TECHNICAL REPORT 9104

THE POLLUTION HAZARD ASSESSMENT SYSTEM

VERSION 20: DOCUMENTATION AND USERS MANUAL

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This report describes an upgraded revision of software described in Technical Report 9003 (The Pollution Hazard Assessment System: Documentation and Users Manual) which was issued in December 1989. The upgraded software, referred to as PHAS20, is programmed in BASIC code. The system is sufficiently compact to be handled on personal computer configurations, and can be supported with a computer with 640K memory, a monochrome monitor, and a line printer.

PHAS20 is designed for general use in risk assessments, such as the "baseline assessment" detailed in the most recent Risk Assessment Guidance for Superfund (EPA/540/1-89/002). PHAS20 performs the risk assessment on the basis of a "unit concentration" algorithm and provides outputs from which hazard indices can be developed. The algorithm is compatible

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with those described in the Guidance, but provides more generalized results so as to be more universal in application. PHAS20 lets the user incorporate information about potential effects to indigenous biota in the environment so that the assessment encompasses both human and biota implications.

PHAS20 guides the user through the system with instructional menus displays provided for specific tasks of data and information processing, modification, and storage. The user can prepare information or data for immediate analysis or store information in off-line files for recall. These files can be rapidly downloaded for system use. Three set of user files are employed: files that store information about scenario exposure pathways; files that store non-chemical data (i.e.: human intake rates, site-specific parameters, time scales, and for meat or dairy intake, livestock characteristics); and files that store chemical-related data (i.e.: physicochemical properties, transfer or partition coefficients, Public Health toxicity information, and environmental biota limits). The exposure pathways presented covers many common water, fish, vegetable, meat or dairy intake situations, as well as (for soil) direct exposure intakes and diffused vapor dispersed in air situations. PHAS20 contains a chemical-related data estimation subroutine package. This package can be accessed from data processing routines directly for the purpose of developing online data for analyses or storage. The package can be also accessed in a "desk-calculator" mode.

The main text provides the user with a discussion of PHAS20 health-effects related concepts and operational instructions. Appendix A presents a glossary of terms and data identifications. Appendix B contains the source code with commentary, but is not included in the DTIC-distributed document; for availability details, refer to the Preface. Appendix C contains the pathway equations used in the assessment along with assumptions involved in their use.

ERRATA

This section will carry any changes to text or software since the technical report was sent to press. Minor typographic errors have been corrected in the text.

1. An .LDS file can be downloaded in CRDES20 as indicated in Sections 3.3 and 10.2. Although the data from a downloaded file in CRDES20 will be online, the associated documentation will not. If the user plans to change data or documentation in a .LDS file, that file should be downloaded in NOCHFL20.

2. Figure 3. The files RUNOFF.SCN and KDINFO.SCN listed in this Figure have been crossed out. They will not appear in the issued PHAS20 software. After PHAS20 operations, the filename CHEMDOC may be added to the disk 1 storage device directory. This is a temporary holding file.

3. Figure 6 (and others). The texts of many information files were edited after the report went to press, and the PHAS?0 software issued may provide a different version from what is presented in the text.

4. Figure 10. The routine performed for entry '2' will read "Download a .DAT file".

5. Page 65. The displays discussed in Section 10.2 do not appear in Figures 23, 24, 26, 28-31. The figures were prepared before the software was modified.

PREFACE

This report documents computer software developed under Work Unit 686 (Hazard Assessment Method Computerization) in the Environmental Quality Research Branch of the Health Effects Research Division.

The author acknowledges the support of Jesse J. Barkley, Jr., Branch Chief, and the programming suggestions of Mr. Jeffry D. Leach. The author also acknowledges the penetrating technical reviews of Mr. James C. Eaton and Dr. Winifred G. Palmer.

The Defense Technical Information Center does not supply software. The author will supply the software to persons who provide either two unmarked two-sided 5-1/4 inch floppy disks or one unmarked 3-1/2 inch diskette and a suitable mailer. The floppy disks may be either double-density or high-density. Send disks to

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Copies of the disk operating system and the GW-BASIC interpreter cannot be supplied.

Due to the size of Appendix B and the anticipated limited-interest audience, this Appendix is not included in reports issued through the Defense Technical Information System. Interested persons can request this appendix directly from the author.

PHAS20 will operate on computer equipment with two floppy disk drives. The installation and startup procedures for such equipment is not discussed in this report, since most systems in use are more sophisticated. Contact the author for startup procedures.

CONTENTS

Figures

* Appendix B is not provided in DTIC-Supplied Documents, see Preface for availability.

Tables

1.0 INTRODUCTION

The Pollution Hazard Assessment System (PHAS) is a suite of programs used to perform exposure assessments for pollutants in soil or water at known or suspected hazardous waste sites. PHAS can assist in the planning, data gathering and exposure assessment exercises of remedial investigations. It includes chemical-related data estimation subroutines (CRDES) to provide approximations when experimental values are not available. The present version, PHAS20, is designed for use on the IBM Personal Computer, its family of successors, and compatible computers. It is an extensive update of PHAS version 1.1, which was developed by Small[1].

This document describes PHAS20. The general exposure assessment problem is discussed in Section 2.0. This discussion is presented to promote an understanding of the system's response to the problem, and its relationship to U.S. Environmental Protection Agency (EPA) risk assessment guidance[2]. The system structure is reviewed in Section 3.0. Operations are presented at two levels, one level for users, the other for programmers. Sections 4.0 through 10.0 present instructions for use of PHAS20 programs. These sections comprise the "user's manual" for PHAS20 and cover the "how to" aspects of PHAS20. After Appendix A, which provides a glossary of terms, Appendix B presents the program code and commentary on program execution. This Appendix is the "programmer's manual" for PHAS20 (see Preface). Appendix C provides a discussion of the exposure pathways used in PHAS20, including assumptions and restrictions.

2.0 PHAS20 EXPOSURE ASSESSMENT CONCEPTS

2.1 Background

Since 1980, considerable legislation and regulations have been devised to manage the process of remediation of hazardous waste sites. A critical point in the process is a remedial investigation. This investigation seeks to define the existing contamination situation at a site and to assess the hazard that the site poses, or could pose in the future to public health and the environment. From this assessment, decisions can be made, at least from the public health/environmental viewpoint, as to the need for remedial actions and the extent to which they are required.

The US Army Biomedical Research and Development Laboratory became involved in the assessment issue in the mid-1970s, when it provided health-effects related information about contaminants in soil and groundwater at Rocky Mountain Arsenal, CO.[3] A complimentary approach was developed to determine safe levels of pollutants in soil or water from a public health viewpoint if the arsenal were to be fully demilitarized. This approach, with improvements, became known as the Preliminary Pollutant Limit Value (PPLV) approach[4], and was used to analyze several military sites[5]. The approach computes a soil or water contamination limit (the PPLV) corresponding to a defined intake, which if attained, would not pose a hazard to an exposed population. This is an answer to the "How Clean is Clean?" question. The PPLV provides a concentration-based guidepost for decision making. The approach has been used for such applications as determining analytical sensitivity limits and setting residual concentration goals as criteria for completing remedial treatment.

2.2 Specific Steps in the Exposure Assessment Process

PHAS2O conceptually follows the PPLV approach. For this discussion, a "site" is a distinct area of land with soil contamination. The approach involves these steps:

o Determine pollutants of concern.

o Define land-use scenarios, and for each scenario, specify component exposure pathways.

o Develop an equation (or equations) for each pathway that relates the human intake of a substance to the substance concentration in soil.

o Collect the data needed to solve such equations.

o For each pollutant and scenario, use the developed equations to compute pathway soil concentration limits corresponding to an "acceptable" intake. From these limits, the PPLV is computed.

o Interpret the results, and

o Determine if non-public health considerations, such as aquatic toxicity or phytotoxic effects, might be more restrictive than public health considerations.

The first two steps above address the questions "What are the contaminants and how are or will people be reasonably expected to be exposed to them?" The contaminants are often tentatively identified from a records study of site operations. For example, at an old explosives production plant, the raw materials, product explosives intermediates, and by-products would be possible contaminants. This study may be augmented by preliminary sampling to identify other contaminants. One could expect that, if production-related substances are peculiar to the site, the substances are contaminants. Sometimes, contaminants have to be distinguished from naturally-occurring or antropogenic substances in terms of concentration or distribution. Chapter 4 of the EPA Guidance[2] discusses this distinction.

In the second step, land-use scenarios are defined in terms of specific pathways which trace exposure from site pollutants to human receptors. A pathway may include more than one specific route by which people can be exposed to a soil pollutant. For example, assume that a community near a hazardous waste site uses groundwater as a domestic water source. Pollutants from the site can percolate to this groundwater. Assume further that the community has a small recreational lake for water activities, and the lake is also used for fishing. Pollutant in soil from the site may be carried in run-off to this lake. Three exposure pathways can be identified: domestic water exposure, recreational water exposure, and fish intake. However, the first two pathways can each include three exposure routes -- ingestion, dermal absorption, and inhalation (of pollutant vapors released from water). Thus, the scenario (which might be titled "resident exposure near a site") consists of three exposure pathways and seven routes. The EPA Guidance[2] further discusses pathways and routes in Chapter 6.

The scenarios may be current activities, or activities projected to occur in the future during or after remedial actions. Scenarios may be defined for different age groups, such as children and adults. They may be specified for specific time frames, such as the expected residence time of adults in the vicinity of a site.

For each proposed route, an equation is needed to describe the relation between human intake and the pollutant level in soil. Section 6.6 of the EPA Guidance[2] presents equations for the most recognizable routes. The presented equations are in the general form:

Dose =	Consumption or ingestion rate of item to which humans are exposed	x	Model exchange and transfer from soil to the exposure item	x	Time adjustment factors	x	Pollutant concentration in soil

(1)

In broad terms, two sets of data are required for assessments: non-chemical data, such as daily intake rates by human receptors and site soil and water characteristics, and chemical-related data, such as public health limit doses*, physico-chemical properties, and partition coefficients between soil, water, and air in the environment and foodstuffs consumed by humans. For many substances, the partition coefficients have not been measured, and must be estimated. Moreover, models are frequently employed to estimate the concentration of pollutant in one medium based on that in another, such as a groundwater dispersion model. Some of these models include both non-chemical site data (in the groundwater dispersion model, dispersion and porosity data describing the aquifer), and chemical-related data (in the groundwater dispersion model, a retardation factor). The results of a model can be fashioned as a "super" partition coefficient, in terms of a ratio of media concentrations.

The interpretation of results depends on the specific problem. For exposure assessments discussed by the EPA[2], the sum of doses from each route's intake equation 1 is divided by a public health limit dose to define a pollutant's hazard index. The index is summed for all pollutants with similar health effects; see Chapters 7 and 8 of the EPA Guidance[2]. If this index is one or less, scenario exposure to the considered pollutants is unlikely to pose a public health concern. In terms of the site situation and the public health standpoint, the site probably is "clean" and needs no remediation.

The conclusion is subject to two contingencies. There is no guarantee that a "clean" site would be safe for indigenous species of the ecosystem. They must be considered in a complete analysis. If the site, left untreated, can be predicted to cause unacceptable adverse effects to other biota, or aesthetic problems, remediation may be needed regardless of the public health concern. A second contingency is that the physico-chemical properties of a substance, particularly water solubility, may limit its transfer to humans. If this is indicated, a hazard index above one must be critically re-examined, since the implied proportionality between dose and concentration in equation 1 may be invalid.

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* The specific dose would be associated with an adverse effect to be avoided (a toxic response, an increased risk of carcinogenicity, teratogenicity effects, etc.). An example of such a dose would be the applicable EPA Guidance RfD.

2.3 Comparison of PHAS20 to EPA Guidance

EPA Guidance has been developed for the specific application of "developing health risk information at Superfund sites."[2] PHAS20 is more generalized in its applications. The two "methods" must not be thought of as exclusive alternatives; PHAS20 is compatible with EPA Guidance.

In the exposure assessment equations presented in EPA Guidance[2], the term "intake" is used in the context of what is commonly called dose (see page 8-2), and is here called DINTAKE. PHAS20 considers "intake" in terms of mass/day. The conversion is: dose x body weight = mass/day intake. PHAS20 uses a "unit concentration" intake algorithm; in the case of soil contamination, the intake equations are solved in terms of 1 mg pollutant/kg soil. Once the intake is computed, results can be "scaled" for exposure assessment needs.

Exhibit 6-14 in EPA Guidance[2] illustrates the comparison. The pathway involved is residential exposure to ambient soil, and the specific route is ingestion of chemical in soil. The following equation is presented:

$$DINTAKE = CS \times IR \times CF \times FI \times EF \times ED / (BW \times AT) \quad (2)$$

DINTAKE = daily ingestion of chemical per unit body weight (mg/kg-day)
CS = chemical concentration in soil (mg/kg)
IR = Ingestion rate (mg soil/day)
CF = Conversion factor (10^{-6} kg/mg)
FI = Fraction of soil ingested from contaminated soil (unitless)
EF = Exposure frequency (days/years)
ED = Exposure duration (years)
BW = Body weight (kg)
AT = Averaging time (time over which exposure is averaged-days)

The product DINTAKE x BW is an intake in mg/day; dividing this intake by CS provides a daily intake for 1 mg/kg chemical in soil. The term IR x CF x FI can be combined into one term, the kg/day of contaminated soil ingested.* The term EF x ED / AT is a time adjustment factor (see equation 1); it converts a daily soil ingestion situation into the specific intake situation hypothesized for the scenario. Equation 2 can be regrouped:

$$(DINTAKE \times BW / CS) = (IR \times CF \times FI) \times (EF \times ED / AT) \quad (3)$$

The PHAS20 version of equation 3 is

$$TAKE(27) = SIR \times S(RS) \quad (4)$$

TAKE(27) = Unit concentration intake for route, mg/day per mg/kg in soil
SIR = oral ingestion of soil from site in kg/day
S(RS) = adjustment factor for scenario conditions, dimensionless

The difference in equations is in location and ordering of variables. This holds true for the other intake equations used in PHAS20.

* A distinction is made between consumption, deliberate intake on the part of an exposed person and ingestion, which is considered unintentional intake.

In PHAS20, a unit concentration intake is computed for each route. These are summed for all routes applicable in a scenario to an overall intake for a specific chemical, here called SUMTAKE. The product RfD x BW is a daily intake limit of that chemical. The daily intake limit divided by SUMTAKE yields a term with concentration units, which is called the PPLV:

$$PPLV = RfD \times BW / SUMTAKE \quad (5)$$

The PPLV is next related to the hazard index, central to exposure assessment analyses. For any route, generically called route "j", by comparing equations 3 and 4, TAKE(j) = DINTAKE x BW / CS. After reordering, a summation process leads to the following relation:

$$Sum(DINTAKE) = CS \times SUMTAKE / BW \quad (6)$$

Both sides can be divided by RfD, and with reordering:

$$\text{Hazard Index} = Sum(DINTAKE) / RfD = CS / PPLV \quad (7)$$

The PPLV is then the concentration for which the hazard index is unity. The hazard index specified in equation 7 is limited to each specific scenario and chemical. Strictly, equation 7 is specific for one mode of human exposure (often oral intake). Its derivation needs to be modified if non-oral intake modes, such as inhalation or dermal absorption are expected. In PHAS20, TAKE(j) values are expressed on an "oral intake basis". The PPLV can still be defined by equation (5), where the RfD is understood to be based on oral intake. This is shown below.

Following the EPA Guidance[2], the hazard index would be computed from a summation of hazard indices by mode of exposure where, for each mode, the hazard index is $Sum(DINTAKE)_{mode}$ / RfD_{mode}. RfD_{mode} is expressed in consistent terms for each mode (see page 8-5 in the Guidance[2]). As an alternate treatment, these indices can be directly combined. For the specific example of oral and inhalation modes, subscripted "$_o$" and "$_i$":

$$\text{Hazard Index} = (RfD_i \times Sum(DINTAKE)_o + RfD_o \times Sum(DINTAKE)_i) / (RfD_o \times RfD_i)$$

The inhalation term can be restated as (RfD_o / RfD_i) x $Sum(DINTAKE)_i$ / RfD_o. From here, it is seen that where the factor RfD_o / RfD_i adjusts non-oral TAKE(j) terms, the relations above still apply.

2.4 PHAS20 Applications

2.4.1. Remedial Investigation Planning and Performance

The term "preliminary" in PPLV also applies to PHAS. It is most useful at the start of a remedial investigation exercise. It can resolve questions of analysis sensitivity; clearly problems can occur in credibility if a proposed analytical method cannot detect the PPLV concentration. Thus, the PPLV can serve a detection goal for selection of analytical methodology.

In the scenario formulation process, PHAS20 provides a "blueprint" to indicate the data inputs for the exposure assessment. The blueprint indicates data that are employed in unit concentration intake equations, as well as data that

may be used for estimation purposes. Thus, while every identified datum may not be necessary for the investigation, the planner is aware of the data requirements for different estimation options. The constraint analyses provide "red flags" that the user may want to address in depth as part of the environmental evaluation in the remedial investigation.

As data is developed in the remedial investigation, files are created with PHAS20 for their storage. Documentation concerning the source of data can be concurrently stored. Generally, the coded pathway equations in PHAS20 are designed to be "safe-sided" (see Appendix C). Thus, the PHAS20 assessment can be used as a check of the results from more refined exposure assessments. PHAS20 may be used directly for a formal remedial investigation exposure assessment with three caveats: first, the exposure pathways are included in the PHAS20 repertoire (see Section 5.0); second, the assumptions involved in PHAS20 exposure pathway equation development apply to the specific site situation; and third, that approval is obtained from the appropriate regulatory authority.

2.4.2 Visualization of Public Health Data

The comparison of PPLV and CS can be extended to more than one chemical substance. Figure 1 shows an example for a site with two contaminants; the concentration of each contaminant can be thought of as a dimension in a mathematical space. The PPLVs (points "A" and "B") are located on the axes. If the contaminants have additive effects (an assumption made in the absence of knowledge to the contrary), a line between the PPLVs defines the unit hazard index, a boundary between what is "clean" and what may not be "clean". Survey results expressed as representative concentrations can be viewed as points in the concentration space. If a point is "inside" the boundary, such as point "C' in Figure 1, the hazard index corresponding to point "C" is less than 1.

2.4.3 Integration of Non-Public Health Effects

PHAS20 provides the user with an elementary analysis of biota data to indicate adverse effects within a hazard index-defined space. Since the criteria for such effects are typically in concentration units (such as mg/L in water causing a certain threshold toxicity to fish within a lifetime), they are more readily contrasted to a PPLV than to a dose or hazard index. Figure 1 shows a simple example of this contrast. The criterion for one effect of "Substance A" appears as the vertical line through points "D" and "E". If there was some adverse effect of "Substance B", it would be shown as a horizontal line. In PHAS20 terminology, if line D-E intersects the triangular area O-A-B, a type 1 constraint situation exists; potentially, the biota criterion may dictate the extent to which remediation is necessary. This situation is shown in Figure 1, where only the area O-B-E-D meets two conditions: (1) hazard index < 1 and (2) the concentration of substance "A" < D.

More complex cases could be advanced, such as $_{96}LC_{50}$ data for fish for both substances. If the substances' toxicities were additive, a line connecting the values on each axis could be constructed. Then, the Type 1 constraint condition occurs when the triangular area O-A-B is intersected by the fish toxicity line.

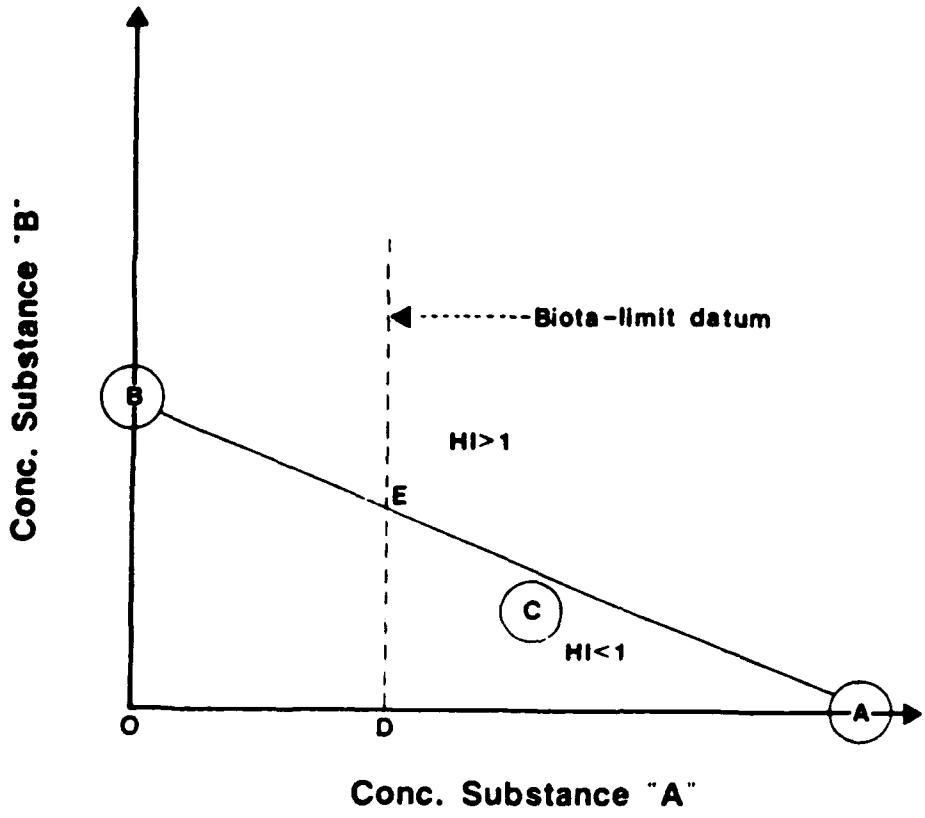

Figure 1. Relation of PPLVs to Hazard Index and Type 1 Constraints

3.0 DESCRIPTION OF PHAS20 STRUCTURE

3.1 Hardware

PHAS20 will operate on a computer system with 640 K capacity, under control of MS-DOS level 3.1 or higher, and with either GW-BASIC or IBM BASICA software. PHAS20 is designed to operate with several different storage device configurations. It can be operated on an elementary system with two 5-1/4 inch floppy disk drives supporting double density disks. A printer with 8.5-inch wide paper is required, and, as a minimum, an 80-column wide monochrome monitor. PHAS20 software is normally supplied on either two 5-1/4 inch floppy disks or on one 3-1/2 inch diskette (see Preface).

3.2 Definitions

To avoid ambiguities, some terms are defined for restrictive use. They are:

BASIC - Either GW-BASIC.EXE or a compatible interpreter of BASIC language.

data - numerical values used in equations. Titles used in PHAS20 to describe data are datanames.

device - either a drive for a floppy disk, mini-disk, or a hard disk.

DOS - MS-DOS used to manage computer operations.

download - As a verb, the act of transferring data or information from an external file for processing in PHAS20 programs. Also used as an adjective (downloaded) to describe the transfer of file contents.

external file - a collection of information or data created and stored for use in PHAS20 programs. Each file has a unique file name.

information - numerical values or text used for purposes other than as inputs to PHAS20 intake equations or estimation methods.

medium - a repository of a pollutant in the environment that is subject to remediation. Thus, the user may process pathways involving exposure via water when soil is the definitive medium.

online - capable of being transferred between PHAS20 programs (programmers refer to data or information with this attribute as COMMON).

3.3 System Structure and External Files

PHAS20 programs are designed to process external files that contain scenario information, non-chemical data, and chemical-related data. These files can be created at one time and recalled for use. Three specific types of files are used and are differentiated by their filename extension. The extensions will be used in the text for description, and are:

.PXX — .PXX files store two numeric information lists. The first keeps track of pathways involved in a given scenario. This list is called the scenario selection table (SST). The second list describes the role of data in route exposure or constraint calculations. It is called the Data Use Status Table (DUST). There are three varieties of this file based on medium: .PWA for water assessments, .PTS for soil assessments, and .PSD for sediment assessments. A text information line can be used to identify and provide commentary about the scenario developed.

.LDS — .LDS files contain 140 numeric entries, the non-chemical data in an exposure assessment analysis. The data include human and livestock consumption factors, site soil parameters, watershed descriptors, non-chemical model parameters for transfers between soil, water, and air, and air dispersion model results. Along with each numeric entry, the user can include information to document the source or derivation of data. A commentary text line is provided to describe the site.

.DAT — .DAT files contain 60 numeric entries, the chemical-related data. The data include public health limit values, input data to CRDES, partition coefficients, soil to air or water transfer model output data as well as physico-chemical data inputs to exposure assessment equations and constraint test equations. Along with each numeric entry, the user can include information to document the source or derivation of data. A commentary text information line is provided to name the pollutant and provide other noteworthy information.

PHAS20 programs can create, download, and store files as well as change file contents. The ERASE or DELETE utilities in DOS, or the KILL command within the GW-BASIC interpreter, can be used to remove files.

Figure 2 is a schematic of PHAS20 structure. Entry to and exit from PHAS20 is via OPEN20. With the exception of CRDES20 and the "satellite" programs, access to other programs in PHAS20 must be through OPEN20. CRDES20 can be accessed from OPEN20 to do estimations in a "desk calculator" mode; in this mode, estimations are not retained online. This access is shown by the solid-line one-way arrow. Section 4.3 and 8.0 detail OPEN20 operations.

In PATWAY20, scenarios for the exposure assessment process are defined. For this purpose, exposure route information is extracted from a satellite PTXXX20 program* based on the route repertoire for a specified medium. Scenario information can be stored in a .PXX file. A .PXX file can be used in the two data-handling programs NOCHFL20 and CHMFIL20 as a "filter", whereby only data required for assessments, or data from which such required data can be estimated, are handled. This is shown by the dashed-line one-way arrow directed from a .PXX file to these programs; information downloaded from a .PXX file in either NOCHFL20 or CHMFIL20 is not retained when these programs are exited. A .PXX file can be either downloaded or created in PATWAY20 for online use. Online information can be passed to OPEN20 as shown by the solid-line single-arrow in Figure 2. PATWAY20 accesses the satellite program PATLLIST, which provides a "blueprint" of the data needs for the selected scenario. The blueprint describes the data significance, and shows how data can be obtained, either from external sources or from CRDES20 routines. Section 5.0 details PATWAY20 operations.

The two data-processing programs are NOCHFL20 and CHMFIL20. Their operations are detailed in Sections 6.0 and 7.0, respectively. NOCHFL20 functions are to download data from .LDS files, alter data online, and store online data in an .LDS file. CHMFIL20 does similar operations with .DAT files. Moreover, CHMFIL20 can access CRDES20 for data estimates via its CRDES, and these estimates are retained online.

COMPUT20 contains the unit concentration assessment equations and computes the PPLV. COMPUT20 accesses the satellite program CONSTR20 to optionally analyze either or both of the two contingencies described in Section 2.2. The COMPUT20 program will not operate unless the contents of a .PXX file, a .LDS file, and a .DAT file are online. Section 9.0 describes these program's operations.

CRDES20 provides background information about chemical-related data and contains estimation subroutines. This program's operations are detailed in Section 10.0. When CRDES20 is accessed from CHMFIL20; data estimated within CRDES20 are retained online. When CRDES20 is accessed from OPEN20; estimates are not retained online when CRDES20 is exited. If chemical-related data are needed in estimation subroutines and CRDES20 is accessed from CHMFIL20, online data are employed. The user supplies chemical-related input data when CRDES20 is accessed from OPEN20. Several subroutines in CRDES20 require data from a .LDS file. CRDES20 can download a .LDS file (see above), and the downloaded file data are online after CRDES20 is exited. This feature is not indicated in Figure 2.

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* PTXXX20 represents the generic name of one of three programs: PTWAT20, which addresses water medium exposure pathways, PTTOPS20, for soil medium exposure pathways, and PTSED20, for sediment medium exposure pathways.

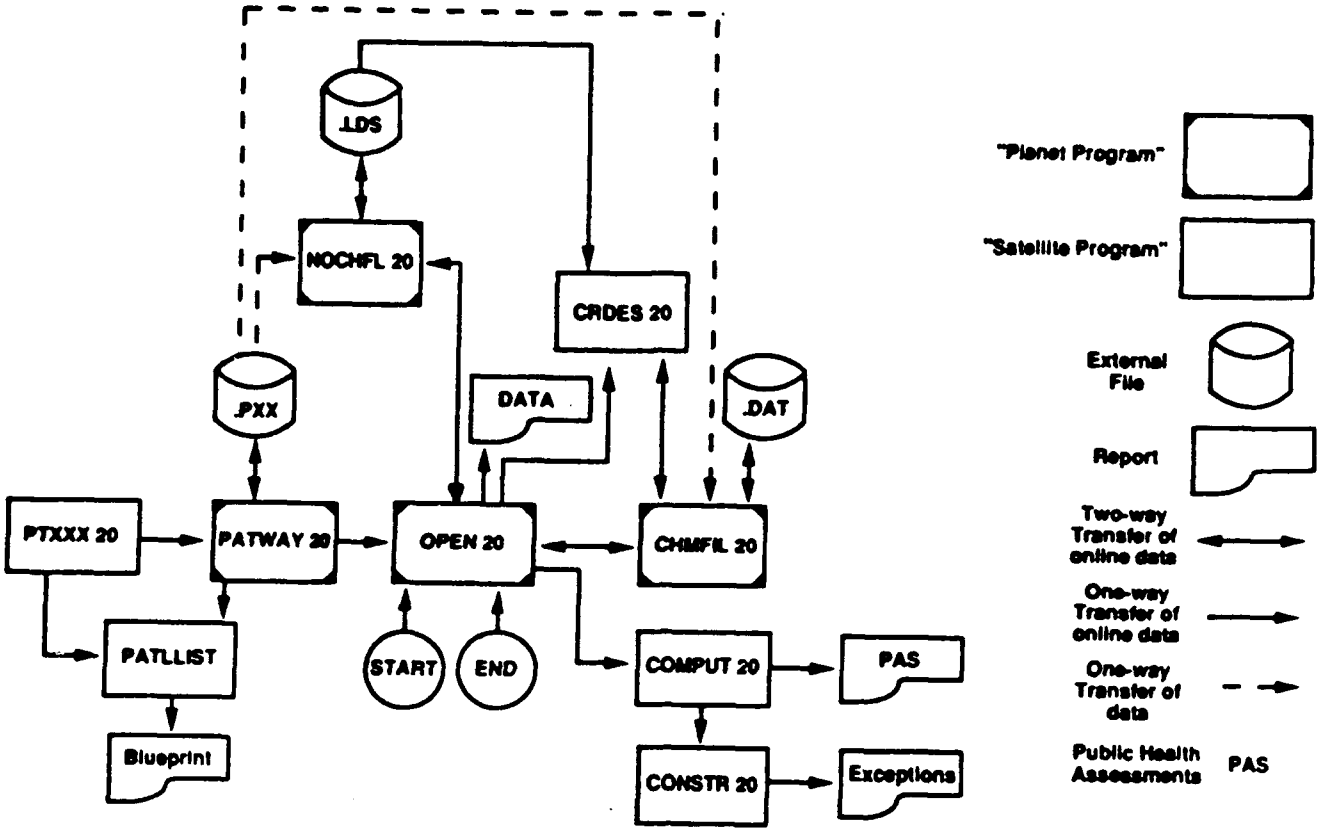

Figure 2. PHAS 20 System Structure and Program-File Relationship

4.0 PHAS20 INSTALLATION AND START UP

4.1 General System Notes

PHAS20 is user-friendly in several respects. It provides online messages describing program subsections, and explains and prompts for user inputs. Operational user inputs are either integer numeric entries, alphanumeric entries, or filenames. After a user input, the return (enter) key is depressed. Many halts are provided to permit the user to review and to optionally print the contents of a screen display ("Shift" - "Print-Screen"). After such halts, the user depresses the return key to continue processing; this keystroke is called a continuation return.

