CalTOX™, A Multimedia Total Exposure Model For Hazardous-Waste Sites

Spreadsheet User's Guide

Version 1.5

Prepared by
The University of California, Davis
in Cooperation with
Lawrence Livermore National Laboratory

for

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Department of Toxic Substances Control
California Environmental Protection Agency
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FOREWORD

The CalTOX risk assessment model is being developed by the Office of Scientific Affairs in the California Department of Toxic Substances Control to improve the risk assessment information used in regulatory decisions. The implementation of this model is occurring in two stages: a technical development phase and a policy formulation phase. The current version of CalTOX represents the completion of the technical development phase. The model has been extensively peer-reviewed by scientists in academia, industry and government. Comments of the reviewers resulted in changes to the model and identification of its scientific limitations. However, issues pertaining to policy development have not been addressed. Therefore, CalTOX is **not** the current risk assessment policy of the Department.

Existing risk assessment policy is inadequate to address the application of CalTOX. The novel methods introduced by CalTOX for predicting transport of a chemical and dealing with uncertainty will require well considered policy decisions before CalTOX can be implemented as a risk assessment method for regulatory purposes. The Department will refine its policy during the first year (1995) of application, as CalTOX is applied to selected sites under the regulatory jurisdiction of the California Department of Toxic Substances Control. Responsible parties may request to use CalTOX at a site regulated by the Department. The Department will use a number of criteria to determine if the site is suitable for CalTOX. The responsible party will then work closely with the Office of Scientific Affairs and other Department staff to implement CalTOX at the chosen site. Policy decisions will be addressed as they arise on these sites and recorded in an evolving policy document, *CalTOX Applications Manual*. Drafts of the applications manual will be available from the computer bulletin board system (BBS) established by the Office of Scientific Affairs (see Appendix B). The BBS will enable users to download files, including the text file of the *CalTOX Applications Manual*, as well as suggest improvements to the document on the BBS. The objective of this is to maintain the open process that was used during the technical development phase. The BBS provides a manageable method of communication with interested parties, including other regulatory agencies, responsible parties, community groups, environmental groups or any person with interest on this subject.

Sites with the following conditions will not be selected for the 1995 trial application of CalTOX if the following conditions exist:

- presence of inorganic chemicals,
- presence of non-aqueous phase liquids (NAPLs),
- a release to soil less than one year ago,
- a source other than contaminated soil, or
- exposure to off-site receptors.

Other restrictions for inclusion during 1995 may apply, but the policy development will be open to all interested parties via the BBS. As with the technical development phase, policy formulation will be guided by the peer-reviewed scientific literature and the existing U.S. EPA site investigation process as defined in the National Contingency Plan.

NOTE:

> **The figures in this manual illustrate Macintosh-versions of the screen displays and outputs from the CalTOX program. These displays will appear somewhat differently on an IBM PC or PC compatible computer operating under Windows. However, the information contained in these displays and the procedures for running CalTOX are the same in both the Macintosh and PC-Windows versions.**

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1. INTRODUCTION

This manual is intended to provide   CalTOX users with a brief overview of the   CalTOX spreadsheet model. This manual is not intended to be an exhaustive description of the model and its potential applications. Detailed information about the   CalTOX model and its development, validation, and potential applications is covered in a number of supporting documents available from the National Technical Information Services (NTIS) and from the California Department of Toxic Substances Control.

What is CalTOX?

CalTOX has been developed as a spreadsheet model to assist in health-risk assessments that address contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water. This spreadsheet model includes three components—a multimedia transport and transformation model, exposure scenario models, and efforts to quantify and reduce uncertainty in multimedia, multiple-pathway exposure models.

The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of contaminants introduced initially to soil layers or for contaminants released continuously to air, surface soil, or water. This model assists the user in examining how chemical and landscape properties and exposure factors impact both the ultimate route and quantity of human contact. Multimedia, multiple pathway exposure models are used in the   CalTOX model to estimate average daily potential doses within a human population in the vicinity of a hazardous substances release site.

The exposure models encompass twenty-three exposure pathways. The exposure assessment process consists of relating contaminant concentrations in the multimedia model compartments to contaminant concentrations in the media with which a human population has contact (personal air, tap water, foods, household dusts soils, etc.). The average daily dose is the product of the exposure concentrations in these contact media and an intake or uptake factor that relates the concentrations to the potential dose within the population.

CalTOX has been designed to provide the user with the options of: (1) making point estimates of average exposure during an exposure duration, (2) applying a sensitivity analysis to these point estimates, (3) using a Monte   Carlo add-in to make stochastic estimates of the distribution of exposure uncertainty/variability, and (4) to apply a sensitivity analysis to determine the variance contributions of model inputs to the overall variance in the estimated distribution of exposure and risk.

Computer Requirements

The minimum hardware requirements for running the   CalTOX spreadsheet are either

- an IBM personal computer (PC) or PC-compatible   capable of running Microsoft Excel 4.0 or Excel 5.0 for Windows and preferably having a mouse,

or

- a Macintosh personal computer capable of running Microsoft Excel 4.0 for the Macintosh[*].

For either computer system, a hard-drive storage device with at least 2 megabytes of available storage is required to store and operate the   CalTOX spreadsheet and supporting files and applications. The   CalTOX spreadsheet cannot be executed from a floppy-disk drive. A black and white monitor is sufficient, but a color screen is preferable.

The CalTOX spreadsheet was designed and assembled using Microsoft Excel 4.0 on Macintosh personal computers. All of the initial testing and debugging has been carried out using Excel 4.0. It was modified to run on a PC compatible computer using Excel 4.0 and Excel 5.0. The PC version has been run on a number of IBM-compatible computers but has not been tested on all possible computers. If you have difficulty viewing, operating, or printing   CalTOX, please see the Problems Section of this manual.

The CalTOX spreadsheet has been imported into a Lotus 123 spreadsheet on an IBM PC and used with Lotus 123 Version 2.1. However, when imported into the Lotus environment, the cell alignment, color displays, and charts intended to increase clarity are lost. It is possible that other spreadsheet programs and newer versions of Lotus 123 will be capable of importing the   CalTOX color formats and graphic results, but the DTSC has not confirmed this.

Technical support for   CalTOX will be exclusively through a computer bulletin board system (BBS). Therefore, a modem and communications program are necessary to obtain that technical support.

Knowledge Requirements

In preparing this guide, we assume that the user has a basic familiarity with spreadsheet calculations and is familiar with the   CalTOX documentation, which describes the theoretical basis for the model. The material included in the   CalTOX

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[*]At the time this version of   CalTOX was prepared, Microsoft Excel 5.0 was not available. Based on the PC version of Excel 5.0, the current version of   CalTOX was found to be capable of running with Excel 5.0. However this capability has not been tested on the Macintosh system.

reports is not repeated in this manual. Users without a solid understanding of the human exposure intake equations and the fugacity-based compartment model will only be able to use the model superficially, if at all.

Excel Spreadsheet Program

All of the CalTOX files, including macro files, worksheet files, and file templates, are designed to work with either Microsoft Excel 4.0 for the Macintosh or Microsoft Excel 4.0 or Excel 5.0 for Windows on an IBM PC or PC-compatible computer. We have tried to design and build macros that allow the user to load data, operate the CalTOX worksheet, and view the results of a CalTOX calculation with a minimum understanding of Excel. Nonetheless, those with a more in-depth understanding of Excel will be able to master the operations of CalTOX more rapidly and be more comfortable making their own modifications to the program execution.

US EPA Risk Assessment Guidance for Superfund (RAGS)

Assessment of human exposure to environmental contaminants requires that we translate environmental concentrations into quantitative estimates of the amount of chemical that contacts individuals within an exposed population. Dose models used in CalTOX are based on those described by the U.S. Environmental Protection Agency (EPA, 1989) in the Risk Assessment Guidance for Superfund (RAGS) documents and by the California Department of Toxic Substances Control (DTSC, 1992a, 1992b). Familiarity with the RAGS documents is necessary for understanding the results produced by CalTOX. The exposure pathway models used in CalTOX are described in detail in Part III of the CalTOX reports (DTSC, 1993c)

Seven Compartment Fugacity Model

CalTOX includes a seven-compartment regional and dynamic multimedia fugacity model. For all chemicals, fugacity and fugacity capacities are used to represent mass potential and mass storage within compartments. The seven compartments used in CalTOX are (1) air, (2) ground-surface soil, (3) plants, (4) root-zone soil, (5) the vadose-zone soil below the root zone, (6) surface water, and (7) sediments. Contaminant concentrations in ground water are currently set equivalent to the predicted vadose-zone soil leachate concentration [*]. In contrast to many models used for assessing environmental fate, CalTOX imposes conservation of mass on the contaminated landscape unit. In addition, the model accounts systematically for gains and losses in each compartment and for the whole system in concert. Understanding the results of the CalTOX spreadsheet requires a basic familiarity with this model, which is described in Part II of the CalTOX reports (DTSC. 1993b).

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[*]Future versions of the CalTOX model will include an option to specify contaminant dilution factors in ground water relative to vadose-zone leachate.

Stochastic Add-in Program

CalTOX was designed to have both sensitivity and uncertainty analyses incorporated directly into the model operation. Parameter values suggested for use in CalTOX are described in terms of mean values and coefficients of variation in place of plausible upper values. Model results are described in terms of the confidence intervals associated with model predictions. CalTOX has its own routine for carrying out a sensitivity analysis on point estimates of exposure and risk. CalTOX is designed to integrate with stochastic add-in programs such as *@Risk* and *Crystal Ball*, which can be used to do sensitivity and uncertainty analyses with the results produced by CalTOX. In order to use one of these add-on programs, the user must be familiar both with the operation of the add-in program and with the techniques of uncertainty/sensitivity analysis. The current version of CalTOX has been used with *Crystal Ball* version 3.0, which is available as an add-in program for both Excel 4.0 for Windows and Excel 4.0 for the Macintosh. In order to use *Crystal Ball* with CalTOX using Excel 5.0, a newer version of *Crystal Ball* that is compatible with Excel 5.0 must be obtained. All of the CalTOX inputs and selected outputs have been formatted for immediate use with *Crystal Ball* Version 3.0. In order to use other add-in programs, such as *@Risk*, the user must assign distributions to each input cell and select the outputs for which distribution results are needed.

Computer Bulletin Board Knowledge

The only means of technical support for CalTOX will be through a computer bulletin board system (BBS). Therefore, to access technical support, users will must have or acquire the equipment and skills necessary to use a BBS.

Applications Limitations

As is the case with any model, CalTOX was designed for use in a limited range of spatial scales, time scales, geographic conditions, and chemical classes. These technical limitations apply to version 1.5 of CalTOX. Future versions of the model may be modified to overcome these limitations.

Chemical limitations

CalTOX is not for surfactants or volatile metals. It should be used for partially ionized organic chemicals only when great care is exercised to adjust the partition coefficients to make sure they are appropriate for the pH of the landscape under consideration. The model is further limited to chemicals for which one has good physical and chemical parameters.

