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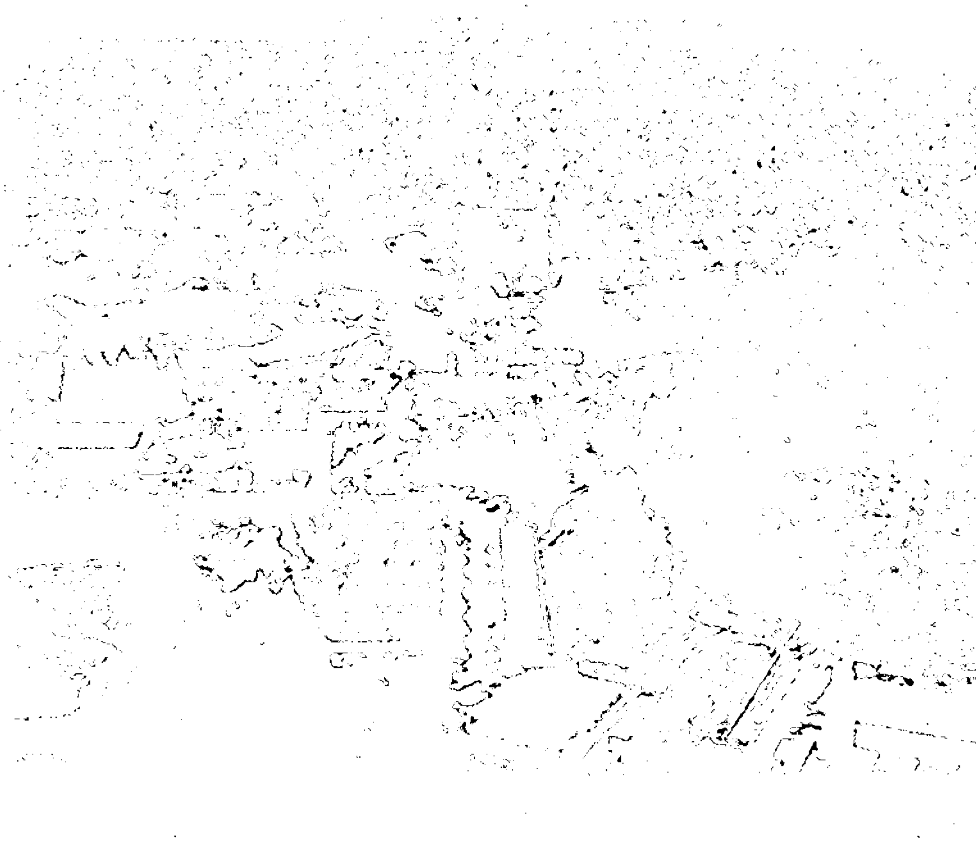
CalTOX™, A Multimedia Total Exposure Model Spreadsheet User's Guide Version 4.0 (Beta)

T.E. McKone and K.G. Enoch

Environmental Energy Technologies Division

August 2002



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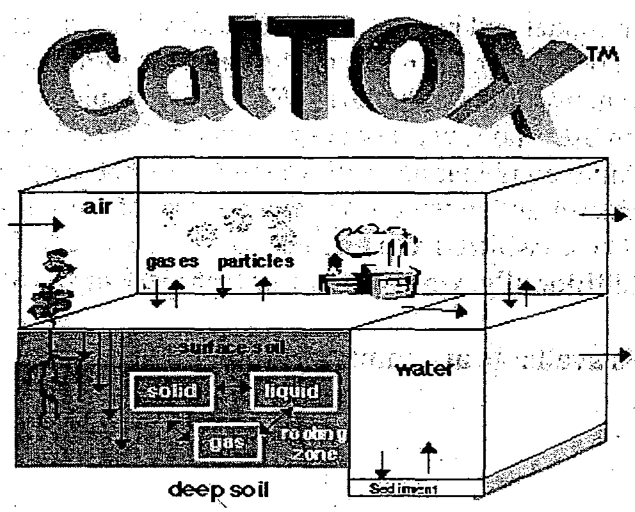


August 2002

List of Trademarks and Copyrights

CalTOX

Crystal Ball

Excel

Microsoft

PC

Visual Basic

Windows

Disclaimer

CalTOX is a research model and has not been fully tested for a broad range of applications. There could be errors in the mathematical algorithms that we have not yet identified. 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. Problems may occur in the execution of macros and in the display and printing of the spreadsheet information. This program should be considered as a research tool, and not used for regulatory decision making. **Additionally, we cannot offer technical support for the program at this point in time.**
More information is available at http://eetd.lbl.gov/ied/era

ABSTRACT

CalTOX has been developed as a set of spreadsheet models and spreadsheet data sets to assist in assessing human exposures from continuous releases to multiple environmental media, i.e. air, soil, and water. It has also been used for waste classification and for setting soil clean-up levels at uncontrolled hazardous wastes sites. The modeling components of CalTOX include a multimedia transport and transformation model, multi-pathway exposure scenario models, and add-ins to quantify and evaluate uncertainty and variability. All parameter values used as inputs to CalTOX are distributions, described in terms of mean values and a coefficient of variation, rather than as point estimates or plausible upper values such as most other models employ. This probabilistic approach allows both sensitivity and uncertainty analyses to be directly incorporated into the model operation. This manual provides CalTOX users with a brief overview of the CalTOX spreadsheet model and provides instructions for using the spreadsheet to make deterministic and probabilistic calculations of source-dose-risk relationships.

KEYWORDS: Exposure assessment, mass-balance model, multi-pathway exposure, probabilistic models

TABLE OF CONTENTS

1. INTRODUCTION

This manual provides CalTOX users with an overview of the CalTOX spreadsheet model and instructions for making calculations with this spreadsheet. We explain the layout of the spreadsheet and explain the use of Visual Basic algorithms that have been included to assist in making CalTOX calculations. This manual does not provide an extensive description of the model algorithms and its potential applications. Technical support documents provide more detailed information about the CalTOX model and its development, validation, and potential applications. These documents are available from the Technical and Electronic Information Department (TEID) at Lawrence Berkeley National Laboratory or from our web site: **<http://eetd.lbl.gov/ied/era>.**

What is CalTOX?

Environmental Scientists at the University of California campuses and national laboratories developed CalTOX as a spreadsheet model to assist in health-risk assessments that address multimedia pollutants. That is, pollutants that are emitted to and transferred among air, soil, surface water, sediments, and ground water. This spreadsheet model includes three components—a multimedia transport and transformation model, exposure scenario models, and components that quantify and evaluate parameter variability and uncertainty.

The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of contaminants that are placed in soil layers at a time-zero concentration or contaminants released continuously to air, 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 linked to a pollutant source. 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 users with the options of: (1) making point estimates of average exposure during an exposure duration, (2) applying a sensitivity analyses to these point estimates, (3) using a Monte Carlo add-in to make stochastic estimates of the distribution of exposure uncertainty/variability, and (4) applying a sensitivity analysis to the results of the Monte Carlo 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 a personal computer (PC) with a mouse, capable of running Microsoft Excel 97 or Excel 2000 for Windows, and able to "unzip" files compressed using "zip".

CalTOX requires approximately 2 megabytes of storage space. Additional storage space is required to save and store specific CalTOX sheets. 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 2000. All of the initial testing and debugging has been carried out using Excel 2000. This version has been run on a number of PCs 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.

Knowledge Requirements

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

CalTOX is designed to work with either Microsoft Excel 97 or Microsoft Excel 2000. We have developed macros that allow you 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.

Fugacity Mass-Balance Models

CalTOX includes an eight-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 eight compartments used in CalTOX are (1) air, (2) ground-surface soil, (3) plant leaves, (4) plant leaf surfaces, (5) root-zone soil, (6) the vadose-zone soil below the root zone, (7) surface water, and (8) sediments. Contaminant concentrations in ground water are currently based on a simple mass balance. CalTOX 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 the CalTOX reports (DTSC, 1993a, 1993b, 1993c; McKone at al., 2002).

Probabilistic 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 the add-in program *Crystal Ball*, which can be used to carry out sensitivity and uncertainty analyses with the results produced by CalTOX. In order to use *Crystal Ball*, the user must be familiar both with the operation of *Crystal Ball* and with the techniques of uncertainty/sensitivity analysis. The current version of CalTOX has been set up for use with *Crystal Ball* version 4.0, which is available as an add-in program for both Excel 97 or 2000.

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 4.0 of CalTOX. Future versions of the model may be modified to overcome these limitations.

Chemical Limitations

CalTOX is designed primarily for non-ionic organic chemicals and inorganic chemicals with linear and reversible distribution coefficients in soil and sediments. CalTOX was also designed to model emissions that can be treated as uniform over a region. CalTOX has not been designed or tested for surfactants or volatile metals. It can be used for partially ionized organic chemicals only when great care is exercised to adjust the partition coefficients to confirm that they are appropriate for the pH of the landscape under consideration. The model is further limited to chemicals for which one has reliable values for physical and chemical parameters.