User inputs are monitored to detect common errors. When such an error occurs the user is so informed and can repeat the input process. Common errors which can be detected and resolved include:

* An integer input outside the range of accepted values.
* A non-integer input when an integer is specified.
* An unspecified alphanumeric entry (typographical error).
* A filename input that violates DOS specifications.
* A filename input with a missing or incorrect extension.
* A filename input for a nonexistent file.

If an alphanumeric entry is entered when a numeric entry is expected, or vice versa, the interpreter issues the message "?Redo from start". When this

happens, the disputed input should be checked, the error determined, and the corrected input re-entered (followed by a return).

Specific conventions are followed in the instructions. Program names, file extensions, and specific filenames are shown in capital letters. PHAS20-generated messages or prompts are in compressed pitch font (compressed pitch font). They are in full quotes when used within text narrative or are set apart from the text. User responses to PHAS20 prompts are shown in single quotes; in practice, they are entered without quotation marks, and are followed by pressing the return (enter) key. Alphanumeric responses are shown in lower case; either case can be used. If a term is shown in braces "<term>", the specific contents of the displayed term will be determined by PHAS20. The text term explains or paraphrases the display.

4.2 Installing PHAS20

The supplied PHAS20 program hardware (see Preface) should be copied for day-to-day operations or for installation purposes. The issued hardware can then be stored. Figure 3 shows PHAS20 files supplied on Disks 1 and 2 when software is provided on 5-1/4 inch double density floppy disks. If 5-1/4 inch high-density floppy disks or a 3-1/2 diskette is used, the .NCI files shown in Figure 3 will be placed on Disk 1 instead of Disk 2. In either case, all Disk 1 software shown in Figure 3 and the .NCI files will be in a subdirectory named \PHAS20\DISK1. All other Disk 2 software will be in a subdirectory named \PHAS20\DISK2.

Computer systems are configured to operate with different magnetic storage devices. PHAS20 can be operated on many of these. Before operation, PHAS20 has to be installed so that its programs will "know" where external files will be located. This location is called the "Disk 2 device". Here, installation details are limited to computers with a hard disk (see Preface).

Hard Disk and a Double Density Floppy Disk

This section applies if PHAS20 programs and supporting files are to reside on a hard disk. First, create a subdirectory for these program and files on the hard disk. Copy the contents of Disk 1 to that subdirectory. If software is provided on double-density floppy disks, the .NCI files on Disk 2 are also copied to that subdirectory. After this step, the .NCI files can be removed from Disk 2. GWBASIC.EXE should be on the hard disk, either in the same subdirectory as the PHAS20 programs or as designated in a PATH statement.

Set the subdirectory assignment to the PHAS20 subdirectory. At the DOS prompt, type: 'gwbasic install'. The program INSTALL starts (see Appendix B for details), and this menu is displayed:

```
********** INSTALLATION MENU **********

This program assigns a disk drive or subdirectory for
external data files of the PHAS system. Once assigned, the drive
or subdirectory will be accessed by the system until this program
is again run. Enter an option from 1 to 4....
```

```
Input '1' for B: drive (good for a dual-floppy disk system).
Input '2' for A: drive (good for hard disk/floppy disk system).
     or programs in C: drive/data in A: drive configuration)
Input '3' to put all files on this subdirectory
Input '4' to put .PIX, .LDS, and .DAT files on a different subdirectory.
Enter your selection:
```

Respond with '2'. No further action is required by the user, and the user is returned to DOS. During PHAS operations, Disk 2 is placed in the "A" drive.

Hard Disk

All files can be stored on a hard disk. The contents of Disk 1 are copied to a designated hard disk subdirectory. All PHAS20 programs and files can be placed in one subdirectory, or the execution programs and supporting files can be placed in one subdirectory and external files in another. If all PHAS20 software is to reside in one subdirectory, option '3' is selected when INSTALL is executed. No further action is required by the user, and the user is returned to DOS. After INSTALL is completed, the contents of Disk 2 are copied to that subdirectory. If the external files are to reside on another subdirectory of the hard disk, option '4' is selected in INSTALL execution. The program prompts for the full subdirectory name in which the contents of Disk 2 will reside. For example, if the user wants to use the subdirectory designation of the supplied 3-1/2 inch diskette on a hard disk in the "D" drive, the entry in INSTALL would be ' d:\phas20\disk2\ '. Note that a final backslash is required. After the subdirectory name entry, the user is returned to DOS.

```
D>dir a:/w

 Volume in drive A is PHAS20DISK1
 Directory of  A:\

INSTALL  BAS     PTSED20  BAS     PATWAY20 BAS     CRDES20  BAS     NOCHFL20 BAS
OPEN20   BAS     CHMFIL20 BAS     PTTOPS20 BAS     COMPUT20 BAS     PTWAT20  BAS
CONSTR20 BAS     PATLLIST BAS     ASSIGN   OPE     OVERVIEW OPE     DIAGNOST OPE
NOCHFL   OPE     COMPUTE  OPE     PARAM    OPE     PATHWAY  OPE     CHEMFILE OPE
CHEMPROP OPE     FISH     SCN     DOMWAT   SCN     GWDOMWAT SCN     OPENWAT  SCN
MILK     SCN     LIVESTOK SCN     PATINFO  SCN     PATPMP   SCN     BASEVAP  SCN
SITEVAP  SCN     CONTSOIL SCN     RESSOIL  SCN     TOFFSITE SCN     VEGGIE   SCN
MILTBOIL CMP     VPFACTOR CMP     MILLERM  CMP     STOREIT  CMP     FOCINFO  CMP
HENRY    CMP     PHYTOTOX CMP     KPATINFO CMP     KPDINFO  CMP     KD1INFO  CMP
KOCINFO  CMP     MKSW6    CMP     KSPKSV   CMP     MOLWT    CMP     KWPVINFO CMP
MKSW5    CMP     LOGKOW   CMP     LEBASA   CMP     MKSW1    CMP     ORGLEP   CMP
VPTABLE  CMP     KPMINFO  CMP     PERMINFO CMP     CATLIST  CMP     AQUATOX  CMP
BCFINFO  CMP     CATTOX   CMP     CFDOINFO CMP     CFIOINFO CMP     VAPMENU  CMP
STATDEX  CMP     CONTTALK CMP     DTOCINFO CMP     DTOINFO  CMP     TBOIL    CMP
DWINFO   CMP     TMELT    CMP     VAPRINFO CMP     WATERSOL CMP     MKSW3    CMP
DAINFO   CMP
       76 File(s)     86016 bytes free

D>dir a:/w

 Volume in drive A is PHAS20DISK2
 Directory of  A:\

FILE7    NCI     FILE6    NCI     FILE5    NCI     FILE3    NCI     FILE4    NCI
FILE1    NCI     FILE2    NCI     PROMPT   OPE     DEFAULT  LDS     DEFLPWA  PWA
DEFLPSD  PSD     DEFLPTS  PTS     DEFCHEM  DAT     PTSAMPLE PTS
       14 File(s)    264192 bytes free
```

Figure 3. PHAS20 Files as Supplied on 5-1/4 inch Double-Density Floppy Disks

If PHAS20 is supplied on double-density floppy disks, after completion of INSTALL, the .NCI files on Disk 2 should be copied to the Disk 1 subdirectory, the .NCI files removed from Disk 2, and the remaining contents of Disk 2 copied to the external file subdirectory. With the other supplied hardware, the contents of Disk 2 are simply copied to the external file subdirectory.

The user may want to retain and operate PHAS20 on a copy of the supplied 3-1/2 inch diskette or 5-1/4 inch high-density diskette. In these cases, the INSTALL program can be performed, and option '4' selected. If the supplied subdirectory assignments are used, the entry in INSTALL is '<diskette device address>:\phas20\disk2\'.

4.3 OPEN20

Before starting PHAS20 execution, the user should ensure that the files DEFLPWA.PWA, DEFLPTS.PTS, DEFLPSD.PSD, DEFAULT.LDS, DEFCHEM.DAT, and PROMPT.CMP are on the Disk 2 device. Their absence will trigger error traps, such as discussed Section 4.3.2, and may cause PHAS20 execution to be aborted when attempts are made to store files in PATWAY20 or CHMFIL20.

4.3.1. Operating Procedures

If the computer is to be operated with a hard disk and a floppy disk, ensure that the correct floppy disk is in the Disk 2 device. Ensure that the hard disk assignment is the subdirectory containing Disk 1 files. If the computer is operated with all files on one hard disk, one floppy-disk or one diskette, ensure that the assignment is the subdirectory containing Disk 1 files. At the DOS prompt, enter 'gwbasic open20'. The initial display is the "OPEN20 Main Selection Menu" shown in Figure 4. Otherwise, an error message is displayed, indicating an error condition and the probable remedial action; see Section 4.3.2.

The menu accepts a prompt value between 1 and 10 (except 6 and 8) to start a specific function. Entries '2', '3', '4', '7', and '9' access, respectively, the programs PATWAY20, NOCHFL20, CHMFIL20, COMPUT20, and CRDES20. The '5' entry accesses a series of routines in OPEN20 used for viewing specific online data and information, and modifying data "on the fly"; these routines are discussed in Section 8.0. With the exception of Section 8.4, this section can be omitted in initial readings and then read after confidence is gained with PHAS20 operation.

If entry '1' is selected, the display shown below appears:

```
********** PROGRAM EXPLANATION MENU **********
 ENTER              EXPLANATION
   0     None, exit to Main Function Selection Menu
   1     Overall system description
   2     Scenario and pathway processing (PATWAY20)
   3     Non-chemical data processing (NOCHFL20)
   4     Chemical-related data processing (CHMFIL20)
   5     Hazard Assessment and Constraint Analyses (COMPUT20)
   6     The DIAGNOSTIC UTILITY routines
   7     Chemical-related data estimation methods (CRDES20)
ENTER YOUR SELECTION:
```

```
************** POLLUTANT HAZARD ASSESSMENT SYSTEM (PHAS) *********
                    Version 20, February 1991
******************** OPEN20 MAIN SELECTION MENU *****************

  ENTER            FUNCTION PERFORMED BY ENTRY
  1       Descriptions of PHAS and its component programs.
  2       SCENARIO definition and PATHWAY selections.
  3       NON-CHEMICAL data processing.
  4       CHEMICAL-RELATED data processing.
  5       Diagnostic utility.  Review scenarios, review
             or alter online data, or printout data.
  7       EXPOSURE ASSESSMENT and optional constraint analysis.
  9       Chemical data estimation methods, results not online.
  10      Exit the system to DOS.
  ENTER YOUR SELECTION:
```

Figure 4. The OPEN20 Main Selection Menu

The number is entered for the desired explanation message. At the conclusion of any message, a continuation return is entered. The "Program Explanation Menu" will reappear.

PHAS20 is exited by responding with '10' to the OPEN20 Main Selection Menu prompt. The prompt must be confirmed by responding 'yes' to the query " Are you leaving PHAS? " A 'no' response directs the user to the OPEN20 Main Selection Menu. A 'yes' response directs the user to DOS.

4.3.2 OPEN20 Error Traps and Resolution

OPEN20 has error traps designed to detect situations which otherwise would cause abortion of PHAS20 with a terse interpreter-supplied explanation. The traps diagnose the probable cause of errors related to PHAS20 operation, and suggest corrective action. In all but one trap, PHAS20 must be exited to perform corrective action. The trapped situations are described below:

1. The file PARAM.OPE is not on the Disk 1 device. The user is returned to DOS to find this file and copy it to the device.

2. INSTALL has not been executed. The user is returned to DOS to do the required execution.

3. OPEN20 cannot access the Disk 2 device. There are three likely causes. If the error involves an apparently empty floppy disk drive, the program will pause and allow the user to insert the absent disk. If file PROMPT.OPE cannot be accessed, the user is returned to DOS to copy that file to the Disk 2 device. Finally, if OPEN20 can't find the subdirectory INSTALL has specified for Disk 2 files, the user is returned to DOS. The error is most probably caused by failure to create the subdirectory or incorrect identification of the subdirectory in INSTALL.

5.0 PATWAY20

PATWAY20 is accessed when '2' is entered at the OPEN20 Main Selection Menu prompt. The initial display is shown in Figure 5. The status report indicates the last downloaded file, last stored file, last file operation, and current medium selection. The selection menu presents six functions in PATWAY20, and the option to exit to OPEN20. With the exception of selection '0', after the completion of any function operation, either the entire format in Figure 5 or the PATWAY20 Main Selection Menu is displayed.

5.1 Source Medium Selection

PATWAY20 initially displays the surface water medium. If a different medium is wanted, first select this function. The following message will appear:

```
********** SOURCE MEDIUM SELECTION **********

   In PHAS20, a preliminary pollution limit value (PPLV) is computed for
each specific environmental medium which contains one or more pollutants
and can provide these pollutants through exposure pathways to groups of
people or the ecosystem, and which would be subject to remediation.  PHAS20 has
exposure pathways for each of the environmental media listed below.
   Note that PHAS20 does not model inter-media transfers from one medium
to another.  Input the integer between 1 and 3 to select an environmental medium...
INTEGER      MEDIUM
   1         Surface water or groundwater
   2         Surface or near-surface soil
   3         Sediment (as a contamination source for surface water only).
Enter your selection here :
```

Enter the integer for the desired medium. The PATWAY20 Main Selection Menu will then appear. The change in medium is indicated at the menu's option line:

```
    6       Store SST/DUST in a <.pxx> - extension file
```

5.2 Stored Filenames Review

The selection of '2' at the PATWAY20 Main Selection Menu prompt produces a list of existing files on the Disk 2 device with the current .PXX extension. If no file with that extension is present, this error trap message appears:

```
No <.pxx> files were found on Disk 2 device.  Although you return
to the main menu, advise that you exit PHAS20 and copy the default
<.pxx> from issued disks.
```

At least one of each .PXX file (typically DEFLPTS.PTS, DEFLPSD.PSD, and DEFLPTS.PTS) must on the Disk 2 device or PHAS20 will not be able to store an online .PXX file (see Section 5.6).

5.3 Stored File Downloading

Initially, selection '3' to the "PATWAY20 Main Selection Menu" produces the list of files described above. This list is followed by a query:

```
******* WELCOME TO PATWAY20, THE SCENARIO OPERATIONS MODULE *******
******************** FILE STATUS REPORT **********************
Last downloaded file was...   .pwa
Last stored file was...   .pwa
Last file manipulation was...
Current medium selection is... Surface water pathways
***************** PATWAY20 MAIN SELECTION MENU *****************
 ENTER            FUNCTION PERFORMED BY ENTRY
   1              Select a different environmental medium
   2              Review files with current extension
   3              Download file with current extension
   4              Create a scenario SST and DUST
   5              Produce scenario report on hard copy (need LP!)
   6              Store SST/DUST in a  .pwa-extension file
   0              Exit to OPEN20 Now
   Enter function number: 0
```

Figure 5. PATWAY20 File Status Report and Main Selection Menu

"Enter your pathway input file (without extension): " Unless an error in the entered filename is detected*, the file is downloaded, and this message is displayed:

Scenario information downloaded from file <filename.pxx>
********** PATHWAYS IN FILE <disk or subdirectory:filename.pxx>
Scenario Title: <alphanumeric>
Medium is <medium>
MKsw selection sequence is <blank space or a number>

The last line appears only when the medium selection is "surface or near surface soil" (see below). Execution pauses for a continuation return, after which a short narrative of pathways involved in the downloaded scenario appears. After another continuation return, the routine ends.

PATWAY20 attempts to resolve improper filename inputs.* If the file name specified is not on the Disk 2 device, an explanation message is issued, the current list of files is displayed, and the file name input prompt is again displayed. If the file name entered has illegal characters (for example, periods in a file name), the same procedure will occur. If the Disk 2 device does not contain any of the specific .PXX files, an error message is issued, and the PATWAY20 Main Selection Menu appears. The resolution of this error will depend upon the Disk 2 device. If it is a floppy disk drive, the most probable causes are that the wrong disk is inserted or the drive is empty. If all PHAS20 files are on one device, the most probable causes are that either some Disk 2 files never copied to the specified subdirectory or they were deleted from that subdirectory. The user will probably have to exit PHAS20 to resolve this problem.

* PATWAY20 will return the user to a file input prompt for these errors:
the filename entered is greater than 8 characters in length;
the filename entered is zero characters in length (a blank);
the filename specified is not available on the Disk 2 device; or
the filename entered has illegal characters (such as punctuation marks)

5.4 Scenario Creation

Function '4' is used to create files. When selected, the following lines are displayed:

********** SCENARIO CONSTRUCTION ROUTINE **********
Enter Scenario Title Line:

The user can enter any scenario title information desired up to 255 spaces. Each line on the monitor is 80 spaces long, so the entry can be as long as the rest of the prompt line plus 2-1/2 additional lines. As the user completes a line on the display, the display "wraps-around" to the next line. The cursor back, cursor forward, backspace, insert and delete keys suffice for most editing purposes. The return key terminates input regardless of cursor position.*

After the title line entry, the user is guided through a series of exposure pathway selection displays. Each display explains the pathway and prompts for an entry. The pathway is omitted from consideration by the '0' entry. Based on the pathway options, the pathway can be included (with no options, this is always the '1' entry) or, with multiple exposure route options, one option is selected (the input will range from '1' to as high as '4'). Table 1 summarizes the pathways and routes in order of appearance.

At the conclusion of the scenario construction routine, PATWAY20 assesses if the user has omitted all pathways. The user could go through the exposure pathway selection displays and respond '0' at each prompt. In that case, the message "WARNING! Null scenario(no paths)!" is displayed, and the user is returned to the main selection menu.

Scenario Creation: Surface and Near Surface Soil

For this medium, some inputs differ. With PHAS20, a site can be divided into two subsites allowing the user to process a large site where topsoil properties may differ markedly. Alternately, the user can process a site that includes more than one drainage watershed, where exposure routes could involve different watersheds (homes could be located in one watershed and crop fields in another). Footnote "b" in Table 1 identifies the pathways that are assigned a subsite designation. For these pathways, the selection prompt discussed above is followed by a second prompt:

Which subsite is involved , #1 or #2? Enter '1' or '2':

The domestic water use - surface water supply pathway is automatically assigned to subsite #1. Other selections must agree with this assignment. If this pathway is not included in a scenario, subsites can be assigned in any consistent order. If the beef consumption pathway is included, its subsite designation will be assumed for the dairy consumption pathway. If the dairy consumption pathway is also selected, the subsite prompt is not displayed. If the beef consumption pathway is not selected, but the dairy consumption pathway is, the subsite prompt for the dairy consumption pathway is displayed.

* The size of text entry and the editing specifications also apply to title lines and documentation messages entered in NOCHFL20 and CHMFIL20.

TABLE 1. Exposure Pathways of PHAS20 in Order of Presentation

PATHWAYS	Environmental Medium		
(Routes shown in parentheses)	Water	Topsoil	Sediment
Domestic water use, surface water supply. (consumed water alone or with either or both inhaled vapor intake and dermal absorption)	Yes	Yes[a]	Yes
Water recreation (ingested water alone or with either or both inhaled vapor intake and dermal absorption)	Yes	Yes[b]	Yes
Fish consumption	Yes	Yes[b]	Yes[d]
Vegetable consumption	Yes	Yes[b]	
Beef consumption (water alone or with plant intake included)[c]	Yes	No	
(plant alone or with either or both soil and water)[c]	No	Yes[b]	
Milk consumption (water alone or with plant intake included)[c]	Yes	No	
(plant alone or with either or both soil and water)[c]	No[d]	Yes[b]	
Dust intake in vicinity of on-site residence		Yes	
Dust intake at an on-site work setting		Yes	
Inhaled pollutant in house from vapors diffused from soil		Yes	
Inhaled pollutant at on-site location from vapors diffused from soil		Yes	
Inhaled pollutant at off-site location from vapors diffused from soil		Yes	
Domestic water use, groundwater supply. (consumed water alone or with either or both inhaled vapor intake and dermal absorption)		Yes[a]	

a. Portion of site contributing to pollution is called the #1 subsite
b. Portion of site contributing to pollution to be selected by user, subject to restriction for domestic water.
c. Reference is to exposure routes to the steer or cow.
d. No further exposure pathways for this medium.

5.5 The Scenario Data Needs Report

When function '5' is selected at the "PATWAY20 Main Selection Menu" prompt, this message appears:

> PATHWAY INFORMATION FOR SCENARIO <user input information> IN MEDIUM <medium>
> Make sure your line-printer is operating!
> Hit enter (return) to continue..

After the continuation return, the satellite program PATLLIST provides the printout, which is discussed in detail below. The processing time for PATLLIST execution will be faster for a scenario that has just been created in PATWAY20 than for either a downloaded .PXX file or for a situation where PATWAY20 has been exited and re-entered after scenario creation. The differences in program execution are discussed in Appendix B.

To illustrate PHAS20 operations, the following hypothetical problem is processed. It is also employed in subsequent illustrations of PHAS20 displays and printouts. The problem statement is:

" There is an area of a former ammunition plant where soil is contaminated with 'trinitroanything', a persistent organic compound, at concentrations up to 2 mg/kg. A decision is needed as to whether this concentration is 'safe' for current land use; if not, remediation may be necessary. The area consists of farm residences and grazing areas for cattle, raised primarily for beef. The portion of the area used for cattle grazing drains to a creek, from which water is diverted to feed the animals. There is concern about vapor exposure due to diffusion of trinitroanything from soil to the living area in homes, and about exposure to dust in and about homes. The residents raise some of their vegetables in gardens near their homes."

At the PATWAY20 Main Selection Menu prompt, '1' is entered to access the pollutant source medium change routine. In this routine (Section 5.1), selection '2' specifies the "surface and near surface soil" medium. The scenario creation routine (Section 5.4) is entered by responding with '4' to the next display of the PATWAY20 Main Selection Menu. The following pathways (see Table 1 for order of appearance) are selected :

* Vegetable consumption. Gardens are designated to be within the #1 subsite.

* Beef consumption. There are 3 options, and the option to include all routes is chosen. The specific area for grazing is assumed to be in the #2 subsite.

* Dust intake in the vicinity of on-site residence

* Inhaled vapors in house from vapors diffused from soil

Portions of the printed "Pathway Selection And Data Needs Summary" report are in Figure 6. After the scenario title and medium are listed, "global data" are identified. These data are used to determine the limiting intake from which the PPLV and hazard index are computed (equation 5 in Section 2.3). After this listing, each exposure pathway is identified. After each pathway identification, datanames are listed in three groups. The first group appears

after the "DATA USED IN ROUTE INTAKE EQUATIONS ARE.." title line. The user needs these data to solve an intake equation. The next group appears after the "DATA USED IN CONSTRAINT EQUATIONS RELATED TO THE ROUTE ARE.." title line. The user will need these data to solve a type 1 constraint related to the route (in the case of beef consumption, toxicity to animals and their foodstuffs would be involved). The same datanames may be cited in both these groups.

The last group appears after the "DATA WHICH CAN BE USED TO ESTIMATE EQTN. DATA ARE..." title line. These data may be needed in CRDES20 routines to provide estimates for one or more of the route intake equation data. After each exposure pathway is processed, the following message appears on the monitor:

End listing for pathway <description message for pathway>

Each dataname line is preceded by a number. The number is an index assigned in PHAS20. This index is used in the OPEN20 diagnostic utility to manually change data (see Section 8.5). Table 2 shows the index and datanames used in PHAS20. At the conclusion of pathway processing, an information message is printed for all identified datanames. The messages follow the sequence of the numerical index. The index from 1-140 is for non-chemical data. Each message printed indicates the significance of data, its value in DEFAULT.LDS, the basis for this value, and information on how it can be evaluated. The index from 141-200 is for chemical-related data. For these, each message printed out indicates the significance of the data, and what, if any, estimation methods are available in CRDES20. Otherwise, information is presented on how data can be obtained. At the conclusion of the information messages for non-chemical data, the following message appears on the monitor:

End of information messages for non-chemical data

At the conclusion of the information message for chemical-related data, the message appears on the monitor: End of information messages for chemical-related data

If the "surface and near surface soil" medium is chosen, and any of the pathways involve selection of a subsite, additional lines are printed, and each has the format: "Subsite selection for <short pathway identification> is <1 or 2>"

5.6 Scenario Information Storage

When this function is selected at the PATWAY20 Main Selection Menu prompt, the procedure for selection 2 is first executed to let the user review existing filenames. Next, the user is prompted:

> Enter an allowable name up to 8 characters.
> Please don't use the name - defl<pxx>

In response to this prompt, a filename is entered. As with all MS-DOS filenames, it cannot exceed 8 characters in length (extension excluded). The filenames DEFLPWA.PWA, DEFLPTS.PTS, and DEFLPSD.PSD are "reserved" in PHAS20. PHAS20 will prevent attempts to use these filenames to store information. At the completion of the storage algorithm, the message "SST/DUST stored in file on <disk 2 assigned> device." appears, followed by the updated File Status Report and the PATWAY20 Main Selection Menu display.

```
SCENARIO DATA NEEDS REPORT
For the Sample problem described in Technical Report/User's Manual scenario
in Surface and near-surface soil

************ SPECIAL ABBREVIATIONS ************
dwb  = dry weight basis
nodim = dimensionless
p.c. = partition coefficient

      GLOBAL DATA INVOLVED IN ALL PATHWAYS INTAKES ARE...
1   BWa, adult body weight, kg
21  BWc, child body weight, kg
141 DTo, Long term NOAEL dose estimate, oral route, mg/kg-day
142 DTos, Short term NOAEL dose estimate, oral route, mg/kg-day

PATHWAY 8 consume contaminated vegs. grown at designated subsite (1 or 2)

DATA USED IN INTAKE EQUATIONS ARE...
10  Wva, adult vegetable consumption, kg dwb/day
30  Wvc, child vegetable consumption, kg/day
45  S(Wv), Adjustment factor/vegetable consumption
82  rh1, bulk density, topsoil #1 subsite, kg/L
83  th1, average moisture capacity, topsoil #1 subsite, L/L
166 Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L
170 Kd1 soil/water p.c. for #1 subsite pathways, mg/kg / mg/L
                    **********
DATA USED IN CONSTRAINT EQUATIONS ARE...
82  rh1, bulk density, topsoil #1 subsite, kg/L
83  th1, average moisture capacity, topsoil #1 subsite, L/L
166 Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L
170 Kd1 soil/water p.c. for #1 subsite pathways, mg/kg / mg/L
194 PHLW, Phytoxicity limit in water, mg/L
195 PHLS, Phytoxicity limit in soil, mg/kg
196 focPS, foc for soil used to detemine phytotoxicity limit
                    **********
DATA WHICH CAN BE USED TO ESTIMATE EQTN. DATA ARE...
81  focl, fraction organic carbon, topsoil #1 subsite
146 MW, Molecular weight, g/mol
147 Tm, Normal or extrapolated melting point, deg C
148 LogP, Log (basel0) octanol-water partition coefficient
149 Wsol, Water solubility, mg/L
152 Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)
153 Ksv, Soil/vegetable p.c., mg/kg (dwb) per mg/kg soil
154 Ksp, Soil/plant (forage) p.c., mg/kg (dwb) per mg/kg soil
155 foc for soil used to determine soil/veg p.c.
156 foc for soil used to determine soil/forage p.c.
167 Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L
                    **********

PATHWAY 9 consume beef, livestock grazes on forage grown at designated
subsite(1 or 2).  Allowance is made for livestock ingestion of soil and for
livestock watering on surface supply which gets cont. runoff from sub-site.

DATA USED IN INTAKE EQUATIONS ARE...
11  Wma, adult beef consumption, kg/day
31  Wmc, child beef consumption, kg/day
46  S(Wm), Adjustment factor/beef consumption
63  Uwm, water intake by steer, L/day
64  Upm, plant (forage) intake by steer, kg (dwb)/day
65  Usm, soil intake by steer, kg/day
97  rh2, bulk density, topsoil #2 subsite
98  th2, average moisture capacity, topsoil #2 subsite, L/L
167 Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L

168 Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb)
171 Kd2 soil/water p.c. for #2 subsite pathways, mg/kg / mg/L
182 MKro2, model soil-water p.c., #2 subsite runoff, mg/kg / mg/L
                    **********
```

Figure 6. Portion of Scenario Data Needs Report for Sample Problem. (page 1 of 3 pages)

1 BWa, adult body weight, kg
For BW, the DEFAULT.LDS value is 70 kg (about 154 pounds), a widely-used weight based on the averaged weight of the adult man and woman across an age spectrum from 18 years to 75 years. Based on EPA's Exposure Factor Handbook (EPA 600/8-89-043, 1989) , a more precise value is 71.8 kg (not adjusted for population within age group). This reference may be consulted for more specific sex or age group data.

10 Wva, adult vegetable consumption, kg dwb/day
Wva is the vegetable consumption for adults from produce grown at a contaminated site (or with contaminated water). It is cited on a dry-weight basis. The report: Small, M.J. 1988. The Preliminary Pollutant Limit Value Approach: Manual for Users. USAMBRDL Technical Report 8918, DTIC AD-A206976 describes approaches to developing an estimate as does EPA/600/8-89/043. The value 0.017 kg/day in DEFAULT.LDS represents intake by adults in rural, non-farm areas of vegetables (including potatoes). Estimates for other generic locales are in Table 13 of the Small, 1988 report. The EPA report may be consulted for fruit intake estimates.

11 Wma, adult beef consumption, kg/day
Wma is the adult daily consumption of beef from animals raised at a contaminated site. A value of 0.044 kg/day is in DEFAULT.LDS, from the presentation in EPA 600/8-89/043. This is developed primarily for farm households. Further guidance about obtaining estimates for particular locales is in the EPA report.

13 SIRa, adult oral intake of soil, residential, kg/day
SIRa is the adult daily ingestion of soil at a residence. While most people don't purposely ingest soil, events such as particulate matter being swallowed directly, smoking soiled cigarettes or consumption of food held in dirty hands can occur. A value of 1e-4 kg/day is provided in DEFAULT.LDS, which is in keeping with EPA guidance concerning soil ingestion (Soil Exposure-EPA guide seeks more uniform vaste site analysis. Superfund Report, March 29, 1989,pp 7). This is a highly conjectural value.

.....

118 Qa3, volume air through basement, m^3/day
Qa3 is the volume of air passing through a basement per day. The product MKdb (averaged flux) x area is a mass/day, which multiplied by MXb yields a concentration term for pollutant in respirable basement air. In NOCHFL20, the estimation method for MXb is simply Qa3 = 1 / MXb. In DEFAULT.LDS, Qa3 = 2400 m^3/day, a default value. The actual value will depend on a representative basement volume and the number of air changes per day provided by ventilation.

119 Ab3, basement area contacting soil diffusing vapors,m^2
Ab3 is the area of a basement that is normal to diffusing vapors from subsoil. This area should include at least the floor area of a basement. Depending on whether a basement is sunk below grade and the initial top depth db (#113), Ab3 may also include wall area. The product MKdb x Ab3 yields a mass/day averaged pollutant source that can mix in basement air. In DEFAULT.LDS, Ab3 = 125 m^2, a default value. NOTE: The intake equation does not reduce Ab3 as a function of time (wall effects due to decreased pollutant thickness). This is a conservative simplification. For relatively non-volatile substances, any decrease << Ab3 and can be ignored.

137 MXb, dilution air factor for vapor flux in basement, day/m^3
MXb is a reciprocal volume/day of air that mixes with flux diffusing into a basement. The product (flux x area x MKb) yields a nominal pollutant concentration in inhaled basement air. The method in NOCHFL20 is that MXB = 1/Qa3, and the default value in DEFAULT.LDS is 4.17e-4, or 1/2400. The user can input a value from a more elaborate model expressed in day/m^3.