Time scale limitations

The CalTOX transport model is intended for application over long time scales, several months to decades. It should be used cautiously for time periods less than one year and then only when properly time-averaged landscape properties are employed. When this is not the case,   CalTOX can be used, but some discount of model reliability must be considered.

Landscape Limitations

CalTOX should not be used for landscapes in which water occupies more than 10% of the land surface area.   CalTOX should not be used on areas of less than 1000 m ^{2}.

Concentration Limitations

CalTOX is designed for modeling very low concentrations of contamination. When the contaminant concentration exceeds the solubility limit in any phase, the results of the model are no longer valid. There is a warning in the program to advise the user when this happens. It is possible that high existing concentration of chemical may preclude the ability of CalTOX to estimate baseline risk, but a health-based soil clean-up level can usually still be estimated.

Receptor Location Limitations

CalTOX should not be used when the primary source is not contaminated soil. It is not designed to estimate exposure to off-site receptors.

As stated above, these technical limitations may be overcome in future versions of CalTOX, but they apply to version 1.5. In addition to the technical limitations, policy must be developed so that the model is applied to sites and facilities in a fashion which yields meaningful risk estimates. Policy limitations for sites and facilities regulated by the California Department of Toxic Substances Control have only begun to be addressed. They will be described in the forthcoming   *CalTOX Applications Manual* which will be written during the Department's limited application of   CalTOX during 1995 (see foreward).

Computer Bulletin Board Knowledge

The only means of technical support for   CalTOX will be through a computer bulletin board system (BBS). Therefore, to access technical support, users must have or acquire the equipment and skills necessary to use a BBS.

Technical Support

Support for CalTOX users will be supplied exclusively through a computer bulletin board system (BBS). There will be no telephone support or any other support for CalTOX users. The BBS enables the Department to provide technical support which it can maintain with limited resources. Users may send a message to the system operator asking questions about the model. The user should log back on to the BBS in three working days to obtain an answer. Refer to Appendix B for instructions on logging on and using the BBS.

The BBS is not only for technical support, it is also a means of maintaining your copy of CalTOX. The BBS has files which may be downloaded. Among the files that can be downloaded from the BBS will be updated versions of the EXCEL file Datcal.xls. Datcal.xls came with your purchased copy of CalTOX and contains the default parameter values required by the CalTOX model. The Department envisions these default parameter values changing as new scientific information is published in the peer-reviewed literature. Therefore, you should check the BBS periodically to determine if you have the most current Datcal.xls file. Other files are available for downloading as well. These files include text files (in Word for Windows) which describe the basis for default distributions, validation reports, and the evolving drafts of the *CalTOX Applications Manual*.

Philosophy of CalTOX

The ultimate objective of CalTOX is to improve the quality of risk information incorporated in regulatory decision-making. This requires that estimates of risk be provided to decision makers in a timely fashion. More importantly, these risk estimates should be accurate portrayals of potential risks which incorporate the best appropriate science. CalTOX has been subjected to extensive scientific peer review, and we believe that CalTOX truly represents a state-of-the-art model for the early- to mid-1990s. Undoubtedly, the science of risk assessment will progress. As new information becomes available, it should be incorporated into CalTOX. For example, the default parameter values found in the Datcal.xls file are based on the best estimates we could find in the peer-reviewed literature. We anticipate that they will change as new information is obtained. The structure of the model will also change. If publications appear in the peer-reviewed literature relevant to CalTOX, please call our attention to these publications. Please provide your comments on the computer bulletin board.

Overview of this Manual

The remainder of this document is divided into nine sections. Sections 2 and 3 give the user a step-by-step set of instructions for loading the program and using the spreadsheet without the custom macros. The fourth section explains how to start and run a sample problem using the CalTOX macro and worksheet files. Following this is a

section that provides a summary of the   CalTOX worksheet and identifies what is included in each of the eighteen pages of this worksheet. In section 6, we describe the calculation of risk and soil clean up goals. The next two sections deal respectively with sensitivity and uncertainty analyses. The last section of the report is an appendix that provides a complete listing of the eighteen-page   CalTOX worksheet. This listing is referred to several times in this report.

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2. GETTING STARTED

The CalTOX files come on a single 720 K (Macintosh) or 800 K (IBM) diskette. This disk is locked and should not be used to run the program, since there is not sufficient room on this disk to contain the files created during the execution of the CalTOX macros.

Hard disk Configuration

Before copying any files onto your hard disk, create a new sub-directory or folder on your hard disk. The name CalTOX is an obvious choice, but any name will do. Copy all the files from the CalTOX floppy disk into the new sub-directory or folder of your hard disk. Store the master disk in a safe place. Open the directory or folder in which you have copied the CalTOX files.

The CalTOX files

There are six files in the CalTOX disk which should all be copied into the CalTOX directory (folder). Names of these files follow the naming convention of the IBM-PC and PC compatible computers, but the files work with either a PC-compatible or Macintosh computer. After you copy files into your folder (directory) you should have the following files:

> RunCal.xls
> CalTOX.xlt
> DatCal.xls
> SEN.xlt
> CalMACS.xlm
> Cal5FIX.xls

The type, contents, and purpose of each file are as follows:

> *RunCal.xls* is a worksheet that is used as a home file to orchestrate other CalTOX operations. When you open this file, it automatically sets up the working environment for CalTOX within Excel (including custom tools, macro buttons, and menu bars) and loads and creates the needed files. This file also provides a flowchart that illustrates the basic steps of the CalTOX calculation process and carries out each step automatically when the appropriate button is clicked using the mouse key.

> *CalTOX.xlt* is a worksheet template. When this template is opened, the user creates a spreadsheet that serves as the central component of the CalTOX files. This is a very large spreadsheet and includes the scenario-specific input tables,

output tables, graphical outputs and all intermediate calculations that are involved in the process of estimating the environmental distribution of a chemical, transfer to exposure media, human contact, and potential health risk.

DatCAL.xls is worksheet file that contains a listing of chemical properties, landscape properties, and human exposure factors required as input for   CalTOX. Mean values and coefficients of variation for each input are listed for several chemicals and several California landscapes (see Philosophy of   CalTOX). This worksheet is normally hidden from view. The chemical data and land-use/exposure factors data in this worksheet can be automatically loaded into the main CalTOX spreadsheet by macro commands that are initiated from   RunCal.xls or from the CalTOX toolbar.

There are blank columns in this file in which the user can enter new chemical data and landscape data/exposure factors. The file must be unhidden before it is edited (use the " Unhide" command in the "Window" menu of Excel). Hiding the file again before it is used with CalTOX speeds up the operation of CalTOX.

Changes to the file, DatCal.xls, should not be made in conjunction with the RunCal.xls window, since any changes to this file that have not been saved will be lost when the "Quit" button is used.

SEN.xlt is a worksheet template. This template is used by the sensitivity analysis macro to display the results of the sensitivity analysis. A row is included for each parameter used in the sensitivity analysis. Each row includes a column to summarize the mean (or reference) value of the parameter, its coefficient of variation, the measure of local sensitivity, and the overall sensitivity score.

CalMACS.xlm is a macro sheet that includes all of the macros used for making and executing the custom menu, custom menu bar, custom toolbar, and dialog boxes that assist the user in making calculations on the   CalTOX worksheet.

Cal5FIX.xls is a worksheet file that contains instructions used by   CalMACS.xlm to adjust the working environment of Excel 5.0 so that   CalTOX works properly under this newer version of Excel. (At the time this document was prepared, this file had only been tested with the PC-version of Excel 5.0 and has not been tested with the Macintosh version of Excel 5.0.)

3. USING THE CALTOX SPREADSHEET WITHOUT MACROS

The CalTOX worksheet can be run without using the associated macros. In the   CalTOX files, macros are used for making and executing the custom menu, custom menu bar, custom toolbar, and dialog boxes that assist the user in making calculations on the CalTOX worksheet. In order to start a   CalTOX worksheet without automatically loading the CalTOX inputs, CalTOX templates, and the macros; simply open the template file *CalTOX.xlt* using Excel version 4.0 or higher on the Macintosh or Excel version 4.0 or higher for Windows on the PC and PC-compatible machines. When this template is opened, the user creates a spreadsheet that has a number added to the name. It becomes CalTOX.xlt1 on a Macintosh and CalTOX1.xls on PC and PC compatible machines. This is a very large spreadsheet and includes the input tables, output tables, graphical outputs and all intermediate calculations that are involved in the process of estimating the environmental distribution of a chemical, transfer to exposure media, human contact, and potential health risk. The layout of this spreadsheet is described in more detail in Section 5 below.

This spreadsheet can be used with any of the Excel functions. The user can manually enter data into this worksheet, one cell at a time, or can open and " unhide" the *DatCal.xls* file and copy and paste the columns of inputs from this input file. Many of the cells in this file are locked in order to prevent the user from either entering data in a formula column or from incorrectly modifying equations. Each adjustment cell next to the data input fields has a predefined probability density function assigned to it for use with the *Crystal Ball* add-in program.

4. USING CalTOX WITH CUSTOM MACROS

Starting the CalTOX Macros

To start CalTOX using the CalTOX macros, launch the file named RunCal.xls. This can be done in both Macintosh and Windows by double clicking on the icon for this file or by opening the RunCal.xls file from within the Excel application. On **Macintosh** computers, the RunCal.xls file will be marked by the following icon:

RunCal.xls

After the program is initiated, you will see a number of operations taking place. The status bar in lower left corner informs the user of what operations are taking place. In order to carry out any operations, you must choose whether you want to **create** a new CalTOX working file from the template worksheet or load an existing file. If this is the first time you are running CalTOX, the only option you will have is to create a new file. The dialog box below will appear on the screen and prompt you to either create a file or open an existing file.
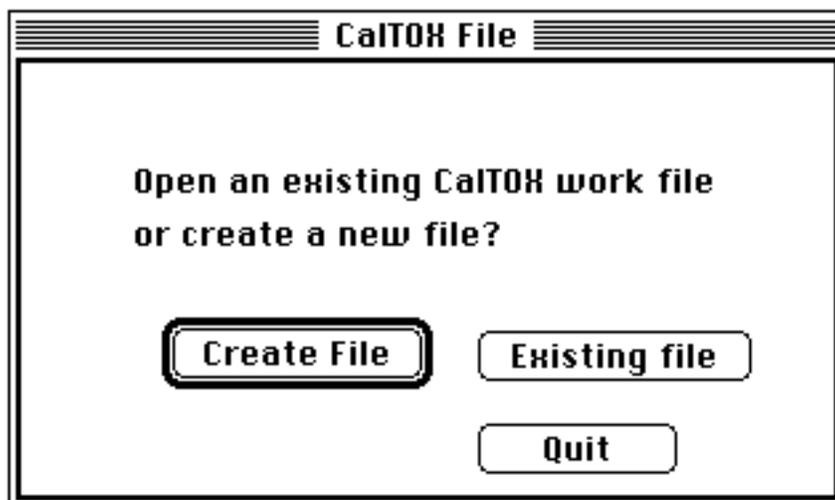
This display shows the Macintosh-version of this dialog box. These dialog boxes will be somewhat different in appearance on an IBM PC or PC compatible computer operating under Windows. The figure on the following page shows the display that appears on the (Macintosh) computer screen once the RunCal.xls file has been loaded.

figure 1 goes here

If you select the option of opening an existing file, you will be asked to select a file from the CalTOX directory. **Do not select a file from outside the CalTOX directory or else the macros will not work, since moving outside the CalTOX directory causes the directory path to be reset.** If the file you select is not a worksheet file or does not match the CalTOX worksheet template, it will be rejected.