Time Scale Limitations

The CalTOX transport model is intended for application over long time scales, months to years. It should be used cautiously for time periods less than one month 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. If an area is too small, it is flagged by an error message in the program.

The Philosophy of CalTOX

CalTOX has been subjected to extensive scientific peer review, and we believe that CalTOX is a state-of-the-art model for making regional multimedia exposure assessments. The objective of CalTOX is to improve the transparency of exposure information used in support of regulatory decision-making. This objective requires a model in which the user can track calculations and assumptions, a model that is relatively easy to use and flexible, a model that provides output in a timely and reliable fashion, and an explicit treatment of parameter uncertainty. We anticipate that the science supporting risk assessment will continue to evolve and that common assumptions will change. CalTOX was planned so that new information and algorithms can be readily incorporated in the spreadsheet templates as this information becomes available.

Overview of this Manual

The remainder of this document is divided into seven sections. Section 2 gives the user a step-by-step set of instructions for loading the program and using the spreadsheet. Section 3 explains how to start and run a sample problem using the CalTOX macro and worksheet files. Section 4 identifies a number of common problems and provides remedies. Section 5 provides a summary of the CalTOX worksheet and identifies what is included in each of the eighteen pages of this worksheet. Section 6 explains the calculation of risk and soil clean up goals. Sections 7 and 8 deal respectively with sensitivity and uncertainty analyses.

2. GETTING STARTED

The CalTOX file can be downloaded from <http://eetd.lbl.gov/ied/era> or obtained as a zip file on a 1.44 Megabyte disk. 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 the zip file 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 the zip file from the CalTOX floppy disk or from our download site 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 CalTOX.zip and extract all of the files into this subdirectory or folder using an unzipping program such as Winzip. The files that will be extracted are *CalTOXtemplate.xls, userinfo.txt, CalTOXmanual.pdf,* and any other currently available support files.

IMPORTANT:
The name of the CalTOX file must remain "CalTOXtemplate.xls". This name should not be changed. If it is renamed, the macros written for CalTOX will no longer work.

If you would like to store multiple copies of CalTOX, place them in different locations so that the name can remain "CalTOXtemplate.xls". If you create copies of CalTOX, you must also copy the file "userinfo.txt" into the same subdirectory or folder. If this is not done, the help option in the CalTOX menu will not work.

The CalTOX Workbook

The CalTOX workbook contains eight worksheets. Most of these sheets are used only by the Visual Basic macros and do not need to be view or modified by the user. When you start the program, there are only two sheets that will be visible to you. These sheets are the following:

RunCal

CalTOX

There are six other sheets that are used by CalTOX which are not visible and they are the following:

Contaminated Soil

Continuous Emission

DatCal

InputLists

Sensitivity

AllChemicals

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

RunCal is a worksheet that is used as a menu to easily perform the CalTOX operations. This sheet contains several different buttons that carry out different operations when activated. These buttons are explained in the next section.

CalTOX is the primary worksheet used for making user-specified calculations. The actual "CalTOX" worksheet is built up from one of two templates. 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.

Contaminated Soil is a worksheet template. This template contains a spreadsheet that uses algorithms applied to soil compartments that are already contaminated. This template is one of the two sheets (the other being Continuous Emission) used to create a "CalTOX" spreadsheet.

Continuous Emission is a second worksheet template. This template contains a spreadsheet that applied to soil and other compartments that are initially clean and then contaminated over time due to continuous emissions to air, soil, and/or water. This template is one of the two sheets (the other being Contaminated Soil) used to create a "CalTOX" spreadsheet.

DatCal is a worksheet 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 numerous chemicals, several landscapes in the United States, and several exposure factors (see Philosophy of CalTOX). This worksheet is hidden from view. The chemical, landscape, and exposure factor data in this worksheet will be automatically loaded into the main CalTOX spreadsheet by macro commands that are initiated from the use of drop down menus on the CalTOX spreadsheet. New chemical data, landscape properties, and exposure factors can be added with the use of buttons on the RunCal sheet.

InputLists is a worksheet that contains a list of the names of chemicals, landscape properties, and exposure factors. This worksheet is used by the drop down menus on the CalTOX sheet to cross reference and select data from DatCal and load it into CalTOX.

Sensitivity 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.

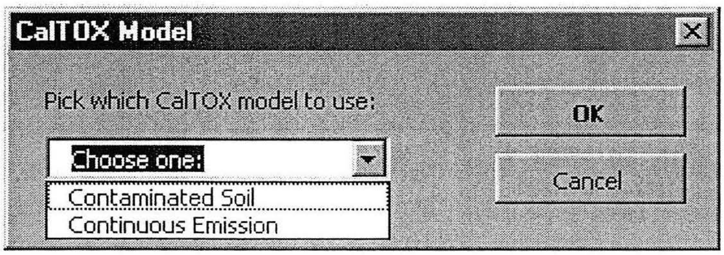
AllChemicals is a worksheet template. This template is used by a macro that runs through all the chemicals contained in the DatCal sheet. For each chemical, the data is entered into the CalTOX spreadsheet and the resulting risk and hazard ratio values are recorded into a copy of this template.

3. USING CalTOX

Starting CalTOX

To start CalTOX, launch the file named CalTOXtemplate.xls. This can be done in Windows by double clicking on the icon for this file or by opening the CalTOXtemplate.xls file from within the Excel application.

After the program is initiated, a dialog box will appear asking you which CalTOX template you would like to use to create a new scenario. There are two models that you can choose from. These models are Contaminated Soil and Continuous Emission. The Contaminated Soil model uses algorithms that assume the soil is initially contaminated. The Continuous Emissions model uses algorithms that assume the soil is initially clean and is contaminated over time due to the continuous emission of a chemical into ail, soil, or water. After you have selected the desired template, press the "OK" button. This will create a sheet called "CalTOX". The CalTOX spreadsheet will contain a copy of the template that was selected from the dialog box below.



If you prefer to use a CalTOX sheet that has been saved previously, press the "Cancel" button. RunCal will be the only sheet open. To use a previously saved sheet, click the "Import Saved Scenario" button.

Once you have made your selection on the dialog box, the CalTOX Control Panel will appear. If you selected a model to begin a new scenario, there will also be a sheet named "CalTOX" open, indicated by the tab at the bottom of the screen called "CalTOX". If you chose not to begin a new scenario, there will not be a sheet named "CalTOX" open. The picture below is a sample of what the Excel window will look like once the dialog box is gone.