Figure 6. Portion of Scenario Data Needs Report for Sample Problem. (page 1 of 3 pages)

183 MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m^2-day

MKdb and MKdo are 'pseudo' soil-air p.c. for diffusion of pollutant from a contaminated soil mass to bulk air. They indicate the mg/kg in soil which generates a time-averaged flux of 1 mg/m^2-day. This flux is mult. by an area (the area normal to the flux) to yield a mg/day time averaged source term. The source term is divided by a volume/time term. For basement exposure, the divisor is MTb. For outdoors exposure at a site, the divisior is Mton. For outdoors exposure distant from a site, the divisior is MTof. The division yields a time-averaged air concentration term.

The estimation method uses landfarming equations cited in the Superfund Exposure Assessment Manual (EPA/540/1-88/001), April 1988, pages 20-21. The underlaying diffusion model is discussed is the user's manual, Section 5.3.5. A 'dryout' test determines if pollutant is removed from soil prior to the end of exposure time. If so, the averaged flux computed is the initial pollutant per area/exposure time. NOTE: **1** If you use this method and enter CHMPRP20 from OPEN20, you must manually enter the factors Kd, Da and Kh. **2** If you access this method from the CRDES20 Selection Menu, both the long and short term MKdb or MKdo values are estimated.

194 Phytotoxicity limit in water, mg/L
195 Phytotoxicity limit in soil, mg/kg

This limit indicates the mg/kg of substance in soil or mg/L in water which would be of concern in plant life. If this limit is below that indicated by the PPLV, a Type 1 constraint may exist. The specific effect end-point is not-specified. The user may wish to use a limit indicating reduced yield in a food crop or forage or a more subtle threshold such as a given level of leaf discoloration. Toxic effect levels differ for different plants, so phytotoxic data derived for one species may not apply to others at a specific site. Generally, most information for substances other than well-known weed-control agents or pesticides is in journals.

If a phytotoxic limit in soil is used, a reference soil fraction organic carbon value must be supplied. The constraint analysis algorithm converts a soil limit to a water limit, ie: Water Limit = Soil Limit / Kd , where Kd=foc(reference soil) x Koc. Thus, ensure that foc data is available; its prompt follows the 'phytotoxicity limit in soil' prompt in CHMFIL20; or if you provide data in OPEN20, the foc index is 196. If 'phytotoxicity limit in water' data is used, ensure that the 'in soil' value is set to -1.

196 focPS, foc for soil used to detemine phytotoxicity limit
See above message for use of this parameter for conversion from phytotoxicity on a soil basis to phytotoxicity on a water basis

197 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day

This is the analog of a reference dose for humans. The product of this dose and a representative cattle weight is a daily intake limit. A Type 1 constraint may occur if this limit is exceeded by the intake of pollutant computed for a cow from plant, soil, and water (whichever are involved a exposure pathway) if the PPLV were in effect.

Information about chronic cattle toxicity under controlled conditions is rare except for persistent pesticides. More often, poisoning incidents are reported, and in these incidents, plant or soil conc. data are often not accurate. Thus, resort is made to back extrapolations from either long-term human dose (DTo for non-carcinogenic effect avoidance) or mammalian toxicity data. The following suggestion is made - select the lowest of:

100 x DTo
NOEL(2 year mammalian toxicity test)/10
NOEL(90-day mammalian toxicity test)/100

Note that the extrapolation (safety) factors suggested are less severe than those often applied for humans. The rationales for lover factors are: cattle form a more homogeneous population and subtle low-level effects may be tolerated as long as the animals produce.

******* OPTION SELECTIONS ********
Subsite selection for Vegetable Intake Pathway is 1
Subsite selection for Beef and/or Milk Intake Pathways is 2

Figure 6. Portion of Scenario Data Needs Report for Sample Problem. (page 3 of 3 pages)

Table 2. Datanames and Symbols Used in PHAS20. (page 1 of 4 pages)

Index	Identification of Dataname
1	BWa, adult body weight, kg
2	IWa, adult drinking water intake, L/day
3	EIWa, adult oral water equiv. for inhaled pollutants, L/day
4	DAWa, adult body surface for dermal exposure to water, m^2
5	DETa, adult dermal exposure time to domestic water, hr/day
6	OIWa, swimwater ingested by adult, L/TA day
7	ORWa, adult respiration rate during water activity, m^3/TA day
8	ODTa, adult water activity immersion time, hour/TA day
9	Wfa, adult fish consumption, kg/day
10	Wva, adult vegetable consumption, kg dwb/day
11	Wma, adult beef consumption, kg/day
12	Wda, adult milk consumption, L/day
13	SIRa, adult oral intake of soil, residential, kg/day
14	SARa, adult exposure area to dust on skin, residential, m^2
15	PLa, adult perspiration rate, L/m^2/day
16	RIa, adult respiration rate, residential, m^3
17	CSI, construction area-related dust intake, kg/workday
18	BIRa, adult respiration rate, basement vapors, m^3/day
21	BWc, child body weight, kg
22	IWc, child drinking water intake, L/day
23	EIWc, child water oral water equiv. for inhaled pollutant, L/day
24	DAWc, child body surface for dermal exposure to water, m^2
25	DETc, child dermal exposure time to domestic water, hr/day
26	OIWc, swimwater ingested by child, L/TA day
27	ORWc, child respiration rate for water activity, m^3/TA day
28	ODTc, child water activity immersion time,hr/TA day
29	Wfc, child fish consumption, kg/day
30	Wvc, child vegetable consumption, kg/day
31	Wmc, child beef consumption, kg/day
32	Wdc, child dairy consumption, L/day
33	SIRc, child oral intake of soil, residential, kg/day
34	SARc, child exposure area to dust on skin, residential, m^2
35	PLc, child perspiration rate, L/m^2/day
36	RIc, child respiration rate, residential, m^3
38	BIRc, child respiration rate, basement vapors, m^3/day
41	S(DWa), Adjustment factor/adult domestic water exposure pathways
42	S(DWc), Adjustment factor/child domestic water exposure pathways
43	S(OW), Adjustment factor/water activity pathways
44	S(Wf), Adjustment factor/fish consumption
45	S(Wv), Adjustment factor/vegetable consumption
46	S(Wm), Adjustment factor/beef consumption
47	S(Wd), Adjustment factor/dairy consumption
48	S(RSa), Adjustment factor/adult daily soil residential intake
49	S(RSc), Adjustment factor/child daily soil residential intake
50	S(CSa), Adjustment factor/construction area soil intake

Table 2. Data Names and Symbols Used in PHAS20. (page 2 of 4 pages)

Index	Identification of Dataname
51	S(BIR), Adjustment factor/basement vapors exposure
52	BTa, Time exposure for adult on-site residence occupancy, days
53	BTc, Time exposure for child on-site residence occupancy, days
54	S(EIR), Adjustment factor/external vapor exposure
55	OTa, Time exposure for adult off-site receptors, days
56	OTc, Time exposure for child off-site receptors, days
61	fm, fat content in beef
62	fd, fat content in milk
63	Uwm, water intake by steer, L/day
64	Upm, plant (forage) intake by steer, kg (dwb)/day
65	Usm, soil intake by steer, kg/day
66	Uwd, water intake by dairy cow, L/day
67	Upd, plant (forage) intake by dairy cow, kg (dwb)/day
68	Usd, soil intake by dairy cow, kg/day
69	BWM, representative steer body weight, kg
70	BWD, representative dairy cow body weight, kg
71	foc5, fraction organic carbon content of sediment
72	rh5, bulk density of sediment, kg/L
73	th5, void fraction of sediment, L/L
74	dp5, initial top of pollution layer in sediment below grade, m
75	hp5, bottom depth of pollution layer in sediment below grade, m
76	STa, adult exposure time, sediment-based pollutant, days
77	STc, child exposure time, sediment-based pollutant, days
78	As5, surface area of contaminated sediment in waterway, ha
79	Qu5, annual flow of waterway below polluted sediment locale, m^3/sec
81	foc1, fraction organic carbon, topsoil #1 subsite
82	rh1, bulk density, topsoil #1 subsite, kg/L
83	th1, average moisture capacity, topsoil #1 subsite, L/L
84	Acw1, contaminated area of #1 subsite, ha
85	Aw1, total watershed area at #1 subsite outfall, ha
86	WP1, wilt point, topsoil #1 subsite
87	FC1, field capacity, topsoil #1 subsite
88	K1, erodability factor for #1 subsite
89	LS1, length-slope factor for #1 subsite
90	C1, crop cover factor for #1 subsite
91	P1, erosion control factor for #1 subsite
92	RO1, runoff from #1 subsite, inches/year
93	Qu1, Annual ave. flow above #1 subsite outfall, m^3/sec
94	R1, rain/runoff factor for contaminated site
96	foc2, fraction organic carbon, topsoil #2 subsite
97	rh2, bulk density, topsoil #2 subsite
98	th2, average moisture capacity, topsoil #2 subsite, L/L
99	Acw2, cont. area for watershed #2 site,ha
100	Aw2, total watershed area at #2 subsite outfall, ha

Table 2. Datanames and Symbols Used in PHAS20. (page 3 of 4 pages)

Index	Identification of Dataname
101	WP2, wilt point, topsoil #2 subsite
102	FC2, field capacity, topsoil #2 subsite
103	K2, erodability factor for #2 subsite
104	LS2, length-slope factor for #2 subsite
105	C2, crop cover factor for #2 subsite
106	P2, erosion control factor for #2 subsite
107	RO2, runoff from #2 subsite, inches/year
108	Qu2, Annual ave. flow above #2 subsite outfall, m^3/sec
109	SLA, soil loading rate on exposed skin, kg/m^2/day
110	RSPA, particulate conc. in air, residential, kg/m^3
111	CWTF, weather&time factor for construction site soil pathway
112	foc3, fraction organic carbon, soil contiguous with basement
113	rh3, bulk density, soil contiguous with basement, kg/L
114	th3, soil fraction voids with water, basement model, L/L
115	ep3, soil fraction voids with air, basement model, L/L
116	db, initial top of pollution layer below grade, basement model, m
117	hb, lower depth of pollution layer, basement model, m
118	Qa3, volume air through basement, m^3/day
119	Ab3, basement area contacting soil diffusing vapors,m^2
120	UW3, wind-speed for on-site exposure to diffusing vapors, m/sec
121	foc4, fraction organic carbon, outside diffusion
122	rh4, bulk density, soil for outside diffusion, kg/L
123	th4, soil fraction voids with water, outside diffusion, L/L
124	ep4, soil fraction voids with air, outside diffusion, L/L
125	do, initial top of pollution layer below grade, outside diffusion, m
126	ho, lower depth of pollution layer, outside diffusion, m
127	AO4, area of site with diffusing vapors, ha
128	UW4, wind-speed for off-site exposure to diffusing vapors, m/sec
129	MH, rep. mixing height, on-site, m
130	DW4, distance from site to off-site receptors, m
131	MH4, rep. mixing height for off-site receptor, m
132	TK6, initial thickness of pollutant in soil, m
133	RI6, infiltration of rainwater to aquifer, m/year
134	VGW6, velocity of groundwater flow, m/year
135	TAQ6, thickness of aquifer, m
136	th6, effective porosity in aquifer, L/L
137	MXb, dilution air factor for vapor flux in basement, day/m^3
138	MXon, dilution air factor for vapor flux to outside on-site, day/m^3
139	MXof, dilution air factor for vapor flux to off-site, day/m^3
141	DTo, Long term NOAEL dose estimate, oral route, mg/kg-day
142	DTos, Short term NOAEL dose estimate, oral route, mg/kg-day
143	DTi, NOAEL dose estimate, inhalation basis, mg/kg/day
144	DTd, NOAEL dose estimate, dermal basis, mg/kg/day
146	MW, Molecular weight, g/mol
147	Tm, Normal or extrapolated melting point, deg C
148	LogP, Log (base10) octanol-water partition coefficient
149	Wsol, Water solubility, mg/L
150	Tb, Normal or extrapolated boiling point, deg C

Table 2. Datanames and Symbols Used in PHAS20. (page 4 of 4 pages)

Index	Identification of Dataname
151	VP, Saturated vapor pressure, mm Hg
152	Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)
153	Ksv, Soil/vegetable p.c., mg/kg (dwb) per mg/kg soil
154	Ksp, Soil/plant (forage) p.c., mg/kg (dwb) per mg/kg soil
155	foc for soil used to determine soil/veg p.c.
156	foc for soil used to determine soil/forage p.c.
157	Kpat, Plant(forage) to adipose tissue p.c.,mg/kg per mg/kg dwb
161	Da, Molecular diffusivity in air, m^2/sec
162	Dw, Molecular diffusivity in water, m^2/sec
163	Kh, Henry Law constant, dimensionless [conc./conc.]
164	PC, Dermal permeability constant, cm/hr
165	BCF, Fish bioconcentration factor, mg/kg fish per mg/L
166	Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L
167	Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L
168	Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb)
169	Kpd, Plant (forage) to milk p.c., mg/L milk per mg/kg (dwb)
170	Kd1, soil/water p.c. for #1 subsite pathways, mg/kg / mg/L
171	Kd2, soil/water p.c. for #2 subsite pathways, mg/kg / mg/L
172	Kd3, soil/water p.c. for basement subsoil, mg/kg / mg/L
173	Kd4, soil/water p.c. for outside diffusion, mg/kg / mg/L
174	Kd5, sediment/water p.c., mg/kg / mg/L
181	MKro1, model soil-water p.c., #1 subsite runoff, mg/kg / mg/L
182	MKro2, model soil-water p.c., #2 subsite runoff, mg/kg / mg/L
183	MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m^2-day
184	MKdbc, soil flux p.c., basement model short-term, mg/kg per mg/m^2-day
185	MKdoa, soil flux p.c., outdoors long-term, mg/kg per mg/m^2-day
186	MKdoc, soil flux p.c., outdoors short-term, mg/kg per mg/m^2-day
187	MKdwa, sediment-openwater p.c. long-term, mg/kg per mg/m^2-day
188	MKdwc, sediment-openwater p.c. short-term, mg/kg per mg/m^2-day
189	MKgwa, topsoil-groundwater p.c. long-term, mg/kg per mg/L
190	MKgwc, topsoil-groundwater p.c. short-term, mg/kg per mg/L
191	TOL, Organoleptic limit - taste in water, mg/L
193	AQTL, Aquatic toxicity limit in water, mg/L
194	PHLW, Phytotoxicity limit in water, mg/L
195	PHLS, Phytotoxicity limit in soil, mg/kg
196	focPS, foc for soil used to determine phytotoxicity limit
197	CTAEL, Cattle toxicity adverse effects limit, mg/kg-day

6.0 NOCHFL20

NOCHFL20 handles the creation, modification and storage of non-chemical data files. The datanames for non-chemical data are listed in Table 2, and are indexed from 1 to 140. NOCHFL20 data processing is performed under what is called "DUST control". Not every datum is required for a given scenario, and one DUST function is to remove those definitely not required from the processing steps. Another DUST function is to indicate the role of data in a given analysis. Some non-chemical data enter directly into input equations while other data are used in estimation methods to approximate values of non-chemical or chemical-related data used in such equations. The DUST is obtained from a .PXX file or online scenario information.

The datanames MXb, MXon, and MXof are indexed respectively 137, 138, and 139. They are processed differently from the other non-chemical data in NOCHFL20. They respresent air dispersion model results, and the user can either input a dataname value directly (from an externally-executed model), or use a provided estimation method within NOCHFL20 for their evaluation.

NOCHFL20 is accessed when '3' is entered at the OPEN20 Main Selection Menu prompt. The NOCHFL20 initial display is shown in Figure 7. The status report is updated as NOCHFL20 operations are executed. The NOCHFL20 selection menu presents five functional routines, and the option to exit directly to OPEN20. The user enters the integer for the desired routine.

6.1 .LDS File Retrieval, Data Review and Change Routines

Options '1', '3', or '4' in the NOCHFL20 Selection Menu are similar; the major difference between them is when and from where online data are obtained for modification. All data review and changes performed in NOCHFL20 start with a downloaded .LDS file. When a routine to "create" a file is selected, NOCHFL20 automatically downloads DEFAULT.LDS as a starting point, which is then subject to modification. Otherwise, the user specifies the file to be downloaded. The steps common to these routines are: 1. Obtain the online data from a .LDS file, 2. Obtain a DUST, and 3. Do the data review and change routine.

<u>Obtain the online data from a .LDS file</u>

Option 1: Data are online if an .LDS file has been previously downloaded (either in NOCHFL20 or in CRDES20). NOCHFL20 checks for this condition. If online data are not available, the message: "No valid online info, select another option" appears, and the NOCHFL20 Selection Menu is displayed again.

Option 3: The current listing of .LDS files is displayed. The prompt: "Enter file name:" then appears. The user enters the filename to be downloaded without the extension .LDS. Unless an error is detected*, the specified file is downloaded. As a double-check, the following message appears:

---

* NOCHFL20 will return the user to a file input prompt whenever:
the filename entered is greater than 8 characters in length;
the filename entered is zero characters in length;
the filename specified is not available on the Disk 2 device; or
the filename entered has illegal characters (such as punctuation marks).

```
***** WELCOME TO THE NON-CHEMICAL DATA PROCESSING PROGRAM (NOCHFL20) *****
***************** FILE STATUS REPORT *****************
Last downloaded file was ...
Title of current online file (if any) is:
Last stored file was...
Last file operation was...
********** NOCHFL20 SELECTION MENU **********
 ENTER      ROUTINE PERFORMED
   1        Modify online information under DUST control.
   2        Download a stored .LDS file and return to OPEN20
   3        Modify a stored .LDS file under DUST control.
   4        Create a file for online use or storage
   5        Go to Storage options routine
   0        Exit NOCHFL20; return to OPEN20
  Enter selection: 3
********** CURRENT INVENTORY OF .LDS FILES AT DEVICE...
E:\THEMOD20\DISK31
DEFAULTX.LDS      DEFAULT .LDS      DEFAULXX.LDS
 921600 Bytes free

 Enter file name: defaulxx
 Downloading of file defaulxx.lds completed...
 Enter 'yes' or 'no'.
 Want to continue?: yes
```

Figure 7. Opening Display in NOCHFL20. Routine '3' Operations Shown.

```
Downloading of file <filename> completed
Enter 'yes' or 'no'
Want to continue? :
```

appears. A 'no' response returns the user to the NOCHFL20 Selection Menu. This display sequence is also shown in Figure 7.

Option 4: The file DEFAULT.LDS is downloaded and the above message appears.

Obtain a DUST

After the online data from a .LDS file are obtained, the following menu is displayed:

```
****** DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU ******
You will need a DUST to process data.  Select 1 of 3 options.
Option '1' to use the online scenario DUST
Option '2' to use the DUST from a stored file.
        The program will prompt you for a file name
Option '3' to use default DUST for selected enviornmental medium
Enter the desired option integer
```

A scenario's DUST was developed in PATWAY20, and if stored, resides in a .PXX file. A user may download a .PXX file in PATWAY20 so that its DUST is online, but this operation is not necessary. A DUST may be obtained in one of three ways: from online information, a .PXX file to be selected by the user, or a default file.

Following selection of option '1' to the DUST Loading Process Menu, this message appears:

Your online DUST is for medium... <medium description>
and scenario titled...<alphanumeric supplied by user>
OK to continue? (yes or no) :

If the user responds 'no', the Data Use Status Table (DUST) Loading Process Menu is again displayed. Otherwise, the "data review and change routine" described in the next subsection starts.

If the user selects either option '2' or '3' from the DUST Loading Process Menu, the Source Medium Selection display appears. This display is shown in Section 5.1, and the instruction given there apply to the response. After the user selects a medium, this message is displayed:

YOU HAVE SELECTED MEDIUM <medium description>
OK to continue? (yes or no):

If the user responds 'no', the process is repeated. If option '2' was selected, a listing of files with the extension <.pxx> is displayed next. The user is prompted: "Input name of DUST file:" The user provides the filename without the .PXX extension. See the footnote in Section 5.3 for filename error resolution.

If option '3' was selected, the "data review and change routine" described in the next subsection starts. A "default" .PXX file is downloaded (one of the reserved files mentioned in Section 5.6). This will provide a DUST based on selection of all pathways available for exposure from a medium.

The DUST downloaded in response to either option '2' or '3' at the DUST Loading Process Menu is <u>not</u> retained for use in other programs when NOCHFL20 is exited. Moreover, if a different DUST is online when either of these options is chosen, that DUST will be retained online. The medium selected in response to the Source Medium Selection display is <u>not</u> retained for use in other programs when NOCHFL20 is exited. If a different medium selection is online, it will be retained online.

<u>Data Review and Change Routine</u>

The following instructions are valid for datanames indexed from 1 to 136. See Section 6.4 for special instructions for MXb, MXon, and MXof.

After the header display in Figure 8, the line: "The last file processing action was...<message>" appears. The message will summarize the last file processing done with an .LDS file, either in response to the NOCHFL20 Selection Menu or in CRDES20 (see Section 3.3). The first prompt in this routine is:

The current title line for the downloaded file is <user-supplied title>
Should this line be changed (yes or no)?:

If the response is 'yes', the prompt: "Enter revised title line:" is issued. An informative title of up to 255 spaces (3 lines of screen) can be entered; see Section 5.4. The routine then proceeds sequentially through the online data according to DUST control. A sample portion of the dataname review sequence is shown in Figure 8. The data message includes: 1. the dataname, 2. the current value, 3. user-supplied documentation of the value basis, and 4. the

```
 Input name of BOOT file: pto
****************** DATA REVIEW AND CHANGE ROUTINE ******************
 The last file processing action was... Online data in review/change mode
 The current title line for the downloaded file is  Brand new title line
 Should this line be changed (yes or no)? : yes
 Enter revised title line  This is where you would put information concerning th
e non-chemical data base such as the location and any other items deemed worthy
of interest for storage
 ......
 1   BWa, adult body weight, kg  =  70
 Documentation: This is the revision to the revision
 Main input variable to intake pathway eqtn.
 Select '1' to accept current value and documentation message.
 Select '2' to replace value
 Select '3' to change documentation message
 Select '4' to get info message about variable. Input selection: 2
     Enter revised value. ? 60

 ......
 1   BWa, adult body weight, kg  =  60
 Documentation: This is the revision to the revision
 Main input variable to intake pathway eqtn.
 Select '1' to accept current value and documentation message.
 Select '2' to replace value
 Select '3' to change documentation message
 Select '4' to get info message about variable. Input selection: 1
 ......
 10  Wva, adult vegetable consumption, kg dwb/day  =  .017
 Documentation:  default file, see writeup in filexx.nci file
 Main input variable to intake pathway eqtn.
 Select '1' to accept current value and documentation message.
 Select '2' to replace value
 Select '3' to change documentation message
 Select '4' to get info message about variable. Input selection: 4

   Wva is the vegetable consumption for adults from produce grown at a
 contaminated site (or with contaminated water).  It is cited on a dry-weight
 basis.  The report: Small, M.J. 1988. The Preliminary Pollutant Limit Value
 Approach: Manual for Users. USAMBRDL Technical Report 8918, DTIC AD-A206976
 describes approaches to developing an estimate as does EPA/600/8-89/043.
 The value 0.017 kg/day in DEFAULT.LDS represents intake by adults
 in rural, non-farm areas of vegetables (including potatoes).  Estimates for
 other generic locales are in Table 13 of the Small, 1988 report.  The EPA
 report may be consulted for fruit intake estimates.

 ......
 10  Wva, adult vegetable consumption, kg dwb/day  =  .017
 Documentation:  default file, see writeup in filexx.nci file
 Main input variable to intake pathway eqtn.
 Select '1' to accept current value and documentation message.
 Select '2' to replace value
 Select '3' to change documentation message
 Select '4' to get info message about variable. Input selection: 3
     Enter revised documentation message : This is where you would put the basis
 for a new value of Wva if you replaced the current value.

 ......
 10  Wva, adult vegetable consumption, kg dwb/day  =  .017
 Documentation:
 This is where you would put the basis for a new value of Wva if you replaced th
e current value.
 Main input variable to intake pathway eqtn.
 Select '1' to accept current value and documentation message.
 Select '2' to replace value
 Select '3' to change documentation message
 Select '4' to get info message about variable. Input selection:
```

Figure 8. Sample Display of the NOCHFL20 Data Review and Change Routine

role of the datum in the assessment analysis. The role message has one or more of the following statements:

> Main input variable to intake pathway eqtn.
> Var. may be needed to estimate intake main input variable.
> Variable is used in constraint analysis equation.

The user has four options: accept the current datum value ('1'), replace the value ('2'), replace the current documentation message ('3') or see the information message about the datum ('4'). If the current value is accepted, the next datum indicated by the DUST is reviewed. Until option '1' is selected, values and documentation messages for a datum can be changed. If option '2' (replace value) is chosen, the message: "Enter revised value:" is displayed, and the replacement value is entered. If the user wants to change documentation, the message "Enter revised documentation message:" appears, and the user can enter up to 255 spaces (3 lines of screen) of information; See Section 5.4. If the user chooses option '4', a message of up to ten lines in length will be displayed. This message is also issued in the Scenario Data Needs Report and serves to documents data selections for DEFAULT.LDS. This usually will be different from the "Documentation" entry, which is provided for the user's data. At the conclusion of options '2', '3' or '4', the data message (revised) appears, and the user is prompted for another option.

6.2 The "Load and go" Routine

Selection '2' allows the user to download a specified .LDS file and return to OPEN20. This is useful when an assessment is to be performed with an established non-chemical data base, or when the user prefers to modify data in OPEN20 (see Section 8.5) rather than in NOCHFL20. The names of available files are shown, and filename input (without the .LDS extension) is prompted. After the file is downloaded, the OPEN20 Main Selection Menu will appear next. The file status summary will have the format:
"Your last file operation was...Downloaded 'to go' file."
This summary can be viewed in OPEN20 (Section 8.3), the next time NOCHFL20 is entered, or in COMPUT20 (Section 9.0).

If no .LDS files are present, this error trap message appears:

> No .LDS files were found on Disk 2.
> Although you are returned to the main menu, advise that you exit PHAS
> and copy DEFAULT.LDS to storage from issued disks.

6.3 The Data Storage Routine

This routine, accessed by selection '5', is announced by the display:

```
********** STORAGE DISPOSITION MENU **********
    You have three options available.
    Select '0' if you don't want to store data on Disk 2 device.
    Select '1' if you want to store data in a file with the same filename as
        the downloaded file had. This is recommended for MODIFYING a file.
    Select '2' to store data under a different filename than the downloaded
        file had. This is recommended for storing NEW files.
```

NOTE: Database will be in online storage until a different file with the specified extension (.LDS or .DAT) is subsequently downloaded.
Enter your selection:

If '0' is entered, the File Status Report and the NOCHFL20 Selection Menu displays appear. The last line of the status report will read:
"Your last file operation was...any changes to online data are not stored."
If '1' is entered, the downloaded filename automatically becomes the filename for storage. The online data and title are written to that file. The File Status Report and NOCHFL20 Selection Menu will then appear. The filename on the first two lines of the status report will be the same and the last line will state: "Your last file operation was...Replacing last downloaded file with online mod."
If '2' is entered, the current list of .LDS files on the Disk 2 device are displayed. The user is prompted: "Please enter filename (8 alphanums or less, no punct):"
The user supplies a filename (see footnote in Section 5.3 for filename error resolution). The online data and title are written to that file. In this case, the last line of the File Status Report will read:
"Your last file operation was...File stored with user-given name."

DEFAULT.LDS should not be modified. The user may accidently attempt this by downloading DEFAULT.LDS, changing data, and selecting option '1' at the Storage Disposition Menu prompt. If this happens, the message:
"Can't use default.lds. Try another name." is issued, and the user is prompted for an alternate filename.

6.4 Data Review and Change Routine for MXb, MXon, and MXof

These data are peculiar to the surface or near-surface soil medium pathways. MXb is used in the intake equation for the "inhaled pollutant in house from vapors diffused from soil" pathway. MXon is used in the intake equation for the "inhaled polutant at on-site location from vapors diffused from soil" pathway. MXof is used in the intake equation for the "inhaled pollutant at off-site location from vapors diffused from soil" pathway.

The "MX" variables have units of reciprocal volumes/day. These volumes/day refer to dilution air that mixes with a mass/day flux per mg/kg pollutant in soil to provide a nominal air concentration per mg/kg pollutant in soil. The MXon and MXof are estimated by variants of box or dispersion model equations. The models in PHAS20 are, by necessity of software size, elementary, and the reader should review the assumptions associated with their use in the following subsections. In terms of external dispersion models, MXon and MXof are equal to the ratio χ/Q in the notation employed by Turner[6].

Figure 9 shows a sequence of processing for MXon. When these datanames are accessed, a fifth option is available, indicated by the additional line
"Select '5' to access estimation method routine." before the "Input selection :"
prompt. After responding with '5' to this prompt, the user can then select a method routine for the designated dataname. The subsections below describe the methods in NOCHFL20. At the completion of the routine, the estimation provided by the routine is online, and will appear in the result line:
"<index number, dataname> = <estimate>"

```
.....
138 MXon, dilution air factor for vapor flux to outside on-site, day/m^3 =
.0000001
Documentation:  default file, select '4' for information message.
Main input variable to intake pathway eqtn.
Select '1' to accept current value and documentation message.
Select '2' to replace value
Select '3' to change documentation message
Select '4' to get info message about variable
Select '5' to access estimation method routine. Input selection: 4


   MXon is a reciprocal volume/day of air that mixes with flux diffusing into
outside air on-site. Two methods are provided in NOCHFL20 to estimate MXon
They are 'box models'. In method 1: MXon = 1 / (86400*MH*UW3*23.2 AO4^0.5)
The on-line data data are used. In method 2, MH is estimated from
23.2 AO4^0.5 as a 'pseudo' sigma-y, and assumptions about long-term stability
categories. The default value in DEFAULT.LDS is 3.94e-9 day/m^3, based
on method 1 with DEFAULT.LDS MH, UW3, and AO4 data. Users can
input a value from a more elaborate dispersion model in day/m^3 units.

.....
138 MXon, dilution air factor for vapor flux to outside on-site, day/m^3 =
.0000001
Documentation:  default file, select '4' for information message.
Main input variable to intake pathway eqtn.
Select '1' to accept current value and documentation message.
Select '2' to replace value
Select '3' to change documentation message
Select '4' to get info message about variable
Select '5' to access estimation method routine. Input selection: 5
************ Estimation methods for MXon **********************
Select '1' for 'box model' with file-supplied mixing height
Select '2' for 'box model' with computed mixing height
Enter your selection: 1
127 AO4, area of site with diffusing vapors, ha =  10
120 UW3, wind-speed for on-site exposure to diffusing vapors, m/sec =  2
129 MH, rep. mixing height, on-site, m =  20
.....
138 MXon, dilution air factor for vapor flux to outside on-site, day/m^3 =
3.944012E-09
Documentation:  default file, select '4' for information message.
Main input variable to intake pathway eqtn.
Select '1' to accept current value and documentation message.
Select '2' to replace value
Select '3' to change documentation message
Select '4' to get info message about variable
Select '5' to access estimation method routine. Input selection: 5
************ Estimation methods for MXon **********************
Select '1' for 'box model' with file-supplied mixing height
Select '2' for 'box model' with computed mixing height
Enter your selection:
```

Figure 9. Sample Display and Processing Sequence for MXon in NOCHFL20.

6.4.1 MXb

After the '5' selection is made, the program proceeds automatically to the next "Input selection :" prompt. The estimate for MXb is 1/Qa3. This approach assumes that basement air is rapidly mixed with diffusing vaporized pollutant, and that persons in the basement do not stay in "hot spots" where concentrations can build up.

6.4.2 MXon

MXon has two online estimation methods. After method selection is made, the program proceeds automatically to the next "Input Selection :" prompt.