Once you have created a new file or loaded an existing file, you will be prompted to name and save the file in your current directory. The following dialog box will appear on the screen to solicit this information.
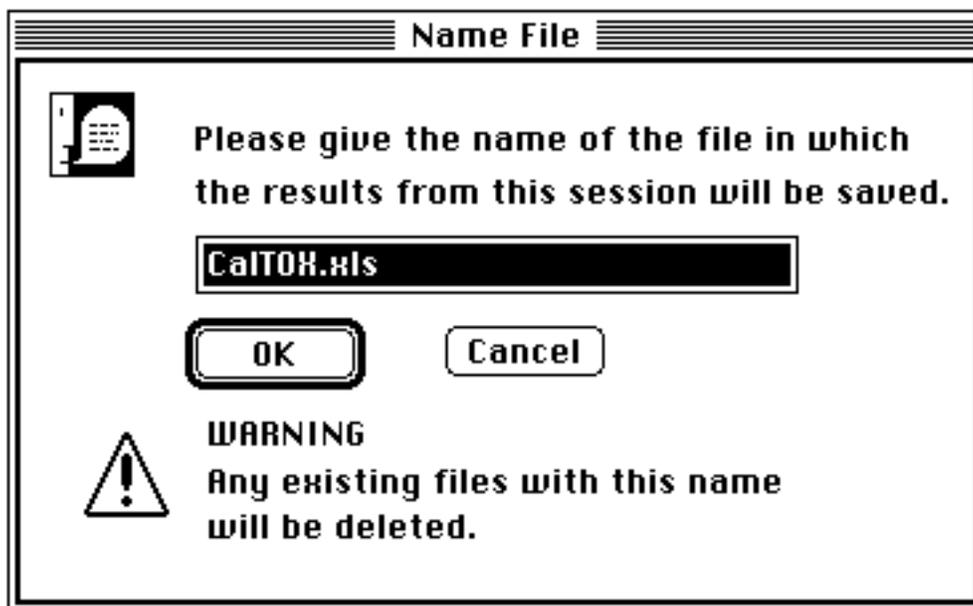
The default name is CalTOX.xls. However, this file can be given any name (within the name-size limit) on a Macintosh and any eight-character name followed by ". xls" on PC or PC-compatible machine. **Characters that are not allowed as parameter names in Excel, such as, blanks, commas, hyphens, plus signs, etc., canNOT be used in this name. (Consult the Excel manual for a full list of restricted characters. The underline character "_" and numbers ARE allowed in this name.)**

*Importa*nt: If you select a name that already exists in the current directory, any file with that name will automatically be overwritten.

CalTOX is currently configured to use only a one main worksheet at a time. Other CalTOX-type spreadsheets can be opened using the "File Open" command in Excel, but only the worksheet opened initially by RunCal.xls or a file opened using the "New Problem" button on the RunCal window will be used in combination with the command macros that load new data into the spreadsheet and carry out the sensitivity and uncertainty analyses.

Using CalTOX with Macros

Once the CalTOX work environment has been established, the CalTOX worksheet and the data files are loaded, and you will be ready to carry out calculations using CalTOX. You should now see the display shown in Figure 1. This flow chart illustrates the typical flow of tasks in a CalTOX calculation and provides buttons that operate macros that automatically carry out CalTOX calculations. Figure 2 illustrates which boxes in this flow chart are linked to CalTOX macros.

The CalTOX worksheet files, created from the CalTOX.xlt template file by choosing the "create file" option from the "start-up" or "new-problem" dialog boxes, come pre-loaded with a default set of data, which are generic and not representative of any chemical or California landscape.

Selecting a Chemical

In order to select a chemical to use in a CalTOX calculation, click on the button labeled "Pick a Chemical". The following dialog box will appear on the screen.
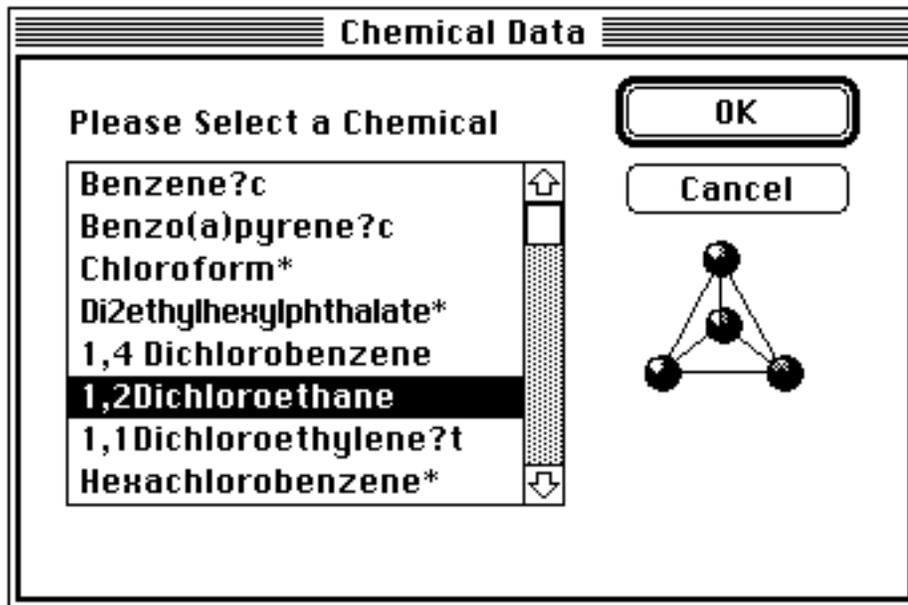
This dialog box provides a scrolling menu of the chemicals currently available in the file DatCal.xls. Updated DatCal.xls files may be downloaded from the computer bulletin board (see Technical Support Section and Appendix) and will contain additional chemicals as they are approved for use in CalTOX. The DatCal.xls file on the computer bulletin board should be checked frequently to get the most current parameter values. Also, the computer bulletin board has a conference for users to leave messages and opinions on chemical parameters (conference #5).

The symbols that are placed after the chemical name are used to designate the source of the chemical properties. Currently, two references are being used for chemical properties input. The first reference, which is indicated by the absence of the * symbol, consists of a series of chemical-properties reviews prepared at the University of California, Davis, during 1993-1994, specifically to support the   CalTOX model. The second reference, indicated by the presence of the   *symbol, is based on
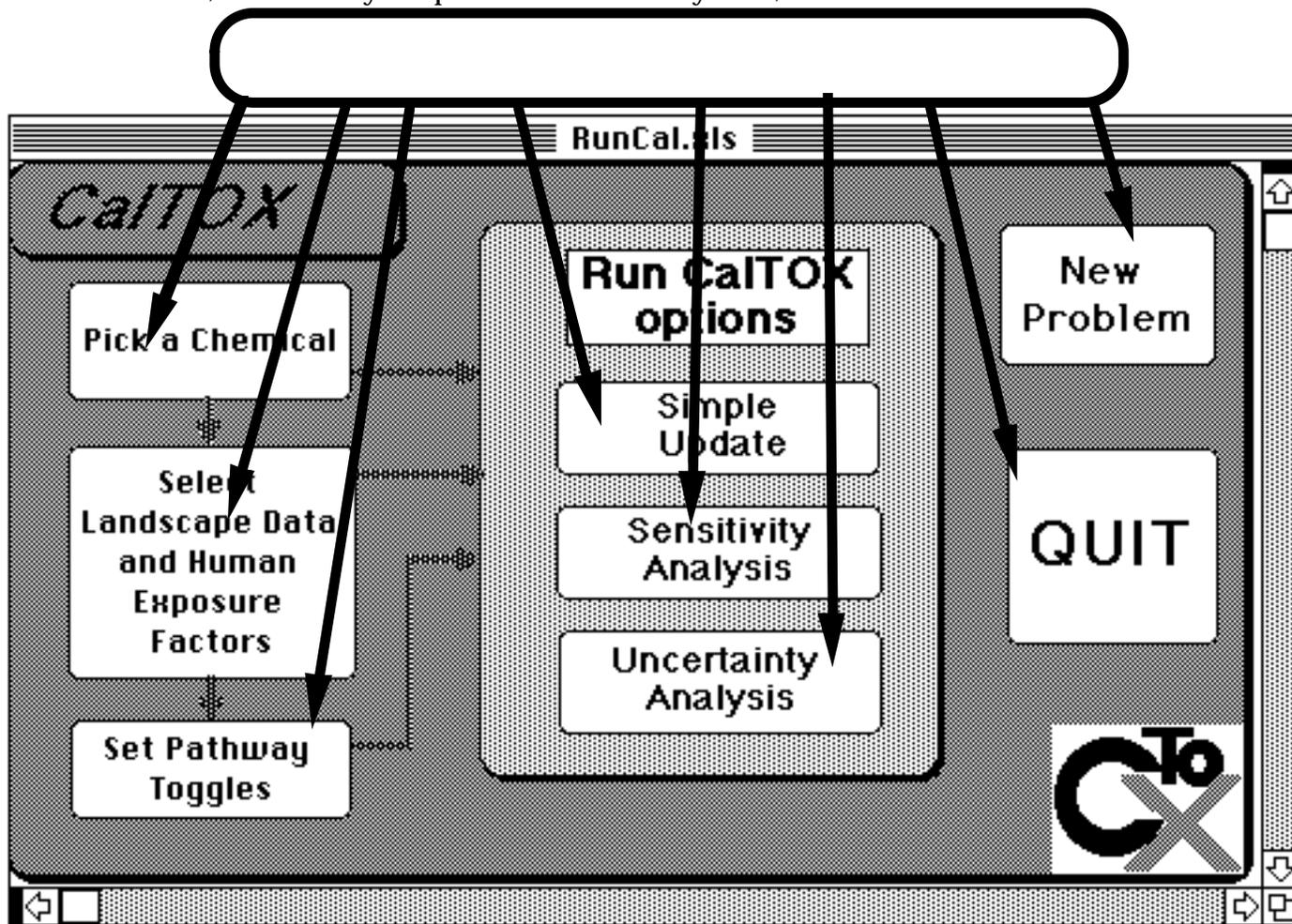
Figure 2. The macro buttons on the   CalTOX flow-chart worksheet.

information included in a report prepared by Lawrence Livermore National Laboratory (McKone et al., 1994) for the State of California Office of Environmental Health Hazard Assessment and the Air Resources Board. A   *?c* symbol indicates a chemical for which the chemical-properties data have not yet been audited and approved for application by the DTSC. The chemical-properties data provided for these chemicals should be considered as preliminary and subject to revision. A   *?t* symbol indicates a chemical for which the toxicity data have not yet been audited by the DTSC for consistency with current Cal/EPA guidelines and recommendations. The toxicity data provided for these chemicals should be considered as preliminary and subject to revision.