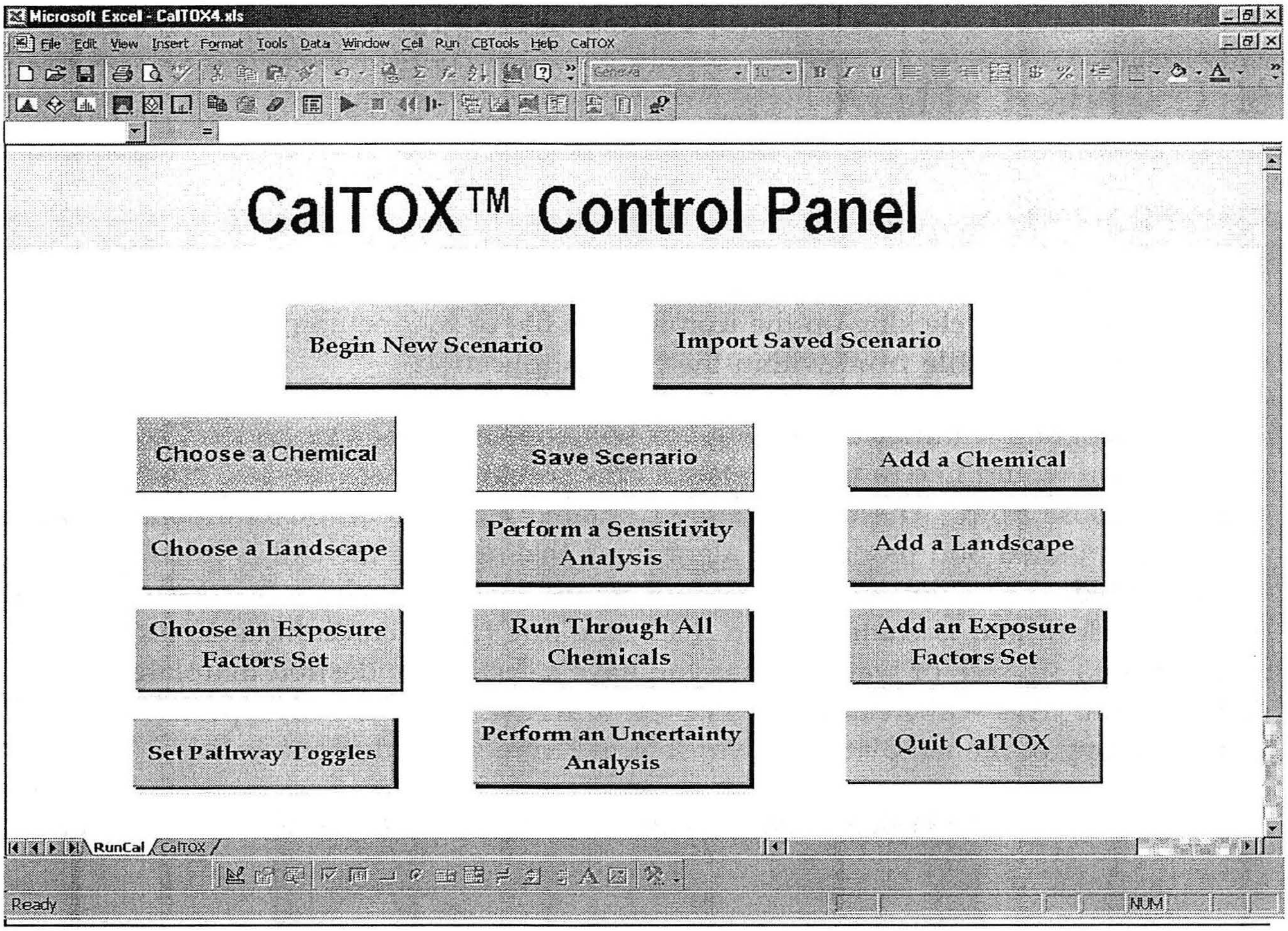


Figure 1. CalTOX Control Panel

Using the CalTOX Control Panel

The buttons on the CalTOX Control Panel operate macros that automatically carry out CalTOX operations. The following sections give explanations on how to use these buttons.

Begin New Scenario

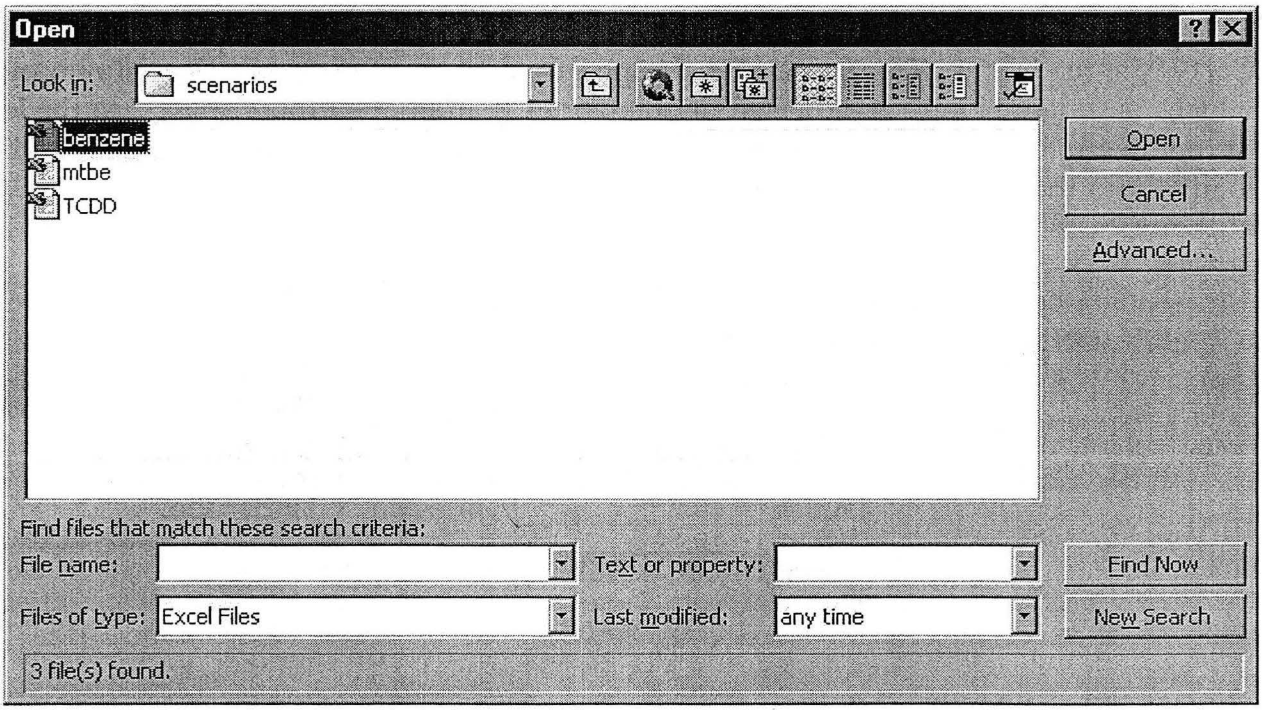
When the "Begin New Scenario" button is selected, a dialog box will appear on the screen. It is the same dialog box that appears when CalTOX is first loaded. Use the menu to select the template you would like and click the "OK" button. This will open a sheet called "CalTOX" containing the template that was chosen with the use of the dialog box.

IMPORTANT:
If a sheet called "CalTOX" already exists, it will automatically be overwritten with the new sheet. If you wish to save the current CalTOX spreadsheet and have not done so already, click the "Save Scenario" button before beginning a new scenario.

Always use the "Save Scenario" button to Save a CalTOX spreadsheet. DO NOT use the Excel "Save" commands. Using the Excel "Save" or "Save As" commands can over-write or alter the CalTOXtemplate workbook. Always make sure you store an original version of the CalTOXtemplate in a safe place as a backup.

Import Saved Scenario

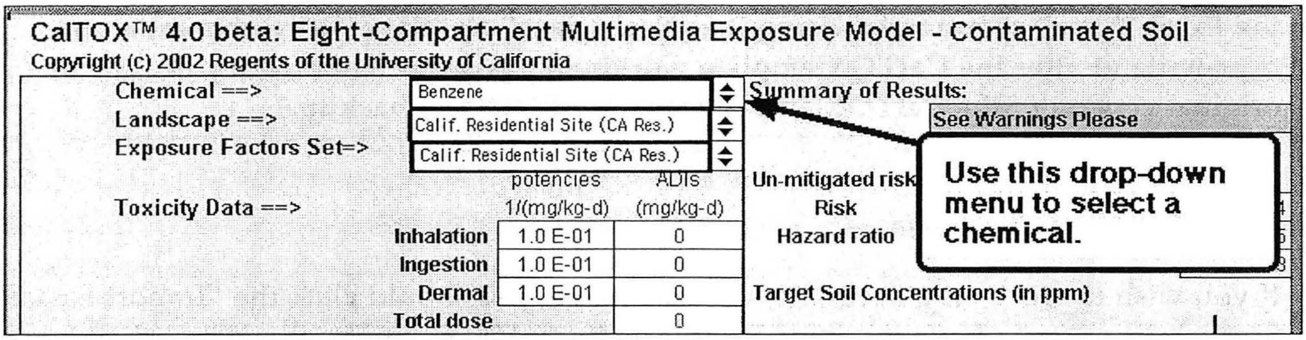
If you wish to work on a sheet that already exists, you should click the "Import Saved Scenario" button to have it copied back into the CalTOX workbook. When the "Import Saved Scenario" button is activated, you will be asked to select the file that contains the sheet on which you want to work.



After you choose the file, the sheet will be copied into CalTOX and named "CalTOX". **If a sheet called "CalTOX" already exists, it will automatically be overwritten with the new sheet.** If you wish to save the current "CalTOX" sheet and have not done so already, click the "Save Scenario" button before importing a saved scenario.

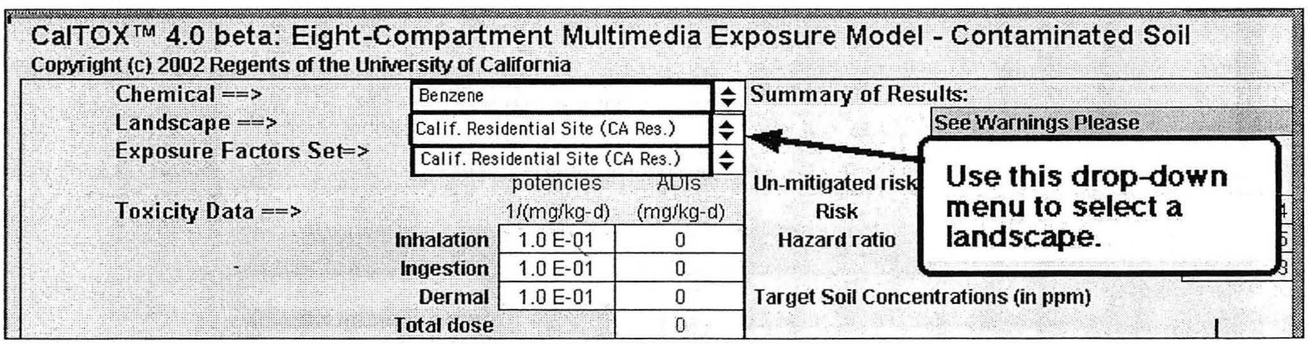
Choose a Chemical

Selecting the "Choose a Chemical" button transports you to the first page of the CalTOX spreadsheet. To choose a chemical, use the top-most drop down menu, which, as shown below, is indicated by the words "Chemical ==>" to the left of the drop down. Once you choose a chemical from the menu, the data will be loaded into the CalTOX spreadsheet and the algorithms will be recalculated automatically.