Method 1 is the following relation:

$$MXon = 1 / (86400 \times MH \times UW3 \times 23.2\ A04^{0.5})$$

The term 86400 converts from seconds (used in UW3) to days. The last term is based on Turner's approximation[6] for the Gaussian horizontal dispersion coefficient (HDC) at the edge of a square uniform source area. If the width of the square is L, the HDC is $(L)^{0.5}/4.3$. The width here is assumed to be the square root of the contaminated area A04, and the 23.2 accounts for the denominator and conversions to meters from $(\text{hectares})^{0.5}$. The MXon estimate is considered conservative in that the dispersion term is in terms of 3 minutes time-averaged exposure, and that the exposed person, when exposed, is always at the edge of the area downwind the prevailing wind direction.

Method 2 uses a similar equation, but internally estimates MH. HDC is assumed to equal $23.2\ A04^{0.5}$. A pseudo-distance in kilometers, Xpd, conceptually the downwind distance from a point source with similar characteristics to the area source, is back-computed from the C stability curve for the downwind distance-HDC.* The relation is:

$$Xpd = (HDC/105)^{1.11}$$

Next, a vertical dispersion coefficient (VDC) is computed from an approximate Xpd - VDC relation for the E stability curve:

$$VDC = 20\ Xpd^{0.7}$$

and VDC replaces MH in the calculation. This method is subject to the assumptions stated above for the first method. Moreover, the E stability conditions to estimate VDC from Xpd is a conservative approach since most outside exposure is expected to occur during the daytime.

---

* Turner[6] uses six stability categories (A through F) as parameters to describe prevailing weather conditons for dispersion calculations. Parametric curves are available for dispersion coefficients as a function of distance downwind from a point source. For the short-term curves and an explanation of conditions, see Section 3.3 in the Superfund Exposure Assessment Manual.[7] HDC is often referred to as σy and VDC as σz.

6.4.3 MXof

MXof has two online estimation methods. After method selection is made, the program proceeds automatically to the next "Input Selection :" prompt.

Method 1 is the following relation:

$$MXof = 1 / (86400 \times MH4 \times UW4 \times [\pi\ DW4/8 + 23.2\ A04^{0.5}])$$

The term 86400 converts from seconds (used in UW4) to days. The term in braces is the sum of two lengths. The first length accounts for uniform wind direction in the area of concern. The second length is the VDC discussed above in the MXon method 1. This equation was suggested by McKone[8]. The MXof estimate is considered conservative in that the dispersion term is in terms of 3 minutes time-averaged exposure.

Method 2 does not require MH4. It uses the following Gaussian equation:

$$MXof = 0.316 / (\pi \times 86400 \times UW4 \times VDC \times HDC)$$

where $VDC \times HDC = 1900 (Xpd + DW4/1000)^{1.6}$, and

$$Xpd = (1/70) \times (23.2\ A04^{0.5})^{1.11}$$

The VDC x HDC product is based on Turner's[6] curves for D stability. The product follows a downwind distance$^{1.6}$ power law, and 1900 represents the intercept at 1 km downwind. Here, the user-provided downwind distance DW4 (input is in meters) is augmented by a pseudo-downwind distance Xpd. Xpd is back-calculated from A04. It has the same significance as discussed in Section 6.4.2. The back-calculation is based on the D stability curve. The 0.316 attempts to adjust for longer-term dispersion coefficients than those presented by Turner[6], and is the one-day adjustment that he suggests. This results is expected to be conservative, since downwind exposure is always assumed, and D stability dispersion coefficients are lower than those expected for exposure during mainly daylight conditions.

7.0 CHMFIL20

CHMFIL20 is accessed when '4' is entered at the OPEN20 Main Selection Menu prompt. The initial display is the status report and the selection menu shown in Figure 10. The status report indicates the last downloaded file, the title of the current online file, the last stored file, and the last file operation with respect to downloaded or stored .DAT files. The selection menu presents six optional routines in CHMFIL20, and the option to exit to OPEN20 without further processing. CHMFIL20 resembles NOCHFL20 in many respects, and in these cases, reference will be made to subsections in Section 6.0. Data modification procedures in CHMFIL20 are more complex than in NOCHFL20. First, the user can access the CRDES20 program to estimate data. Moreover, the user can access specific CRDES20 subroutines in two different ways; either under DUST control, or by direct selection from a chemical property menu. The "Load and Go" option of NOCHFL20 is not available in CHMFIL20.

7.1 .DAT File Retrieval, Data Review and Change Routines

Routines '1', '3' and '4' shown in Figure 10 are discussed here.

Download the online data from a .DAT file

If option '4', is selected, the program operates as discussed in Section 6.1. The file DEFCHEM.DAT is downloaded. For options '1' and '3', the program follows the sequence discussed in Section 6.1. Figure 10 shows sample displays with option '3'.*

Obtain a DUST

The program operates as discussed in Section 6.1. The comments concerning the online status of a DUST downloaded at the DUST Loading Process Menu also applies to CHMFIL20.

Data Review and Change Routine

A sample display from this routine is shown in Figure 11. First, the user can change the chemical name information line. The display:
"Is chemical name: <user supplied information> OK? (yes or no) "
appears. If the user responds 'yes', the data review and change routine proper begins. If the user responds 'no', the prompt:
" Input revised name and other info. (up to 3 lines can be used): "
is issued. The user can enter a message of up to 255 spaces; see Section 5.4 for input details.

After processing the chemical title, data are processed under DUST control. As each datum is accessed, its dataname, current value, and current documentation message are displayed. The role of the datum in the assessment is cited; see Section 6.1 for role messages. Four processing options are provided. The first two options operate as described in Section 6.1.

---

* CHMFIL20 returns the user to a file input prompt when: the filename entered exceeds 8 characters in length; the filename entered is a blank (no characters); the file specified is not available on the Disk 2 device ; or the filename entered has illegal characters (such as punctuation marks).

```
*WELCOME TO CHMFIL20, THE CHEMICAL DATA PROCESSING SUBROUTINE*
***************** FILE STATUS REPORT *****************
Last downloaded file was ...
Last stored file was...
Chemical name for online data is...
Last file operation was...
****************** CHMFIL20 SELECTION MENU ******************
 ENTER      ROUTINE PERFORMED
   1        Modify online information under DUST control.
   2        Download a [illegible] .DAT file
   3        Modify a stored .DAT file under DUST control.
   4        Create a file for online use or storage.
   5        Go to storage options routine
   6        Modify *online* data via the CRDES20 selection menu.
   0        Exit CHMFIL20; return to OPEN20.
  Enter selection: 3
********** CURRENT INVENTORY OF .DAT FILES ON ...
E:\THEMOD20\DISK31
NEWCHEM .DAT       DEFCHEM .DAT
 892928 Bytes free

 Enter file name: newchem
 File newchem.dat downloaded.
 Want to continue? (yes or no): yes
 ****** DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU
 You will need a DUST to use this [illegible]
```

Figure 10. Opening Display in CHMFIL20. Routine '3' Operations Shown.

Option '1' advances processing to the next DUST-control selected datum. Option '2' lets the user manually change the existing data value. When option '3' is selected, CHMFIL20 accesses CRDES20 for a specific subroutine. Below this option's statement line, a message will indicate whether the corresponding CRDES20 subroutine contains an estimation method or only provides an information display. After the completion of the CRDES20 subroutine, the line: "<dataname> = <value>" appears. Option '4' is provided so the user can change documentation messages; this process is also shown in Figure 11. The user can consult Section 5.4 for input details.

When the data review and change routine is completed, the File Status Report and the CHMFIL20 Selection Menu reappear and further processing can be done. The last line of the status report will read:
"Last file operation was...Data change and review routine completed, changes to data are not stored"

7.2 Download a .DAT File

The monitor displays the current listing of .DAT files on the Disk 2 device. When prompted, the user specifies a .DAT file to be downloaded. After the file is downloaded, the File Status Report and the CHMFIL20 Selection Menu reappear for the next routine selection or return to OPEN20. The last line of the status report will read:
"Last file operation was...Downloaded file for return to OPEN20 or option '6' processing"

If no .DAT files are present, this error trap message will be displayed:

> No .DAT files were found on Disk 2.
> Although you are returned to the main menu, advise that you exit PHAS
> and copy DEFCHEM.DAT to storage from issued disks.

7.3 The Data Storage Routine

The procedures parallel those discussed in Section 6.3, with the substitution of .DAT files for .LDS files. DEFCHEM.DAT is not protected; the user can modify data online and store the altered data in DEFCHEM.DAT.

```
********** DATA REVIEW AND MODIFICATION ROUTINE **********
 The last file processing action was...
 User-specified file downloaded for review/change mode.
 Is chemical name:
 2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
 OK? (yes or no)
? no
 Input revised name & other info. (up to 3 lines can be used) This is where the
user can replace the default name or update existing information in his file.
 **********
 141 DTo, Long term NOAEL dose estimate, oral route, mg/kg-day =  .001
 Documentation: This is anew message
Main input variable to intake pathway eqtn.
 Select '1' to accept current value.
 Select '2' to replace value
 Select '3' for variable's info/estimation subroutine in CRDES20.
 Informational message only available
 Select '4' to replace documentation message
 Enter your selection: 1
 **********
 142 DTos, Short term NOAEL dose estimate, oral route, mg/kg-day =  .01
 Documentation:  default file
Main input variable to intake pathway eqtn.
 Select '1' to accept current value.
 Select '2' to replace value
 Select '3' for variable's info/estimation subroutine in CRDES20.
 Informational message only available
 Select '4' to replace documentation message
 Enter your selection: 2
    Enter revised value. ? .003
 **********
 142 DTos, Short term NOAEL dose estimate, oral route, mg/kg-day =  .003
 Documentation:  default file
Main input variable to intake pathway eqtn.
 Select '1' to accept current value.
 Select '2' to replace value
 Select '3' for variable's info/estimation subroutine in CRDES20.
 Informational message only available
 Select '4' to replace documentation message
 Enter your selection: 4
    Enter revised documentation message: This is where the user would replace t
he default documentation message "default file" or would modify the message prev
iously provided for data entry
 **********

 142 DTos, Short term NOAEL dose estimate, oral route, mg/kg-day =  .003
 Documentation:
This is where the user would replace the default documentation message "default
file" or would modify the message previously provided for data entry
Main input variable to intake pathway eqtn.
 Select '1' to accept current value.
 Select '2' to replace value
 Select '3' for variable's info/estimation subroutine in CRDES20.
 Informational message only available
 Select '4' to replace documentation message
 Enter your selection: 1
```

Figure 11. Sample Display of the CHMFIL20 Data Review and Change Routine

7.4 Modify Online Data via the CRDES20 Selection Menu

Before this routine ('6') in the CHMFIL20 Selection Menu can be exercised, a .DAT file must be online or the message: "No valid online info, select another option" will appear followed again by the menu. If a .DAT file is not online, the download routine of Section 7.2 must be first performed.

Access to CRDES20 is recognized when the CRDES20 Selection Table appears (Figure 12). The user accesses a specific subroutine by entering the subroutine code number. At the completion of the CRDES20 subroutine, CRDES20 returns processing to CHMFIL20, at which point the message:

*** END CRDES FOR SELECTED DATA ***
Current status of value for <dataname> is <value>.

usually appears. The message will be slightly different for the "model" soil partition coefficients indexed between 183 and 190 (see Table 2). Their specific subroutines calculate both long-time and short-time values, and both these values are displayed within the CRDES20 program and within the CHMFIL20 program (for an example, see Section 10.4.5). Moreover, when "the phytotoxicity constraint" subroutine is selected, following the information display, the current values of both the water-based and soil-based phytotoxicity limits online will appear.

After the "*** END CRDES FOR SELECTED DATA ***" message appears, the user has the option to change the documentation message. The following prompt is issued: "Do you want to change documentation (yes/no)? :" If the user responds 'no', a continuation return is requested, which is followed by the File Status Report and the CHMFIL20 Selection Menu display. If the response is 'yes', the prompt: "Enter revised documentation message:" appears, after which the updated documentation can be entered. See 5.4 for input details.

The documentation replacement for partition coefficients indexed between 183 and 190 and the phytotoxicity limits is restricted. For the partition coefficients, only the short-time data documentation can be replaced. For the phytotoxicity limits, only the soil-based data documentation can be replaced. The user can change the other messages in OPEN20 through the Online Data Review and Change Utility explained in Section 8.5.

7.5 Chemical-Related Data

The user should be aware of chemical-related data order to avoid "unpleasant surprises" in CRDES20 data processing. The data in a .DAT file are those indexed from 141 to 200; see Table 2. The indices 141-145 are reserved for toxicological data. The indices 146-151 are reserved for conventional physical properties of substances. The data indexed from 161 to 190 are used in at least one pathway intake equation. The index has been arranged so data that serve as inputs to specific estimation subroutines are obtained before the subroutine is executed. As examples, some vapor pressure estimation methods require boiling point data as input; some fish bioconcentration factor estimation methods require the octanol-water partition coefficient as input.

When the data review and change routine discussed in Section 7.1 is used, the index order ensures that input data to estimation methods are available. When

```
********** WELCOME TO THE CHEMICAL PROPERTIES ESTIMATION MODULE **********

******* CRDES20 SELECTION MENU OF DATA DESCRIBED AND ESTIMATED ********
The chemical-related data selected may require data inputs which have to be
estimated.  Consult the user's guide. [D] indicates description only.
* indictes selection of one specific datum in estimation module.
 0. QUIT w/o any selection              17. PC (dermal perm. const.)
 1. DTo and DTos (toxicity limits) [D]  18. BCF (fish bioconc. factor)
 2. DTi and DTd (toxicity limits) [D]   19. Kwv (water->vegetable p.c.)
 3. MW (molecular weight)[D]            20. Kwp (water->forage plant p.c.)
 4. Tmi (melting point)[D]              21. Kpm (forage plant->meat p.c.)
 5. Tbi( boiling point)                 22. Kpd (forage plant->milk p.c.)
 6. LogP (octanol-water p.c.)[D]        23. Kd  (soil->water p.c.)*
 7. Wsol (water solubility)             24. MKro1 or MKro2 (model soil->
 8. VP (Saturation vapor pressure)          surface water p.c.)*
 9. Koc (OC->water p.c.)                25. MKdb (soil->basement flux p.c.)
10. Ksv (Soil->vegetable p.c.)              or MKdo (soil->onsite flux p.c.)*
11. Ksp (Soil->plant(forage) p.c.)      26. MKgw (soil->groundwater p.c.)
12. Reference foc for Ksv & Ksp [D]     27. MKdw (sediment->water flux p.c.)
13. Kpat (plant->adipose tissue p.c.)   28. Organoleptic constraint [D]
14. Da (molecular diffusivity in air)   29. Aquatic toxicity constraint [D]
15. Dw (molecular diffusivity in water) 30. Phototoxic constraint [D]
16. Kh (Henry's Law constant)           31. Livestock toxicity constraint [D]
Input the number of your selection: 6
```

Figure 12. The CRDES20 Selection Menu

the routine discussed in Section 7.4 is selected, the user assumes this responsibility. PHAS20 has two features to assist the user:

* The Scenario Data Needs Report presents datanames in index order, and provides guidance as to what data input are required for specific methods.

** The selection code in the CRDES20 Selection Menu is ordered such that the most fundamental data are listed first.

The estimation methods for data indexed from 166 to 197 involve non-chemical data inputs. The Scenario Data Needs Report will identify these. In CRDES20, the non-chemical data can be accessed only from a .LDS file. Section 10.4 includes several examples of the accession procedure.

Data indexed from 181-190 can be considered model results expressed as partition coefficients. To stress this, their datanames have the prefix with "MK". The CRDES20 subroutines will provide estimates of these data. If the values are manually entered from a model performed outside of PHAS20, the user should be clear as to the units expected.

The CRDES20 subroutines for MKdb, MKdo, MKdw and MKgw provide time-dependent estimates, since the estimation methods account for diminished pollutant content in the medium source with passage of time. The time inputs for these data are contained in the .LDS file, and the user must ensure that the time frame data are in the intended .LDS file prior to entry to CRDES20.

Data indexed from 191-197 are reserved for inputs to the Type 1 constraint analysis. If these data are not available, or the user does not want to include a constraint in his analysis, a negative data value should be assigned. The negative value serves as a "flag".

8.0 Diagnostic Utility Routines in OPEN20

These routines allow the user to review online data, alter data rapidly, and printout data. The user must understand the index system for datanames, which is in Table 2. The Diagnostic Utility is accessed when '5' is entered at the OPEN20 Main Selection Menu" prompt. The following menu appears:

```
********** DIAGNOSTIC UTILITY MENU **********
 ENTRY          FUNCTION
   0    Quit utility and return to main menu
   1    Display pathway status (SST) for online scenario
   2    Display data use status table (DUST) for scenario
   3    Display online non-chemical data (.LDS data)
   4    Display online chemical-related data (.DAT data)
   5    Printout of online data, datanames supplied
   6    Review specific data name/value with option to
            change online data.
 Enter your selection:
```

The '0' entry to this menu returns the user to the OPEN20 Main Selection Menu. At the end of any function, the above menu reappears. The subsections below discuss these functions. The information in the figures shown apply to the problem developed in Section 5.5.

8.1 Display Pathway Status (SST) for Online Scenario

This display appears when '1' is entered, and is shown in Figure 13. The SST is presented in two columns, each under a "Paths " heading. The left column holds a code for pathways 1 to 10; the rightmost column holds a code for pathways 11 to 20. The pathway numbering for location in these columns is:

Domestic water ingestion (1)
Inhalation of vapors from domestic water(2)
Domestic water dermal absorption (3)
Water recreation\ water ingestion (4)
Water recreation\ vapor inhalation (5)
Water recreation\ dermal absorption (6)
Fish consumption (7)
Vegetable consumption (8)*
Beef consumption (9)*
Milk consumption (10)
Dust intake in vicinity of on-site residence (11)*
Dust intake at an on-site work setting (12)
Inhaled pollutant in house from vapor diffused from soil (13)*
Inhaled pollutant at on-site location from vapor diffused from soil (14)
Inhaled pollutant at off-site location from vapor diffused from soil (15)
Domestic water-groundwater supply\ ingestion (16)
Domestic water-groundwater supply\ vapor inhalation (17)
Domestic water-groundwater supply\ dermal absorption (18)

An asterisk indicates that the pathway is in the sample problem. If the code for a pathway is zero, the pathway is not included in the scenario. For pathways 1 through 8, when a pathway has been selected, the pathway number is the code number. Note that for the sediment medium, selections are only to

```
     Enter your selection: 1
       Paths 1-10  Paths 11-20
1        0           15
2        0           0
3        0           17
4        0           0
5        0           0
6        0           0
7        0           0
8        8           0
9        11          0
10       0           0

 Read down column for pathway status: 0 = not used
 Online scenario title is ...
Sample problem described in Technical Report/User's Manual
 Environmental medium of scenario is...  Surface and near-surface soil
 Last downloaded file was ... ptsample.pts
 Last stored file was... .pts
 If no downloaded or stored file shown above, data is only online
 Last file processing was...  File downloaded
 For topsoil medium only, site selection 'word' is  12
 Hit enter (return) to continue....

 ten ten+1 ten+2 ten+3 ten+4 ten+5 ten+6 ten+7 ten+8 ten+9 ten+10
(tens)
 0    1     0     0     0     0     0     0     0     0     1
 1    1     0     1     1     1     1     0     1     0     0
 2    1     0     0     0     0     0     0     0     0     1
 3    1     0     1     1     1     1     0     1     0     0
 4    0     0     0     0     1     1     0     1     1     0
 5    1     2     2     0     0     0     0     0     0     0
 6    2     2     5     5     5     0     0     0     4     0
 7    0     0     0     0     0     0     0     0     0     0
 8    2     5     5     0     0     0     0     0     0     0
 9    0     0     0     2     0     2     5     5     2     2
 10   2     2     2     2     2     2     2     2     1     1
 11   0     2     2     2     2     2     2     2     1     0
 12   0     0     0     0     0     0     0     0     0     0
 13   0     0     0     0     0     0     1     0     0     0
 14   1     1     1     1     0     2     2     2     2     2
 15   2     2     2     2     2     2     2     0     0     0
 16   2     0     2     0     0     7     3     1     2     5
 17   5     2     0     0     0     0     0     0     0     0
 18   0     5     1     1     0     0     0     0     0     0
 19   0     0     0     4     4     4     4     0     0     0
 To locate DUST entry index, read down 'tens' column, then across.
 Hit enter (return) to continue....
```

Figure 13. Diagnostic Utility Display of PTSAMPLE.PTS SST and DUST Information

pathway 7. For the "surface water or groundwater" medium, if beef consumption has been selected and water intake by livestock alone is selected, the code for pathway 9 is "9". Otherwise, it is "10". If milk consumption has been selected, the code for pathway 10 is "11' when water intake by the animal alone is selected. Otherwise, it is "12".

For the "surface and near surface soil" medium, if beef consumption has been selected, the code for pathway 9 can be one of three values:

"9" for plant intake by livestock alone
"10" for plant intake with soil ingestion
"11" for plant intake, soil ingestion, and water intake

If milk consumption has been selected, the code for pathway "10" will be either "12", "13", or "14", based on the respective option of intake by dairy cows selected. For selected pathways that are in the right-most column, their appearance in a scenario is indicated by the pathway number plus 4. Thus, if the pathway "dust intake in vicinity of onsite residence" is selected, the code value will be "15" at its position (the top of the right-most column). After the column display, the following narrative appears:

Read down column for pathway status: 0 = not used
Online scenario title is ....<title supplied by user>
Environmental medium of scenario is <medium selected>
Last downloaded file was...<filename + extension, if any>
Last stored file was...<filename, if any + extension>
If no download or stored file shown above, data is only online
Last file processing was...<statement indicating operation>

If the "surface or near surface soil" medium has been selected, an additional line appears: "For topsoil medium only, site selection 'word' is <number>"
This numerical value is a code, translated as follows:

Let the number equal "abcd", where each letter stands for the number 0, 1, or 2. Leading zeros do not appear, following zeros do appear. If the "a" position is not blank, at least of the one water recreation exposure routes was chosen. If the value is '1', subsite 1 was selected. If the value is '2', subsite 2 was selected. If the "b" position is not zero (or blank), the fish consumption pathway was selected, with subsite assignments as above. If the "c" position is not zero (or blank), the vegetable consumption pathway was selected, with subsite assignments as above. In Figure 13, this is the digit '1' in '12'. If the "d" position is not zero (or blank), either the beef or milk consumption pathways or both were selected. Again subsite assignments correspond to the number shown. In Figure 13, this is the '2' in '12'.

8.2 Display Data Use Status Table (DUST) for a Scenario

This display appears when '2' is entered, and is also shown in Figure 13. The display has ten columns and 20 rows. The status codes are read from left to right and then down. Thus, the right-most code in the first row is the status of the datum with index '10' (adult vegetable consumption). For other data, the table is read down to find the tens position and then across to find the unit position. The status codes are integers from "0" to "7", and can be interpreted by statements shown below:

0 The datum is not needed.
1 The datum is used in at least one exposure pathway equation.
2 The datum is used to estimate other data that appear in at least one exposure pathway equation.
3 Both statements 1 and 2 apply
4 The datum is used in a constraint equation.
5 Both statements 1 and 4 apply.
6 Not used
7 Both statements 2 and 5 apply

In Figure 13, the DUST code entry for the datum with index 166, the water to vegetable partition coefficient, Kwv, is '7'. Thus, the roles of this dataname in the example scenario is indicated by statements 1, 2, and 4.

8.3 Monitor Data Displays

Non-chemical data can be reviewed by responding with '3' to the Diagnostic Utility Menu. The display is presented as two screens. Figure 14 shows the display for DEFAULT.LDS. The data are read from left to right in each row. The first entry in the row indicates the base for the row. Thus in the row with base "65+", the value 16.6 under the column "two" corresponds to the dry plant intake in kg/day for dairy cattle, the datum with index 67.

The first screen shows data indexed from 1 to 80. The second screen shows data indexed from 81 to 140. These listing are followed by a narrative indicating the title line for the .LDS file, the name of the last downloaded file, the last file to which data were stored (if any), and the last file operation performed.

Chemical-related data can be reviewed by responding with '4' to the Diagnostic Utility Menu. Figure 15 shows this display for DEFCHEM.DAT. The location of indices follows the pattern discussed for the .LDS file above. The data table is concluded by a narrative which follows the sequence indicated for .LDS files.

8.4 Online Data Printouts

This routine is invoked in response to the '5' entry to the Diagnostic Utility Menu. The program checks if certain global data are valued as zero, which indicates that neither a .LDS file or a .DAT file was downloaded. In this case, a warning message is issued:

```
WARNING: You may not have valid data.
         Answer yes or no
         Do you wish to continue:
```

A response of "no" sends the user back to the Diagnostic Utility Menu.
A response of "yes" presents the user with the Printout Options Menu shown below:

```
    Enter your selection: 3
 Adult person variable values (1-20); Child values (21-40)
line       one              two              three            four             five
 0 +     70               1.6              3.4              1.8              .3
 5 +     8.999999E-03     .45              .18              .0065            .017
 10 +    .044             .18              .0001            .62              .35
 15 +    13               .0004            1.5              0                0
 20 +    13               .5               1.05             .6               .3
 25 +    8.999999E-03     .18              .18              .0022            .007
 30 +    .02              .56              .0002            .26              .35
 35 +    6.4              0                .63              0                0
 Variables indexed 41-80
line       one              two              three            four             five
 40 +    1                1                1                1                1
 45 +    1                1                1                1                1
 50 +    1                25600            365              1                25600
 55 +    365              0                0                0                0
 60 +    .2               .04              15.3             6.6              .35
 65 +    78               18.6             .87              250              520
 70 +    .04              1.5              .4               .5               5
 75 +    25600            365              100              1                0
 For location, read down side for multiple of 5, then across.
 More to come...
 Hit enter (return) to continue....


 Variables indexed 81-140
line       one              two              three            four             five
 80 +    .02              1.4              .1               10               100
 85 +    .08              .25              .35              1                .12
 90 +    1                8                .2               150              0
 95 +    .03              1.4              .1               20               260
 100 +   .08              .25              .35              1                .12
 105 +   1                10               .2               .0145            7E-08
 110 +   .44              .003             1.8              .15              .2
 115 +   .1               3                2400             125              2
 120 +   .003             1.8              .15              .2               .1
 125 +   5                10               2                20               500
 130 +   50               10               .1               365              10
 135 +   .35              .000417          3.94E-09         7.140001E-10     0
 For location, read down side for multiple of 5, then across.
 Title assigned from downloaded/online file is...'
Default file for starting new .LDS file.  Check user's guide for parameter value
 derivation. '
 Last downloaded file was ...default.lds
 Data stored in ...
 Last file operation:  Downloaded 'to go' file
 Hit enter (return) to continue....
```

Figure 14. Diagnostic Utility Display of DEFAULT.LDS Data

```
     Enter your selection: 4
line        one            two          three          four          five
 140 +    .001           .01          1              1             0
 145 +    227            92           2.32           .001          303
 150 +    .0004          1000         .02            .2            .02
 155 +    .02            .005         0              0             0
 160 +    .55            .000055      .00003         .0008         200
 165 +    1.5            15           .001           .0002         20
 170 +    10             2            15             50            0
 175 +    0              0            0              0             0
 180 +    1765 728       11111        30             50            100
 185 +    200            1567.391     1550           500           1000
 190 +    .01           -1            .05            5            -1
 195 +   -1              .01          0              0             0
For location, read down side for multiple of 5, then across.
Data is for substance
2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
Last downloaded file was ...defchem.dat. Data stored in ...
Last file operation:
Downloaded file for return to OPEN20 or option '6' processing
Hit enter (return) to continue....
```

Figure 15. Diagnostic Utility Display of DEFCHEM.DAT Data

ENTER	OPTION
0	For no printout, return to Diagnostic Utility Menu
1	Printout ALL data online
2	Printout ALL data that may be scenario-related
3	Printout ONLY data used in intake/constraint equations

Enter your selection here:

Respond '0' to exit this routine. The other entries cause a printout of datanames followed by their online values. The extent of the printout is more restrictive as the response value is increased. If the response is '1', the printout includes all datanames which are used in PHAS2D. If '2' or '3' is entered, the routine checks the online DUST. If a DUST is missing or defective, the message "DUST either not available or defective" is issued, and the user is returned to the Printout Options Menu. If a valid DUST is online, a printout is issued. If the response is '2', the printout includes only those datanames that have a non-zero entry in the DUST. If the response is '3', the printout includes only those data that appear either in the intake equations in COMPUT2D or in the constraint equations in CONSTR2D. Figure 16 is the sample problem printout for entry '3'. After each dataname and value is printed, the data documentation message appears. The printout is concluded with the title lines for the scenario, the non-chemical data file, and the chemical-related data file.

