SOFEA© (SOil Fumigant Exposure Assessment system)

User's Guide

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ABSTRACT

SOFEA© (SOil Fumigant Exposure Assessment system), a stochastic numerical modeling tool, was developed by Dow AgroSciences as a regulatory tool to evaluate and manage human inhalation exposure potential associated with the use of soil fumigants. SOFEA calculates fumigant concentrations in air arising from volatility losses from treated fields for entire agricultural regions using multiple transient source terms (treated fields), GIS information, agronomic specific variables, user specified buffer zones and field re-entry intervals. A modified version of the USEPA Industrial Source Complex Short Term model (ISCST3) is used for air dispersion calculations. SOFEA uses field observed (or numerically generated) fumigant flux profiles from soil as transient source terms for both shank injection and drip-irrigation applications. Reference flux observations are scaled based upon depth of incorporation and the time of year to map the complete flux response surface from field/numerical observations. Weather information, field size, application date, application rate, application type, depth, pesticide degradation rates in air, tarp presence, ag-capable land, field re-treatment, buffer setbacks, and other sensitive parameters are varied stochastically using Monte Carlo techniques to mimic region and crop specific agronomic practices. Agricultural regions up to 19,000 mi^2 can be simulated for temporal periods ranging from 1 day to more than 70 years for the purpose of assessing acute, sub-chronic, or chronic exposure. Multi-year, multiple field simulations are conducted using random field placement in all agricultural capable areas or by selectively placing fields in historical or prospective use areas. Regional land cover, elevation, and population information can be used to refine source placement (treated fields), dispersion calculations, and exposure assessments. Both current and anticipated/forecasted fumigant scenarios can be simulated to provide risk managers the necessary information to make sound regulatory decisions. SOFEA has been successfully used for regulatory decision making in California. Algorithms used by SOFEA to refine exposure predictions and manage acute, sub-chronic, and chronic risk associated with the use of soil fumigants on a local or regional basis are presented. Although SOFEA was generated specifically to describe air concentrations of the soil fumigant 1,3-dichloropropene, the model is readily adaptable to generically describe the post-fumigation air concentration of other soil fumigants.

Details of SOFEA algorithms can be found in the companion programmers guide (Cryer, 2004). In addition, references are provided for peer reviewed literature articles or 3rd party user manuals (eg. ISCST3) for more detailed technical explanation and theory of the modeling components.

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1.0 INTRODUCTION

1.1 Model Overview and Capabilities

The generation of a generic methodology to determine fumigant air concentrations in large and diverse air sheds has been developed. Directionally averaged air concentrations within entire air sheds are determined using a multiple source Gaussian dispersion model that has been modified to include Monte Carlo sampling techniques and ties to Geographic Information System databases, and agronomic practices. Time averaged transient air concentrations via a numerical model can be used in exposure procedures for risk determination for unlimited number of scenarios.