Selecting a Landscape and Exposure Factors

To select a set of landscape data and human exposure factors that define an exposure scenario to be used with chemical data in a   CalTOX calculation, click on the button labeled "Select Landscape Data and Human Exposure Factors". The following dialog box will appear on the screen. The user can scroll among the list of scenarios to select the data set to be loaded into the main   CalTOX spreadsheet. Additional scenarios will be available in the future via updated   DatCal.xls files placed on the computer bulletin board (see Technical Support Section).
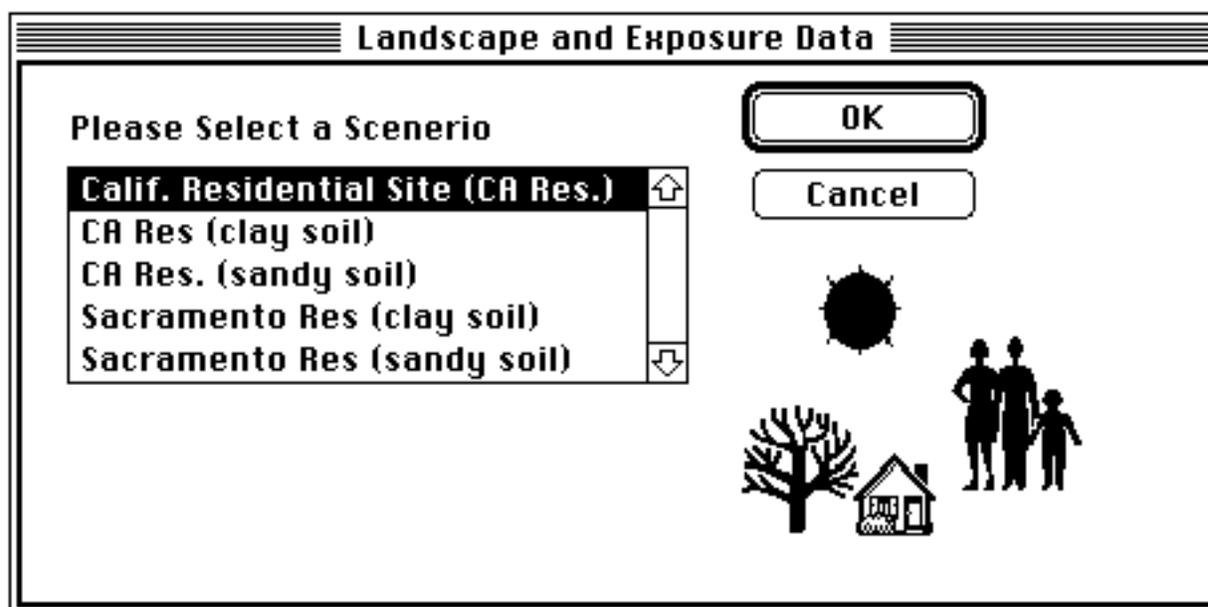
Setting Pathway Toggles

Each update of the   CalTOX spreadsheet values can be modified to include and exclude exposure pathways and/or exposure and environmental media. On page 8 of the CalTOX worksheet is a list of the exposure pathways that can be set off or on for any calculation. When activated, the "Set Pathways Toggles" button moves the window to page 8 of the CalTOX spreadsheet so the user can select the pathways to be included in a given calculation. On this page are two large columns that contain brief descriptions of the pathways that can be turned on or off. Next to these columns are narrow columns, which contain either a "1" or a"0". A "1" indicates a pathway or exposure medium that is "on" and a "0" indicates a pathway that is "off".   **Only "1" or "0" should be entered in these columns.** The CalTOX worksheet is pre-loaded with all pathway toggles "on".

Updating the Spreadsheet Values

To update the calculations in the CalTOX worksheet after any data/input modifications—that is, selecting a new chemical, selecting a new landscape and exposure data set, making changes to the pathway toggles, or changing the target risk, the time, or the initial concentrations—it is necessary to **either** activate one of the buttons in the column with the heading "Run CalTOX Options" in the main flow-chart (see Figure 1) or activate the "recalculate" button on the CalTOX toolbar. The "recalculate" button makes a simple update of the cell values.

Simple Update

Pressing the "Simple Update" button causes the CalTOX spreadsheet to update all the cells to reflect any changes in values that have been made. Once the spreadsheet has been updated using this button, the window is reset to the "home" page (page 1) on the active CalTOX worksheet. The following dialog box appears on the screen to let the user know that the spreadsheet has been updated to reflect current values.
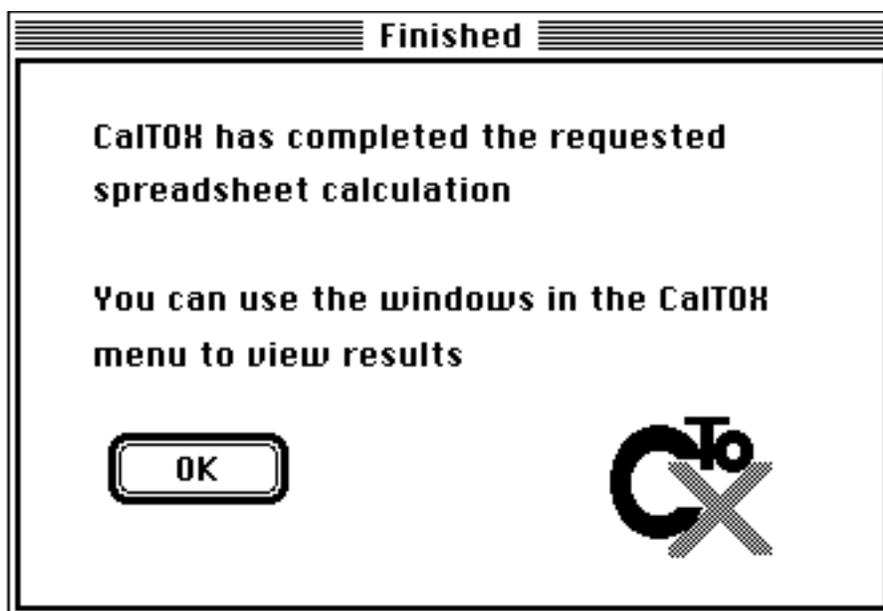
When the "recalculate" button on the CalTOX toolbar is used to update spreadsheet values, this dialog box does not appear.

Sensitivity Analysis

The "Sensitivity Analysis" button is used to carry out sensitivity analyses on the current CalTOX worksheet. More details on what actions this macro initiates are described in the section below on sensitivity analysis with CalTOX. The sensitivity analysis creates a file in which the results of the sensitivity analysis are stored. When the sensitivity

analysis is started, the following dialog box appears and the user is asked to provide a name of a file in which to display the results of the sensitivity analysis.
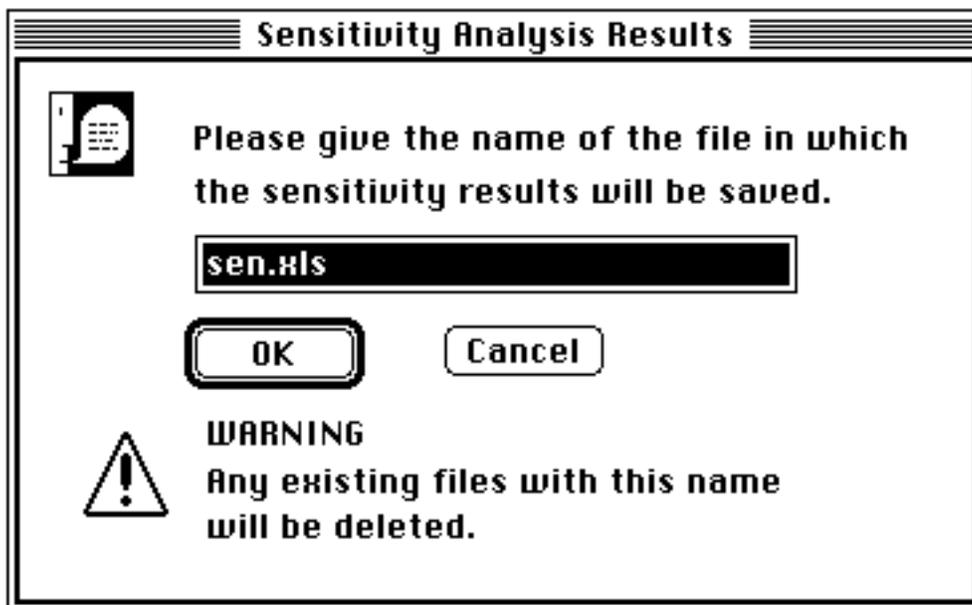
```
╔═══════════ Sensitivity Analysis Results ═══════════╗
║                                                     ║
║    ┌──┐   Please give the name of the file in which ║
║    │▤ │   the sensitivity results will be saved.    ║
║    └──┘                                              ║
║          ┌─────────────────────────────────┐        ║
║          │ sen.xls                         │        ║
║          └─────────────────────────────────┘        ║
║                                                     ║
║          ┌────────────┐    ┌──────────┐             ║
║          │     OK     │    │  Cancel  │             ║
║          └────────────┘    └──────────┘             ║
║                                                     ║
║    ╱╲     WARNING                                    ║
║   ╱ !╲    Any existing files with this name          ║
║  ╱────╲   will be deleted.                            ║
║                                                     ║
╚═════════════════════════════════════════════════════╝
```

Characters that are not allowed as parameter names in Excel, such as, blanks, commas, hyphens, plus signs, etc., canNOT be used in this name. (Consult the Excel manual for a full list of restricted characters. The underline character "_" and numbers ARE allowed in this name.)

Important:	If you select a name that already exists in the current directory, any file with that name will automatically be overwritten.

At the conclusion of the sensitivity analysis, the window switches to the sensitivity results file.

Uncertainty Analysis

Activating the "Uncertainty Analysis" button creates a file called " UNSCal.xls" into which the current CalTOX spreadsheet is saved. All other CalTOX files as well as the CalTOX menu, the CalTOX menu bar, the CalTOX toolbar, and the CalTOX macro file are closed for the uncertainty analysis. Once this button is activated, the current CalTOX session is closed and the only way to return to the CalTOX working environment is to restart the CalTOX using the RunCal.xls file.

The file " UNSCal.xls" includes all the current information contained in the active CalTOX worksheet, but excludes all graphics displays in order to speed up the Monte Carlo calculations. An uncertainty analysis can be performed on the file " UNSCal.xls" by adding in a Monte Carlo program, such as *Crystal Ball* or *@Risk.* More details on

what actions this macro initiates are described in the section on uncertainty analysis with CalTOX.