8.5 Review and Change Online Data

These functions are initiated by responding with '6' at the Diagnostic Utility Menu prompt. The following menu appears:

```
********** ONLINE DATA REVIEW AND CHANGE UTILITY **********
In this utility, you review a dataname and value by citing
the data index. Then you can change a value or select another
datum to review. Exit is to the Diagnostic Utility Menu.
```

```
OPTION          FUNCTION PERFORMED
  0       Return to DIAGNOSTIC UTILITY MENU
  1       Review a dataname and value
  2       Change the reviewed value
  3       Change the documentation message
Enter your selection here:
```

The entry '0' exits this routine. Option '1' must be exercised before any of the other options can be exercised, otherwise the message "You must enter an index first!! Try again." will appear. After the entry '1', the prompt: "Enter the index number for the datum:" appears, to which the user provides the index (from 1 to 200). One of two messages will appear. If the datum is not used at all, the message is "<index number> index datum not used. Try again." Otherwise the message is in the form:

```
The dataname is.... <title line from Table 1>
It value is... <data value>
Documentation: <current documentation message>
```

The menu is again displayed. If option '2' is selected, the user is prompted: "Enter the new value desired for the datum:" The user enters a value. The program displays the revised information in the format shown above followed by the option selections. If option '3' is selected, the user is prompted "Enter new documentation for the datum: " The user can enter up to 3 lines of documentation information (see Section 5.4 for editing specifications). Figure 17 presents a display sequence that demonstrates the various optional responses.

```
1   BWa, adult body weight, kg  70
Documentation:  default file, select '4' for information message.
10  Wva, adult vegetable consumption, kg dwb/day  .017
Documentation:  default file, select '4' for information message.
11  Wma, adult beef consumption, kg/day  .044
Documentation:  default file, select '4' for information message.
13  SIRa, adult oral intake of soil, residential, kg/day .0001
Documentation:  default file, select '4' for information message.
14  SARa, adult exposure area to dust on skin, residential, m^2 .52
Documentation:  default file, select '4' for information message.
15  PLa, adult perspiration rate, L/m^2/day .35
Documentation:  default file, select '4' for information message.
16  Rla, adult respiration rate, residential, m^3/day 13
Documentation:  default file, select '4' for information message.
18  BIRa, adult respiration rate, basement vapors, m^3/day 1.5
Documentation:  default file, select '4' for information message.
21  BWc, child body weight, kg  13
Documentation:  default file, select '4' for information message.
30  Wvc, child vegetable consumption, kg/day  .007
Documentation:  default file, select '4' for information message.
31  Wmc, child beef consumption, kg/day  .02
Documentation:  default file, select '4' for information message.
33  SIRc, child oral intake of soil, residential, kg/day .0002
Documentation:  default file, select '4' for information message.
34  SARc, child exposure area to dust on skin, residential, m^2 .26
Documentation:  default file, select '4' for information message.
35  PLc, child perspiration rate, L/m^2/d  / .35
Documentation:  default file, select '4'   or information message.
36  Ric, child respiration rate, residential, m^3 6.4
Documentation:  default file, select '4' for information message.
38  BRIc, child respiration rate, basement vapors, m^3/day .63
Documentation:  default file, select '4' for information message.
45  S(Wv), Adjustment factor/vegetable consumption 1
Documentation:  default file, select '4' for information message.
46  S(Wm), Adjustment factor/beef consumption 1
Documentation:  default file, select '4' for information message.
48  S(RSa), Adjustment factor/adult daily soil residential intake 1
Documentation:  default file, select '4' for information message.
49  S(RSc), Adjustment factor/child daily soil residential intake 1
Documentation:  default file, select '4' for information message.
51  S(BIR), Adjustment factor/basement vapors exposure 1
Documentation:  default file, select '4' for information message.
63  Uwm, water intake by steer, L/day 15.3
Documentation:  default file, select '4' for information message.
64  Upm, plant (forage) intake by steer, kg (dwb)/day 6.6
Documentation:  default file, select '4' for information message.
65  Usm, soil intake by steer, kg/day .35
Documentation:  default file, select '4' for information message.
69  BWM, representative steer body weight, kg 250
Documentation:  default file, select '4' for information message.
82  rh1, bulk density, topsoil e1 subsite, kg/L 1.4
Documentation:  default file, select '4' for information message.
83  th1, average moisture capacity, topsoil e1 subsite, L/L .1
Documentation:  default file, select '4' for information message.
97  rh2, bulk density, topsoil e2 subsite 1.4
Documentation:  default file, select '4' for information message.
98  th2, average moisture capacity, topsoil e2 subsite, L/L .1
Documentation:  default file, select '4' for information message.
109 SLA, soil loading rate on exposed skin, kg/m^2/day .0145
Documentation:  default file, select '4' for information message.
110 RSPA, particulate conc in air, residential, kg/m^3  7E-08
Documentation:  default file, select '4' for information message.
119 Ab3, basement area contacting soil diffusing vapors,m^2 125
Documentation:  default file, select '4' for information message.
137 MXb, dilution air factor for vapor flux in basement, day/m^3 .000417
Documentation:  default file, select '4' for information message
```

Figure 16. Diagnostic Utility Printout of Online Data With Option '3' Control (page 1 of 2 pages)

```
141 DTo, Long term NOAEL dose estimate, oral route, mg/kg-day .001
Documentation: default file, select '6' to see information messages.
142 DTos, Short term NOAEL dose estimate, oral route, mg/kg-day .01
Documentation: default file, select '6' to see information messages.
143 DTI, NOAEL dose estimate, inhalation basis, mg/kg/day 1
Documentation: default file, select '6' to see information messages.
144 DTd, NOAEL dose estimate, dermal basis, mg/kg/day 1
Documentation: default file, select '6' to see information messages.
166 Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L 1.5
Documentation: default file, select '6' to see information messages.
167 Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L 15
Documentation: default file, select '6' to see information messages.
168 Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb) .001
Documentation: default file, select '6' to see information messages.
170 Kd1 soil/water p.c. for e1 subsite pathways, mg/kg / mg/L 20
Documentation: default file, select '6' to see information messages.
171 Kd2 soil/water p.c. for e2 subsite pathways, mg/kg / mg/L 10
Documentation: default file, select '6' to see information messages.
182 MKro2, model soil-water p.c., e2 subsite runoff, mg/kg / mg/L 11111
Documentation: default file, select '6' to see information messages.
183 MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m^2-day 30
Documentation: default file, select '6' to see information messages.
184 MKdbc, soil flux p.c., basement model short-term, mg/kg per mg/m^2-day 50
Documentation: default file, select '6' to see information messages.
194 PHLW, Phytoxicity limit in water, mg/L 5
Documentation: default file, select '6' to see information messages.
197 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day .01
Documentation: default file, select '6' to see information messages.
Substance is
2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
Site data file is:
Default file for starting new .LDS file.  Check user's guide for parameter value
derivation.
Scenario title is: Sample problem described in Technical Report/User's Manual
```

Figure 16. Diagnostic Utility Printout of Online Data With Option '3' Control (page 2 of 2 pages)

```
Enter your selection: 6
********** ONLINE DATA REVIEW AND CHANGE UTILITY **********
In this utility, you review a data name and value by citing
the data index.  Then you can change value or select another
datum to review.  Exit is to the DIAGNOSTIC UTILITY MENU

   OPTION          FUNCTION PERFORMED
     0             Return to DIAGNOSTIC UTILITY menu
     1             Review a dataname and value
     2             Change the reviewed value
     3             Change the documentation message
Enter your function number: 2
You must enter an index first!! Try again.

   OPTION          FUNCTION PERFORMED
     0             Return to DIAGNOSTIC UTILITY menu
     1             Review a dataname and value
     2             Change the reviewed value
     3             Change the documentation message
Enter your function number: 1
Enter the index number for the datum :24
The dataname is....
24  DAWc, child body surface for dermal exposure to water, m^2
Its value is.....6
Documentation:  default file, select '4' for information message.

   OPTION          FUNCTION PERFORMED
     0             Return to DIAGNOSTIC UTILITY menu
     1             Review a dataname and value
     2             Change the reviewed value
     3             Change the documentation message
Enter your function number: 2
Enter the new value desired for the datum: 0.4
24  DAWc, child body surface for dermal exposure to water, m^2
Its value is... .4
Documentation:  default file, select '4' for information message.

   OPTION          FUNCTION PERFORMED
     0             Return to DIAGNOSTIC UTILITY menu
     1             Review a dataname and value
     2             Change the reviewed value
     3             Change the documentation message
Enter your function number: 3
Enter new documentation for the datum: You can change the message to indicate t
he basis of the 0.4 value inserted.  This change is online, so you can store the
 revised documentation in the applicable data file (here, a .LDS file).


The dataname is....
24  DAWc, child body surface for dermal exposure to water, m^2
Its value is... .4
Documentation:
You can change the message to indicate the basis of the 0.4 value inserted.  Thi
s change is online, so you can store the revised documentation in the applicable
 data file (here, a .LDS file).

   OPTION          FUNCTION PERFORMED
     0             Return to DIAGNOSTIC UTILITY menu
     1             Review a dataname and value
     2             Change the reviewed value
     3             Change the documentation message
Enter your function number: 0
```

Figure 17. Diagnostic Utility Review and Changes to Data and Documentation Display

9.0 POLLUTION ASSESSMENT PROGRAMS

9.1 COMPUT20

COMPUT20 processes .LDS and .DAT data in the context of information from a .PXX file to assess pollutant hazard in terms of Public Health considerations. COMPUT20 is accessed when '7' is entered at the OPEN20 Main Selection Menu prompt. This preamble is displayed:

```
*** WELCOME TO THE ASSESSMENT AND CONSTRAINT ANALYSIS PROGRAMS ***

COMPUT20 does the assessment for the SST, non-chemical data set and
chemical-related data set currently on line. Then you have the option
to do the constraint analysis. First, a check is made for online information
and data. If there are problems, they will be identified, and you will be
sent back to OPEN20 to do further processing as required.
```

The online data and information are reviewed to ensure that all data essential to performing the assessment are present. If not, omitted data sets and missing data are identified. Then, after a continuation return, the OPEN20 Main Selection Menu appears.

If online information and data are in order, the following message appears:

```
You have valid online information and data available. A status
summary is listed. Then you can choose to continue or not.
Hit enter (return) to continue....
```

After the continuation return, a summary report on the scenario, non-chemical data and chemical-related data is presented. This report includes the title of the scenario, site information, or chemical in the respective online database. The report states the last files downloaded and stored, and the last PHAS20 data processing operation in PATWAY20, NOCHFL20 or CHMFIL20, respectively. The user is then queried:

```
Answer yes or no
Do you wish to continue...
```

If the user responds 'no' at this prompt, control is transferred to OPEN20, and the OPEN20 Main Selection Menu is displayed. This "escape" is provided in case unwanted files were online. If the user responds 'yes' at this prompt, this message is displayed:

```
Ready to begin analysis. If you have not done so already, you
should consider a printout of display of your database in the
DIAGNOSTIC UTILITY in OPEN20.
********** HUMAN TARGET SELECTION **********
    Input '1' for adult-based analysis
    Input '2' for child-based analysis
    Input '3' for both analyses:
```

In Sections 2.2 and 2.3, the assessment process was discussed. A consumption or ingestion rate term was included in pathway equations represented by Equation 1. The relative impact of this term with respect to body weight can

differ considerably between adults and children. Moreover, equation 5 indicated that hazard index or PPLV calculations involve a public-health limit value (reference dose). This dose may differ for children and adults, often reflecting subchronic vs. chronic exposure concerns. PHAS20 can perform exposure assessments on the basis of either adult data, child data or both. If the human target selection input is '3', the adult-based analysis precedes the child-based analysis.

The analysis continues without further inputs by the user other than continuation returns. Figure 18 is the analysis for the sample problem for an adult-based limit dose (response '1' at the Human Target Selection Menu prompt. After a listing of scenario pathways, the display starts with either
(for adults): "ANALYSIS FOR ADULTS: INTAKE CRITERION IS = <adult value> mg/day"
or (for children): "ANALYSIS FOR CHILDREN: INTAKE CRITERION IS = <child value> mg/day"

The Assessment Computations Table follows. For each pathway (identified in the table by the number cited in the list described above), three numerical results appear.* The "unit intake" is the TAKE(j) described in Section 2.3. The "medium concentration at limit intake" has not been previously identified; it is the mg/kg (in soil) or mg/L (in water) of substance in medium which would "provide" the Public Health Limit Intake by each pathway in the absence of all others. The last value, the "LIMIT INTAKE" is the product TAKE(j) x PPLV. The sum of limit intakes equals the Public Health Limit Intake. Below the tabulated results is the PPLV (equation 5 in Section 2) and the hazard index per unit concentration.

If the analysis is for the "surface or near-surface soil" medium, the above information will be followed by a breaker line "********** OPTIONS **********"
If any the scenario pathways require an option selection (either a subsite option or air dispersion model option), a note will appear indicating the selected option.

9.2 THE CONSTRAINT ANALYSES

After the Assessment Computations display(s) provided by COMPUT20 are presented, a continuation return is entered. There is a pause as the satellite program CONSTR20 is accessed. The initial CONSTR20 display briefly explains the two types of constraints, and prompts for an integer input of 0, 1, 2, or 3. The input '0' bypasses the constraint analyses. This closeout display appears:

```
Ready to return to OPEN20
Hit enter (return) to continue...
```

After the prompted return, the OPEN20 Main Selection Menu is accessed.

Alternately, the input '1' at this prompt starts the Type 1 constraint analysis; the input '2', the Type 2 constraint analysis. The input '3' specifies both routines, starting with the Type 1 constraint analysis. If only one assessment analysis was specified in COMPUT20, the constraint analysis is also performed on that basis. If the option to select both the adult-based and child-based assessment analysis was exercised in COMPUT20, the message:

---

* The results in Figure 18 and in subsequent displays are based upon the contents of DEFAULT.LDS (Figure 14) and DEFCHEM.DAT (Figure 15).

```
 Hit enter (return) to continue....
 ****************** SCENARIO STATUS ******************
 Your current environmental medium is... Surface and near-surface soil
 Your current scenario is titled...
Sample problem described in Technical Report/User's Manual
 Your last data operation was... File downloaded
 Your last file down-loaded was...ptsample.pts
 Your last file used to store an on-line SST was....pts
 ************* NON-CHEMICAL DATA STATUS ***************
 Your last down-loaded file was...\phas20\disk2\default.lds
 Your last stored file was...
 Your last file manipulation was... Downloaded 'to go' file
 On-line title for data is...
Default file for starting new .LDS file.  Check user's guide for parameter value
 derivation.
 *************** CHEMICAL DATA STATUS ******************
 Your last down-loaded file was...\phas20\disk2\defchem.dat
 Your last stored file was...
 Your last file manipulation was...
 Downloaded file for return to OPEN20 or option '6' processing
 The chemical name for on-line data is...
 2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
 Enter 'yes' or 'no'.
 Do you want to continue...yes

 Ready to begin analysis.  If you have not done so already, you
 should consider a printout or display of your database in the
 DIAGNOSTIC UTILITY in OPEN20.
************** HUMAN TARGET SELECTION ***************
     Input '1' for adult-based analysis
     Input '2' for child-based analysis
     Input '3' to do both analyses:  1
 Scenario is... Sample problem described in Technical Report/User's Manual
 Medium being analyzed is...  Surface and near-surface soil
 Non-chemical data file title is...
Default file for starting new .LDS file.  Check user's guide for parameter value
 derivation.
 Scenario pathways are...
 PATHWAY 8 consume contaminated vegs. grown at designated subsite (1 or 2)
 PATHWAY 9 consume beef, livestock grazes on forage grown at designated
 subsite(1 or 2).  Allowance is made for livestock ingestion of soil and for
livestock watering on surface supply which gets cont. runoff from sub-site.
 PATHWAY 11 exposure to dirt at residence (oral, dermal, respired)
 PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house.
 Exposure assumed to be primarily caused by inhalation of vapors in basement.
                          **************

 Hit enter (return) to continue....

 ANALYSIS FOR ADULTS: INTAKE CRITERION IS... .07  mg/day

**************** ASSESSMENT COMPUTATIONS ****************
    SUBSTANCE NAME IS
 2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
PATH NUMBER              UNIT INTAKE        MEDIUM CONC      LIMIT INTAKE
                         mg/day per         AT LIMIT INTAKE  mg/day at Limit Conc.
                         mg/kg              mg/kg
 *  8                     1.270E-03          5.510E+01        6.154E-02
 *  9                     6.787E-05          1.031E+03        3.288E-03
 *  11                    1.041E-04          6.723E+02        5.044E-03
 *  13                    2.606E-06          2.686E+04        1.262E-04

 PPLV* IS   4.844E+01                    mg/kg
 Hazard index per unit concentration is  2.064373E-02
 PUBLIC HEALTH LIMIT INTAKE (reference dose x body weight) is  .07 mg/day
 * PPLV is medium conc for which intake is ADI.
 ********* OPTIONS **********
 Vegetable intake pathway computed for subsite #1
 Meat or milk intake pathways computed for subsite #2
 Hit enter (return) to continue....
```

Figure 18. Public Health Assessment for Sample Problem

Adult limit = <PPLV for adult analysis> Child limit = <PPLV for child analysis>
Enter '1' to use adult limit in analyses, '2' for child limit:

is issued. Based on the response, the appropriate basis and PPLV display follows. Note that if both bases were selected in the COMPUT20 program, only one basis at a time can be performed in CONSTR20. Generally, the basis corresponding to the lowest PPLV should be selected for use in CONSTR20.

When the Type 1 Constraint Analysis is selected, CONSTR20 selects pathways with identified constraints. For each pathway-constraint selection, the message presented reads:

PPLV = <value and appropriate concentration units> vs.
Critical conc. = <value and appropriate concentration units> based on CONSTRAINT
<dataname for value from which critical conc. is computed> = <constraint value>
Pathway: PATHWAY <number, followed by narrative pathway description>
<Conclusion (either "NO TYPE 1 CONSTRAINT" or "POTENTIAL TYPE 1 CONSTRAINT")>
Hit enter (return) to continue...

Figure 19 is the analysis for the sample problem. The user provides a continuation return after each pathway-constraint message. This procedure continues until all pathway-constraint combinations are processed. The message: "End Type 1 Constraint Analyses" then appears. It is followed by either the closeout display if only the Type 1 analysis was selected or by the Type 2 Constraint header:

" ********** TYPE 2 CONSTRAINT ANALYSIS FOR <medium>"

The Type 2 constraint analyses for the "surface water and groundwater" and "sediment" media are straightforward. In the first case, the PPLV is compared to solubility. If the PPLV exceeds solubility, this message appears:

Type 2 constraint exists. Public health limit conc.
may not be relevant for this analysis since
Wsol, Water solubility, mg/L = <value of Wsol (index 149)> is less than limit.

If solubility exceeds the PPLV, this message appears:

Public health conc. limit not subject to Type 2 constraint.

After either of these messages, the closeout display appears, and OPEN20 is again accessed. In the case of sediment, the water concentration corresponding to the PPLV in sediment is computed, and the described analysis occurs based on that water concentration.

The Type 2 constraint analysis for the "surface and near surface soil" pathways is more complicated, since corresponding water contents have to be calculated for pathways where a soil-water transfer occurs. For each of these pathways, the one of the following message is issued:

PATHWAY <number, followed by narrative>
Water conc. corresponding to PPLV is <value>
Type 2 constraint detected for pathway

```
********** TYPE 1 CONSTRAINT ANALYSIS **********
******** PPLV =  48.44086 mg/kg vs.
Critical conc. =  100.3571 mg/kg based on CONSTRAINT
194 PHLW, Phytoxicity limit in water, mg/L =  5
Pathway:
PATHWAY 8 consume contaminated vegs. grown at designated subsite (1 or 2)
NO TYPE 1 CONSTRAINT
Hit enter (return) to continue....
******** PPLV =  48.44086 mg/kg vs.
Critical conc. =  50.35714 mg/kg based on CONSTRAINT
194 PHLW, Phytoxicity limit in water, mg/L =  5
Pathway:
PATHWAY 9 consume beef, livestock grazes on forage grown at designated
 subsite(1 or 2).  Allowance is made for livestock ingestion of soil and for
livestock watering on surface supply which gets cont. runoff from sub-site.
NO TYPE 1 CONSTRAINT
Hit enter (return) to continue....

******** PPLV =  48.44086 mg/kg vs.
Critical conc. =  .2455515 mg/kg based on CONSTRAINT
197 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day =  .01
Pathway:
PATHWAY 9 consume beef, livestock grazes on forage grown at designated
 subsite(1 or 2).  Allowance is made for livestock ingestion of soil and for
livestock watering on surface supply which gets cont. runoff from sub-site.
POTENTIAL TYPE 1 CONSTRAINT
Hit enter (return) to continue....
Pathway 11 & 12: Direct soil exposure constraint test not available
Pathways 13, 14 & 15: Diffused vapor constraint not available
 If no paths appear, no Type 1 limits were identified related to pathways select
ed in scenario
End Type 1 Constraint Analysis
Hit enter (return) to continue....
```

Figure 19. Type 1 Constraint Analysis for Sample Problem

or "Type 2 constraint not detected for pathway".

Figure 20, a portion of the Type 2 constraint analysis for the sample problem, illustrates these displays. The user then provides a continuation return to continue the analysis. At the conclusion of one pass through all pathways, one of three possible summary outcome messages is displayed:

* If NO pathways incur a TYPE 2 constraint, a message to this effect is displayed, followed by the closeout display.

* If ALL pathways incur a TYPE 2 constraint, the message displayed is:

> TYPE 2 CONSTRAINT BREAKDOWN OF EXPOSURE ROUTES COMPLETE
> No adjustment in soil limit possible. Soil limit may be inappropriate based on human health effects.

This message is followed by the closeout display.

* If SOME pathways incur a Type 2 constraint, the message displayed is:

> TYPE 2 CONSTRAINT BREAKDOWN OF EXPOSURE ROUTES COMPLETE
> Revised soil limit is <new value>
> Now testing for need for further adjustment
> Doing another iteration

The Type 2 constraint analysis is repeated. After the iteration, either the above message is displayed again, or the message:

> TYPE 2 CONSTRAINT BREAKDOWN OF EXPOSURE ROUTES COMPLETE
> Revised soil limit is <new value>
> No further adjustment needed.

This is the final message for the third situation, which is followed by the closeout display.

```
********** TYPE 2 CONSTRAINT ANALYSIS FOR  Surface and near-surface soil

Most analyses based on criterion that water conc. at PPLV
exceeds solubility limit of  .ØØ1  mg/L.  After each test
you will be prompted to enter a return to continue.
PATHWAY 8 consume contaminated vegs. grown at designated subsite (1 or 2)
Water conc. corresponding to PPLV is  2.413424 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....
PATHWAY 9 consume beef, livestock grazes on forage grown at designated
subsite(1 or 2).  Allowance is made for livestock ingestion of soil and for
livestock watering on surface supply which gets cont. runoff from sub-site.
Water conc. corresponding to PPLV is  4.ØØ9731 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....
PATHWAY 9 consume beef, livestock grazes on forage grown at designated
subsite(1 or 2).  Allowance is made for livestock ingestion of soil and for
livestock watering on surface supply which gets cont. runoff from sub-site.
Water conc. corresponding to PPLV is  4.359721E-Ø3 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....

PATHWAY 11 exposure to dirt at residence (oral, dermal, respired)
Water conc. corresponding to PPLV is  2.413424 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....
PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house.
Exposure assumed to be primarily caused by inhalation of vapors in basement.
Water conc. corresponding to PPLV is  3.46ØØ62 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....
TYPE 2 CONSTRAINT BREAKDOWN OF EXPOSURE ROUTES COMPLETE
Revised soil limit is  683.7761
Now testing for need for further adjustment
Doing another iteration.
PATHWAY 8 consume contaminated vegs. grown at designated subsite (1 or 2)
Water conc. corresponding to PPLV is  34.Ø6714 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....

PATHWAY 9 consume beef, livestock grazes on forage grown at designated
subsite(1 or 2).  Allowance is made for livestock ingestion of soil and for
livestock watering on surface supply which gets cont. runoff from sub-site.
Water conc. corresponding to PPLV is  6.154Ø46E-Ø2 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....
PATHWAY 11 exposure to dirt at residence (oral, dermal, respired)
Water conc. corresponding to PPLV is  34.Ø6714 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....
PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house.
Exposure assumed to be primarily caused by inhalation of vapors in basement.
Water conc. corresponding to PPLV is  48.84115 mg/L
Type 2 constraint detected for pathway.
Hit enter (return) to continue....
TYPE 2 CONSTRAINT BREAKDOWN OF EXPOSURE ROUTES COMPLETE
Revised soil limit is  683.7761
Now testing for need for further adjustment
No further adjustment needed
Ready to return to OPEN2Ø
Hit enter (return) to continue....
```

Figure 20. Type 2 Constraint Analysis for Sample Problem

10.0 CRDES20

CRDES20 provides information and methods to estimate chemical-related data. CRDES20 consists of a central processing routine and several subroutines. Each data estimation subroutine is discussed in either Section 10.3 or 10.4. The estimation methods incorporated in CRDES20 were selected for wide applicability, minimal input requirements, and ability to be executed without extensive coding. They are not necessarily the most accurate estimation methods available. Many methods have been adapted from Lyman et al.[9]; and that reference provides many other methods and additional background information.

10.1 General CRDES20 Access and Exit Procedures

CRDES20 is accessed from OPEN20 by responding '9' at the OPEN20 Main Selection Menu Prompt. CRDES20 is accessed from CHMFIL20 with either self-guided entry (routine '6', see Section 7.4) or under DUST control (selection '3' from the data review and change routine, see Figure 11). For convenience, these modes will be referred to as accession modes 1, 2, and 3 respectively. With accession modes 1 and 2, the CRDES20 Selection Menu, Figure 12, is initially displayed. The user enters a specific subroutine by entering an integer in response to the menu's "Input the number of your selection: " prompt. With accession mode 3, the subroutine is directly entered.

CRDES20 has two general types of subroutines, those which only have an information message and those which have both an information message and estimation methods. The information message indicates the significance of each datum in PHAS20 pathway assessments, a summary of how data may be evaluated either externally or in the subroutine, and special processing notes. After an information-only subroutine is accessed, the "Central Processing Routine" prompt will immediately appear. The prompt is:

***** Central Processing Routine *****
Wish to Do More? (enter 'yes' or 'no')

The result of 'yes' or 'no' responses will depend upon the accession mode. With accession mode 1, after a 'yes' response, the CRDES20 Selection Menu reappears. Otherwise, the Main Selection Menu in OPEN20 is accessed. In other words, for each prompt at the CRDES20 Selection Menu, the user is limited to one estimation method within a subroutine. With accession mode 2, after a 'yes' response, the user is routed back to that subroutine. After a 'no' response, the user is routed back to CHMFIL20 as indicated in Section 7.4. With accession mode 3, after a 'yes' response, the user is also routed back to the subroutine. After a 'no' response, the user is routed back to the data review and change routine of CHMFIL20.

DTo, DTos, DTi, and DTd are the four public health limit inputs used in PHAS20. CRDES20 provides information-only subroutines for them. When these subroutines are entered by accession mode 3, only the specific information message for the specific datum is displayed. If CRDES20 is otherwise accessed, both the DTo and DTd information messages are displayed when '1' is entered at the CRDES20 Selection Menu prompt. The information for DTo is displayed first, followed by a request for a continuation return. After the return, the DTos information is displayed. The DTi and DTd information is

displayed when '2' is entered at the CRDES Selection Menu prompt, and the presentation is in the order DTi followed by DTd.

10.2 Estimation Method Subroutines Procedures

In most subroutines with estimation methods, after the information message, an explicit method selection prompt display appears. Based on message length, the user may have to issue a continuation return to proceed from the information message to the method selection prompt display. The user selects a method by input of a specified integer. The user may select an "escape" prompt of '0', after which the "Central Processing Routine" prompt appears, and is responded to as discussed [redacted] in Section 10.1.

When a method is selected within a subroutine, input data are collected. If CRDES20 is accessed from OPEN20, all chemical-related data must be provided by the user; a prompt is provided for each input. If CRDES20 is accessed from CHMFIL20, online chemical-related data are used without any prompts. If non-chemical data inputs are needed (see Section 10.4), the user must either download a file (the choice of DEFAULT.LDS or a user-selected file) or use online data. Once an .LDS file is downloaded, the data from the file are online for use in other PHAS20 programs.

After an estimation method is completed, all input data to the estimation equations are displayed. The estimation will appear in the following format:

<index number dataname> = <estimate>
Estimate by method # <number from method selection menu>

If the user entered by subroutine accession mode 1, the Central Processing Routine prompt is next encountered. Otherwise, the display will continue with the following formatted message and prompt:

CHMFIL20 Online value is: <current value>
Do you want to replace online value with estimate? (yes/no):

The value of the dataname from CHMFIL20 remains online until the user enters a 'yes' response here to replace it with the CRDES20 estimate. After the 'yes' or 'no' response, the Central Processing Routine prompt is encountered.

10.3 Estimation Subroutines Requiring Only Chemical-Related Data Inputs

10.3.1 Water Solubility (Wsol)

Four equations options are available. When CREDS20 is accessed from CHMFIL20, the only user input is the option selection. The equations are octanol-water partition coefficient-based correlations, and have been presented in Lyman et al.[9]. Equations 2.2 and 2.15 from Lyman et al.[9] compute a molar water solubility, thus molecular weight data is required to convert to a mg/L basis. Equation 2.15 is presented in two formats; one includes a melting point correction term. This additional term is claimed to be somewhat more accurate for substances that are crystalline solids above 25 ^{o}C[9]. If this option is selected, the melting point in ^{o}C is requested. If the melting point is below 25 ^{o}C, the input is ignored in calculations.

10.3.2 Boiling Point (Tb)

Two methods are presented. Method '1' is an inverse form of the Lorenz and Herz correlation[10] which predicts the melting point from the boiling point. The inverse form is: Tb = 1.713 x Tm , where Tb and Tm are the boiling and melting point temperatures in degrees Kelvin. It is not recommended for aldehydes, alcohols, and polar hydrocarbons.

Method '2', developed by Miller, is discussed in Section 12-5 of Lyman et al.[9]. The user must know structure substance to apply this method. Figure 21 shows the information message for the method followed by the presentation tableau indicating the applicable fragment and structures. After the message and tableau, the prompt:

```
Enter 'yes' or 'no'
Do you wish to continue analysis?
```

appears. If the user responds 'no', the subroutine is terminated. If the user responds 'yes', the presentation tableau is displayed. This tableau follows the order of Table 12-12 in Lyman et al.[9]. The subroutine prompts for a fragment identifier number (FIN) input followed by the number of times an identified fragment occurs in the pollutant molecule. After their input, the tableau display is updated to reflect the last input. Then the message:

```
   The CRT will display 41 different structure fragments in a table.
You will be prompted to enter the identification number for a given
fragment (FIN) of the subject pollutant and then the number of times that
fragment occurs in the pollutant molecule. Your entry will be echoed back.
You will be queried if you wish to do more. If you select yes, the table
will re-display with the previous selection posted. This sequence is
repeated until you respond 'no' to the 'Do you want to do more?' query.
   In the table, there are coded abbreviations. 'NR' indicates a non-
ring structure, 'RG' a ring. Rings can be either aliphatic or aromatic.
Other abbreviations are alc=alcohol, phl=phenol, ald= aldehyde, est=ester.
A triple bond is shown as '-='. As examples of input, dinitrophenol would
appear as 3FIN14 (=CH- in a ring), 3FIN15 (=C< in a ring), 1FIN22
(phenolic OH), and 2FIN37 (nitro groups). 1,2-dibromo-3-chloropropane or
CH2Br-CHBr-CH2Cl appear as 2FIN2 (-CH2- non-ring), 1FIN3 (-CH< non-ring),
2FIN1  (bromine), and 1FIN18 (chlorine). FIN order of entry is not required.
    E ter 'yes' or 'no'.
   Do you wish to continue analysis? yes

                  MILLER BOILING POINT METHOD FRAGMENTS ID TABLE
 ØFIN1 -CH3 [NR]     2FIN2 -CH2-[NR]     1FIN3 -CH< [NR]     ØFIN4 >C<  [NR]
 ØFIN5 =CH2 [NR]     ØFIN6 =CH- [NR]     ØFIN7 =C<  [NR]     ØFIN8 =C=  [NR]
 ØFIN9 -=CH [NR]     ØFIN1Ø -=C- [NR]    ØFIN11 -CH2- [RG]   ØFIN12 -CH< [RG]
 ØFIN13 >C<  [RG]    ØFIN14 =CH- [RG]    ØFIN15 =C<  [RG]    ØFIN16 =C=  [RG]
 ØFIN17 -F           ØFIN18 -Cl          ØFIN19 -Br          ØFIN2Ø -I
 ØFIN21 -OH alc      ØFIN22 -OH phl      ØFIN23 -O- [NR]     ØFIN24 -O- [RG]
 ØFIN25 >C=O [NG]    ØFIN26 >C=O [RG]    ØFIN27 -CH=O ald    ØFIN28 -COOH acid
 ØFIN29 -COO- est    ØFIN3Ø =O other     ØFIN31 -NH2         ØFIN32 >NH [NR]
 ØFIN33 >NH [RG]     ØFIN34 >N- [NR]     ØFIN35 >N- [RG]     ØFIN36 -CN
 ØFIN37 -NO2         ØFIN38 -SH          ØFIN39 -S- [NR]     ØFIN4Ø -S- [RG]
 ØFIN41 =S

When promoted, enter FIN. Enter number of units next
Enter FIN (from 1 to 41) here: 19

Enter number of specified fragments in molecule. 2

    Enter 'yes' or 'no'.
Do you want to do more? yes
```

Figure 21. Sample Miller Boiling Point Method Displays.

Enter 'yes' or 'no'
Do you want to do more?

is displayed. If the user responds with 'yes', the subroutine again requests a FIN and the number of FIN fragments. For example, in Figure 21, the user is about to substitute 2 of 3 positions on a propane substrate with bromine. The user provides paired entries until the structure is complete. The user can correct errors, or replace a non-zero value with zero. After all entries have been made, the above message is answered with 'no'.

The molecular weight used in Miller's method is computed from fragment inputs. If CRDES20 is from accessed CHMFIL20, the online molecular weight also is displayed. If these weights differ other than for round-off (in computations, fragment weights are to the nearest 0.1 units), either the user's inputs are not correct for the structure or the online molecular weight is in error.

10.3.3 Vapor Pressure (VP)

Five methods are provided for vapor pressure, and are summarized in the information message (Figure 22). Before the user selects a method option selection, the prompt "Enter temperature in DegC for calculation result:" is displayed, and the user enters the calculation temperature. Vapor pressure inputs must be in mm Hg or torr.