Choose a Landscape

Selecting the "Choose a Landscape" button transports you to the first page of the CalTOX spreadsheet. To choose a landscape property, use the middle drop down menu which, as shown below, is indicated by the words "Landscape Property ==>" to the left of the menu. Once you choose the landscape property from the menu, the data will be loaded into the CalTOX spreadsheet and the algorithms will be recalculated automatically.



Choose an Exposure Factors Set

Selecting the "Choose an Exposures Factor Set" button transports you to the first page of the CalTOX spreadsheet. Similar to the process for selecting chemical and landscape properties, to choose an exposure factor set, use the last drop down menu as indicated by "Exposure Factor ==>" to the left of the menu. Once you choose an exposure factor from the menu, the data will be loaded into the CalTOX spreadsheet and the algorithms will be recalculated automatically.

Set Pathway Toggles

Selecting the "Set Pathway Toggles" button transports you to page 8 of the CalTOX spreadsheet. On this page, there is a list of the exposure pathways that can be turned on or off for any calculation by setting cell values to 1 or 0. There 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.** By default, the CalTOX spreadsheet is pre-loaded with all pathway toggles set equal to 1, that is, in the "on" position.

Save Scenario

The "Save Scenario" button allows you to save the CalTOX spreadsheet in a separate workbook. When the "Save Scenario" button is activated, you will be asked to select the location in which you want the workbook saved and the name of the workbook. **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.

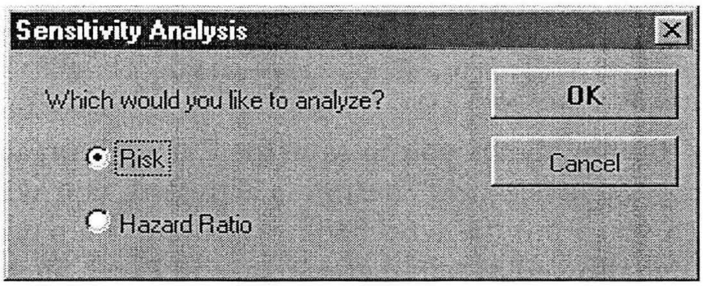
And as noted above:
Always use the "Save Scenario" button to Save a CalTOX spreadsheet. DO NOT use the Excel "Save" commands. Using the Excel "Save" or "Save As" commands can over-write or alter the CalTOXtemplate workbook. Always make sure you store an original version of the CalTOXtemplate in a safe place as a backup.

After you specify the location and name of the file, click the "Save" button. The CalTOX spreadsheet will then be copied into the specified workbook and saved. The drop down menus cannot be used in the saved files. Therefore, the only choices from the drop down menus are the chemical, landscape, and the exposure factors set that were selected in CalTOX. The workbook will remain open after this process is complete. Remember to save this new CalTOX workbook if you make any changes to the spreadsheet.

IMPORTANT:
Always use the Save Scenario button before using the Sensitivity Analysis or Run Through All Chemicals buttons.

Perform a Sensitivity Analysis

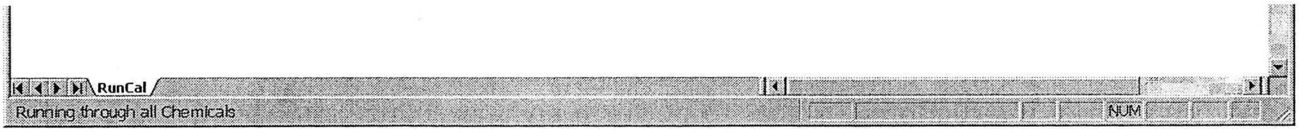
The "Perform a Sensitivity Analysis" button is used to carry out sensitivity analyses on a saved CalTOX spreadsheet. More details on what actions this macro initiates are described in the section below on sensitivity analysis with CalTOX. When the sensitivity analysis is started, the following dialog box appears and the user is asked choose to perform an analysis on either the Risk or the Hazard Ratio of the chemical.



The CalTOX spreadsheet must already be saved to perform a sensitivity analysis on it. After the "OK" button is clicked, you will be asked to specify the file on which you would like to perform the sensitivity analysis. This file should be a saved workbook that contains the CalTOX spreadsheet. Once the sensitivity analysis is finished, it will be saved in the same workbook as the CalTOX spreadsheet on which it was performed. This new spreadsheet will be named "Sensitivity – Risk" or "Sensitivity – Hazard Ratio", depending on which end point was analyzed. **If a sensitivity analysis has already been saved in the workbook, it will automatically be overwritten by the new analysis.**

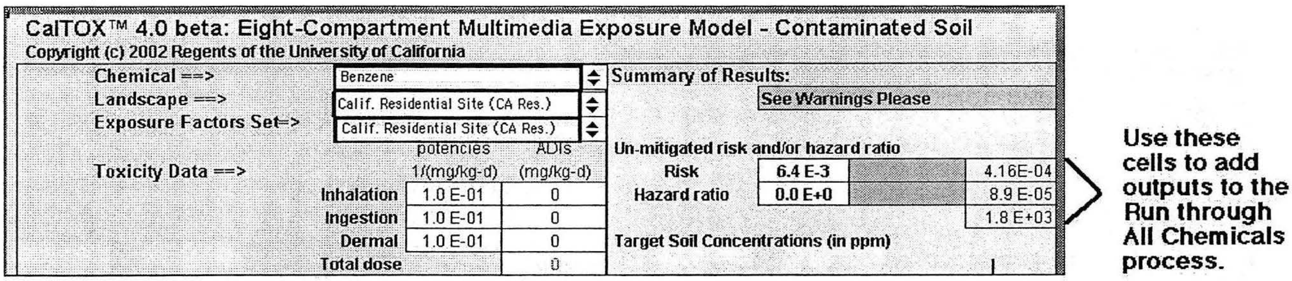
Run Through All Chemicals

When the "Run Through All Chemicals" button is pressed, it will begin the process of recording the Risk and Hazard Ratio of every chemical contained in the DatCal sheet. The Save Scenario button should be used before using to Run Through All Chemicals. After the "Run Through All Chemicals" process starts, you will be prompted to choose the location and file name for the workbook in which you wish to save the new worksheet that will be generated by this process. Choosing the location and naming the file should be done in the same manner as the "Save Scenario" process. After you indicate the location and name of the workbook, the process of running through every chemical will begin. Because this takes some time to complete, the status bar at the bottom of the Excel window will indicate that the new sheet is being generated as shown below.



Once the process is complete, the status bar will say "Ready". The workbook in which you saved the sheet will remain open, and the visible sheet will be named "ChemicalRun."

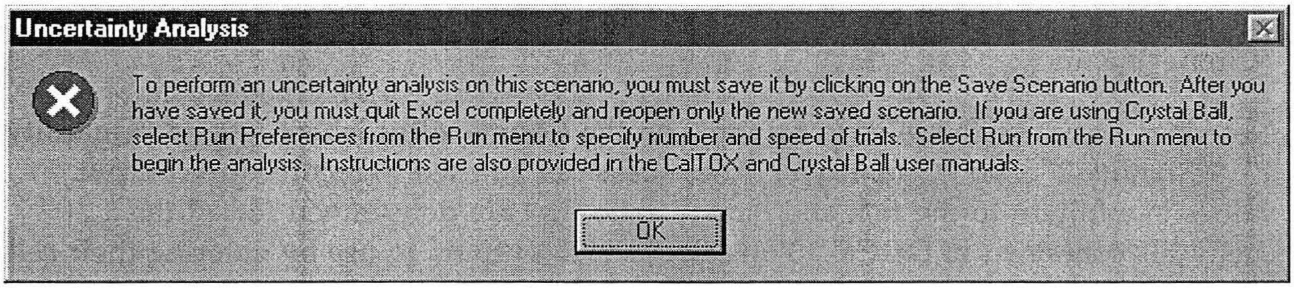
Note that there are three extra columns on the ChemicalRun sheet named "Quantity 1", "Quantity 2", and "Quantity3". These cells can be used to record three output values in addition to the risk and hazard ratio that are determined for all the chemicals contained in DatCal. You select which outputs to use by entering their cell locations on the CalTOX spreadsheet into three cells in the column next to the risk and hazard ratio values. These three cells are J8,J9, and J10. As an example, if you want to see the fugacity capacity of pure air, the offsite air concentration, and the concentration limit for ground water for all chemicals, you would enter "=AE3", "=P181", and "=H24" into the cells J8, J9, and J10, respectively. This example is shown in the figure below.