Starting a New Problem

At any point during the operation of   CalTOX, the user can create a new   CalTOX worksheet from the CalTOX template, or open an existing file that is on the hard disk by using the "New Problem" button. The file selected using the "New Problem" button becomes the file that is operated on by any macro operation associated with (a) the buttons in the RunCal flow chart, (b) the tools on the   CalTOX tool bar, or (c) menu commands in the CalTOX menu. When the "New Problem" button is activated, the last file opened at start-up or opened by a previous "New Problem" action and any   *sen.xls*-file are saved and closed. Other   CalTOX files remain open. When the user activates the "New Problem" button, the following dialog box appears. Selecting the "cancel" button in this dialog box stops a new file from being loaded and the existing   CalTOX worksheet retains priority for all macro operations.
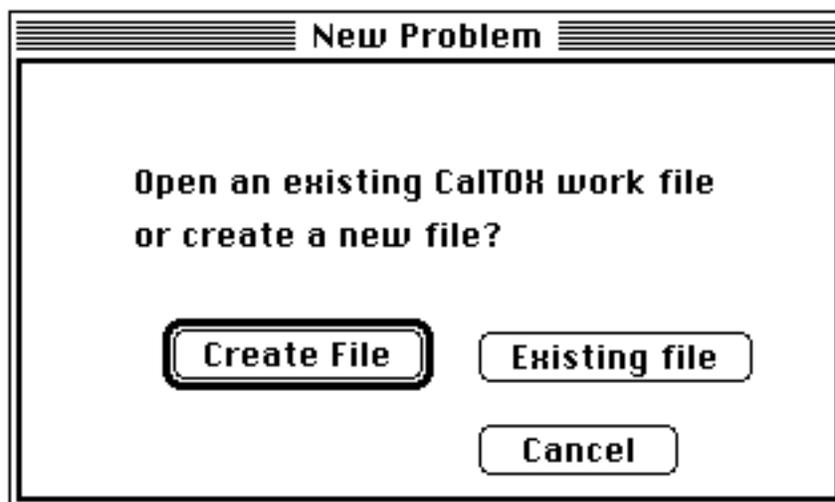
Quitting CalTOX

The "Quit" button causes the   CalTOX worksheets and macro sheets to be closed and causes Excel to quit. Changes to the file,   DatCal.xls, should not be made in conjunction with the RunCal.xls window, since any changes to this file that have not been saved will be lost when the "Quit" button is used.

Viewing the Spreadsheet Results

A number of macros and macro-initiating buttons and commands are included in the CalTOX environment so the user can quickly and easily load data, switch from one spreadsheet window to another and locate inputs and outputs in the   CalTOX worksheet. There are three items that can be used to operate these macros—the

"RunCal.xls" worksheet that was described above, the   CalTOX menu on the CalTOX menu bar, and the CalTOX toolbar. The latter two items are described here.
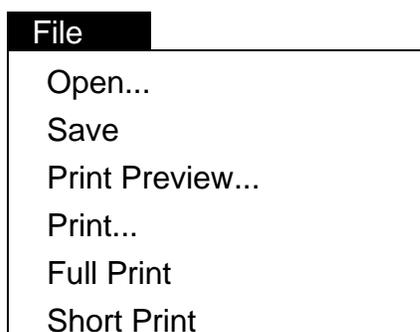
The CalTOX Menu Bar

The CalTOX menu bar differs from the standard Excel menu bar by the presence of the "CalTOX" menu, by modifications to the "File" menu, and by the absence of standard menus that are not required in the   CalTOX environment. This menu is created automatically when the file " RunCal.xls" is loaded. The appearance of the   CalTOX menu bar is illustrated below.
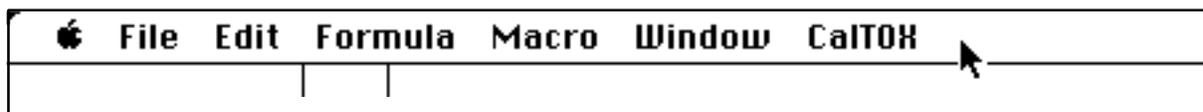
The Modified File Menu

The "File" menu in the   CalTOX environment is modified by being shortened and by the addition of two custom-print commands. The modified menu contains no "Save As..." command and no "Quit" or "Exit" command. Exiting or Quitting   CalTOX is accomplished by either using the "Quit" button on the flowchart or by pressing the   +Q key combination on a Macintosh or the   **ctrl**+**Q** key combination on a PC. The "Print Preview" and "Print" commands operate as they would on any Excel file. The "Full Print" command is used to automatically print all 18 pages of the current   CalTOX worksheet. The "Short Print" command is used to print out the first 8 pages of the CalTOX worksheet, which contain all the input information. Printing the worksheet takes a considerable amount of time. The modified "File" Menu is illustrated below.

The CalTOX Menu

The CalTOX menu includes a list of commands that can be used to view different parts of the CalTOX worksheet. Each command name includes a brief description of the table or object in the   CalTOX worksheet that can be viewed using that command. Also

listed is the worksheet page number corresponding to the table or object. The status bar in the lower left of the Excel window gives a longer description of what is found by a high-lighted command. The CalTOX menu can also be used to reset the window view to either the " RunCal" flow chart or the home page of the CalTOX worksheet. An illustration of how the CalTOX menu looks is provided below.

CalTOX
Reset to flow-chart CalTOX home window (p1)
Chemical properties (p2) Landscape data (p3) Exposure factors (p5)
Exposure histogram (p7) Pathway toggles (p8) Potential dose matrix (p9) Exposure media conc. (p10) Cumulative dose (p11) Chemical fate (p12)
Warnings! (p14) Fugacities and Z values (p15) Gain-loss table (p17) Conc. vs time graph (p18)
Quit CalTOX

Printing Results

The "File Print" in the menu bar can be used to print out any of the CalTOX files that can be located in the "Window" menu. Any file created from the CalTOX worksheet template has both the print area and page setup already defined so that the print command causes all pages of the CalTOX worksheet to be printed out in landscape format on 8 1/2 by 11 inch paper. The "Full Print" command automatically prints all 18 pages of the current CalTOX worksheet, and the "Short Print" automatically prints out the first 8 pages of the worksheet.

The CalTOX Toolbar

The CalTOX toolbar is placed in the upper right of the computer screen when   CalTOX starts. Currently, this toolbar can be used to begin three different   CalTOX macros. The left-most tool activates the " RunCal" (or flow-chart) worksheet and is marked by the CalTOX icon. The middle tool (with the diamond shape) can be used to activate the "home" window of the   CalTOX worksheet. The third, tool recalculates all the cells on the CalTOX worksheet and can be used in place of the "Simple Update" button on the flowchart to make a simple update of worksheet values. This is a "floating" toolbar and thus can be moved to any location on the screen by dragging it with the mouse.

This tool recalculates all the cells on the CalTOX worksheet and can be used to make a simple update of spreadsheet values

This tool activates the RunCal (flow-chart) worksheet

This too activates the CalTOX worksheet and goes to the "home" page on that worksheet

---
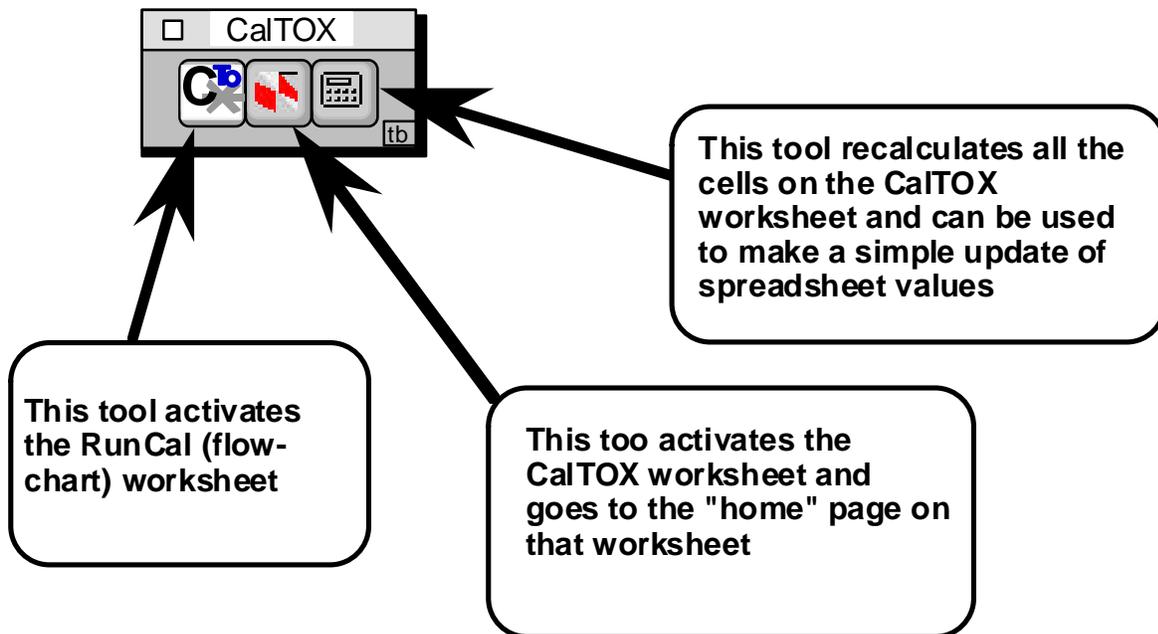
5. PROBLEMS

There are many different brands of PCs and multiple versions of Windows and Excel currently in use, and it was not possible to test CalTOX on the full spectrum of machine/software/printer combinations with which it could be used. Thus, problems may occur in the execution of macros and in the display and printing of the spreadsheet information.

What to do if a Macro-Interrupt Occurs

In Excel for Macintosh and for Windows, an error during the execution of a macro causes the "macro-interrupted" message to be displayed. When this happens, the user is given the option to "Halt," "Step," or "Continue." If this display appears, the user should select "Halt" and get back to the " RunCal" flowchart and try to run the macro again. If problems continue, quit CalTOX and restart.

Multiple CalTOX Tool Bars

If CalTOX starts up and displays more than one CalTOX toolbar, quit the program, delete the file " oldtool.xlb" and restart the program.

Screen Displays and Zoom Scaling

On PC computers, the CalTOX worksheet is preset for display at 90% of full size. On the Macintosh, the CalTOX worksheet is preset for display at 100%. On some computer screens this scaling is too large, whereas, it is too small on others. On some machines this scaling leads to distortions in the display. If the worksheet is distorted or appears too large or small, it may be necessary to use the Excel "Zoom" function to change the display scaling. When printing, the scaling should not be set above 100%. In Excel 4.0, the "Zoom" function is under the "Window" menu, and in Excel 5.0, the "Zoom" function is under the "View" menu.

On some PC computers, the words appear chopped off or #### is found instead of a number. This is because personal computers do not handle video displays identically. This is an annoying situation, but we have not seen a PC display in which one cannot see all important information. You may "uncover" words or numbers by increasing the column width. This is most easily done by moving the pointer to the column heading letter area. Point at the line on the right hand side of the column to be widened (the pointer will become another symbol), press the mouse button, and "pull" the column wider. This will affect how much of the page you will see on the screen and printed on

a single page, but it will affect only the current worksheet. Future worksheets will appear with the chopped off words and ### symbols.

Print-Preview, Print-Scaling, and Page Setup

The CalTOX worksheet is preset to print on 18 pages at 90% of full size in black and white. Sometimes these settings can result in loss of information or can cause distortion on the printed pages or in Excel "Page Review." These settings are built into the "short print" and "full print" options. The "Page Setup" function in the "File" menu can be used to change these settings on the "Print" function under the "File." However, when print scaling goes above 90%, the automatic page breaks in the   CalTOX worksheet may not work, resulting in more than 18 pages being created and page breaks in the wrong places.