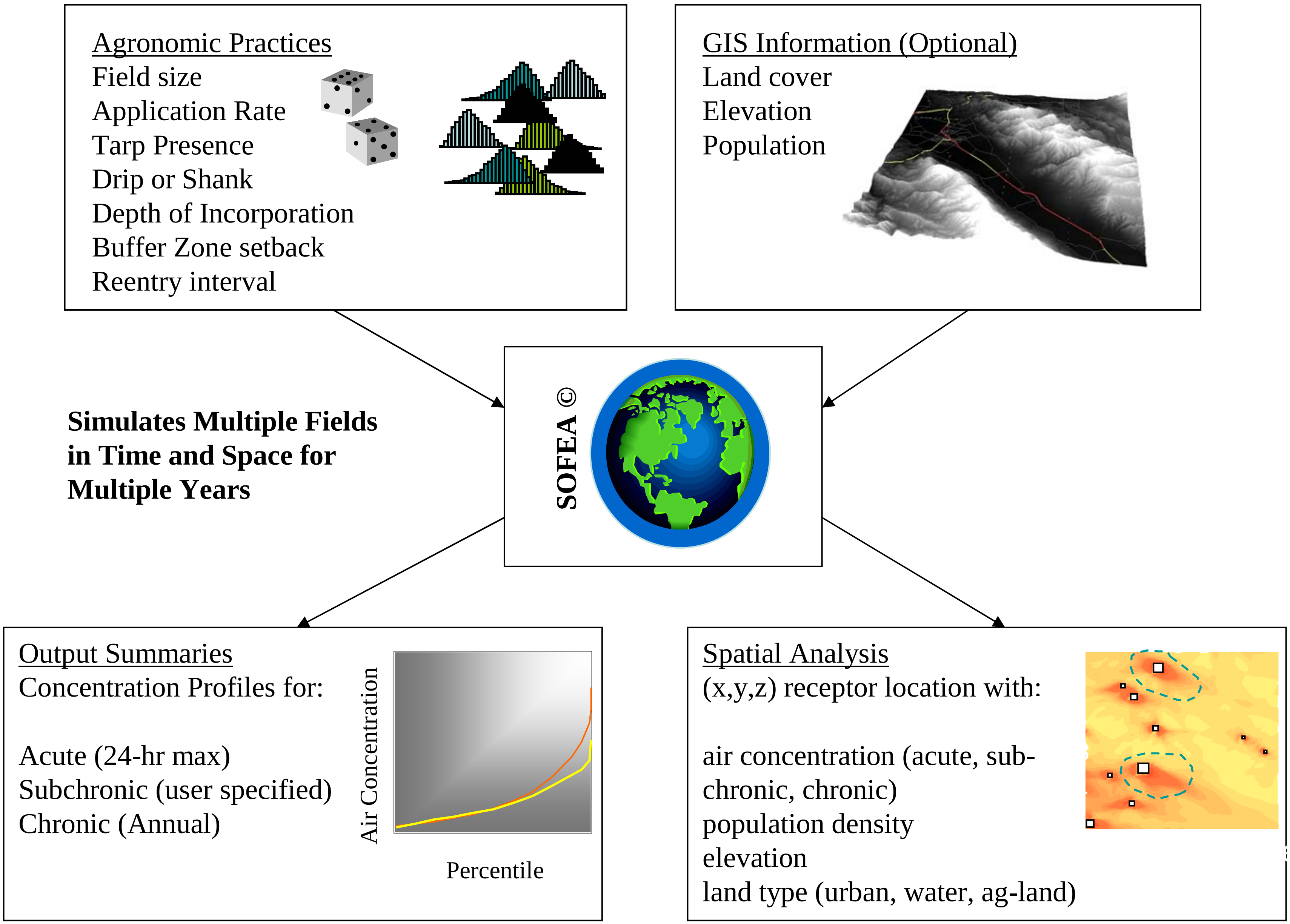
SOFEA enables the determination of 'area-wide' concentration profiles for user specified buffer distances that account for multiple field applications. Thus, the effect of fields 'off-gassing' at different points in time and space are accounted for in simulations conducted using SOFEA. By specifying a buffer distance fro the edge of treated fields, the user can evaluate the impact of the buffer on the acute exposure of residents and by-standers. By specifying the total mass applied within a specific use region on an annual basis, the user can determine the chronic exposure to individuals residing in the use area.

SOFEA inputs and outputs are contained within EXCEL spreadsheets, allowing model output to easily be exported to other file formats or programs. Concentrations of soil fumigants in air are associated with x,y,z co-ordinates and can thus be associated with proximity to treated fields as well as human populations, if census data are available.

Although SOFEA was generated specifically to describe air concentrations of the soil fumigant 1,3-dichloropropene, the model is readily adaptable to generically describe the post-fumigation air concentration of other soil fumigants.

1.1.1 Air Dispersion Model

The Industrial Source Complex Short-Term (ISCST3, 1995) model was developed by USEPA as a regulatory tool for predicting concentrations of air contaminants in diverse air sheds. ISCST3 is a Gaussian plume model useful for estimating air quality surrounding contaminant release sites. Examples include vehicle exhausts in urban areas (Hoa *et al*, 1999), industrial sulfur dioxide emissions (Kumar *et al*., 1999), methyl bromide concentrations resulting from soil fumigation in rural areas (Honganahalli and Seiber, 2000), and 1,3-D township wide air concentrations for multiple transient agricultural sources within a California township (Cryer and van Wesenbeeck, 2001).
Modifications to ISCST3 deal with buffer zones and reentry periods (Johnson, 2001). The user can now specify a buffer zone around source terms (treated fields). Any receptors within the field or within the buffer zone are excluded from analysis until the user supplied reentry period (e.g., 7-days) has expired, at which point the receptors are reactivated. This modification addresses the impact of buffer setbacks on acute air concentrations.



Soil Fumigant Exposure Assessment Model

1.2 Air Shed Domain

An air shed is defined as a volume of air overlying a square surface area, where source terms throughout the air shed can contribute to overall air concentrations at specific locations. SOFEA focuses on air concentrations in either a single township or a 3x3 township domain.

