RTECS Registry of Toxic Effects of Chemical Substances*.

Si Generic dilution factor term in a SPLV equation.

SOC Soil organic carbon.

SPHEM Superfund Public Health Evaluation Manual*.

SPLV Single pathway limit value; for soil, in mg/kg, for water, in mg/L. SPLV_{ij} used to denote the value for the medium "i" and pathway "j".

SW Solubility limit in water, mg/L; SW_m, limit in moles/L.

T Time, usually in days. T₁ refers to a "lifetime period"; T₀ to an initial time for exposure sometime after the onset of volatilization from a plot.

TAC Time per air change, days.

T_{ij} Matrix element to indicate presence of pathway in a PPLV scenario.

TLV Threshold Limit Value, mg/m³.

Up_d Dairy cow consumption of plant matter, kg/day**.

Up_m Beef steer consumption of plant matter, kg/day**.

USDA United States Department of Agriculture.

Us_d Dairy cow intake of soil during the process of grazing, kg/day.

Us_m Beef steer intake of soil during the process of grazing, kg/day.

Uw_d Dairy cow consumption of water, L/day.

Uw_m Beef steer consumption of water, L/day.

VAR Volume to area ratio of basement, m.

VP Saturation vapor pressure, mm Hg. VP_l, for supercooled liquid; VP_s, for substance normally a solid at reference temperature.

VW Representative windspeed across contaminated site, m/day.

W_d Adult human consumption of milk, L/day.

W_f Adult human consumption of fish, kg/day.

W_m Adult human consumption of beef, kg/day.

W_s Human intake of soil, subscripted a for adult, c for child, or i intake at a specific age, kg/day.

WS6	Lifetime-averaged human intake of soil under ordinary conditions, kg/day.
WSa7	Worker's average intake of soil at a "dusty" work site, kg/day.
Wv	Adult human consumption of vegetables, kg/day.
Ww	Adult human consumption of water, L/day.
ϵ	Fractional volume of soil filled with air.
θ	Fractional volume of soil filled with water.
ρ	Density of bulk soil, kg/L.
$\Phi(T)$	Instantaneous diffusional vapor flux ($\text{mg}/\text{m}^2\text{-day}$) from soil with an initial 1 mg/kg contamination level.

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