Mackay's method #1. This was presented in Mallon, et al[11]. The equation involved is:

$$\ln VP = -(4.4 + \ln Tb) \times (1.803 [Tbr-1] - 0.803 Tbr) - 6.8 (Tmr-1)$$

where Tb is the boiling point, Tbr is the relative boiling point Tb/Tcalc, and Tmr is the relative melting point Tm/Tcalc. Tcalc is the temperature for which VP is being calculated. All temperatures are in degrees Kelvin, and the calculated VP is in atmospheres. When CRDES20 is entered from OPEN20, the user supplies the melting point and boiling point in ^{o}C. When entry is from CHMFIL20, no inputs are required.

Watson's boiling point method. This is described in Lyman et al.[9], sections 14-3 and 14-4. When CRDES20 is accessed from OPEN20, the user supplies the substance's boiling point in ^{o}C and the substance's physical state at the calculation temperature. The prompt for physical state is: "Is substance a liquid at calculation temp? " For the liquid state, the response is 'yes'; 'no' for the solid state. After this prompt, an informative message and the Watson Method Index Table is displayed; see Figure 23. This table identifies classes of compounds, and the user enters the index number corresponding to the classification that best describes the substance (in Figure 23, '19' has been entered, the index for a "nitro compound"). A default index number (35) is also provided. A value of K_F corresponding to the index number is used to evaluate equation 14-16 from Lyman et al.[9] These values are in Table 14-4 of Lyman et al.[9]. The six-carbon entries are used.

When CRDES20 is accessed from CHMFIL20, the online stored boiling point is employed to determine the physical state (solid or liquid) of the substance. Here, the first prompt for input is the "Enter identification number:" query after the index table presentation. Execution continues as noted above.

```
*************** VAPOR PRESSURE METHOD SELECTION MENU ******************
Select '0' to exit without estimation
Select '1' for Mackay's Method #1 for both liquid and solids. If you're
    here from OPEN11, you must input Tmelt and Tboil.
Select '2' for Watson's boiling point method for both liquids and solids.
    If you're here from OPEN11, you must input the liquid boiling point and
    the state of the substance (liquid or solid) at ambient conditions.
Select '3' for simple interpolation. You enter two data pair sets of
    saturation vapor pressure/ temperature. The sets must be for either
    the solid or liquid state, but not one of each. If you're here from
    OPEN11, and your data pair sets are for the liquid state, but you want
    a solid state VP, you will be prompted for Tmelt. You can't estimate
    a liquid-state VP by this method from solid state data.
Select '4' for Mackay's Method modified for input of only the melting point.
    Tboil is approximated internally. This is the least accurate of the
    methods. No additional inputs are needed if you're here from CHMFIL11.
Select '5' for Watson's reduced pressure method. This is similar to
    selection '2' above but uses a reduced saturation vapor pressure
    and temperature input in place of the boiling point.
Enter your selection (from 0 to 5):  2
```

Figure 22. The Vapor Pressure Method Selection Menu

```
Enter your selection (from 0 to 5):  2
Enter temperature in DegC for calculation result: 18
Enter boiling point temp. in degC: 90
Enter 'yes' or 'no'.
Is substance a liquid at calculation temp? no
You will be shown a table of general compound groups. Choose the
number of the group describing your compound. Note, for mixed
aromatic constituents,-OH takes precedence. For simple aromatics
consider the phenyl group as a n-Alkane (selection #1).
Press enter (return) key to continue....



******* WATSON METHOD INDEX TABLE FOR VAPOR PRESSURE ESTIMATIONS *******
*** Aliphatic or Carbocyclic/ Heterocyclic Cmps. with Aliphatic Properties
1. n-Alkanes              2. Other alkanes          3. Olefins
4. Cyclic sat. hydrocarbs 5. Alkylated cyclic sat. hydrocarbs
6. Monochloride           7. Monobromide            8. Monoiodide
9. Polyhalide (not entirely halogenated)  10. Totally halogenated cpd.
11. Perfluorocarbon       12. Ester (R-COO-R')      13. Ketone
14. Aldehyde              15. Primary amine         16. Secondary amine
17. Tertiary amine        18. Nitrile               19. Nitro compound
20. Mercaptans            21. Sulfides
22. Alcohol(single OH)    23. Diols                 24. Triols
25. Cyclohexanol, cyclohexyl methyl alcohol, etc.
26. Aliphatic ethers                          27. Oxides (cyclic ethers)
*** Aromatic Compounds (use phenol values if mixed function on ring)
27. Monophenols                               28. Other phenols(2 or more -OH)
29. Monoaniline                               30. Other aniline(2 or more -NH2)
31. N-sub. anilines (C6H5NHR)                 32. Naphthols (one -OH)
33. Naphthylamines (one -NH2)                 34. N-Substitued naphthylamines
35. ANY OTHER COMPOUND(Default value)
   Enter identification number: 19
KFCAL=  1.05
Boiling Point (C) =  90          Ambient state of substance is solid
151 VP, Saturated vapor pressure, mm Hg =  34.2216
VP computed at  18  degC.

***** Central Processing Routine *****
Wish to do more? (enter 'yes' or 'no'): no
```

Figure 23. Sample Watson Vapor Pressure Method Calculation. CRDES Accessed from OPEN20.

Simple interpolation. This is based on the Clausius-Clapeyron equation, which which states that, within a short range of temperature, log $P \propto T^{-1}$, where T is in Kelvin. The program prompts for two sets of temperatures and pressures, first for the lower end of the range, and next for the upper end of the range. The next query is:

> Enter '1' if substance is liquid at calc. temp & in range.
> Enter '2' if substance is solid at calc. temp but liquid in range.
> Enter '3' if substance is solid at calc. temp & in range.

The user enters the applicable integer. The vapor pressure is computed and displayed directly if the entry response is '1' or '3'. If the response is '2', when CRDES20 is accessed from OPEN20, the user supplies the pollutant's melting point in ^{o}C. Then, the routine computes (but does not display) the vapor pressure of the substance as a "supercooled liquid". The corresponding solid vapor pressure is then computed by equation 14-10 of Lyman et al.[9].

The simple interpolation method is most accurate when the calculation temperature is inside the range. In case of an extrapolation of more than about 25 ^{o}C outside of the range, Watson's reduced pressure method (see below) may be more accurate; moreover it only requires one data set.

Mackay's method (modified). This method uses the Lorenz and Herz equation (see Section 10.3.2) to estimate the boiling point from the melting point. Then, the melting point and estimated boiling point are entered into Mackay's Method #1. The user enters the melting point when prompted if CRDES20 is accessed from OPEN20.

When CRDES20 is accessed from CHMFIL20, a boiling point is computed from the online melting point, and that computed boiling point is displayed. However, that computed boiling point does NOT replace the online boiling point.

Watson's reduced pressure method. This routine is based on equations 14-24 and 14-26 in Lyman et al.[9]. In place of the boiling point (the temperature corresponding to a 1 atmosphere vapor pressure), a paired set of vapor pressure-temperature data are entered. Usually, the vapor pressure used is below 1 atmosphere, hence the term "reduced pressure". The user provides the reference temperature and pressure at the two prompts:

> Enter reference temperature for reduced pressure:
> Enter VP at reference temperature:

When CRDES20 is entered from OPEN20, this query is then issued: "Is substance a liquid at calculation state?" The response is 'yes' for liquid or 'no' for solid. Then the Watson Method Index Table (see Figure 23) is displayed. After the index number is entered, the conditions of the problem and estimated vapor pressure are displayed.

10.3.4 Soil Organic Carbon-Water Partition Coefficient (Koc)

This subroutine provides seven different correlation equations. The display screen shown in Figure 24 identifies these equations and the requisite inputs. When CRDES20 is accessed from OPEN20, the user is prompted to supply the requisite data, after which the estimated Koc is displayed. This is the

```
152 Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)
    Koc is the ratio between the equilibrium pollutant concentration
on soil organic carbon (OC) and its concentration in water. Koc indicates
the relative distribution of pollutant between soil and water assuming
that pollutant in soil is primarily physically adsorbed on OC. Then Kd can
be estimated from Koc: Kd= foc x Koc where foc is the fraction of OC in
soil. Kd is input to many soil pathway intake equations involving soil-
water transfers and in constraint tests where water-based data are used for
comparison to soil results.
    Seven methods are presented here. The first six were presented in the
Lyman and Loreti (L/L) Final Report, Task 15, EPA Contract 68-01-6951.
The 7th is equation 4-5 in Lyman, et. al. Chemical Property Estimation
Methods. See menu below for specific equation inputs (LogP, Wsol, MW)
Select     Eqtn                    Needs      Select   Eqtn                    Needs
 0     Exit w/o Calculation                     1     L/L general eqtn.       LogP
 2     L/L non-aromatic eqtn.     LogP          3     L/L aromatic eqtn.      LogP
 4     L/L general eqtn.          MW, Wsol      5     L/L non-aromatic eqtn.  MW, Wsol
 6     L/L aromatic eqtn.         MW, Wsol      7     Kenaga eqtn.            Wsol
Enter your selection (from 0 to 7): 2
Enter LogP: 3.26
152 Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)  =  1219.158

***** Central Processing Routine *****
Wish to do more? (enter 'yes' or 'no'):
```

Figure 24. Koc Estimation Subroutine Display. CRDES20 is Accessed From OPEN20, and Method '2' is Selected.

situation shown in Figure 24, where the second equation is selected. Otherwise, the only input required is the method selection integer.

10.3.5 Soil to Vegetable and Plant Partitition Coefficients (Ksv and Ksp)

Although each variable has a separate option code in the CRDES Selection Menu, one subroutine processes both of them. Two methods are cited. The first is the Travis and Arms equation[12]. This equation, proposed for "vegetation", is used to estimate Ksv.

$$\log Ksv = 1.588 - 0.578 \times \log P$$

The second method estimates Ksp as 10 x Ksv. When CRDES20 is accessed from OPEN20, the logP value is requested; otherwise there are no further inputs.

There are some restrictions within this subroutine. If the second method (Ksp = 10 x Ksv) is selected when Ksv is the specified datum, the subroutine issues an error message and reissues the initial Ksv/Ksp Estimation Menu display. When CRDES20 is accessed from CHMFIL20 and Ksp is the specified datum, the subroutine does not automatically replace the online value of Ksv with the value from the above equation; this replacement is only done when Ksv is the specified datum. When Ksp is the specified datum, the selection of either method leads to the same result.

10.3.6 Plant to Adipose Tissue Partition Coefficient (Kpat)

Two equations are provided, both from Garten and Trebalka[13]:

$$Kpat = 10^{(\ -3.935 + 0.511 \log P\ )}$$
$$Kpat = 10^{(\ -1.633 - 0.608 \log Wsol\ )}$$

When CRDES20 is accessed from CHMFIL20, no inputs are needed other than the method selection input. Otherwise, logP is requested for the first selected method; water solubility is requested for the other.

10.3.7 Diffusivity in Air (Da)

Two options are presented: an empirical equation and the Fuller, Schettler and Giddings (FSG) method discussed in Section 17-4 of Lyman et al.[9]. The empirical equation was suggested by Small[2]

$$Da = 8 \times (Tcalc / 298.2)^{1.75} / (MW)^{0.5}$$

where Da is in m^2/day, and Tcalc is in degrees Kelvin.

After the user selects a method, the computation temperature (^oC) is requested. The empirical equation requires a molecular weight. When CRDES20 is accessed from OPEN20, the molecular weight is provided by the user when prompted. Otherwise, the online value is used.

The FSG method computes a "LeBas Volume" as an intermediate result. This volume is estimated from factors based upon a pollutant's empirical formula and structure. These factors appear in Table 17-5 of Lyman et al.[9] The instructions for LeBas Volume estimation are shown in Figure 25, as are the atoms/structures of Table 17-5. At the prompt: "Enter ID# of constituent here: " the user furnishes the atom/structure constituent index number. Then the cursor moves to the right of the indexed item in the tableau; here the user enters the number of times the given item appears in the molecule. Then the prompt (near the bottom of the screen): "Do you want to do more (yes or no) ?" appears. When the user responds 'yes', the routine to enter information continues. In the Figure 25 example, the user had previously entered C_3H_4, and has just added O_2 as carboxylic oxygen atoms (see the instruction example in Figure 25. The user intends to add more information to the tableau.

When the user responds 'no', the Da computation continues. If the LeBas Volume is less than 1, the user has probably omitted some structural components, and an error message is issued. Then, the program returns to the FSG method instruction message. The subroutine determines and displays the molecular weight from tableau inputs. When CRDES20 is accessed from CHMFIL20, the online molecular weight is also displayed. If there is considerable difference between them (other than round-off errors; in PHAS20, weights are to the nearest 0.1 units), either the tableau entries or the online molecular weight are incorrect.

10.3.8 Diffusivity in Water (Dw)

Two methods are presented. In the first, Dw is approximated as 0.0001xDa. When CRDES20 is accessed from OPEN20, the user enters Da when prompted. Otherwise, no additional input is required.

The second method is based on the Hayduk and Laudie equation described in Section 17-7 of Lyman et al.[9]. Calculations are specific to one temperature (20 ^oC) for two reasons: the pathway intake equations that use Dw also use the

```
   Two methods are available in PHAS to estimate Da.  The first, a rough
approximation, only requires MW. The second method is the that of Fuller,
Schettler and Giddings (FSG), see Section 17.4 of Lyman et al. Chemical
Property Estimation Methods. It requires MW, and structural inputs. It is
restricted to compounds with C,H,O,N,S,P,F,Cl,Br & I elemental constituents.
**************** Da ESTIMATION MENU SELECTIONS ***************
Select '0' to exit without calculation
Select '1' for rough approximation
Select '2' for FSG method
Enter your selection: 2
Enter temperature of computation in Deg C: 25
***** INSTRUCTIONS FOR FSG METHOD WITH LEBAS VOLUME *****
The CRT will display the FSG method structure units in a tableau.
You are prompted to enter the index number for an element or
structural component in the pollutant molecule.  The cursor will
move to that item in the tableau.  There, you enter the
number of units in the pollutant molecule.  For example,
if your molecule was CH2Cl-CHBr-COOH, you would enter:
IDe1 [C] - 3; IDe2 [H] - 4; IDe4 [Br] - 1; IDe6 [Cl],1 ; and
IDe9 [Carboxylic O] - 2.  At the end of each entry sequence, you
are prompted to continue with entries. The sequence is repeated
if you respond 'yes' to this prompt.
Press enter (return) key to continue....

                    LEBAS VOLUME ELEMENTS/COMPONENT INDEX
IDe1 (C)                          3   IDe2 (H)                    4
IDe3 (O in Meth esters/ethers)    0   IDe4 (Br)                   0
IDe5 (O in Eth ester/ethers)      0   IDe6 (Cl)                   0
IDe7 (O in other esters/ethers)   0   IDe8 (Fl)                   0
IDe9 (O in carboxylic acids)      2   IDe10 (I)                   0
IDe11 (O bonded to S,P or N)      0   IDe12 (S)                   0
IDe13 (other bonded O)            0   IDe14 (3 member ring)       0
IDe15 (Double bonded N)           0   IDe16 (4 member ring)       0
IDe17 (N in primary amines)       0   IDe18 (5 member ring)       0
IDe19 (N in sec. amines)          0   IDe20 (6 member ring)       0
IDe21 (P)                         0   IDe22 (Anthracene ring)     0
IDe23 (Naphthalene ring)          0
 Enter IDe when prompted. Then cursor will move to IDe location
 in the tableau. At that location, enter the number of units.
     Enter IDe here: 9
```

Figure 25. LeBas Volume Information and Tableau Displays

datum EIW (see Table 2), which is computed for 20 ^{o}C, and at 20 ^{o}C, the viscosity term in the Hayduk and Laudie equation is nearly unity.

The second method requires calculation of the LeBas Volume, and the procedure is identical to that described in section 10.3.7. After the LeBas Volume is computed, the statement "Going back to Dw subroutine" appears, which is followed by the computed Dw.

10.3.9 Henry's Law Constant (Kh)

Here, the dimensionless Kh is evaluated as the saturation vapor pressure divided by the water solubility, both evaluated at a given temperature. After the initial display, this prompt appears: "Is temperature of calculation 25C (298.2K) ? " If the answer is 'no,' the user is prompted to enter a temperature. When CRDES20 is accessed from CHMFIL20, there are no further inputs, and the result is displayed. When CRDES20 is accessed from OPEN20, the user is first queried for molecular weight. Then the user is queried for the <u>units</u> of the water solubility datum to be entered:

Water solubility units for input. Enter '1' for mg/L units,
'2' for mole/L units, '3' for millimole/L units:

After the user enters the correct integer, the water solubility data is requested. This sequence is repeated for saturation vapor pressure. The accepted units are torr or mm Hg ('1'), atmospheres ('2'), and pascals ('3').

10.3.10 Dermal Permeability Coefficient (PC)

One method is presented to estimate PC. It is based on the following equation presented by Fiserova-Bergerova and Pierce[14]:

$$flux = Wsol/15 \times (0.038 + 0.153\ P) \times \exp(-0.016\ MW)$$

where flux is the transfer of substance in mg/cm^2-hr, Wsol is in mg/cm^3 and P is the octanol-water partition coefficient. The term flux/Wsol has units of cm/hr, and corresponds to PC.

When CRDES20 is accessed from OPEN20, the user enters, in order, the log octanol-water partition coefficient and molecular weight. No entries are required for access from CHMFIL20.

10.3.11 Fish Bioconcentration Factor (BCF)

Three estimation options are presented, corresponding to equations 5-2, 5-3 and 5-4 in Table 5-1 of Lyman, et al.[9]. These equations respectively require an input of logP, water solubility or Koc, which the user supplies when CRDES20 is accessed from OPEN20. No entries are required for access from CHMFIL20.

10.3.12 Water to Vegetable and Plant Partition Coefficients (Kwv and Kwp)

Kwv and Kwp are handled in one subroutine with four method options. The first two methods involve use of Ksv and Ksp, respectively, to compute Kwv or Kwp, with the internal assumption that the forage partition coefficient is 10 times higher than the vegetable coefficient, as mentioned in Section 10.3.5. For Kwv, these relations can be summarized as the following:

$$Kwv = [\ Ksv \text{ or } Ksp/10\ ] * foc(experimental) * Koc$$

When CRDES20 is accessed from OPEN20, the user enters the experimental soil Ksv (or Ksp), the foc(experimental), and the substance Koc. The third method uses the Travis and Arms equation (see Section 10.3.5) to estimate Ksv, and then the above equation, with an arbitrary foc(experimental) of 0.015. When CRDES20 is accessed from OPEN20, the user must provide the substance Koc. The last method uses the "modified" Briggs equation[15]:

$$Kwp = 5 \times (\ 0.82 + 10^{E1}\ ) \times 10^{E2}\ ;\ \text{where } E1 = 0.95 \times logP - 2.05 \text{ and } E2 = -0.178 \times (\ logP - 1.78\ )^2$$

The user enters logP when CRDES20 is accessed from OPEN20. If this equation is used to estimate Kwv, it uses the default conversion that Kwv = Kwp/10.

If CRDES20 is accessed from CHMFIL20, the subroutine only replaces the specified datum (Kwv or Kwp) with the computed value, even if the calculation internally computes the other value. For example, if Kwv is being estimated by the "modified" Briggs Equation, the online Kwp will not be replaced by the value calculated in the equation.

10.4 Subroutines Requiring Both Non-chemical and Chemical-Related Data.

Several of these subroutines, particularly those which estimate "MK" partition coefficients, require a considerable amount of non-chemical data. Thus, PHAS20 has been designed to access non-chemical data from .LDS files. The user has three file accession options: to use the default file DEFAULT.LDS, to specify the .LDS file to be used, or to use online data (which have been previously downloaded from a .LDS file). The options are stated in the "Non-Chemical Data Accession Subroutine" menu, which appears in Figure 26. A summary of past .LDS operations is presented. The .LDS files on the Disk 2 device are then listed. Following that, the three accession options are presented. In the example in Figure 26, accession option '2' has been selected, and DEFAULTXX.LDS has been selected for downloading. The selection '0' at the accession option prompt returns the user to the exit prompt in the Central Processing Routine.

After non-chemical data accession, non-chemical data that are inputs to a selected estimation method are checked for missing values. If such a condition is found, a message is issued with the format:

Missing non-chemical data for <specified non-chemical dataname>
Leaving estimation routine for <dataname associated with subroutine>

and the user is returned to the exit prompt in the Central Processing Routine.

If the user accesses CRDES20 from OPEN20, chemical-related data are manually entered. If the user accesses CRDES20 from CHMFIL20, the subroutine also checks online chemical-related data that are inputs to the selected estimation method for missing values. If such data are found, a similar process to that for missing non-chemical data occurs.

Each of the below sections that describe "MK" partition coefficients has a concluding "Methods Detail" subsection.

10.4.1 Plant to Beef Partition Coefficient (Kpm)

Two options are available for estimating Kpm. The first option uses Kpat as a starting point; the estimate is Kpm = Kpat x fm . The other option uses Kpd as a starting point; the estimate is Kpm = Kpd x fm / fd . Option 1 requires Kpat input if CRDES20 is accessed from OPEN20. Option 2 requires Kpd input if CRDES20 is accessed from OPEN20. If this subroutine is accessed from CHMFIL20, the Kpd datum must be online. If this is not the case, the user can return to CHMFIL20 and process Kpd, and then either use option '6' in CHMFIL20 or the Review and Change Online Data subroutine described in Section 8.5 to process Kpm. Figure 26 demonstrates Kpm processing with CRDES20 entry from CHMFIL20 (DEFCHEM.DAT data are online).

```
***************** Kpm ESTIMATION METHOD OPTIONS ****************
          Enter value for desired method
 Select '0' to exit without any calculation
 Select '1' to estimate Kpm from Kpat
 Select '2' to estimate Kpm from Kpd
 Enter your selection: 1
 ************* NON-CHEMICAL DATA ACCESSION SUBROUTINE ************
 Last .LDS file downloaded was... defaulxx.lds
 Last .LDS file operation was...  File downloaded in CRDES20
 Last .LDS file stored was...
 Title for online non-chemical data file is...  Brand new title line
 REVIEW OF .LDS FILES AVAILABLE
E:\THEMOD20\DISK3
DEFAULTX.LDS       DEFAULT .LDS       DEFAULXX.LDS
 1114112 Bytes free

 HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
 Select '0' to exit without any selection
 Select '1' to use DEFAULT.LDS non-chemical data
 Select '2' to use non-chemical data from a .LDS file you select
 Select '3' to use non-chemical data which are online.
 Enter your selection: 2
 ENTER .LDS FILE: defaulxx
 ------------------------------------------------------------
 Title for downloaded file is...  Brand new title line
 157 Kpat, Plant(forage) to adipose tissue p.c.,mg/kg per mg/kg dwb =  .005
 61  fm, fat content in beef =  .2
 168 Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb) =
 9.999999E-04

 ***** Central Processing Routine *****
 Wish to do more? (enter 'yes' or 'no'):
```

Figure 26. Sample Kpm Subroutine Processing. CRDES20 Access From CHMFIL20.

10.4.2 Plant to Milk Partition Coefficient (Kpd)

Two options are available for estimating Kpd. They are "mirror images" of those used for Kpm, where fm and fd are switched in equations. Thus, the equations involved are: Kpd = Kpat x fd and Kpd = Kpm x fd / fm . Option 1 requires Kpat input for CRDES20 access from OPEN20. Option 2 requires Kpm input for CRDES20 access from OPEN20.

10.4.3 Soil to Water Partition Coefficient (Kd)

The routine estimates Kd from the relation Kd = foc x Koc. There are five Kd data that may be evaluated in PHAS, and each may have a different foc associated with it. Thus, the first prompt is:

```
Which Kd do you want? (enter '1' for Kd1, '2' for Kd2, etc.)
Enter your selection:
```

If CRDES20 is accessed from OPEN20, the user will have to know which foc corresponds to which subscript. After this prompt, the Non-Chemical Data Accession Subroutine menu appears. IF CRDES20 is entered from OPEN20, after the response to that menu, Koc data is manually entered. For entry from CHMFIL20, only the response to the Non-Chemical Data Accession Subroutine menu is required.

10.4.4 Soil to Surface Water Runoff Coefficients (MKro1 and MKro2)

The surface runoff partition coefficient indicates the mg/kg pollutant in soil at a contaminated site required to provide 1 mg/L in a surface water body. For simplicity, the subscripts will be dropped (they refer to the subsite watershed designation). Prior to the method selection step, the user must designate the subsite. This message appears:

For which subsite is MKro to be computed?
Enter '1' for subsite #1 - '2' for subsite #2
Enter your selection here:

Three methods are available to value these coefficients. KD1 (or KD2) is the chemical-related datum required. The non-chemical data are obtained from a .LDS file via the Non-Chemical Data Accession Subroutine menu described above.

Methods Detail

The first method is the "adjusted" Kd model. Here, MKro = Kd + thav/rh . This equation assumes that all runoff water has attained equilibrium with contaminated soil, which can be considered the "worst case" situation.

The second method uses the relation: MKro = (Acw / Aw) x (Kd + thav/rh) . This equation assumes that all the runoff water from the contaminated site attains equilibrium with contaminated soil as in the first method. However, the runoff water is "diluted" by clean water from non-contaminated portions of the surface water body watershed. The runoff water volume per unit area is the same in all parts of the watershed.

The third model is the "USLE-Haithe" approach. The "USLE", the acronym for Universal Soil Loss Equation, is discussed in Section 2.4.3 of the Superfund Exposure Assessment Manual (SEAM)[7]. This empirical equation was developed by Wischmeier and Smith[16], and provides an estimate of sediment runoff (SOILLD)*. In terms of kg/year, this runoff is:

$$SOILLD = 2240\ Acw \times (K \times LS \times C \times P \times R)$$

Acw, K, LS, C and P are unique for a given watershed. The rain/runoff factor for a contaminated site (R) is site-specific. R factors have been determined for the United States East of the Rocky Mountains, and appear in Figure 27.

The next step within the method is to partition pollutant between sediment and runoff with the "Haithe" model[17]. This model is based on a mass balance between rain and contaminated soil and assumes that the partitioning is restricted to the surface soil to a 1 cm depth. For convenience, a term KFACT = Kd x rh/(FC-WP) is defined. Then, a 1 mg/kg pollutant concentration in topsoil provides a corresponding concentration in sediment (KSFACT) and in runoff water (KWFACT):

$$KSFACT = KFACT/(1+KFACT)$$
$$KWFACT = 1/(1+KFACT)$$

* Here, and in subsequent sections, the symbols used are either those shown in Table 2 or those used in the COMPUT20 program code (see Appendix B).

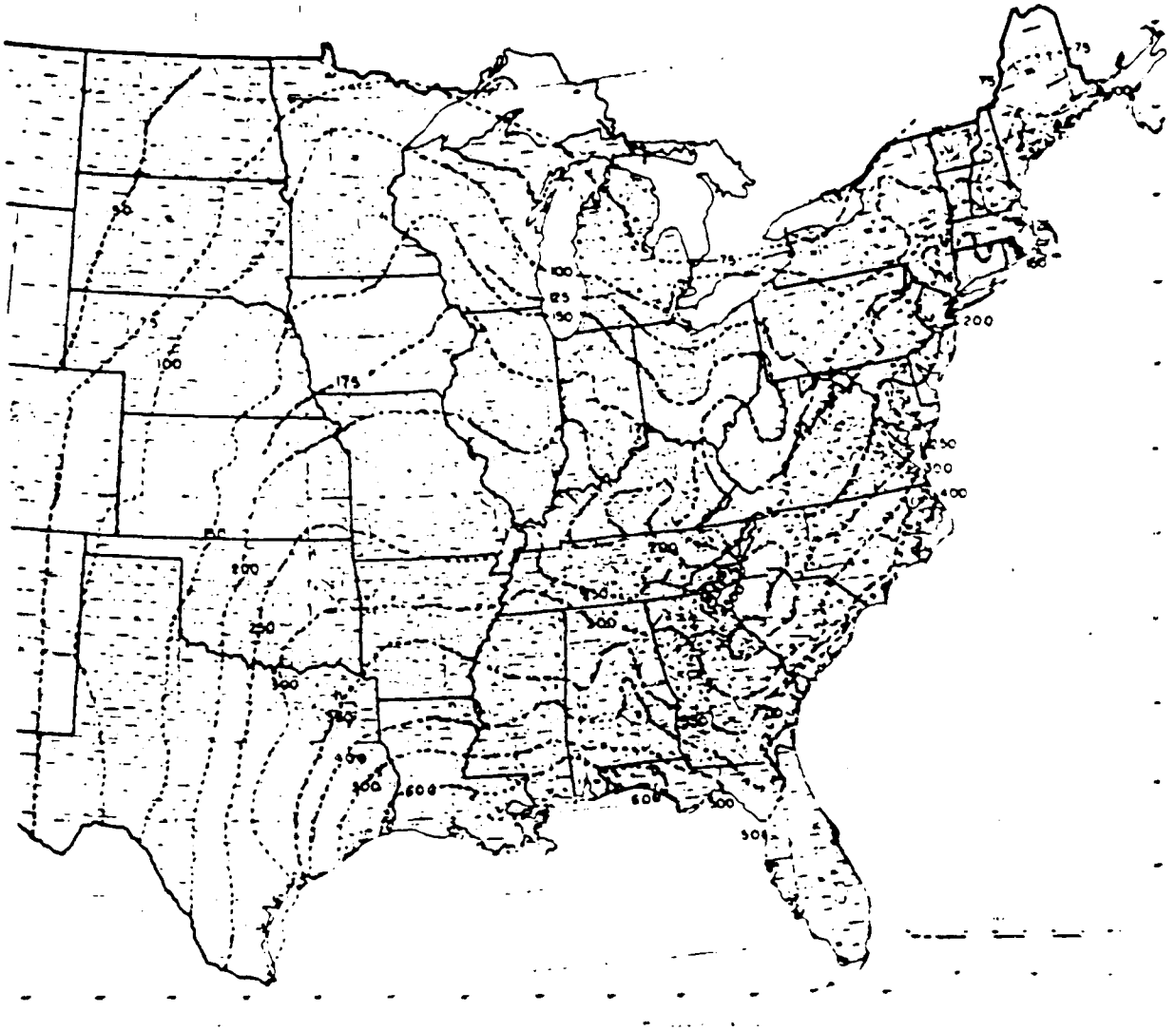

Figure 27. Rain/Runoff Factors for the Eastern United States[16]

The mg/year of pollutant in sediment carried off in runoff water is given by the product SOILLD x KSFACT. The yearly runoff (RUNOF) in liters/year is: RUNOF = $1x10^7$ Acw x RO / 39.37. The coefficient converts from hectares to m^2 and m^3 to liters, while 39.37 converts meters to inches. Haithe[17] makes an "adverse case" assumption that all runoff water from the contaminated site attains the concentration KWFACT. Then, the dissolved pollutant transported in this runoff is the product RUNOF x KWFACT. The total pollutant transported from a site is POLLOAD, which in mg/year, is

SOILLD x KSFACT + RUNOF x KWFACT

A conservative assumption made in PHAS20 is that the surface soil concentration of pollutant remains at 1 mg/kg. This differs from the presentation in SEAM[7], and that of Haithe[17].

As in the second method, there may be inputs of non-contaminated water to the surface water body. The yearly input of such water is called UPFLOW:

UPFLOW = $3.16x10^{10}$ Qu

The coefficient converts from years to seconds and m^3 to liters. Then, MKro = (UPFLOW+RUNOF)/POLLOAD. Figure 28 is a sample of the method display on the monitor. In this example, CRDES20 is accessed from OPEN20.

10.4.5 Soil Flux Partition Coefficients (MKdb and MKdo)

These partition coefficients indicate the mg/kg in soil needed to produce a vapor flux of 1 mg/m^2-day from a uniformly contaminated area. As with MKro1 and MKro2, one subroutine handles both coefficients. The 'db' subscript refers to vapor diffusion in a basement, while the 'do' subscript refers to vapor diffusion to the outdoors. In terms of the diffusion from soil to air step per se, the methodology is similar for both coefficients. The next step is the dilution of diffused pollutant with bulk air, and the "MX" factors discussed in Section 6.4 account for this step.