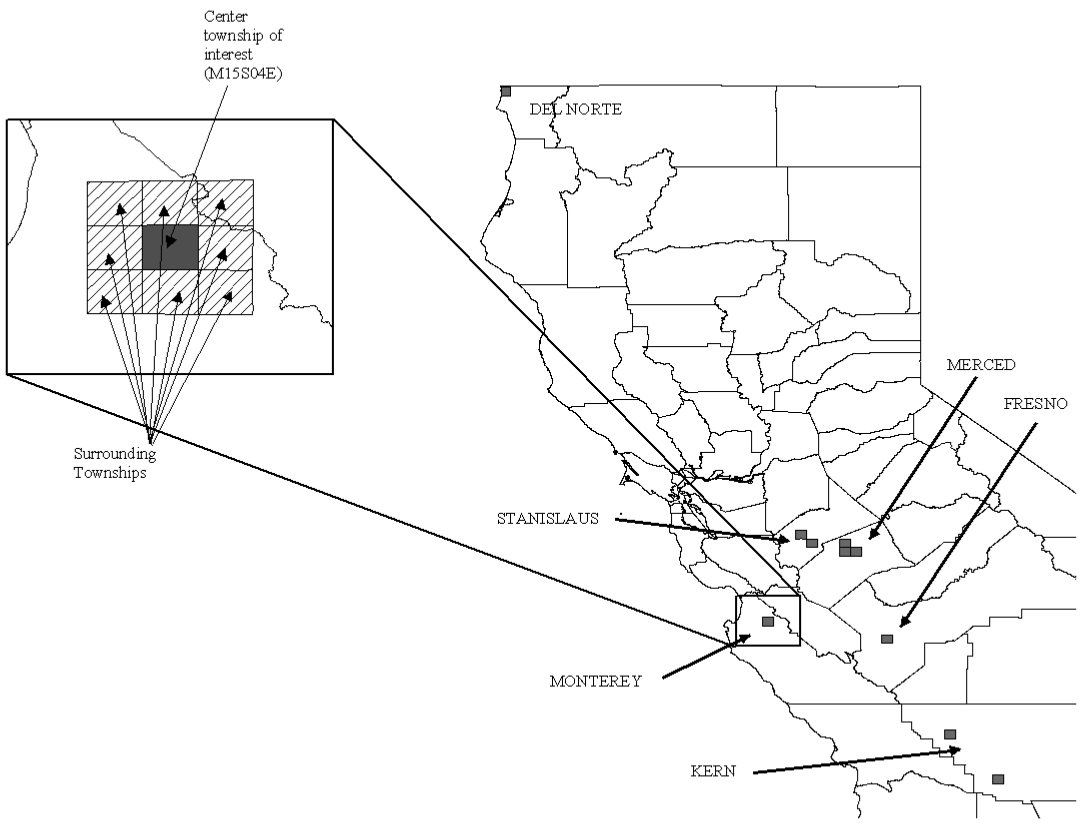


Figure 1. Example of a 9x9 township air shed for SOFEA simulation.

Larger air sheds can be simulated (up to 23x23 townships), although fumigant air concentrations are only determined for the central township or the central 3x3 townships (user can choose this). Thus, townships outside the central 3x3 can have source terms and can contribute "drift" to the central townships as depicted in Figure 1.

1.2 Parameter Representation

1.2.1 GIS Data/Representation

GIS data (land-cover, population, elevation) can be entered for a single township or up to a 3x3 township domain. *The user can still run a simulation without GIS information, but they must first set all land to ag-capable, and null entires for population and elevation. Buttons that are* *linked to macros on the appropriate worksheets are provided for the user.* An example for land cover is given in Figure 2 for the worksheet “LandCover”. The worksheet “Population” and “Elevation” follow the same general format. The upper cells represent a 3x3 township domain, and cell values can be entered by the user to denote land cover. Integer values of 0, 1, 2, or 3 denote agricultural land, water, urban, and mountains (plus other such as wetlands, quarries, etc.). The three buttons at the bottom of Figure 2 are linked to macros that automate the process of GIS entry. The first button ‘Set All Landcover to Ag Capable” places all zeros in the above matrix of data entries. The second button “Update Land Cover Graphics Using data from “GIS_Data” reads in the GIS data found in the worksheet “GIS_Data” and does appropriate checks for land type, interpolation, etc. and generates appropriate integer values to list in the cells above the button describing the 3x3 township domain. The last button called “Update Land Cover Graphics Using User Data” simply takes the values in the cells representing the 3x3 township grid and generates the color graphic using these values as seen in the bottom of Figure 2. Descriptions of the GIS worksheets and the buttons found in these worksheets are summarized in Tables 1-2, respectively. Additional details of the GIS worksheets are discussed in Section 14.