Memory Problems

Memory allocation may be a problem when using   CalTOX on IBM-compatible computers. This generally occurs when you try to run   CalTOX after opening other spreadsheets. This is not unique to   CalTOX but is a general problem affecting Windows and Excel. If you get an error message like "Insufficient Memory", quit the applications and exit from Windows to DOS. Then enter Windows again. This should enable you to run CalTOX.

6. SPREADSHEET STRUCTURE

The CalTOX worksheet has 18 pages arranged in six rows and three columns. Page breaks in the worksheet display are marked by heavy gray lines. Page one is the "home page" and contains summary results and some of the inputs relating to target risk, time to start the calculation, and initial concentrations. Pages 2 through 6 make up the remainder of the first column and serve as input fields for chemical properties, landscape properties, and human exposure factors used in the model.

The second column is devoted to the display of results from the   multipathway exposure assessment. At the top of this column is the exposure histogram that relates potential doses by route to the environmental medium that contributes to that potential dose. The remainder of this column includes the table of toggles to turn pathways on and off, the potential-dose matrix, the matrix of exposure media concentrations, the cumulative-dose table, and the chemical-fate diagram. The chemical-fate diagram is not available in the PC version of   CalTOX. The information in the diagram is tabulated in the gain-loss table on page 17 of the spreadsheet.

The third column is devoted principally to the multimedia   fugacity model. However, the first page in this column includes a list of all secondary input parameters. These are model parameter values that are calculated from model inputs listed on pages 2 through 6. This is followed by a list of any warnings and error messages that have been triggered by the calculation. The remainder of the column is devoted to the fugacity model and includes tables of   fugacities and fugacity capacities, diffusion and advection rate constants, gain-loss tables for each compartment, compartment-specific rate constants, and a table and graph of concentration versus time in the root-zone and vadose-zone compartments.

Figure 3 is a schematic of the 18-page   CalTOX worksheet.

Home page	Exposure histogram	Calculated properties
◆ Inputs Outputs		
page 1	page 7	page 13
Chemical properties	Exposure pathway on/off toggles	Warnings and error messages
page 2	page 8	page 14
Landscape properties	Potential-dose matrix	Fugacities, compartment volumes, and fugacity capacities
page 3	page 9	page 15
Landscape properties (continued)	Exposure-media concentrations table	Diffusion and advection rate constants
page 4	page 10	page 16
Exposure factors	Table of time-dependent cumulative doses within the population	Compartment gains and losses, residence times, inventories, and concentrations
page 5	page 11	page 17
Exposure factors (continued)	Environmental fate diagram (Not available in PC version)	Time dependent compartment inventories in the soil layers
page 6	page 12	page 18

Figure 3. The 18 pages in the   CalTOX worksheet and how these pages are arranged into three columns and six rows in the worksheet.

The "Home" Page

The home page of the CalTOX worksheet is marked by a diamond and contains summary results and some of the inputs relating to target risk, time to start the calculation and initial concentrations. At the top of the page is information on the version of the CalTOX template used. Below this is the problem summary that includes the name of the chemical used in the calculation and the name of the site-data set used for landscape properties and exposure scenarios.

Inputs on the Home Page

The remainder of the page lists important inputs that control the calculation of risk and soil clean-up goals and the summary of outputs describing the forward calculation of risk and the reverse calculation of soil clean-up values. Figure 4 illustrates the input displays on the home page.

Inputs:

Chemical name   Tetrachloroethylene (PCE)

Site name   California Residential Site

Toxicity Criteria

	Cancer potencies (kg-d/mg)	Non-cancer RFDs (mg/kg-d)
Inhalation	3.0 E-03	0
Ingestion	5.1 E-02	0
Dermal	3.0 E-03	0
Total dose		0.1
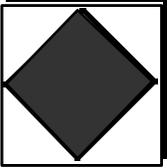
Target Risk/Hazard =

Risk	Hazard quotient
1.0 E-06	0.20

Time after measured concentrations when exposure begins   3.65 E+02 days

Measured Concentrations   (at time = 0)

Root-zone soil	1	ppm (mg/kg)
Vadose-zone soil	1	ppm (mg/kg)
Ground water	n/a	ppm (mg/L)

Continuous inputs

Source term to air (mol/d)	0.0 E+00	Sa
Source term to ground-surface soil (mol/d)	0.0 E+00	Sg
Source term to surface water (mol/d)	0.0 E+00	Sw

Constants

Gas Constant (Pa-m^3/mol-K)	8.31 E+00	Rgas

Outputs on the Home Page

The major outputs from a   CalTOX calculation are summarized on the right side of the home page and include a window for any warning messages and a summary of soil clean-up targets based on the target risk and the target hazard ratio. Soil clean-up numbers based on risk are calculated   **both** for the individual exposed for the exposure duration **without** having any exposure to breast milk and for the individual who is exposed for the first year of the exposure duration to contaminants in breast milk. Similarly, clean-up goals for non-cancer end points are based separately on the breast-feeding infant and the adult. Recommended target soil concentrations at the far right are minimum values in root and   vadose soil of target concentrations based on risk and hazard and infant and adult exposures.

```
Outputs:  ▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒▒
Target Soil Concentrations (in ppm)
Based on cancer risk:
                    w/o b-milk   w b-milk
         Root soil │ 2.4 E-1  │ 2.4 E-1 │
        Vadose soil│ 7.9 E-2  │ 7.8 E-2 │
Based on hazard
                      Adult       Infant
         Root soil │ 4.2 E-1  │ 2.8 E+2 │
        Vadose soil│ 1.4 E-1  │ 9.0 E+1 │
                               │root soil  │ 2.4 E-1 │
                               │vadose soil│ 7.8 E-2 │


Un-mitigated risk and/or hazard ratio
    Risk     │░░1.7E-5░░│ 1.7 E-5 │
Hazard ratio │░░1.9E+0░░│ 3.0 E-3 │


Concentration limits (ppm-solid) without NAPL
         Root soil    866.32
        Vadose soil   600.02
         Sediments   1187.77
Concentrations in environmental media
        Air          │ 3.9 E-05 │ mg/m3
        Plants       │ 8.1 E-02 │ mg/kg(FM)
Grnd-surface soil    │ 1.4 E-04 │ mg/kg(total)
   Root-zone soil    │ 4.1 E-02 │ mg/kg(total)
 Vadose-zone soil    │ 3.6 E-02 │ mg/kg(total)
   Ground water      │ 1.8 E-02 │ mg/L(water)
   Surface water     │ 4.4 E-06 │ mg/L
      Sediment       │ 8.8 E-06 │ mg/kg
```

The soil clean-up goal is based on a target risk or hazard. The estimated lifetime risk is based on a time-weighted average over the exposure duration. The hazard is based on the maximum value computed over the exposure duration. The soil clean-up goal is based on how much the initial soil concentration must be reduced to meet the target risk. Thus, this output column specifies both the estimated risk without soil cleanup and as well as the soil concentrations required to meet the target health goals. Because the forward or reverse calculation of risk is meaningless if the concentration of contaminant in soil exceeds the solubility limit in soil solution, these solubility limits are listed in this output summary.

Target soil concentrations will be labeled "invalid" when: 1) the target soil concentration exceeds the solubility limit in a soil layer (the term "> conc. limit" will appear in the boxes for target clean-up concentrations); 2) the recharge value is negative; or, 3) the recharge value is too large.

The unmitigated risk is labeled "invalid" when: 1) the initial concentration of contaminant exceeds the solubility limit; 2) some other parameter in the model is detected to be out of range; or, 3) the estimated risk exceeds 0.1. An error message appears in the error window as shown below.

When the unmitigated risk exceeds 0.1, the forward calculation of risk cannot be estimated as the product of dose and potency because of non linearity in this range.

However, the calculation of target soil clean up values is usually valid, even when the forward calculation of risk has been labeled as invalid. In this case the display at the top of the following page appears.

When there are no potency values or allowable daily intakes specified for a chemical, the term " n/a" appears in the appropriate box for the clean-up value.

The warning message is also triggered to display a less severe message, when non critical-parameter values go beyond limits that are stated in the model assumptions of the CalTOX reports.

Outputs: See Warnings Please
Target Soil Concentrations (in ppm)

This is often not a critical problem. Using the   CalTOX menu bar to select the "Warnings" command or double clicking on this message will take the user to the table of warning messages to identify the source of the problem.

Parameter Value Inputs

All inputs to the CalTOX worksheet are entered in the seven-column format shown in Figure 5. The first column is used to describe the input parameter including units. The second column lists the symbol used in the spreadsheet to represent that parameter. Symbols in bold with a "-" adjacent indicate parameters whose values can be estimated from default estimation methods when the mean value is set to -99. The third column

is a formula column and displays the value used in a   CalTOX calculation based on the mean value, estimation methods and/or the value selected for adjusting this input as part of the sensitivity or uncertainty analysis. The first three input columns are locked and cannot be modified by the user. The fourth column lists the expected value of an input based on uncertainty and/or variability. The fifth column lists the coefficient of variation, the ratio of standard deviation to the mean, that reflects the variance in the input parameter. Columns four and five are open to modification by the user. Column six includes an adjustment factor to the value of a parameter that is used in a given calculation. On the computer screen, this column contains different colors or shades of gray. No background color indicates no   preassigned distribution; light gray means a preassigned, log-normal independent distribution; cross-hatched means a distribution correlated with some other variable; and dark gray means a truncated log-normal distribution. These gradations will look different on different computers. This cell is provided as a location to modify the value used for the sensitivity and uncertainty analyses. The last column is locked and is for use to make any internal modifications to value units and to list additional input information.

Multimedia Transport Model Inputs

The CalTOX multimedia transport and transformation model uses two sets of input data, one describing the properties of the contaminant and the other providing properties of the environment or landscape receiving the contaminants.
The needed physical-chemical properties include molecular weight;   octanol-water partition coefficient; melting point; solubility, Henry's law constant or vapor pressure; diffusion coefficients in pure air and water; and   intermedia distribution coefficients, such as K_d and K_{oc}. Also required are media-specific transformation rates. The types of data needed to construct a landscape data set include meteorological data, hydrological data, and soil properties. The chemical inputs are on page 2 of the CalTOX worksheet and the landscape data are on pages 3 and 4 of the worksheet (see Appendix A).

The Human Exposure Model

The types of data needed to carry out the exposure assessment include exposure duration and averaging time, anatomical and dietary properties, food consumption patterns, activity patterns and exposure times, household parameters, other human factors such as soil ingestion and breast milk intake, and parameters associated with food crops and food producing animals. In addition, the calculation of   intermedia transfer factors requires that a number of partition factors be available.
The exposure factor data are on pages 5 and 6 of the   CalTOX worksheet (see Appendix A).