A message similar to that presented for MKro1 and MKro2 appears:

For which situation is MK(diffusion) to be computed?
Enter '1' for basement - '2' for outdoors
Enter your selection here:

The chemical-related data inputs are Kd3 (for MKdb) or Kd4 (for MKdo), Da, and Kh. When CRDES20 is entered from OPEN20, these inputs are manually entered. When this subroutine is accessed from the CRDES20 Selection Menu, both the long-term and short-term MKdb or MKdo data will be estimated and displayed. If CRDES20 is accessed via CHMFIL20 option '6', when CHMFIL20 is re-entered, the long-term and short-term data are displayed a second time (see Figure 29 for a demonstration). This subroutine does not have an explicit "exit without calculation" selection prompt. To exit, enter '0' at the Non-Chemical Data Accession Options prompt.

```
********** MKro1 and MKro2 ESTIMATION METHOD OPTIONS **********
Note, for brevity, suffix for watershed site (1 or 2) is 'j'
Select '0' to exit this subroutine without calculation
Select '1' to compute MKswj as adjusted Kdj
Select '2' to compute KKswj as Kdj adjusted for watershed area;
   uses above data and total and contaminated watershed area data
Select '3' for 'USLE-Haith' approach for runoff & sediment
Enter your selection here: 3
************* NON-CHEMICAL DATA ACCESSION SUBROUTINE *************
Last .LDS file downloaded was... defaulxx.lds
Last .LDS file operation was...  File downloaded in CRDES20
Last .LDS file stored was...
Title for online non-chemical data file is...  Brand new title line
REVIEW OF .LDS FILES AVAILABLE
E:\THEMOD20\DISK3
DEFAULTX.LDS       DEFAULT .LDS       DEFAULXX.LDS
 1114112 Bytes free

HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
Select '0' to exit without any selection
Select '1' to use DEFAULT.LDS non-chemical data
Select '2' to use non-chemical data from a .LDS file you select
Select '3' to use non-chemical data which are online.
Enter your selection: 1

Title for downloaded file is...
Default file for starting new .LDS file.  Check user's guide for parameter value
derivation.
Enter KD Value : 25
 82  rh1, bulk density, topsoil e1 subsite, kg/L =  1.4
 83  th1, average moisture capacity, topsoil e1 subsite, L/L =  .1
 170 Kd1 soil/water p.c. for e1 subsite pathways, mg/kg / mg/L =  25
 84  Acw1, contaminated area of e1 subsite, ha =  10
 86  WP1, wilt point, topsoil e1 subsite =  .08
 87  FC1, field capacity, topsoil e1 subsite =  .25
 88  K1, erodability factor for e1 subsite =  .35
 89  LS1, length-slope factor for e1 subsite =  1
 90  C1, crop cover factor for e1 subsite =  .12
 91  P1, erosion control factor for e1 subsite =  1
 92  RO1, runoff from e1 subsite, inches/year =  8
 93  Qu1, Annual ave. flow above e1 subsite outfall, m^3/sec =  .2
 94  R1, rain/runoff factor for contaminated site =  150
 181 MKro1, model soil-water p.c., e1 subsite runoff, mg/kg / mg/L =  26566.54

***** Central Processing Routine *****
Wish to do more? (enter 'yes' or 'no'):
```

Figure 28. Sample Display for the USLE-Haithe Estimation Method of MKro1

Method Details

The method uses the Farino adaptation of the Thibodeaux and Hwang equation discussed in SEAM, Section 2.3.2.1.(4)[7]. The equation is a solution of the one-dimensional, unsteady state partial differential diffusion equation:

$$\partial^2 C / \partial z^2 = D \, \partial C / \partial t$$

where C is the concentration of pollutant in bulk soil (all phases), z is the depth dimension (z = 0 at the surface and increases with depth), D is a soil diffusivity, and T is time. Call C(z,t) the solution to this equation, a concentration for any positive time and position. The surface flux is related to this concentration: $D \times (\partial C(z,t)/\partial t)_{z=0}$

```
 HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
 Select '0' to exit without any selection
  (use for exit from subroutine)
 Select '1' to use DEFAULT.LDS non-chemical data
 Select '2' to use non-chemical data from a .LDS file you select
 Select '3' to use non-chemical data which are online.
 Enter your selection: 1
 Title for downloaded file is...
Default file for starting new .LDS file.  Check user's guide for parameter value
 derivation.
 173 Kd4 soil/water p.c. for outside diffusion, mg/kg / mg/L =  15
 161 Da, Molecular diffusivity in air, m^2/sec =  .55
 163 Kh, Henry Law constant, dimensionless [conc/conc] =  .00003
 122 rh4, bulk density, soil for outside diffusion, kg/L =  1.8
 123 th4, soil fraction voids with water, outside diffusion, L/L =  .15
 124 ep4, soil fraction voids with air, outside diffusion, L/L =  .2
 125 do, initial top of pollution layer below grade, outside diffusion, m =  .1

 126 ho, lower depth of pollution layer, outside diffusion, m =  5
 55  OTa, Time exposure for adult off-site receptors, days =  25600
dryout time,days =  5.413163E+08
 185 MKdoa, soil flux p.c., outdoors long-term, mg/kg per mg/m^2-day =

 2462.334
 Press enter (return) key to continue....
 ****** Calculation for short-term time frame.  Unless specified,
 data inputs are as previously displayed *****
 56  OTc, Time exposure for child off-site receptors, days =  365
dryout time,days =  5.413163E+08
 186 MKdoc, soil flux p.c., outdoors short-term, mg/kg per mg/m^2-day =
 2394.596

 ***** Central Processing Routine *****
 Wish to do more? (enter 'yes' or 'no'): no
 *** END CRDES FOR SELECTED DATA ***
 Current status of value for
 185 MKdoa, soil flux p.c., outdoors long-term, mg/kg per mg/m^2-day is
 2462.334
 Current documentation message:
default file, select '6' to see information messages.

 Current status of value for
 186 MKdoc, soil flux p.c., outdoors short-term, mg/kg per mg/m^2-day is
 2394.596
 Current documentation message:
default file, select '6' to see information messages.
 Hit enter (return) key to continue....
```

Figure 29. Sample Display for MKdo Estimation. CRDES Accessed From CHMFIL20 with Option '6'.

The SEAM flux solution is based on the following assumptions:

(1) only one-dimensional flux to the surface via the air phase is addressed (water-phase diffusion can be neglected).

(2) At an initial time, the pollutant is at a uniform concentration from the surface to a finite depth (an initial condition for solution of a differential equation). This depth is hb in the method for the MKdb coefficients, and ho in the method for the MKdo coefficients.

(3) The concentration of the pollutant in air immediately above the soil surface is initially zero.

(4) In the contaminated soil layer, equilibrium is established between the substance in soil, soil water, and the air in soil voids

(5) Isothermal conditions prevail in the soil column.

(6) No other mechanism of pollution depletion occurs, nor is the soil column physically disturbed.

Immediately after the initial time (assumption 2), diffusion begins. The concentration of substance at the soil surface decreases. As a concentration gradient develops in the soil column, the substance is exhausted from the topmost layer of soil. At the time of sampling, which is not necessarily the initial time mentioned above, the substance is confined to a layer which extends from a distance below grade of db (or do, see above for hb and ho) to hb or ho. The substance has been "flashed" from soil strata above the depth db (or do). The time of sampling is "time zero" for the purpose of the assessment analysis. The analysis addresses an exposure period to human receptors. This exposure period is either BTa or BTc (for the basement, long-term and short-term exposure respectively) or OTa or OTc (for the outside). In the equations below, the exposure period is called BOT.

The initial concentration of pollutant in soil is 1 mg/kg. For evaluation, these terms are defined for the basement situation; the '3' subscript is used to be consistent with equations in the COMPUT20 code:

$$KDA = Kd3 + th3/rh3$$

$$DEI = (Kh \times Da \times ep3^{10/3})/(th3 + ep3)^2$$

$$KDJJ = rh3 \times KDA + th3 + Kh \times ep3$$

DEI is similar to the "phase transfer coefficient" of equation 2-12 in SEAM[7]. However, the Millington- Quirk porosity adjustment term is used here rather than the $ep^{4/3}$ term suggested in SEAM[7]. The author considers that term as unnecessarily conservative. KDJJ corresponds to the term C_S/C_B in equations 2-11 and 2-14 in SEAM[7]. First, a dryout time, TTYME, is computed:

$$TTYME = (KDJJ \times [hb^2 - db^2]) / (2\ DEI)$$

If TTYME < BOT , the pollutant is essentially stripped from the soil layer before the end of the exposure period. In that case, the message " Dryout occurs within <TTYME> days " appears. In this case, the average flux is the pollutant mass in the layer divided by BOT or

$$FLUX = 1000\ rh3 \times (hb - db)/BOT$$

and MKdb = 1/FLUX. The coefficient converts liters to m^3. If BOT > TTYME, the process will be diffusion-limited. In that case, the average flux for the exposure period is

$$FLUX = 2000\ DEI/(KDA \times [db + SQRTERM^{0.5}])$$

where $SQRTERM = db^2 + 2\ DEI \times BOT/KDJJ$. Once more, MKdb = 1/FLUX.

Figure 29 is sample display of method processing for MKdo, where entry to CRDES20 is via option '6' in CHMFIL20.

10.4.6 Sediment Flux Partition Coefficient (MKdw)

MKdw indicates the mg/kg in sediment needed to produce a pollutant in water flux of 1 mg/m^2-day from an uniformly contaminated area. For the method presented, the chemical-related data inputs are Kd5 and Dw. As with MKdb and MKdo, when this subroutine is accessed via the CRDES20 Selection Menu, both the long-term and short-term MKdw values will be estimated and displayed. If CRDES20 is accessed via CHMFIL20 option '6', when CHMFIL20 is re-entered, the long-term and short-term MKdw are displayed a second time. This subroutine does not have an explicit "exit without calculation" selection prompt. To exit, enter '0' at the Non-Chemical Data Access'on Options prompt. Figure 30 demonstrates the monitor display for estimation of MKdwa when CHMFIL20 data processing is under DUST control. The CHMFIL2C-CRDES20 interfaces are shown. The information statement for MKdwa has been abridged.

Method Details

The presented method uses an equation similar to that discussed for MKdb and MKdo, except that diffusion occurs only in the water phase of sediment, and the flux is directed to open water above the sediment. The equation is based on these assumptions:

(1) Only one-dimensional flux to the sediment surface-water bottom interface is considered.

(2) At an initial time, the pollutant is at a uniform concentration in a finite depth layer (an initial condition for solution of a differential equation). This layer extends from the the sediment surface to a depth hp5.

(3) The concentration of pollutant at the sediment-water interface is initially zero.

(4) In the contaminated sediment layer, equilibrium is established between the substance in sediment and water in sediment voids.

(5) Other mechanisms leading to pollutant loss from sediment or sediment scouring by open water turbulence are not addressed.

(6) Isothermal conditions prevail throughout the exposure period.

Immediately after the initial time, diffusion begins, and the concentration of substance at the sediment surface decreases. As a concentration gradient develops in the sediment column, the substance is exhausted from the topmost sediment layer. At the time of sampling, which is again not necessarily the initial time, the substance is confined to a layer which extends from a distance below sediment surface grade, dp5. The substance has been "flashed" from sediment strata above dp5. The time of sampling is the zero time for the the assessment analysis. The analysis is to cover an exposure period of STa (long-term) or STc (short-term).

```
Enter your selection: 1
****************
187 MKdwa, sediment-openwater p.c. long-term, mg/kg per mg/m^2-day =  Ø
Documentation: default file, select '6' to see information messages.
Main input variable to intake pathway eqtn.
Select '1' to accept current value.
Select '2' to replace value
Select '3' for variable's info/estimation subroutine in CRDES2Ø.
Estimation routine available.
Select '4' to replace documentation message
Enter your selection: 3


*************** INFORMATION ON ************************
187 MKdwa, sediment-openwater p.c. long-term, mg/kg per mg/m^2-day
  MKdw is a 'model' sediment-water p.c. for the diffusion of
pollution from a sediment deposit to a waterway, and indicates the mg/kg
of pollutant in sediment which produces a flux of 1 mg/m^2-day pollutant at

  NOTES  **1** If you use this estimation method, and accessed CRDES2Ø from
OPEN2Ø, you must manually enter Kd and Dw. **2** If you access this
method from the CRDES2Ø Selection Menu, both the long and short term MKdw
values are calculated.
Press enter (return) key to continue....
************* NON-CHEMICAL DATA ACCESSION SUBROUTINE ************
Last .LDS file downloaded was...
Last .LDS file operation was...
Last .LDS file stored was...
Title for online non-chemical data file is...
REVIEW OF .LDS FILES AVAILABLE
E:\THEMOD2Ø\DISK3
DEFAULTX.LDS      DEFAULT .LDS      DEFAULXX.LDS
1089536 Bytes free

HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
Select 'Ø' to exit without any selection
 (use for exit from subroutine)
Select '1' to use DEFAULT.LDS non-chemical data
Select '2' to use non-chemical data from a .LDS file you select
Select '3' to use non-chemical data which are online.
Enter your selection: 1


174 Kd5 sediment/water p.c., mg/kg / mg/L =  5Ø
162 Dw, Molecular diffusivity in water, m^2/sec =  .ØØØØ55
72  rh5, bulk density of sediment, kg/L =  1.5
73  th5, void fraction of sediment, L/L =  .4
74  dp5, initial top of pollution layer in sediment below grade, m =  .5
75  hp5, bottom depth of pollution layer in sediment below grade, m =  5
76  STa, adult exposure time, sediment-based pollutant, days =  25600
Washout time =  5.756282E+Ø7
187 MKdwa, sediment-openwater p.c. long-term, mg/kg per mg/m^2-day =  1567.391


***** Central Processing Routine *****
Wish to do more? (enter 'yes' or 'no'): no
****************
187 MKdwa, sediment-openwater p.c. long-term, mg/kg per mg/m^2-day =  1567.391

Documentation: default file, select '6' to see information messages.
Main input variable to intake pathway eqtn.
Select '1' to accept current value.
Select '2' to replace value
Select '3' for variable's info/estimation subroutine in CRDES2Ø.
Estimation routine available.
Select '4' to replace documentation message
Enter your selection:
```

Figure 30. Sample MKdwa Estimation. CRDES20 Accessed From CHMFIL20 Under DUST Control.

The calculation starts with a 1 mg/kg level of pollutant in sediment. For evaluation, these terms are defined:

$$KDJ = KD5 + th5 / rh5$$
$$KDJJ = rh5 \times KDJ$$
$$DEI = DW \times th5^{4/3}$$

Similarly to MKdb, a washout time can be calculated:

$$TTYME = (KDJJ \times [hp5^2 - dp5^2]) / (2\ DEI)$$

The subroutine checks to see if STa or STc, whichever is applicable) exceeds TTYME; in the equations below, the assessment exposure time is called SOT. If so, the message: "Washout occurs before <TTYME> days" appears, and the average flux is computed as FLUX = 1000 rh5 x (hp5 - dp5)/ SOT .

Otherwise, the average flux is computed as

$$FLUX = 2000\ \ DEI/(KDJ \times [dp5 + SQRTERM^{0.5}])$$

where $SQRTERM = dp5^2 + 2\ DEI \times SOT/KDJJ$. Finally, MKdw = 1/FLUX.

10.4.7 Groundwater Infiltration Partition Coefficient (MKgw)

MKgw indicates the mg/kg in topsoil or near surface soil required to produce 1 mg/L in groundwater. In the subroutine method, Kd4 is the only chemical-related datum. When this subroutine is accessed via the CRDES20 Selection Menu, both the long-term and short-term data values will be estimated and displayed. If CRDES20 is accessed via CHMFIL20 option '6', when CHMFIL20 is re-entered, the long-term and short-term data are displayed again (see Figure 29). Figure 31 shows the monitor display of the method when CRDES20 is accessed from OPEN20. This subroutine does not have an explicit "exit without calculation" selection prompt. To exit, enter '0' at the Non-Chemical Data Accession Options prompt.

Method Details

The method presented is an elementary treatment of the removal of pollutant from soil via its transfer to rainwater that infiltrates to the aquifer. This rainwater is called "infiltrate". Assumptions made are:

(1) The infiltration rate is the same each year.

(2) Kd4 relates the concentrations of pollutant in soil and infiltrate.

(3) Infiltrate is thoroughly mixed with groundwater in the aquifer prior to groundwater use for domestic purposes.

(4) The area contaminated, A04, is the same area which would be involved in outside diffusion.

(5) The removal of pollutant from the unsaturated soil column by diffusion to outdoor air or runoff is neglected. This is a conservative assumption.

```
 REVIEW OF .LDS FILES AVAILABLE
E:\THEMOD20\DISK3
DEFAULTX.LDS      DEFAULT .LDS      DEFAULXX.LDS
 1089536 Bytes free

 HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
 Select '0' to exit without any selection
  (use for exit from subroutine)
 Select '1' to use DEFAULT.LDS non-chemical data
 Select '2' to use non-chemical data from a .LDS file you select
 Select '3' to use non-chemical data which are online.
 Enter your selection: 3
 Enter Kd4 value: 5
 122 rh4, bulk density, soil for outside diffusion, kg/L =  1.8
 127 A04, area of site with diffusing vapors, ha =  10
 132 TK6, initial thickness of pollutant in soil, m =  10
 133 RI6, infiltration of rainwater to aquifer, m/year =  .1
 134 VGW6, velocity of groundwater flow, m/year =  365
 135 TAQ6, thickness of aquifer, m =  10
 136 th6, effective porosity in aquifer, L/L =  .35
 52  BTa, Time exposure for adult on-site residence occupancy, days =  25600
 189 MKgwa, topsoil-groundwater p.c. long-term, mg/kg per mg/L =  210070
 Press enter (return) key to continue....

 ****** Calculation for short-term time frame.  Unless specified,
 data inputs are as previously displayed *****
 53  BTc, Time exposure for child on-site residence occupancy, days =  365
 190 MKgwc, topsoil-groundwater p.c. short-term, mg/kg per mg/L =  202208.2

 ***** Central Processing Routine *****
 Wish to do more? (enter 'yes' or 'no'):
```

Figure 31. Sample MKgwa and MKgwc Estimations. CRDES20 Accessed From OPEN20.

---

(6) The exposure time of concern is that employed in the basement diffusion pathways (BTa or BTc). As inputs, they are in day units. In the equations below, the exposure time term BYT is in years.

(7) The removal of pollutant in infiltrate is treated as a step procedure, where each step is a year. The number of steps is BYT. Within each step time interval, the concentration of pollutant in soil remains constant. Changes in concentration are assessed between steps.

(8) Any dispersion or retardation effects during transport to a down-gradient domestic water user are ignored. This is a conservative assumption.

(9) The groundwater flows under the area A04 at a uniform speed. The area approximates a square, and flow is directed normal to two opposite sides of the square.

Initially, the pollutant concentration in soil is 1 mg/kg. The pollutant mass (in mg) in a segment TK6 m deep per unit exposed surface area (in m^2) is MASSINT = 1000 TK6 x rh4. Since TK6 is in m units and rh4 has units kg/L, the 1000 factor is required.

A mass balance after the first step in the process is:

$$MASSINT = 1000\ RI6 \times Cw + MASSINT \times Cs$$

where Cw refers to pollutant concentration in infiltrate (mg/L) and Cs refers to the residual pollutant concentration in soil at the end of the step (mg/kg). The 1000 converts m^3 to L. Cs and Cw are related:

$$Kd4 = Cs/Cw$$

Let LEACHFT = 1000 RI6/KD4. From the above two equations, an attenuation factor, ATTNFACT, can be expressed as:

$$\text{ATTNFACT} = \text{MASSINT}/(\text{LEACHFT} + \text{MASSINT})$$

ATTNFACT equals Cs when the initial concentration is 1 mg/kg. Moreover, ATTNFACT also indicates the relative concentration in soils at the end and start of any subsequent step. After BYT steps, the fraction removal of initial pollutant in infiltrate, TRANSFACT, is given by:

$$\text{TRANSFACT} = 1 - \text{ATTNFACT}^{\text{BYT}}$$

The mass transferred to groundwater in mg for the entire process, MASSTRAN, is

$$\text{MASSTRAN} = 10000\ \text{MASSINT} \times \text{TRANSFACT} \times \text{A04}$$

The 10000 converts hectares to m^2. In BYT years, the total infiltrate volume (in liters), VOLINF, is: $\text{VOLINF} = 10^7\ \text{RI6} \times \text{BYT} \times \text{A04}$. This volume is "diluted" by groundwater. The dilution occurs in a section of aquifer of depth TAQ6 and width LOA, where $\text{LOA} = 100\ \text{A04}^{0.5}$ (TAQ6 and LOA are in m). In BYT years, the volume of groundwater in liters passing through this section is VOLAQF:

$$\text{VOLAQF} = 10^3\ \text{LOA} \times \text{th6} \times \text{TAQ6} \times \text{VGW6} \times \text{BYT}$$

MKgw is the inverse of pollutant concentration in the groundwater plume, or MKgw = (VOLAQF+VOLINF) / MASSTRAN.

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2.0 References Cited in PHAS20 Displays Only

The following references are cited in PHAS20 display messages, but not in the text. After the reference, the first file in alphabetical order that cites the reference is presented. All .CMP files precede .NCI files. All files can be read by a word-processing program that handles ASCII files, or the DOS TYPE utility.

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APPENDIX A. GLOSSARY OF TERMS AND DATANAMES USES IN PHAS20

Table A-1. Frequently-Used Terms and Acronyms.

BASIC - Programming language used to execute PHAS20, such as the Microsoft GW-BASIC, IBM BASICA, or more recent developed BASIC interpreters).

CRDES - Chemical-related data estimation subroutines.

.DAT - Extension for file used to store chemical-specific data.

data - numerical values used in intake or constraint equations.

dataname - title used in PHAS20 to describe a specific datum.

Disk 1 - The magnetic storage hardware containing PHAS20 executable programs and supplemental files.

Disk 2 - The magnetic storage hardware containing PHAS20 external files.

Disk 2 device - The magnetic storage item used to hold .DAT, .LDS, and .PXX files developed by the user. This may be a disk drive for an external diskette or a portion of a hard disk designated by subdirectory assignment.

DOS - Disk Operating System (Microsoft MS-DOS, Version 3.3) for IBM personal computers and compatible hardware systems.

download - As a verb, the act of transferring data or information from a file in storage to program memory. The term downloaded is an adjective to describe the transfer of file contents.

DUST - Data Use Status Table. This is an array of numerical information, each element of which indicates the status of the dataname with the same index in a scenario.

DUST control - use of the DUST from a .PXX file to restrict the data processing program presentations of data to only those items relevant to the scenario in the .PXX file.

dwb - Dry weight basis

EPA - U.S. Environmental Protection Agency

external file - a designated collection of information or data created and stored for use in PHAS20 programs. Each file has a unique file name.

FIN - Fragment identifier number.

HDC - horizontal dispersion coefficient (also known as "sigma-y").

index - A number which identifies a particular element of an array.

information - numerical values or text used for purposes other than as inputs to PHAS20 equations.

.LDS - Extension for file used to store non-chemical specific data

medium - a repository of a pollutant in the environment that is subject to remediation. Thus, the user may process pathways involving exposure via water when soil is the definitive medium.

online - capable of being transferred between PHAS20 programs (programmers refer to data or information with this attribute as COMMON)

p.c. - Partition coefficient

PHAS20 - Pollutant Hazard Assessment System, this version.

PPLV - Preliminary Pollutant Limit Value

.PXX - Generic extension for file used to store scenario information. Based on remedial medium, it can be .PSD, .PTS, or .PWA

SST - Scenario selection table. An array of numerical information, where each element indicates whether a certain pathway is included in a scenario.

TA - Time averaged (usually for an intake exposure parameter restricted to a few days per year divided by a year to express on a per day basis).

variable - The name of an information or data element or single unit used in PHAS20 programs.

Table A-2. Data Names and Symbols Used in PHAS20

Index	Identification of Dataname
1	BWa, adult body weight, kg
2	IWa, adult drinking water intake, L/day
3	EIWa, adult oral water equiv. for inhaled pollutants, L/day
4	DAWa, adult body surface for dermal exposure to water, m^2
5	DETa, adult dermal exposure time to domestic water, hr/day
6	OIWa, swimwater ingested by adult, L/TA day
7	ORWa, adult respiration rate during water activity, m^3/TA day
8	ODTa, adult water activity immersion time, hour/TA day
9	Wfa, adult fish consumption, kg/day
10	Wva, adult vegetable consumption, kg dwb/day
11	Wma, adult beef consumption, kg/day
12	Wda, adult milk consumption, L/day
13	SIRa, adult oral intake of soil, residential, kg/day
14	SARa, adult exposure area to dust on skin, residential, m^2
15	PLa, adult perspiration rate, L/m^2/day
16	RIa, adult respiration rate, residential, m^3
17	CSI, construction area-related dust intake, kg/workday
18	BIRa, adult respiration rate, basement vapors, m^3/day
21	BWc, child body weight, kg
22	IWc, child drinking water intake, L/day
23	EIWc, child water oral water equiv. for inhaled pollutant, L/day
24	DAWc, child body surface for dermal exposure to water, m^2
25	DETc, child dermal exposure time to domestic water, hr/day
26	OIWc, swimwater ingested by child, L/TA day
27	ORWc, child respiration rate for water activity, m^3/TA day
28	ODTc, child water activity immersion time,hr/TA day
29	Wfc, child fish consumption, kg/day
30	Wvc, child vegetable consumption, kg/day
31	Wmc, child beef consumption, kg/day
32	Wdc, child dairy consumption, L/day
33	SIRc, child oral intake of soil, residential, kg/day
34	SARc, child exposure area to dust on skin, residential, m^2
35	PLc, child perspiration rate, L/m^2/day
36	RIc, child respiration rate, residential, m^3
38	BIRc, child respiration rate, basement vapors, m^3/day
41	S(DWa), Adjustment factor/adult domestic water exposure pathways
42	S(DWc), Adjustment factor/child domestic water exposure pathways
43	S(OW), Adjustment factor/water activity pathways
44	S(Wf), Adjustment factor/fish consumption
45	S(Wv), Adjustment factor/vegetable consumption
46	S(Wm), Adjustment factor/beef consumption
47	S(Wd), Adjustment factor/dairy consumption
48	S(RSa), Adjustment factor/adult daily soil residential intake
49	S(RSc), Adjustment factor/child daily soil residential intake
50	S(CSa), Adjustment factor/construction area soil intake

Table A-2. Data Names and Symbols Used in PHAS20

Index	Identification of Dataname
51	S(BIR), Adjustment factor/basement vapors exposure
52	BTa, Time exposure for adult on-site residence occupancy, days
53	BTc, Time exposure for child on-site residence occupancy, days
54	S(EIR), Adjustment factor/external vapor exposure
55	OTa, Time exposure for adult off-site receptors, days
56	OTc, Time exposure for child off-site receptors, days
61	fm, fat content in beef
62	fd, fat content in milk
63	Uwm, water intake by steer, L/day
64	Upm, plant (forage) intake by steer, kg (dwb)/day
65	Usm, soil intake by steer, kg/day
66	Uwd, water intake by dairy cow, L/day
67	Upd, plant (forage) intake by dairy cow, kg (dwb)/day
68	Usd, soil intake by dairy cow, kg/day
69	BWM, representative steer body weight, kg
70	BWD, representative dairy cow body weight, kg
71	foc5, fraction organic carbon content of sediment
72	rh5, bulk density of sediment, kg/L
73	th5, void fraction of sediment, L/L
74	dp5, initial top of pollution layer in sediment below grade, m
75	hp5, bottom depth of pollution layer in sediment below grade, m
76	STa, adult exposure time, sediment-based pollutant, days
77	STc, child exposure time, sediment-based pollutant, days
78	As5, surface area of contaminated sediment in waterway, ha
79	Qu5, annual flow of waterway below polluted sediment locale, m^3/sec
81	foc1, fraction organic carbon, topsoil #1 subsite
82	rh1, bulk density, topsoil #1 subsite, kg/L
83	th1, average moisture capacity, topsoil #1 subsite, L/L
84	Acw1, contaminated area of #1 subsite, ha
85	Aw1, total watershed area at #1 subsite outfall, ha
86	WP1, wilt point, topsoil #1 subsite
87	FC1, field capacity, topsoil #1 subsite
88	K1, erodability factor for #1 subsite
89	LS1, length-slope factor for #1 subsite
90	C1, crop cover factor for #1 subsite
91	P1, erosion control factor for #1 subsite
92	RO1, runoff from #1 subsite, inches/year
93	Qu1, Annual ave. flow above #1 subsite outfall, m^3/sec
94	R1, rain/runoff factor for contaminated site
96	foc2, fraction organic carbon, topsoil #2 subsite
97	rh2, bulk density, topsoil #2 subsite
98	th2, average moisture capacity, topsoil #2 subsite, L/L
99	Acw2, cont. area for watershed #2 site,ha
100	Aw2, total watershed area at #2 subsite outfall, ha

Table A-2. Data Names and Symbols Used in PHAS20

Index	Identification of Dataname
101	WP2, wilt point, topsoil #2 subsite
102	FC2, field capacity, topsoil #2 subsite
103	K2, erodability factor for #2 subsite
104	LS2, length-slope factor for #2 subsite
105	C2, crop cover factor for #2 subsite
106	P2, erosion control factor for #2 subsite
107	RO2, runoff from #2 subsite, inches/year
108	Qu2, Annual ave. flow above #2 subsite outfall, m^3/sec
109	SLA, soil loading rate on exposed skin, kg/m^2/day
110	RSPA, particulate conc. in air, residential, kg/m^3
111	CWTF, weather&time factor for construction site soil pathway
112	foc3, fraction organic carbon, soil contiguous with basement
113	rh3, bulk density, soil contiguous with basement, kg/L
114	th3, soil fraction voids with water, basement model, L/L
115	ep3, soil fraction voids with air, basement model, L/L
116	db, initial top of pollution layer below grade, basement model, m
117	hb, lower depth of pollution layer, basement model, m
118	Qa3, volume air through basement, m^3/day
119	Ab3, basement area contacting soil diffusing vapors,m^2
120	UW3, wind-speed for on-site exposure to diffusing vapors, m/sec
121	foc4, fraction organic carbon, outside diffusion
122	rh4, bulk density, soil for outside diffusion, kg/L
123	th4, soil fraction voids with water, outside diffusion, L/L
124	ep4, soil fraction voids with air, outside diffusion, L/L
125	do, initial top of pollution layer below grade, outside diffusion, m
126	ho, lower depth of pollution layer, outside diffusion, m
127	AO4, area of site with diffusing vapors, ha
128	UW4, wind-speed for off-site exposure to diffusing vapors, m/sec
129	MH, rep. mixing height, on-site, m
130	DW4, distance from site to off-site receptors, m
131	MH4, rep. mixing height for off-site receptor, m
132	TK6, initial thickness of pollutant in soil, m
133	RI6, infiltration of rainwater to aquifer, m/year
134	VGW6, velocity of groundwater flow, m/year
135	TAQ6, thickness of aquifer, m
136	th6, effective porosity in aquifer, L/L
137	MXb, dilution air factor for vapor flux in basement, day/m^3
138	MXon, dilution air factor for vapor flux to outside on-site, day/m^3
139	MXof, dilution air factor for vapor flux to off-site, day/m^3
141	DTo, Long term NOAEL dose estimate, oral route, mg/kg-day
142	DTos, Short term NOAEL dose estimate, oral route, mg/kg-day
143	DTi, NOAEL dose estimate, inhalation basis, mg/kg/day
144	DTd, NOAEL dose estimate, dermal basis, mg/kg/day
146	MW, Molecular weight, g/mol
147	Tm, Normal or extrapolated melting point, deg C
148	LogP, Log (base10) octanol-water partition coefficient
149	Wsol, Water solubility, mg/L
150	Tb, Normal or extrapolated boiling point, deg C

Table A-2. Data Names and Symbols Used in PHAS20

Index	Identification of Dataname
151	VP, Saturated vapor pressure, mm Hg
152	Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)
153	Ksv, Soil/vegetable p.c., mg/kg (dwb) per mg/kg soil
154	Ksp, Soil/plant (forage) p.c., mg/kg (dwb) per mg/kg soil
155	foc for soil used to determine soil/veg p.c.
156	foc for soil used to determine soil/forage p.c.
157	Kpat, Plant(forage) to adipose tissue p.c.,mg/kg per mg/kg dwb
161	Da, Molecular diffusivity in air, m^2/sec
162	Dw, Molecular diffusivity in water, m^2/sec
163	Kh, Henry Law constant, dimensionless [conc./conc.]
164	PC, Dermal permeability constant, cm/hr
165	BCF, Fish bioconcentration factor, mg/kg fish per mg/L
166	Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L
167	Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L
168	Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb)
169	Kpd, Plant (forage) to milk p.c., mg/L milk per mg/kg (dwb)
170	Kd1, soil/water p.c. for #1 subsite pathways, mg/kg / mg/L
171	Kd2, soil/water p.c. for #2 subsite pathways, mg/kg / mg/L
172	Kd3, soil/water p.c. for basement subsoil, mg/kg / mg/L
173	Kd4, soil/water p.c. for outside diffusion, mg/kg / mg/L
174	Kd5, sediment/water p.c., mg/kg / mg/L
181	MKro1, model soil-water p.c., #1 subsite runoff, mg/kg / mg/L
182	MKro2, model soil-water p.c., #2 subsite runoff, mg/kg / mg/L
183	MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m^2-day
184	MKdbc, soil flux p.c., basement model short-term, mg/kg per mg/m^2-day
185	MKdoa, soil flux p.c., outdoors long-term, mg/kg per mg/m^2-day
186	MKdoc, soil flux p.c., outdoors short-term, mg/kg per mg/m^2-day
187	MKdwa, sediment-openwater p.c. long-term, mg/kg per mg/m^2-day
188	MKdwc, sediment-openwater p.c. short-term, mg/kg per mg/m^2-day
189	MKgwa, topsoil-groundwater p.c. long-term, mg/kg per mg/L
190	MKgwc, topsoil-groundwater p.c. short-term, mg/kg per mg/L
191	TOL, Organoleptic limit - taste in water, mg/L
193	AQTL, Aquatic toxicity limit in water, mg/L
194	PHLW, Phytotoxicity limit in water, mg/L
195	PHLS, Phytotoxicity limit in soil, mg/kg
196	focPS, foc for soil used to determine phytotoxicity limit
197	CTAEL, Cattle toxicity adverse effects limit, mg/kg-day

APPENDIX C. PATHWAY AND CONSTRAINT EQUATIONS

Refer to either Table 2, main text or Table A-2 of Appendix A for symbols. Section C.1 contains assumption statements for intake equations, each preceded by a letter. After each intake equation in Sections C.2 through Sections C.4, assumptions implied in the equation are identified by these letters. The pathway titles are those displayed in PATWAY20 or COMPUT20. Sections C.5 and C.6 provide the algorithms used in Type 1 and Type 2 Constraint analyses.