As shown by the formula bar, cell J8 has the value equal to that in cell AE3. On the ChemicalRun sheet, Quantity 1, Quantity 2, and Quantity 3 will be the fugacity capacity of pure air, the offsite air concentration, and the concentration limit for ground water, respectively.

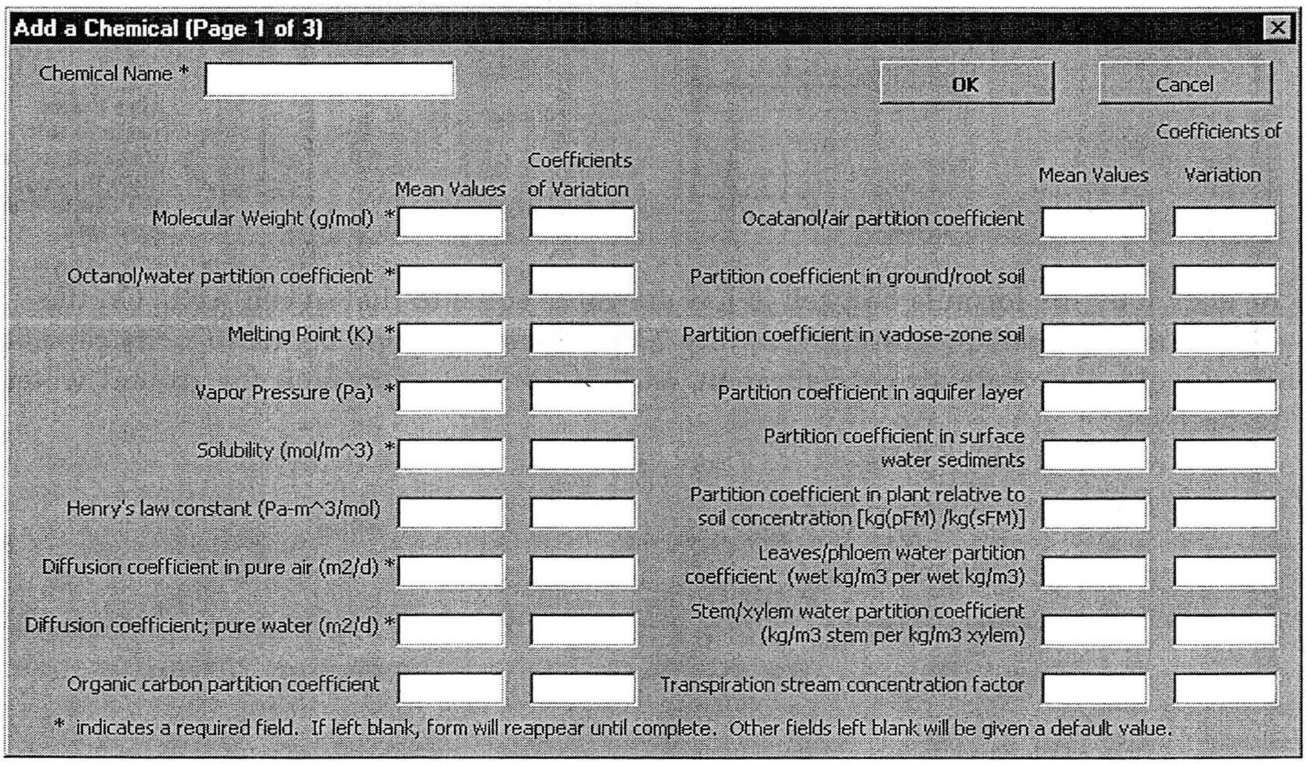
Perform an Uncertainty Analysis

Choosing the "Perform an Uncertainty Analysis" button causes the dialog box below to appear. An uncertainty analysis can be performed on any CalTOX spreadsheet by adding in a Monte Carlo program, such as *Crystal Ball*. More details on how this is done are described in the section on uncertainty analysis with CalTOX. This button only gives brief instructions on how to perform an uncertainty analysis using *Crystal Ball*. It does not perform the actual uncertainty analysis.



Add a Chemical

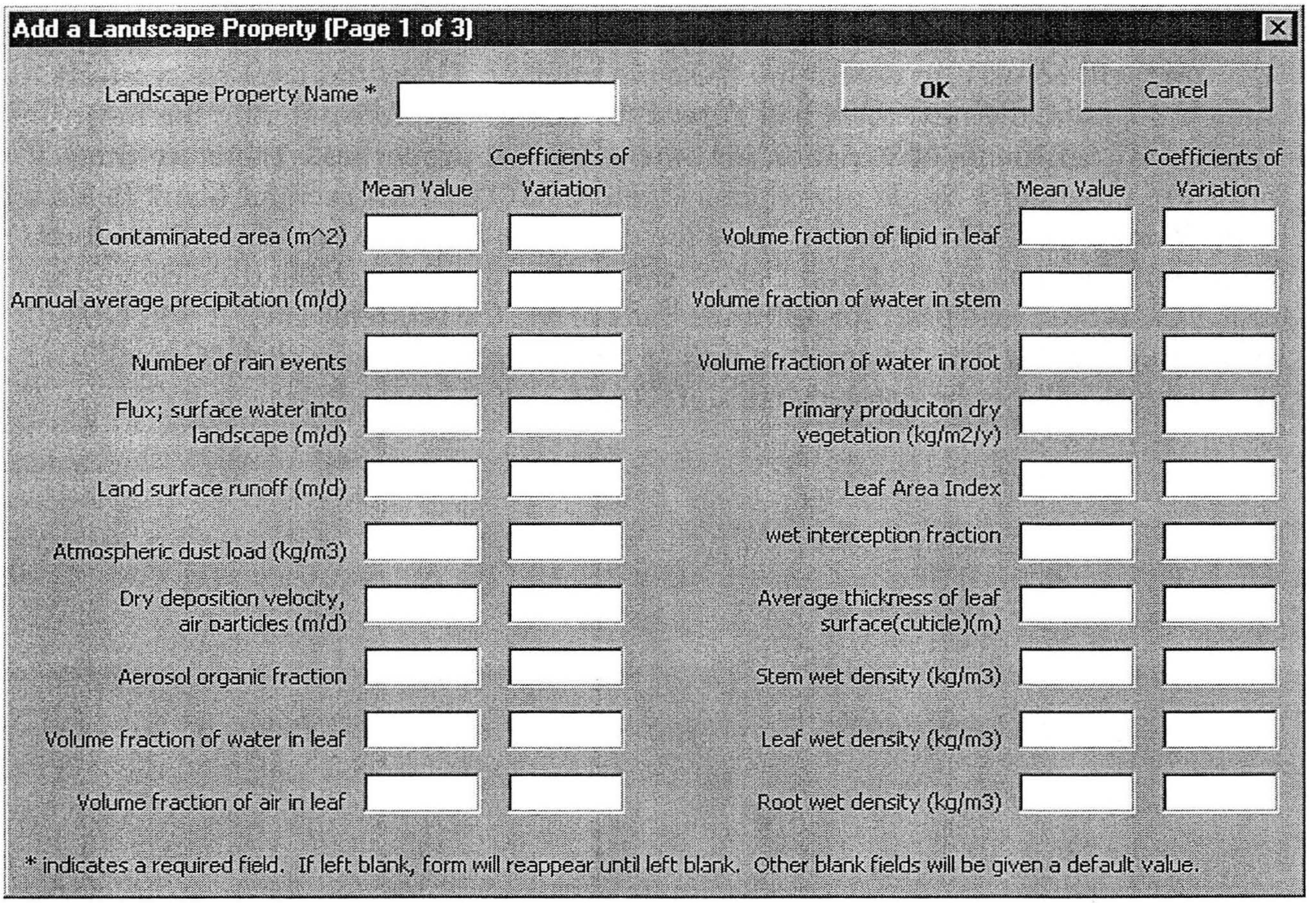
The "Add a Chemical" process is used to automatically add a new chemical into CalTOX. When the "Add a Chemical" button is clicked, the form shown below will appear.