Chemical properties

Compound name Tetrachloroethylene (PCE)		Value used	Mean value	Coeff. Var.	Adjustment	Notes
Molecular weight (g/mol)	MW	1.66 E+02	1.66 E+02	0	1	
Octanol-water partition coefficient	Kow	1.00 E+03	1.00 E+03	1.5	1	
Melting point (K)	Tm	2.52 E+02	2.52 E+02	0.1	1	
Vapor Pressure in (Pa)	VP	2.45 E+03	2.45 E+03	0.1	1	
Solubility in mol/m3	S	9.10 E-01	9.10 E-01	0.5	1	
Henry's law constant (Pa-m^3/mol)	H -	1.99 E+03	1990	0.31	1	
Diffusion coefficient in pure air (m2/d)	Dair	6.60 E-01	6.60 E-01	0.1	1	7.64 E-06
Diffusion coefficient; pure water (m2/d)	Dwater	8.80 E-05	8.80 E-05	0.1	1	1.02 E-09
Organic carbon partition coefficient Koc	Koc -	4.00 E+02	400	1.7	1	m^2/s
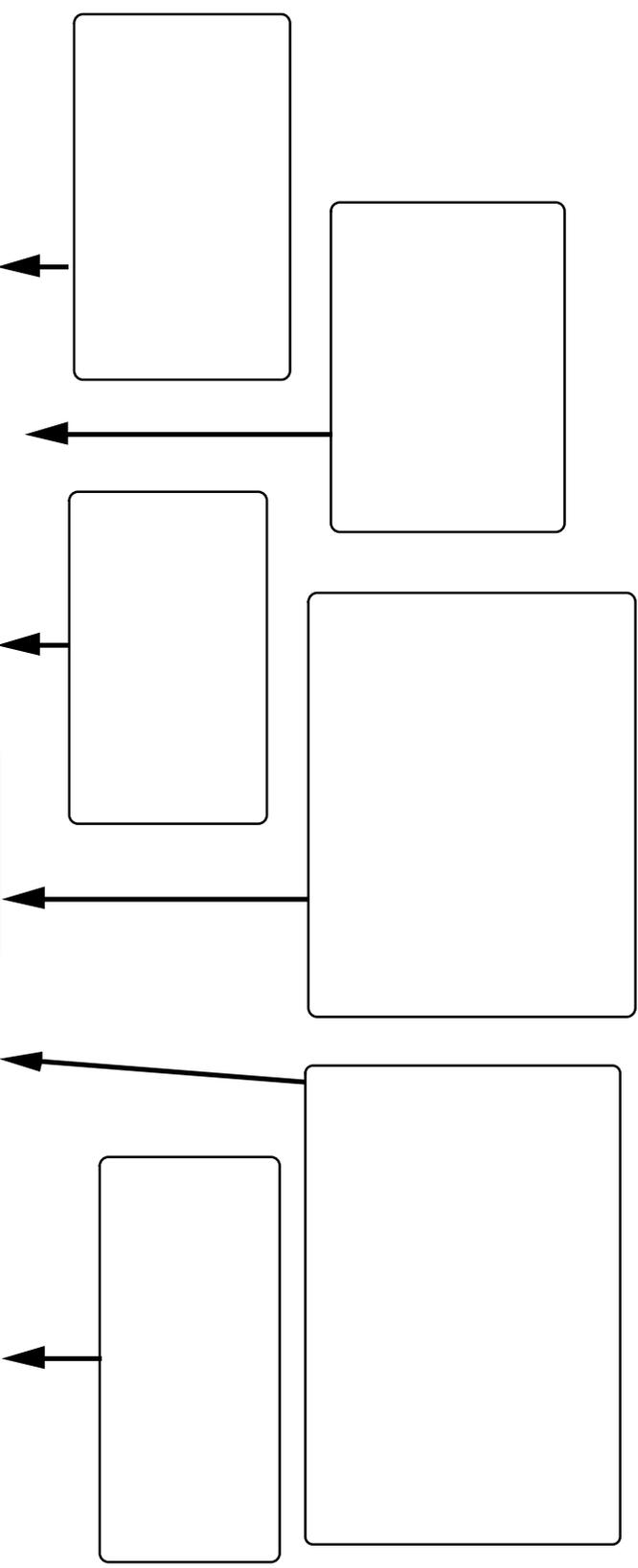
7. THE CALCULATION OF RISK AND SOIL CLEAN-UP GOALS

The Forward Calculation of Potential Dose and Risk

We construct the distribution of individual lifetime risk attributable to exposures over the duration ED (years), to a contaminant in soil at an initial (time zero) concentration, $C_s(0)$ [mg/kg(soil)], by integrating the soil concentration in time and by summing the dose and effect over exposure routes, over environmental media, and over exposure pathways.

$$H(ED) = C_s(0) \times \left\{ \sum_{\substack{j \text{ routes,}}} \sum_{\substack{k \text{ environ-,} \\ \text{mental} \\ \text{media}}} \sum_{\substack{i \text{ exposure} \\ \text{media}}} \left[Q_j\left(ADD_{ijk}\right) \times \left(\frac{ADD_{ijk}}{ED \times C_k} \right) \times \int_0^{ED} \Phi\left[C_s(0) \to C_k, t\right] dt \right] \right\}$$

where $\Phi[C_s(0) \to C_k, t]$ is the multimedia dispersion function that converts the contaminant concentration, $C_s(0)$, mg/kg measured in soil today, into contaminant concentration, C_k, at a time, t, in the future in environmental medium, k (units of C_k are mg/kg for soil, mg/m^3 for air, and mg/L for water). (ADD_{ijk}/C_k) is the unit dose factor, which is the average daily potential dose (over a specified averaging time) from exposure medium, i, by route, j (inhalation, ingestion, dermal uptake), attributable to environmental compartment, k, divided by C_k when C_k is constant over the duration, ED. The exposure media summation is over the number of exposure media that link potential dose by route, j, to contaminants in compartment, k. $Q_j(ADD_{ijk})$ is the dose-response function that relates the potential dose, ADD_{ijk}, by route j to the lifetime probability of detriment per individual within the population, (mg/kg-d)$^{-1}$.

When an environmental concentration is assumed constant over the exposure duration, ED, the population-averaged potential dose (for ingestion or inhalation routes) or absorbed dose (for dermal contact) is the average daily dose rate (ADD_{ijk}), in mg/kg-d given by

$$\left[\frac{}{} \right] \times \left[\frac{}{} \right] \times \frac{\times}{} \times$$

In this expression [C_i/C_k] is the intermedia-transfer ratio, which expresses the ratio of contaminant concentration in the exposure medium i (i.e., personal air, tap water, milk, soil, etc.) to the concentration in an environmental medium, k (ambient-air gases or particles, surface soil, root-zone soil, surface water, and ground water) and [IU_{ij}/BW] is the intake or uptake factor per unit body weight associated with the exposure medium, i, and route j. For exposure through the inhalation or ingestion route, [IU_{ij}/BW] is the intake rate per unit body weight of the exposure medium such as m^3(air)/kg-d, L(milk)/kg-d, or kg(soil)/kg-d. For exposure through the dermal route, [IU_{ij}/BW] is the uptake factor per unit body weight and per unit initial concentration in the applied medium (L(water)/kg-d or kg(soil)/kg-d). EF is the exposure frequency for the exposed individual, in days per year; ED is the exposure duration for the exposed population, in years; AT is the averaging time for the exposed population, in days; and C_k is the contaminant concentration in environmental medium k.

The Reverse Calculation of Soil Clean-Up Goals

CalTOX is designed to also carry out the reverse calculation. That is, what concentration in soil, $C_s(0)$, measured today is acceptable, given that our goal is to maintain our risk, H(ED), within the population at some time, T, in the future at or below a target risk of H^*? In this case, we calculate a target cleanup goal $C_s^*(0)$ according to

$$C_s^*(0) = \frac{H^*}{\displaystyle\sum_{\substack{j \text{ routes,}}} \sum_{\substack{k \text{ environ-,} \\ \text{mental} \\ \text{media}}} \sum_{\substack{i \text{ exposure} \\ \text{media}}} \left[Q_j\left(ADD_{ijk}\right) \times \left(\frac{ADD_{ijk}}{ED \times C_k} \right) \times \int_{T}^{T+ED} \left\{ \Phi\left[C_s(0) \rightarrow C_k, t\right] \right\} dt \right]}$$

CalTOX was designed to make this calculation using a multimedia, multiple pathway approach. In addition, CalTOX is capable of accepting a Monte Carlo add-on function so that the forward projection of risk or the reverse calculation of soil concentration can be determined probabilistically. This allows the specification of a level of certainty associated with the target risk and the target cleanup level.

8. SENSITIVITY ANALYSIS

The goal of a sensitivity analysis is to rank the input parameters on the basis of their contribution to variance in the output. Sensitivity analyses can be either global or local. A global sensitivity analysis quantifies the effects of variation in parameters over their entire range of values. A global sensitivity analysis requires a local uncertainty analysis as a starting point. The variance in the outcome is compared to the variance of the inputs. A local sensitivity analysis is used to examine the effects of small changes in parameter values at some defined point in the range of outcome values. As an example, one can use a local sensitivity analysis to make preliminary sensitivity rankings for model input parameters by using the partial derivatives of each input variable normalized according to the relationship,

$$Ds_i = \frac{\partial Y}{\partial X_i} \times \frac{X_i^o}{Y^o}$$

where Ds_i is the differential sensitivity factor for the ith parameter; $\partial Y / \partial X_i$ is the partial derivative of the output, Y, with respect to the variable, X_i, evaluated at the reference or base-case value of Y and X_i, and Y^o and X_i^o correspond to the base-case values of the variables, X_i, and the output, Y. An alternate normalization procedure is to multiply by $CV_i X_i^o / Y^o$ in place of X_i^o / Y^o, where CV_i is the ratio of standard deviation to mean value for the ith input parameter, that is σ_{X_i}/X_i^o. This alternate normalization gives a sensitivity score as follows
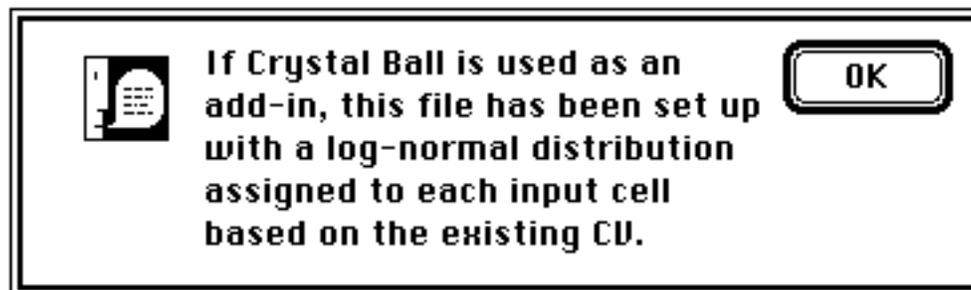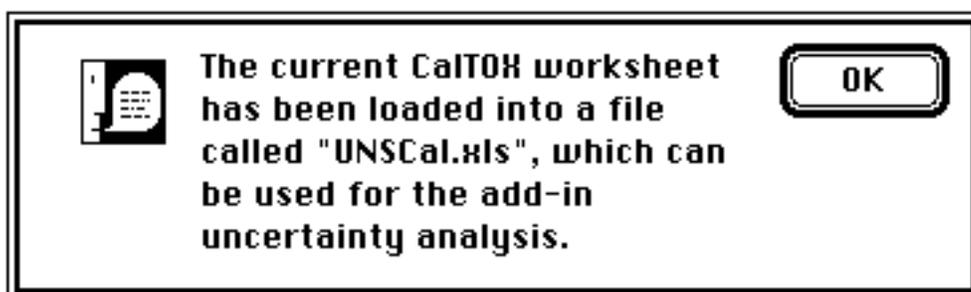
$$\text{sensitivity score} = \frac{\partial Y}{\partial X_i} \times CV_i \frac{X_i^o}{Y^o}$$

The sensitivity analysis calculation in CalTOX compiles a summary of the differential sensitivity factor and the sensitivity score for every model input and lists this information in an output file with a user-specified name.