In addition to the assumptions implied in intake equations, there are assumptions associated with "super" partition coefficients computed in NOCHFL20 and CRDES20. The sections of main text that discuss these coefficients are:

Datanames	Text Section
MXb, MXon, MXof	6.4
MKro	10.4.4
MKdb, MKdo	10.4.5
MKdw	10.4.6
MKgw	10.4.7

C.1 ASSUMPTIONS IMPLIED IN PATHWAY INTAKE EQUATIONS

a. Differences in consumption rates between nominal daily intakes (intake per day of either liquid, food, soil or air) and pathway intakes are accounted for by the S() adjustment factors.

b. No allowance is made for destruction or transformation of pollutants by such processes as photolysis, microbial action, oxidation or reduction, or hydrolysis.

c. Pollutant content in the medium of concern remains constant throughout the scenario exposure time period.

d. The EIWa and EIWc values in DEFAULT.LDS are evaluated according to treatment advanced by McCone[18]. In his model, the concentration of a volatile pollutant is computed for three compartmental parts of a house: the shower, the bathroom, and the rest of the house. Moreover, a "rest of the house compartment" average concentration is determined for the time periods, 7 AM to 11 PM and 11 PM to 7 AM. Specific activities leading to exposure are assigned to time periods. The inhaled intake of the pollutant is then

$$\Sigma \text{ Activity time} \times \text{Concentration} \times \text{Inhalation Rate} \times \text{Uptake efficiency}$$

where the summation is for each activity in a specific house compartment. McCone[18] computes concentrations for a 1 mg/L content of pollutant in water. In PHAS20, perchloroethylene is selected as a reference pollutant. A 50% uptake efficiency is assumed. Intake factors are listed in Table C-1. EIWa, the sum of adult intake factors, is 3.36 mg/day. EIWc factors are also listed in Table C-1. The author has modified some of McCone's values of time and inhalation rate to closely approximate a two-year old child (McCone defines an "infant" as 0-2 years of age, and a "child" as 2-16 years of age.) The result is 1.05 mg/day.

TABLE C-1. Data Used to Estimate EIW Factors in DEFAULT.LDS

EIWa Factors

Function	Time min/day	Concentration mg/L	Inhalation Rate L/min	Intake, mg/day
Shower	10	1.7×10^{-2}	20	1.70
Sleep	480	2.3×10^{-5}	6.6	0.04
Bathroom use	40[1]	3.4×10^{-3}	20	1.36
Other activities	240[2]	1.1×10^{-4}	20	0.26

EIWc Factors

Function	Time min/day	Concentration mg/L	Inhalation Rate L/min	Intake, mg/day
Shower	5[3]	1.7×10^{-2}	7	0.298
Sleep	480	2.3×10^{-5}	2.8	0.015
Bathroom use	40[1]	3.4×10^{-3}	7	0.476
Other activities	675[4]	1.1×10^{-4}	7	0.260

1. McCone[18] assumes 20 minutes bathroom use between 7-9 AM and 20 minutes at other times. An average pollutant concentration in bathroom air is listed by McCone[18] for the 7-9 AM time period, and is higher than for other times. PHAS20 assumes that all bathroom use occurs from 7-9 AM.

2. McCone[18] assumes that adults are home for 4 hours between 7 AM to 11 PM. However, this includes time spent in the shower and in the bathroom. For PHAS20 purposes, "other activities" time remains 240 minutes.

3. The author equates a "shower" to a "bath". McCone[18] assumes that children spend 20 minute/week showering. The author believes this is low, and generation of vapors in a bath should be less than from a shower. A shower time of 5 minutes/day is assumed by the author.

4. McCone[18] assumes that a 2- to 16-year old child spends 60 percent of time from 7 AM to 11 PM at home; and an infant is always at home during this time period. In PHAS20, a compromise time of 675 minutes is used, which is 75 percent of 960 minutes less time for bathroom and shower functions.

e. CFIO or CFDO (whichever is applicable) is the same for children and adults. These factors relate the relative efficacy of inhaled or dermally-absorbed pollutant to oral intake of pollutant (see Section 2.2 in the main text).

f. A highly volatile pollutant concentration in air is related to that in water by Kh, the Henry Law Constant. For less volatile pollutants, the term FLD/(FLD+FDA) indicates the relative importance of air-side and water-side mass transfer control.

g. The absorption of pollutant through skin occurs at a constant rate.

h. The volume of water is sufficient to cover skin at all times through the exposure period.

i. The scenario adjustment factor for adults and children is the same value.

j. The relative pollutant content of all vegetables with respect to soil can be represented by one partition coefficient.

k. For water as the medium of concern, plants obtain pollutant primarily from water applied to crops or pasture as opposed to soil-water.

l. Cows absorb pollutant with equal efficiency from water, forage or soil.

m. In the topsoil medium pathways, vegetables and forage plants obtain pollutant from pollutant in soil solution. An equilibrium exists between pollutant in soil and soil solution.

n. The factor SLA (soil mass/skin area) is the same for adults and children.

o. When pollutant is absorbed from soil on the skin, the pollutant initially in soil that contacts skin is partitioned between soil and perspiration. All pollutant in perspiration is transported through the skin.

p. The inhalation and skin absorption components of exposure included in a augmented oral ingestion term.

q. The factor S(EIR) is the same for residents on-site as for residents off-site.

C.2 SURFACE-WATER RELATED PATHWAYS

PATHWAY 1 ingest water with pollutant from domestic supply

INTAKE = IWa x S(DWa) (adult)
INTAKE = IWc x S(DWc) (child)

Assumptions: a,b,c

PATHWAY 2 inhale pollutant volatilized from household water (all uses)

INTAKE = EIWa x S(DWa) x CFIO x PCEF / (FDA+FDL) (adult)
INTAKE = EIWc x S(DWc) x CFIO x PCEF / (FDA+FDL) (child)

where FDL = 2.5 $(Dw/86400)^{-2/3}$, FDA = $([1/Kh]x[Da/86400])^{-2/3}$, and PCEF = 2879000 (this is FDL for perchloroethylene). CFIO = DTo/DTi for adults or DTc/Dti for children. Assumptions: a,b,c,d,e,f. The constant 2.5 is the cube root of the ratio of air to water viscosity at 20 ^{o}C. The constant 86400 converts days to seconds.

PATHWAY 3 dermal absorption of pollutant from contact with household water.

INTAKE = DAWa x DETa x PC x CFDO x S(DWa) (adult)
INTAKE = DAWc x DETc x PC x CFDO x S(DWc) (child)

where CFDO = DTo/DTd for adults or DTc/DTd for children. Assumptions: a,b,c,e,g,h

PATHWAY 4 ingest water with pollutant while in water sport/play activity.

INTAKE = OIWa x S(OW) (adult)
INTAKE = OIWc x S(OW) (child)

Assumptions: a,b,c,i

PATHWAY 5 inhale vaporized pollutant from open water during water activity.

INTAKE = ORWa x S(OW) x CFIO x Kh x FDL / (FDL+FDA) (adult)
INTAKE = ORWc x S(OW) x CFDO x Kh x FLD/ (FLD+FDA) (child)

Assumptions: a,b,c,e,f,i

PATHWAY 6 absorb pollutant through skin while in water activity.

INTAKE = 10 DAWa x ODTa x S(OW) x PC x CFDO (adult)
INTAKE = 10 DAWc x ODTc x S(OW) x PC x CFDO (child)

Assumptions: a,b,c,e,g,h,i. The constant 10 accounts for m^2 to cm^2 and cm^3 to L conversions.

PATHWAY 7 consume fish from contaminated water.

INTAKE = Wfa x S(WF) x BCF (adult)
INTAKE = Wfc x S(WF) x BCF (child)

Assumptions: a,b,c,i

Pathway 8 consume vegetables watered with contaminated water.

INTAKE = Wva x S(Wv) x Kwv (adult)
INTAKE = Wvc x S(Wv) x Kwv (child)

Assumptions: a,b,c,i,j,k

PATHWAY 9 consume beef, livestock drinks contaminated water (first option).

INTAKE= Wma x S(Wm) x BCWF (adult)
INTAKE= Wmc x S(Wm) x BCWF (child)

where BCWF = Kpm x Uwm / Upm. Assumptions: a,b,c,i

PATHWAY 9 consume beef, livestock drinks contaminated water and grazes on plants irrigated with contaminated water (second option).

INTAKE = Wma x S(Wm) x (BCWF + Kwp x Kpm) (adult)
INTAKE = Wmc x S(Wm) x (BCWF + Kwp x Kpm) (child)

Assumptions: a,b,c,i,k,l.

PATHWAY 10 drink milk, dairy cows drink contaminated water (first option).

INTAKE= Wda x S(Wd) x DCWF (adult)
INTAKE= Wdc x S(Wd) x DCWF (child)

where DCWF = Kpm x Uwd / Upd. Assumptions: a,b,c,i

PATHWAY 10 drink milk, dairy cows drink contaminated water and graze on plants irrigated with contaminated water (second option).

INTAKE = Wda x S(Wd) x (DCWF + Kwp x Kpd) (adult)
INTAKE = Wdc x S(Wd) x (DCWF + Kwp x Kpd) (child)

Assumptions: a,b,c,i,k,l

C.3 SURFACE SOIL-RELATED PATHWAYS

NOTE: In pathways where subsite designation is an option, subsite #1 is designated in presented equations.

PATHWAY 1 ingest water with pollutant from domestic supply; pollutan in runoff from topsoil of #1 subsite.

INTAKE = IWa x S(DWa) / MKrol (adult)
INTAKE = IWc x S(DWc) / MKrol (child)

Assumptions: a,b

PATHWAY 2 inhale pollutant volatilized from household water (all uses); pollutant in runoff from topsoil of #1 subsite.

INTAKE = (1/MKrol) x EIWa x S(DWa) x CFIO x PCEF / (FDA+FDL) (adult)
INTAKE = (1/MKrol) x EIWc x S(DWc) x CFIO x PCEF / (FDA+FDL) (child)

See water pathway 2 for definitions of CFIO, PCEF, FDA, and FDL. Assumptions: a,b,d,e,f

PATHWAY 3 dermal absorption of pollutant from contact with household water; pollutant in runoff from topsoil of #1 subsite.

INTAKE = (1/MKrol) x DAWa x DETa x PC x CFDO x S(DWa) (adult)
INTAKE = (1/MKrol) x DAWc x DETc x PC x CFDO x S(DWc) (child)

where CFDO = DTo/CFdo for adults or DTc/CFdo for children. Assumptions: a,b,e,g,h

PATHWAY 4 ingest water with pollutant while in water sport/play activity; pollutant in runoff from topsoil of designated subsite (1 or 2).

INTAKE = OIWa x S(OW) / MKrol (adult)
INTAKE = OIWc x S(OW) / MKrol (child)

Assumptions: a,b,i

PATHWAY 5 inhale vaporized pollutant from open water during water activity; pollutant in runoff from topsoil of designated subsite (1 or 2).

INTAKE = (1/MKro1) x ORWa x S(OW) x CFIO x Kh x FDL / (FDL+FDA) (adult)
INTAKE = (1/MKro1) x ORWc x S(OW) x CFDO x Kh x FLD / (FLD+FDA) (child)

See water pathway 2 for definitions of CFIO, PCEF, FDA, and FDL. Assumptions: a,b,e,f,i

PATHWAY 6 absorb pollutant through skin while in water activity; pollutant in runoff from topsoil of designated subsite (1 or 2).

INTAKE = 10 DAWa x ODTa x S(OW) x PC x CFDO / MKro1 (adult)
INTAKE = 10 DAWc x ODTc x S(OW) x PC x CFDO / MKro1 (child)

where CFDO = DTo/CFdo for adults or DTc/CFdo for children. Assumptions: a,b,e,g,h,i

PATHWAY 7 consume fish from contaminated water; pollutant is in runoff from topsoil of designated subsite (1 or 2).

INTAKE = Wfa x S(WF) x BCF / MKro1 (adult)
INTAKE = Wfc x S(WF) x BCF / MKro1 (child)

Assumptions: a,b,i

PATHWAY 8 consume contaminated vegetables grown at designated subsite (1 or 2).

INTAKE = Wva x S(Wv) x Kwv / KDJ1 (adult)
INTAKE = Wvc x S(Wv) x Kwv / KDJ1 (child)

where KDJ1 = Kd1 + th1/rh1. Assumptions: a,b,c,i,j,m

PATHWAY 9 consume beef, livestock grazes on forage grown at designated subsite (1 or 2) (first option).

INTAKE = Wma x S(Wm) x Kpm x Kwp / KDJ1 (adult)
INTAKE = Wmc x S(Wm) x Kpm x Kwp / KDJ1 (child)

Assumptions: a,b,c,i,m

PATHWAY 9 consume beef, livestock grazes on forage grown at designated subsite (1 or 2). Allowance is made for livestock ingestion of soil. (second option).

INTAKE = Wma x S(Wm) x Kpm x (Kwp/KDJ1 + Usm/Upm) (adult)
INTAKE = Wmc x S(Wm) x Kpm x (Kwp/KDJ1 + Usm/Upm) (child)

Assumptions: a,b,c,i,l,m

PATHWAY 9 consume beef, livestock grazes on forage grown at designated subsite (1 or 2). Allowance is made for livestock ingestion of soil and for livestock watering on surface supply which gets cont. runoff from subsite (third option).

$$INTAKE = Wma \times S(Wm) \times Kpm \times (Kwp/KDJ1 + Usm/Upm + Uwm/[Upm \times MKrol]) \quad (adult)$$
$$INTAKE = Wmc \times S(Wm) \times Kpm \times (Kwp/KDJ1 + Usm/Upm + Uwm/[Upm \times MKrol]) \quad (child)$$

Assumptions: a,b,c,i,l,m

PATHWAY 10 drink milk, dairy cows graze on forage grown at designated subsite (1 or 2) (first option).

$$INTAKE = Wda \times S(Wd) \times Kpd \times Kwp / KDJ1 \quad (adult)$$
$$INTAKE = Wdc \times S(Wd) \times Kpd \times Kwp / KDJ1 \quad (child)$$

Assumptions: a,b,c,i,m

PATHWAY 10 drink milk, dairy cows graze on forage grown at designated subsite (1 or 2). Allowance is made for dairy cow ingestion of soil (second option).

$$INTAKE = Wda \times S(Wd) \times Kpd \times (Kwp/KDJ1 + Usm/Upm) \quad (adult)$$
$$INTAKE = Wdc \times S(Wd) \times Kpd \times (Kwp/KDJ1 + Usm/Upm) \quad (child)$$

Assumptions: a,b,c,i,l,m

PATHWAY 10 drink milk, dairy cows graze on forage grown at designated subsite(1 or 2). Allowance is made for dairy cow ingestion of soil and for animals watering on surface supply which gets cont. runoff from subsite (third option).

$$INTAKE = Wda \times S(Wd) \times Kpd \times (Kwp/KDJ1 + Usd/Upd + Uwd/[Upd \times MKrol]) \quad (adult)$$
$$INTAKE = Wdc \times S(Wd) \times Kpd \times (Kwp/KDJ1 + Usd/Upd + Uwd/[Upd \times MKrol]) \quad (child)$$

Assumptions: a,b,c,i,l,m

PATHWAY 11 exposure to dirt at residence (oral, dermal, respired).

$$INTAKE = S(RSa) \times (SIRa + [SARa \times PLa \times CFDO \times MGPCC] + [RIa \times RSPA \times CFIO]) \quad (adult)$$
$$INTAKE = S(RSc) \times (SIRc + [SARc \times PLc \times CFDO \times MGPCC] + [RIc \times RSPA \times CFIO]) \quad (child)$$

where MGPCC = SLA / (SLA x KDJ1 + PLa) for adults or SLA/ (SLA x KDJ1 + PLc) for children. MGPCC is the mg/L pollutant in perspiration water per mg/kg pollutant initially in soil deposited on skin. MGPCC is derived from two equations reflecting partitioning between soil and perspiration, and a pollutant mass balance between these substrates.
Assumptions: a,c,e,n,o

PATHWAY 12 exposure to dirt at occupational site (adults only).

$$INTAKE = CSI \times S(CS) \times CWTF$$

Assumptions: a,c,p

PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house. Exposure assumed to be primarily caused by inhalation of vapors in basement.

INTAKE = BIRa x S(BIR) x CFIO x Ab3 x MXb / MKdba (adult)
INTAKE = BIRc x S(BIR) x CFIO x Ab3 x MXb / MKdbc (child)

Assumptions: a,b,e,i

PATHWAY 14 exposure to vapors diffusing from soil outside of house. Exposure assumed to be primarily caused by inhalation of diffusing vapors.

INTAKE = 10000 RIa x S(EIR) x CFIO x A04 x MXon / MKdoa (adult)
INTAKE = 10000 RIc x S(EIR) x CFIO x A04 x MXon / MKdoc (child)

Assumptions: a,b,e,i. The constant 10000 converts ha to m^2.

PATHWAY 15 exposure to vapors diffusing from soil at site to off-site receptors. Pollutant is diffusion-generated, and dispersed in air.

INTAKE = 10000 x RIa x S(EIR) x CFIO x A04 x MXof / MKdoa (adult)
INTAKE = 10000 x RIc x S(EIR) x CFIO x A04 x MXof / MKdoa (child)

Assumptions: a,b,e,i,q

PATHWAY 16 ingest water with pollutant from domestic supply; pollutant infiltrates through soil to groundwater source.

INTAKE = IWa x S(DWa) / MKgwa (adult)
INTAKE = IWc x S(DWc) / MKgwc (child)

Assumptions: a,b

PATHWAY 17 inhale pollutant volatilized from household water (all uses); pollutant infiltrates through soil to groundwater source.

INTAKE = (1/MKgwa) x EIWa x S(DWa) x CFIO x PCEF / (FDA+FDL) (adult)
INTAKE = (1/MKgwc) x EIWc x S(DWc) x CFIO x PCEF / (FDA+FDL) (child)

See water pathway 2 for definitions of CFIO, PCEF, FDA, and FDL.
Assumptions: a,b,d,e,f

PATHWAY 18 dermal absorption of pollutant from contact with household water; pollutant infiltrates through soil to groundwater source.

INTAKE = (1/MKrol) x DAWa x DETa x PC x CFDO x S(DWa) (adult)
INTAKE = (1/MKrol) x DAWc x DETc x PC x CFDO x S(DWc) (child)

where CFDO = DTo/CFdo for adults or DTc/CFdo for children. Assumptions: a,b,e,g,h

C.4 SEDIMENT-RELATED PATHWAYS

PATHWAY 1 ingest water with pollutant from domestic supply. Water source has been in contact with polluted sediment.

INTAKE = IWa x S(DWa) / MKdwa (adult)
INTAKE = IWc x S(DWc) / MKdwc (child)

Assumptions: a,b

PATHWAY 2 inhale pollutant volatilized from household water (all uses) Water source has been in contact with polluted sediment.

INTAKE = (1/MKdwa) x EIWa x S(DWa) x CFIO x PCEF / (FDA+FDL) (adult)
INTAKE = (1/MKdwc) x EIWc x S(DWc) x CFIO x PCEF / (FDA+FDL) (child)

See water pathway 2 for definitions of CFIO, PCEF, FDA, and FDL.
Assumptions: a,b,d,e,f

PATHWAY 3 dermal absorption of pollutant from contact with household water Water source has been in contact with polluted sediment.

INTAKE = (1/MKdwl) x DAWa x DETa x PC x CFDO x S(DWa) (adult)
INTAKE = (1/MKdwl) x DAWc x DETc x PC x CFDO x S(DWc) (child)

where CFDO = DTo/CFdo for adults or DTc/CFdo for children. Assumptions: a,b,e,g,h

PATHWAY 4 ingest water with pollutant while in water sport/play activity Waterbody overlays a polluted sediment site.

INTAKE = OIWa x S(OW) / MKdwl (adult)
INTAKE = OIWc x S(OW) / MKdwl (child)

Assumptions: a,b,i

PATHWAY 5 inhale vaporized pollutant from open water during water activity Waterbody overlays a polluted sediment site.

INTAKE = (1/MKdwa) x ORWa x S(OW) x CFIO x Kh x FDL / (FDL+FDA) (adult)
INTAKE = (1/MKdwc) x ORWc x S(OW) x CFDO x Kh x FLD / (FLD+FDA) (child)

See water pathway 2 for definitions of CFIO, PCEF, FDA, and FDL.
Assumptions: a,b,e,f,i

PATHWAY 6 absorb pollutant through skin while in water activity. Waterbody overlays a polluted sediment site.

INTAKE = 10 x DAWa x ODTa x S(OW) x PC x CFDO / MKdwa (adult)
INTAKE = 10 x DAWc x ODTc x S(OW) x PC x CFDO / MKdwc (child)

where CFDO = DTo/CFdo for adults or DTc/CFdo for children. Assumptions: a,b,e,g,h,i

PATHWAY 7 consume fish from contaminated water; waterbody overlays a polluted sediment site.

INTAKE = Wfa x S(WF) x BCF / MKdwa (adult)
INTAKE = Wfc x S(WF) x BCF / MKdwc (child)

Assumptions: a,b,i

C.5 TYPE 1 CONSTRAINT EQUATIONS

Each applicable term "TEST" is compared to the PPLV. If TEST < PPLV, a Type 1 constraint is identified. A type 1 constraint algorithm is not provided for unlisted pathways. Pathway numbers used in Sections C.2, C.3 and C.4 are also used in this section.

C.5.1 Surface Water or Groundwater

Pathways 1 and 4: TEST = TOL

Pathway 7: TEST = AQTL

Pathway 8: TEST = PHLW
TEST = PHLS / (Koc x focPS)

Pathway 9 (first option): TEST = CTAEL x BWM / Uwm

Pathway 9 (second option): TEST = PHLW
TEST = PHLS / (Koc x focPS)
TEST = CTAEL x BWM / (Uwm + Upm x Kwp)

Pathway 10 (first option): TEST = CTAEL x BWD / Uwd

Pathway 10 (second option): TEST = PHLW
TEST = PHLS / (Koc x focPS)
TEST = CTAEL x BWD / (Uwd + Upd x Kwp)

C.5.2 Sediment

Pathways 1 and 4: TEST = 8640 TOL x QU5 x MKdwa / As5
8640 converts between seconds and days, ha and m^2, L and m^3.

Pathway 7: TEST = 8640 AQTL x QU5 x MKdwa / As5
For a PPLV based on child-limit criteria, the term MKdwc replaces MKdwa in the above equations.

C.5.3 Surface or Near-Surface Soil

All tests for pathways 1 through 10 are listed for the "#1 subsite". For a PPLV based on child-limit criteria, MKgwc replaces MKgwa.

Pathway 1 and 4: TEST = TOL x MKro1

Pathway 7: TEST = AQTL x MKro1

Pathway 8: TEST = PHLW x (Kd1 + th1/rh1)
TEST = PHLS x (KD1 + th1/rh1) / (Koc x focPS)

Pathway 9 (first option):
TEST = PHLV x (Kd1 + th1/rh1)
TEST = PHLS x (Kd1 + th1/rh1) / (Koc x focPS)
TEST = CTAEL x BWM x (Kd1 + th1/rh1) / (Upm x Kwp)

Pathway 9 (second option) See first option for TEST based on PHLV and PHLS
TEST = CTAEL x BWM / (Usm + [Upm x Kwp]/[Kd1+th1/rh1])

Pathway 9 (third option) See first option for TEST based on PHLV and PHLS
TEST = CTAEL x BWM / (Usm + [UpmxKwp]/[Kd1+th1/rh1] + Uwm/MKro1)

Pathway 10 (first option):
TEST = PHLV x (Kd1 + th1/rh1)
TEST = PHLS x (Kd1 + th1/rh1)/(Koc x focPS)
TEST = CTAEL x BWD x (Kd1 + th1/rh1) / (Upd x Kwp)

Pathway 10 (second option) See above option for TEST based on PHLV and PHLS
TEST = CTAEL x BWD / (Usd + [Upd x Kwp]/[Kd1+th1/rh1])

Pathway 10 (third option) See first option for TEST based on PHLV and PHLS
TEST = CTAEL x BWD / (Usd + [Upd x Kwp]/[Kd1+th1/rh1] + Uwd/MKro1)

Pathway 16: TEST = TOL x MKgwa

C.6 Type 2 Constraints

The analysis for the water medium is straightforward: if the PPLV exceeds Wsol, a Type 2 constraint is identified. If sediment is the medium, the term PPLV / (Kd5 + th5/rh5) is compared to Wsol. If Wsol is exceeded, a Type 2 constraint is identified.

The analysis for surface or near-surface soil is more complex. For tested pathways, a water concentration (WSTEST) is computed based on the PPLV and the model used in the intake equation to relate the water to soil contents. WSTEST is compared to Wsol. If WSTEST exceeds Wsol, a Type 2 constraint is identified. The constraint means that the proportionality between intake and pollutant concentration in soil breaks down; no additional intake can be supplied via a constrained pathway with increased pollutant concentration in soil. The constrained limit intake for such pathways is computed as: PPLVTAKE x Wsol/ WSTEST, where PPLVTAKE corresponds to the "LIMIT INTAKE" shown in the last column of the Assessment Computations Table shown in Figure 18. Pathways 9, 10 and 11 have sub-routes. In those pathways, only the PPLVTAKE via each sub-route is so processed. All constrained intakes are computed and their sum is called LMTAKE(31). Other pathways intakes (including portions of pathways with sub-routes that do not involve a soil-water transfer) per unit pollutant concentration in soil are summed; the sum is called ULMTAKE. These unconstrained routes would provide additional intake if the pollutant level in soil were higher.

The total allowable intake for the pollutant is called INTAKE, which corresponds to the RfD x BW discussed in Section 2.3, main text. The

difference INTAKE-LMTAKE(31) is called LIMTAKE. LIMTAKE represents an intake in mg/day which is "allocated" to unconstrained routes. For unconstrained routes, the proportionality between concentration and intake still holds. The PPLV adjusted for Type 2 constraints is LIMTAKE/ULMTAKE, and is called PTEST. Note that PTEST will be higher than the unadjusted PPLV.

The above procedure is repeated for PTEST, since pathways or routes that were not constrained at the unadjusted PPLV may become constrained at the higher concentration PTEST. The procedure leads to a second value of PTEST, which can be compared to the first PTEST value. If they are essentially the same, no further iterations are undertaken. Otherwise, the process continues until two successive PTEST values that are equal are obtained.

The equations presented below for WSTEST are for the "#1 subsite", and if a "MK" partition coefficient has an adult and child-based value, the equation for the adult value is presented. The pathway numbers are those used in previous sections of this Appendix.

Pathways 1 - 7: WSTEST = PPLV / MKrol

Pathway 8: WSTEST = PPLV / (Kdl + thl/rhl)

Pathway 9 (first and second option equations): WSTEST = PPLV / (Kdl + thl/rhl)

The intake subject to constraint is given by the intake equation for Pathway 9, first option. This intake represents the contribution from forage eaten by the beef cow. In the second option equation, Wma x S(Wm) x Kpm x Usm/Upm represents the sub-route contribution from soil ingested by the beef cow, and is never constrained.

Pathway 9 (option 3): The intake has three sub-route components. The WSTEST described above applies to the first intake component. The second component term, discussed above, is never constrained. The last sub-route intake term, Wma x S(Wm) x Kpm x Uwm / (Upm/Mkrol), is constrained if WSTEST = PPLV / MKrol > Wsol.

Pathway 10 (first and second options): WSTEST = PPLV / (Kdl + thl/rhl)

The intake subject to constraint is given by the intake equation for Pathway 10, first option. In the second option equation, Wda x S(Wd) x Kpd x Usd/Upd is never constrained.

Pathway 10 (option 3): The intake has three sub-route components. WSTEST described above is for the first intake component. The second term, which is stated above, is never constrained. The last sub-route intake term, Wda x S(Wd) x Kpd x Uwd / (Upd/Mkrol) is constrained if WSTEST = PPLV / MKrol > Wsol.

Pathway 11: The intake equation has three sub-route components. The intake given by S(RSa) x (SIRa + [RIa x RSPA x CFIO]) is never constrained (these terms correspond to the oral and inhaled soil routes). The intake given by S(RSa) x SARa x PLa x CFDO x MGPCC is constrained if WSTEST = PPLV/(Kdl + thl/rhl) > Wsol.

Pathway 12 is never constrained.

Pathway 13: WSTEST = PPLV / MKdba

Pathway 14 and 15: WSTEST = PPLV / MKdoa

Pathways 16-18: WSTEST = PPLV / MKgwa

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