On this form, there are spaces to enter the name of the chemical, the mean value of the chemical properties, and the coefficients of variation for measurement or estimation of that property. Fields on this form that require an entry are marked with a '*'. When you are finished entering the data on this form, click "OK". When the "OK" button is clicked, there will be a check performed to find any blank fields. If any of these fields left blank are required fields, the form will reappear and you will need to re-enter all of the data. If any fields that are not required are left blank, a default value algorithm will be used to determine these parameters. Once you have successfully entered the data, the next form will appear for you to continue entering the mean values and coefficients of variation for other chemical properties. There are three forms used to enter a single new chemical into CalTOX. The check for blank fields will be performed on all three forms. Once the data have been entered on all three forms, the chemical will be entered into DatCal and will be available in the drop down menu on the CalTOX spreadsheet for all future runs of the CalTOXtemplate. It will be the last chemical in the list. At anytime during this process, you may click "Cancel" and the chemical will not be entered into CalTOX.

Add a Landscape

The "Add a Landscape " process is used to automatically add a new landscape data set into CalTOX. When the "Add a Landscape" button is clicked, the form shown below will appear.



On this form, there are spaces to enter the name of the new landscape properties set, the mean value of the landscape properties, and the coefficients of variation for each property. **All fields on this form require an entry.** When you are finished entering the data on this form, click "OK". When the "OK" button is clicked, there will be a check performed to find any blank fields. If any fields are left blank, the form will reappear and you will need to re-enter all of the data. Once you have successfully entered the data, the next form will appear for you to continue entering the mean values and coefficients of variation for landscape properties. There are three forms used to enter a new landscape into CalTOX. The check for blank fields will be performed on all three forms. Once the data have been entered on all three forms, the new landscape properties set will be entered into DatCal and is available in the drop down menu on the CalTOX spreadsheet. It will be the last landscape in the list. At anytime during this process, you may click "Cancel" and the landscape property will not be entered into CalTOX.

Add an Exposure Factors Set

The "Add an Exposure Factors Set" button is used to automatically add a new set of exposure factors into CalTOX. When the "Add an Exposure Factors Set" button is clicked, a form similar to those for adding a chemical and adding a landscape will appear. On the exposure factors forms, there are spaces to enter the name of the new exposure factors set, the mean values for the various exposure factors, and their coefficients of variation. **All fields on this form require an entry.** When you are finished entering the data on this form, click "OK". When the "OK" button is clicked, there will be a check performed to find any blank fields. If any fields are left blank, the form will reappear and you will need to re-enter all of the data. Once you have successfully entered the data, the next form will appear for you to continue entering the mean values and coefficients of variation for the exposure factors. There are three forms used to enter a new set of exposure factors into CalTOX. The check for blank fields will be performed on all three forms. Once the data have been entered on all three forms, the exposure factors set will be entered into DatCal and is available in the drop down menu on the CalTOX spreadsheet. It will be the last exposure factors set in the list. At anytime during this process, you may click "Cancel" and the exposure factors set will not be entered into CalTOX.

Quitting CalTOX

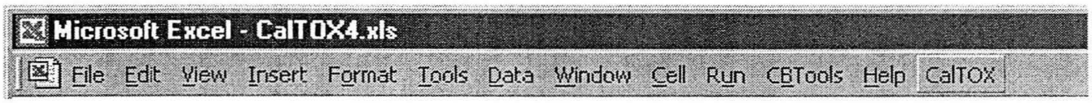
To quit CalTOX properly, you must either use the "Quit CalTOX" button on the RunCal sheet or select "Quit CalTOX" from the CalTOX menu bar (see description under the Viewing Spreadsheet Results section below). Using either of these methods will close the CalTOX workbook, but Excel will remain open. If you do not use either of these methods to quit CalTOX, the CalTOX menu bar may not be removed properly causing problems the next time you run Excel or CalTOX. See the problems section for details on fixing a CalTOX menu problem.

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 spreadsheet. There are two items that can be used to operate these macros—the "RunCal" worksheet that was described above and the CalTOX menu on the CalTOX menu bar. The CalTOX menu is described below.

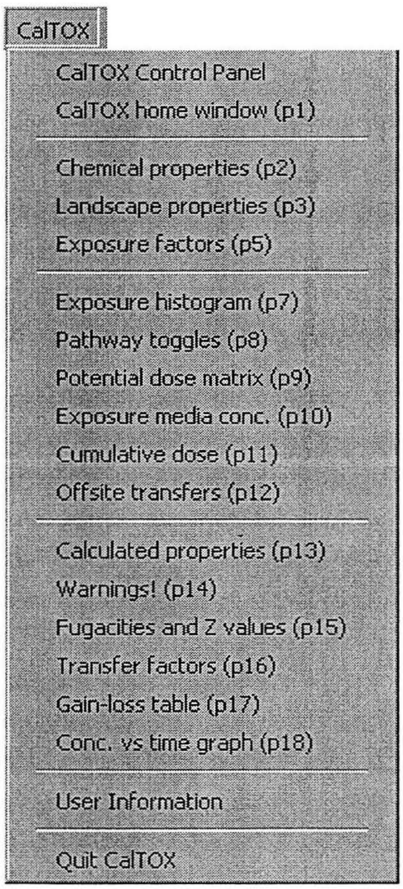
The CalTOX Menu Bar

The CalTOX menu bar differs from the standard Excel menu bar by the presence of the "CalTOX" menu. This menu is created automatically when CalTOX is loaded. The appearance of the CalTOX menu bar is illustrated below. The "Cell", "Run", or "CBTools" menus shown below are for *Crystal Ball*.



The CalTOX Menu

The CalTOX menu includes a list of commands that can be used to view different parts of the CalTOX spreadsheet. 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 spreadsheet page number corresponding to the table or object. The CalTOX menu can also be used to reset the window view to either the RunCal sheet or the home page of the CalTOX spreadsheet. An illustration of the CalTOX menu is provided below.



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 spreadsheet template has the print area 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. To be sure that the whole page fits on each page, select the "Print Preview" option from the File menu. If the pages are too large, decrease the percent of normal size in the scaling section of the "Page Setup" option in the File menu.

4. 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, an error during the execution of a macro causes a "run-time error" message to be displayed. When this happens, the user is given the option to "End," "Debug," or "Help." If this display appears, the user should select "End" and get back to the RunCal sheet and try to run the macro again. If problems continue, quit CalTOX and restart.

Multiple CalTOX Menu Bars

If CalTOX is not quit properly each time, multiple CalTOX menu bars can begin to accumulate in the Excel menu. To get rid of any extra CalTOX menu bars, select "Customize" from the Tools menu. Click on each CalTOX menu bar and drag it into the Customize window and let go. This will delete all CalTOX menu bars. Close CalTOX by selecting File -> Close. Reopen CalTOX to create a fresh menu bar.

Screen Displays and Zoom Scaling

On PC computers, the CalTOX worksheet is preset for display at 90% of full size. 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. On some computers the scaling causes problems with the drop-down menus not scrolling the full set of chemicals or landscapes. If the worksheet or drop-down menus are distorted or appear 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 90%. In Excel 4.0, the "Zoom" function is under the "Window" menu, and in Excel versions 5.0 and later, the "Zoom" function is under the "View" menu.

On some PC computers, the words appear chopped off or #### is found instead of a number in one or more cells. 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 of the important information. You may "uncover" words or numbers by increasing the column width. This is 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 100% 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 "Print Preview." 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.

5. 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 "toggle-switch" cells used to turn pathways on and off, the potential-dose matrix, the matrix of exposure media concentrations, the cumulative-dose table, and information for offsite transfers.

The third column is devoted principally to the information needed and intermediate outputs for the multimedia fugacity mass-balance 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 2 provides a schematic of the 18-page CalTOX worksheet.

The "Home" Page

The home page of the CalTOX worksheet contains summary results and some of the inputs relating to target risk, time to start the calculation of population exposures 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, the name of the landscape-data set, and the name of the exposure factors set used for the calculation.

Home page Inputs Outputs Page 1	Exposure histogram Page 7	Calculated properties Page 13
Chemical properties Page 2	Exposure pathway on/off Toggles Page 8	Calculated properties, warnings, and error messages Page 14
Chemical properties (continued) and Landscape properties Page 3	Potential-dose matrix Page 9	Fugacities, compartment volumes, and fugacity capacities Page 15
Landscape properties (continued) page 4	Exposure-media concentrations table Page 10	Diffusion and advection rate constants Page 16
Landscape properties (continued) and Exposure factors Page 5	Table of time-dependent cumulative doses within the population Page 11	Compartment gains and losses, residence times, inventories, and concentrations Page 17
Exposure factors (continued) Page 6	Information for offsite transfers Page 12	Time dependent compartment inventories in the soil layers Page 18

Figure 2. The 18 pages in the CalTOX worksheet and how these pages are arranged into three columns and six rows in the worksheet.

Inputs on the Home Page

The "input" section of the Home page lists important inputs that control the calculation of risk for both the continuous emission and contaminated soil versions of CalTOX. Figure 3 illustrates the input displays on the home page.