9. UNCERTAINTY ANALYSIS

Uncertainty Analysis with CalTOX

Activating the "Uncertainty Analysis" button causes the creation of a file called "UNSCal.xls" into which the current CalTOX spreadsheet is saved. When this button is pressed the following messages appear in sequence to inform the user that the program is creating a file which can be used with an add-in program for Monte Carlo analysis.

> The current CalTOX worksheet has been loaded into a file called "UNSCal.xls", which can be used for the add-in uncertainty analysis.
>
> **OK**

> If Crystal Ball is used as an add-in, this file has been set up with a log-normal distribution assigned to each input cell based on the existing CV.
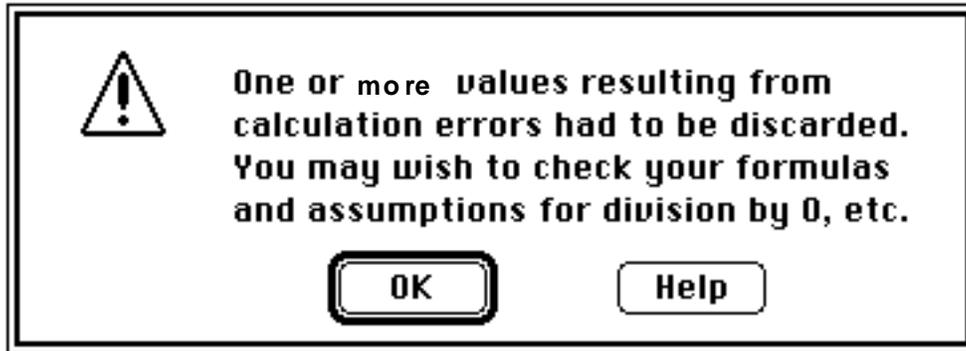>
> **OK**

All other CalTOX files as well as the CalTOX menu, the CalTOX menu bar, the CalTOX toolbar, and the CalTOX macro file are closed for the uncertainty analysis. Once this button is activated, the current CalTOX session is closed and the only way to return to the CalTOX working environment is to restart the CalTOX using the RunCal.xls file.

The file " UNSCal.xls" includes all the current information contained in the active CalTOX worksheet, but excludes all graphics displays in order to speed up the Monte Carlo calculations. An uncertainty analysis can be performed on the file " UNSCal.xls" by adding in a Monte Carlo program, such as *Crystal Ball* or *@Risk*. The CalTOX spreadsheet has been designed to work immediately with the *Crystal Ball* add-in program. All of the adjustment factors have been preassigned log-normal probability density functions with a mean value of 1 and a coefficient of variation read from the

column left of the adjustment column. Also, the outputs or forecasts to be used in the uncertainty analysis well as   correlations among some of the inputs are   preassigned.

Because some of the output cells in the   CalTOX spreadsheet contain non-numerical values the following warning is sometimes generated after the   *Crystal Ball* program runs.

```
⚠   One or more values resulting from
    calculation errors had to be discarded.
    You may wish to check your formulas
    and assumptions for division by 0, etc.

        [ OK ]        ( Help )
```

When this message appears, it is most likely due to this situation. Nonetheless, this message should not necessarily be ignored.   In order to prevent the program from stopping, eliminate the "stop on calculation error" command under the stopping criteria in the "run" menu.

More-detailed information on how to carry out an uncertainty analysis using   *Crystal Ball* and the CalTOX worksheet can be obtained by reading the   *Crystal Ball* version 3.0 User manual (Decisioneering, 1993).

The main steps in a parameter uncertainty analysis

Describing uncertainty in the output variable, Y, involves quantification of the range of Y, its arithmetic mean value, the arithmetic or geometric standard deviation of Y, and upper and lower   quantile values of Y, such as 5% lower bound and 95% upper bound. Convenient tools for presenting such information are probability distributions, such as, the probability density function (PDF) or the cumulative distribution function (CDF) for Y. However, the PDF or CDF of Y can often only be obtained when we have meaningful estimates of the probability distributions of the input variables X_i.

There are five main steps in a parameter uncertainty analysis (IAEA, 1989). These are described below.

(1) Identify the input parameters that could contribute significantly to the uncertainty in the predictions of outcome by a model. Care should be exercised at this point not to discard potentially significant uncertainties without good cause.

(2) Construct for each parameter a probability   density function both to define the range of values that a parameter can take on and to reflect the belief that the parameter will take on the various values within that range.

(3) Account for dependencies (correlations) among the parameters.

(4) Propagate the uncertainties through the model to generate a PDF of predicted outcome values.

(5) Derive confidence limits and intervals from the PDF of predicted values of the outcome variable in order to provide a quantitative statement about the effect of parameter uncertainty on the model predictions.

CalTOX has been designed to carry out these steps using the   CalTOX worksheet and an add-in Monte Carlo program such as *Crystal Ball* (Decisioneering, 1993)

Monte Carlo Analysis

In a Monte Carlo analysis, each of the input parameters is represented by a probability density function that defines both the range of values that the parameter can take on and the likelihood that the parameter has a value in any subinterval of that range. Latin hypercube sampling is a Monte   Carlo method that uses stratified random sampling to select a value from each parameter 's distribution. Whereas for simple random sampling it is often a matter of chance how evenly the selected values cover the range of the input parameter,   latin hypercube sampling places restrictions on possible unevenness. Additional information on   latin hypercube sampling is available in   Iman and Shortencarier (1984) and the users manual for   *Crystal Ball* .

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APPENDIX A: A SAMPLE LISTING OF THE CalTOX WORKSHEET

APPENDIX B: THE COMPUTER BULLETIN BOARD SYSTEM (BBS)

Support for CalTOX users will be supplied exclusively through a computer bulletin board system (BBS) established and maintained by the Office of Scientific Affairs (OSA) in the California Department of Toxic Substances Control. There will be no telephone support or any other support for   CalTOX users. To access the computer BBS,   CalTOX users must have a computer, modem and communications program. The BBS is located in Sacramento, California at (916) 323-3353. The BBS runs using   WildCat BBS software. The user's communications software for gaining access to the bulletin board should be set to 8 data bits, 1 stop bit and no parity. Baud rates up to 14.4   Kbaud are supported. Users must call and "apply" for authorization by answering a number of questions. The "applicant" cannot use the BBS on the first call. The BBS system operator will review the information supplied and authorize the user. This should occur by noon the next working day Once the user is authorized, the user may download files, send or receive messages. The user may send a message to the system operator asking questions about the model. The user should log back on to the BBS in three working days to obtain an answer.

Introduction

A computer bulletin board system is a method for enhancing communications. A BBS lets users obtain and leave information anytime without requiring Department staff be present.   The OSA BBS supporting   CalTOX presently enables users to leave and receive messages and download files. Among the files that can be downloaded from the BBS will be updated versions of the   DatCAL.XLS file containing the most current default parameter values required by the   CalTOX model. Other text documents (in Word for Windows) that will be available on the BBS include validation reports, basis for default distributions, and the evolving   CalTOX Applications Manual (see Foreword).

There are two ways in which most people interact with a BBS: leave/receive messages and download/upload files. One can think of the OSA BBS as a party at a house with several different rooms. You can join the party in one of these rooms (called a conference). Once in the room (conference) you may speak (enter messages), listen (read messages), receive gifts (download files) or bring gifts (upload files). All of these activities are accomplished by giving the appropriate   WildCat commands.

Joining a Conference

The commands are single letters followed by hitting the enter key. The command letters are the first letter (or some letter within) the command name shown as [Q]   uit. Typing [Q] followed by the enter key will send you back to the previous menu in most circumstances. To disconnect from the BBS, type [G]   oodbye. WildCat has menus to help you remember these commands. When you first log on to the BBS, you are in the General Public Messages Conference. You must go to the specific conference in which you are interested by using the [J]   oin command.   Each conference is known to   WildCat by a number, so you must view the list which identifies the conference names and numbers. This is accomplished by using the [L]   ist command. Once you know the number of the conference you give that to the Join command, and you are moved from the General Public Message Conference to the conference of your choice. You may change conferences by using the [J]   oin command at any time.

Leaving/Reading Messages

Once in the conference of your choice, you may read messages other people have left or leave other messages yourself. In order to do either you must use the [M]   essage command. This command will bring up the Message Menu which will direct you in [R]eading or [E] ntering messages. To read messages, you must determine what messages you want to see. All messages are given a number in the order they are received. You may scroll through all the messages, [S]   earch for messages with certain specification or identify only the [N]   ew messages since you last viewed the messages. The [R]ead command enables you to view the messages.

If you want to leave a message for everyone or an individual, you need to use the [E]nter messages command found in the Message Menu. You need to decide who you want to see this message. Type their name or just hit the enter key to allow everyone to see it. Then give the message a subject name. Select the full screen editor and type your message. Once you have finished typing, save your message by hitting the escape key and typing [S] ave to save the message.

Downloading Files

The BBS computer also has files stored on its hard drive that are available for downloading. Going back to the house party analogy, these files (gifts) are located in file areas (closets) associated with the conferences (rooms). More than one room may share the same closet, so that the same gifts may given to people in a number of different rooms. (These closets are somewhat magical, that the identical gift may be

given to an infinite number of people.) The important thing to understand is that you must be in a conference which has access to the file area with the file of interest to you. Therefore, as with messaging, be sure you are in the right room.

Once in the appropriate room, you must go to the [F]   iles Menu. In the File Menu, you must determine which files you want by viewing the [L]   ist of files. Files in a specific file area are identified by a filename and a brief description of the file. Most of the files on the BBS are Word for Windows text files but some are WordPerfect and Word for Macintosh files. There are also some Excel files available, such as, the most current DatCal.xls file. In order to download a file, you must use the [D]   ownload command. Give the filename(s) of the files to be downloaded, prepare your computer to receive the file using the transfer protocol (XMODEM, ZMODEM, etc.) you specified when you registered. Prepare your computer by telling it to get ready to receive a file. This is accomplished in ProComm for Windows in the Current Setup menu. Other communications programs have other methods of alerting your computer to the appropriate communications protocol. It is imperative that your computer have the same protocol setting as the BBS computer is sending.

The OSA BBS computer is currently not taking files via uploading. At some point in the future, we may accept files.