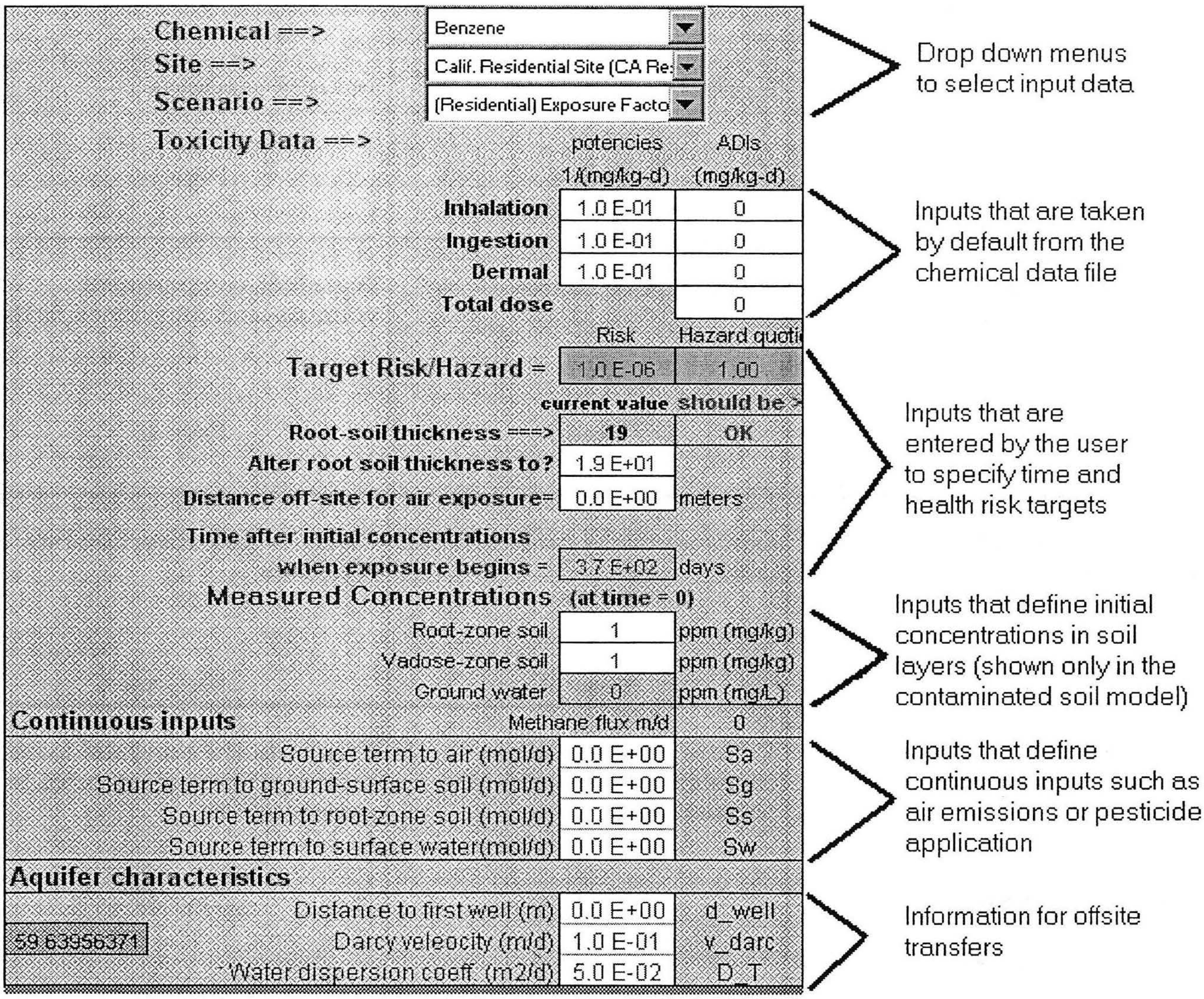


Figure 3. Inputs listed on the home page (based on the contaminated soil model).

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. In the contaminated-soil version of CalTOX there is 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 (these are only shown in contaminated soil model).

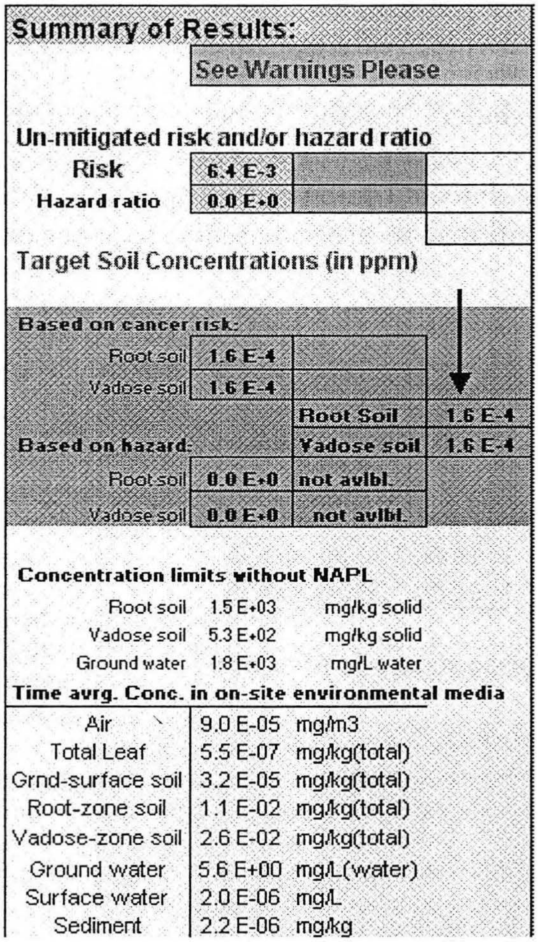
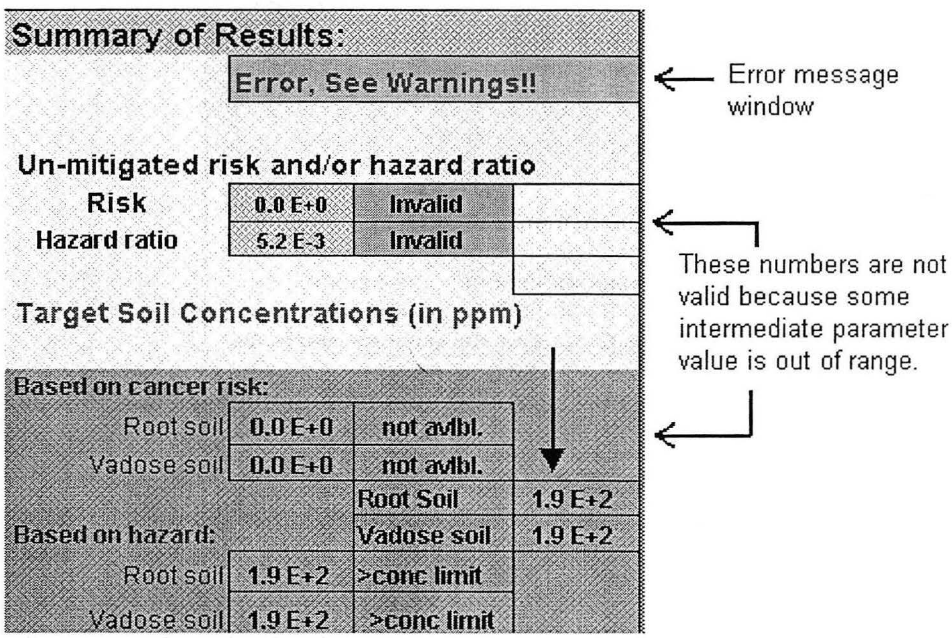


Figure 4. Outputs listed on the home page (this figure is based on the contaminated soil model).

The soil clean-up goal is based on a target risk or hazard. The estimated lifetime risk is based on a time-weighted average exposure over the exposure duration (ED), which is specified among the exposure factors loaded from DatCal and listed on page 6 of the CalTOX sheet. The hazard is based on the maximum exposure rate value computed over the exposure duration (ED). The soil clean-up goal is based on how much the initial soil concentration must be reduced to meet the target lifetime risk. Thus, this output column specifies both the estimated risk without soil cleanup as well as the soil concentrations required to meet the target health goals. Because the reverse calculation of risk is meaningless if the concentration of contaminant in soil solution or groundwater exceeds the solubility limit in water, solubility limits in soil and groundwater are listed in this output summary.

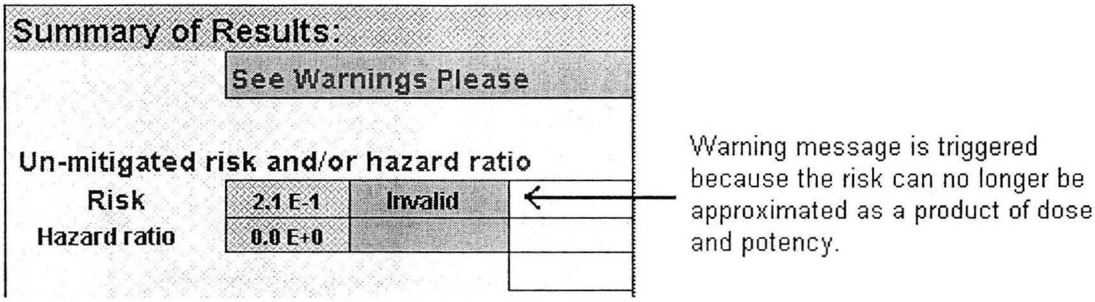
Target soil concentrations are labeled "invalid" when: 1) the target soil concentration exceeds the solubility limit in a soil layer (the term "> conc. limit" will appear in the boxes for target clean-up concentrations); 2) the groundwater-recharge value is negative; or, 3) the groundwater-recharge value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

The unmitigated risk is labeled "invalid" when: 1) the initial concentration of contaminant in the root- or vadose-zone 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. For any of these situations, an error message appears in the error window as shown below.



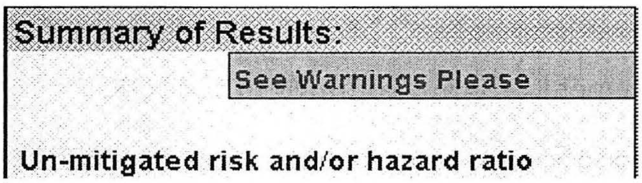
When the unmitigated risk exceeds 0.1, the forward calculation of risk cannot be estimated as the product of dose and potency because of the non-linearity of the dose-response model in this range.

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.



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 "-" to the right 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. Columns four and five are open to modification by the user. The fourth column lists the expected value of an

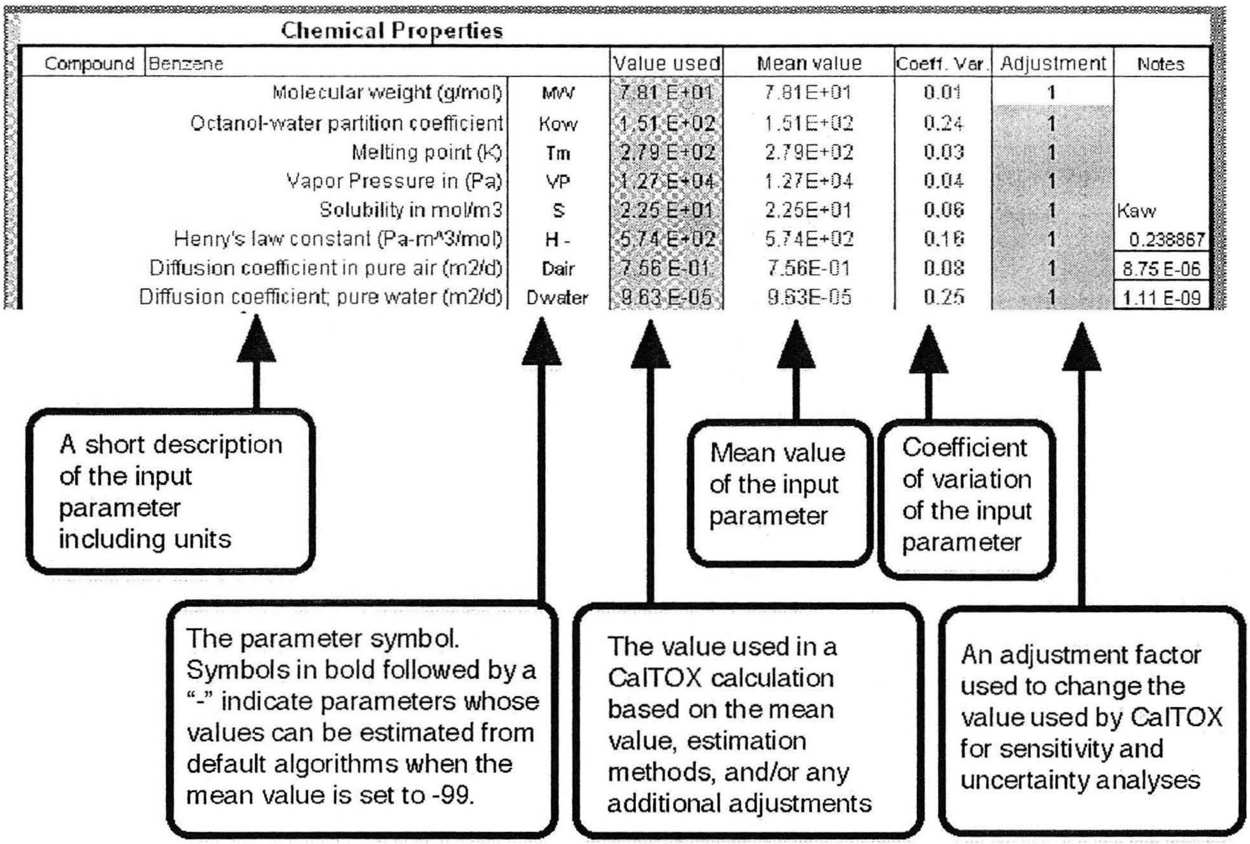


Figure 5. The arrangement of input columns in CalTOX.

input based on uncertainty and/or variability. The fifth column lists the coefficient of variation--the ratio of standard deviation to the mean, which reflects the variance in the input parameter due to uncertainty or variability. Column six can also be modified by the user and includes an adjustment factor to the value of a parameter that is used in sensitivity and uncertainty analyses. On the computer screen, this column contains different colors to indicate the underlying assignment of a distribution. No background color indicates no pre-assigned distribution; light blues means a pre-assigned, independent lognormal distribution; light-blue with a red marker in the upper right corner indicates a distribution correlated with some other variable; and dark gray indicates a truncated lognormal distribution. These colors may look different on different computers. The last column is also not locked and can be used 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.

The Human Exposure Model Inputs

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. Human exposure factors data is listed on pages 5 and 6 of the CalTOX worksheet.

6. THE CALCULATION OF RISK AND SOIL CLEAN-UP GOALS

The Forward Calculation of Potential Dose and Risk

As expressed by the equation below, CalTOX constructs the distribution of individual lifetime risk attributable to cumulative exposures over the duration ED (years), to a contaminant in soil at an initial (time zero) concentration, $C_s(0)$ [mg/kg(soil)]. This is done by integrating the soil concentration in time and then summing the dose and effect attributable to this soil concentration over exposure routes, over environmental media, and over exposure pathways.

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

In the above expression, $\Phi[C_s(0) \rightarrow C_{k,} t]$ is the multimedia dispersion function that converts the contaminant concentration, $C_s(0)$, mg/kg measured in soil at time zero, into contaminant concentration, C_k, at a time, t, 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 the normalizing concentration C_k, which is a constant or representative average concentration 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

$$ADD_{ijk} = \left[\frac{C_i}{C_k}\right] \times \left[\frac{IU_{ij}}{BW}\right] \times \frac{EF \times ED}{AT} \times C_k$$

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 of soil concentration linked to a specified risk. 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

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

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.

7. 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 parameter values over their entire range of values. In a global sensitivity analysis, the variance in the outcome is compared to the variance of the inputs. A global sensitivity analysis often uses a local sensitivity analysis as a starting point. 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 *i* th 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 the 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.

8. UNCERTAINTY ANALYSIS

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.

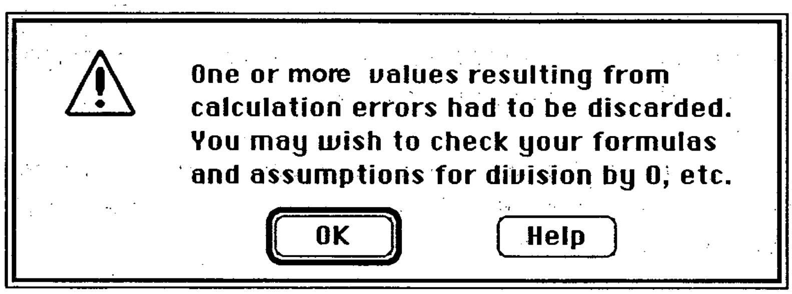
CalTOX has been designed to carry out these steps using the CalTOX worksheet and an add-in Monte Carlo program such as *Crystal Ball* (Decisioneering, 2000).

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 user's manual for *Crystal Ball* .

Uncertainty Analysis with CalTOX

An uncertainty analysis can be performed on any CalTOX spreadsheet by adding in a Monte Carlo program, such as *Crystal Ball.* 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.



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, do not select 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 4.0 User manual (Decisioneering, 2000).

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