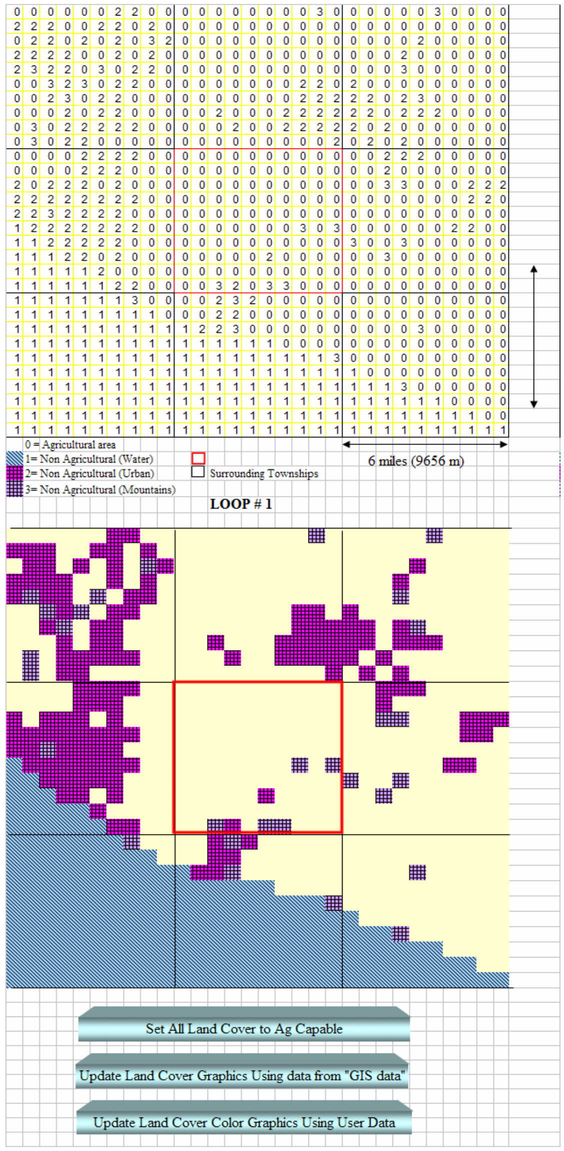


Figure 2. Screen shot of worksheet “LandCover” showing input cells at top, colored contour plot based upon these inputs, and the buttons at the bottom that are linked to macros.

Table 1. Worksheets of SOFEA containing GIS information or where GIS information can be entered.

Worksheet	Description
GIS_data	Contains raw data for township for the 10x10 raster based grid system
LandCover	Worksheet where user can hand enter GIS information for land cover type (ag-capable, urban, water) or read this information from the worksheet “GIS_data”
Population	Worksheet where user can hand enter GIS information for population or read this information from the worksheet “GIS_data”
Elevation	Worksheet where user can hand enter GIS information for elevation or read this information from the worksheet “GIS_data”

Table 2. Worksheet where buttons linked to macros perform GIS driven algorithms.

Worksheet – Macro	Description
LandCover	
Land_null	Sets all land to ag-capable (= 0)
GIS_data_for_LandCover	Gets GIS information from the worksheet GIS_data, populates cells and generates land cover graphic in worksheet "LandCover"
LandCover_update	Uses the user specified cell information in "LandCover" and generates land cover contour graphic
Elevation	
Elev_null	Sets all elevations to zero (i.e. flat terrain)
GIS_data_for_Elevation	Gets GIS information from the worksheet GIS_data, populates cells and generates elevation graphic in worksheet "Elevation"
Elevation_update	Uses the user specified cell information in "Elevation" and generates elevation contour graphic
Population	
Pop_null	Sets all population density to zero
GIS_data_for_Population	Gets GIS information from the worksheet GIS_data, populates cells and generates population contour graphic in worksheet "Population"
Population_update	Uses the user specified cell information in "Population" and generates population contour graphic

The complex terrain algorithms of ISCST3 can take advantage of elevation changes within specific regions should this information be available. Population information (if provided or known) can be used in population based risk assessments. The 2000 U.S. census data lists population densities by census blocks and is a good choice for population information. Receptors can be placed uniformly in the central township or the entire 3x3 domain and the spatial locations for receptors are assigned appropriate land cover, elevation, and population data (from GIS data bases or through manual user input).

Source terms (treated fields) can be placed external to the central 3x3 up to a domain of 23x23 townships (19,000 mi^2), depending on the persistence and drift characteristics of the soil fumigant. The user need only specify the annual fumigant mass applied to any township within a 23x23 township domain, appropriate GIS information (if desired), receptor spacing and heights for the central 3x3 township grid, and appropriate PDFs characterizing agronomic conditions and practices within the region.

1.2.2 Stochastic portrayal

Concentrations of a soil fumigant in air resulting from transient agricultural source terms are also dependent upon meteorological conditions, application timing, and other agronomic properties. A mechanism was required that could propagate parametric uncertainty in sensitive model inputs to air concentration predictions. Monte Carlo (MC) methods provide a straightforward technique to propagate such uncertainty in independent parameters to dependent output variables (Rubinstein, 1981; Yakowitz, 1977). Variability in input is described by probability density functions (PDFs) that are randomly sampled to generate input parameter sequences. If the number of randomly generated input parameter sequences is large enough, then the entire parameter space can be statistically mapped out. Output predictions are no longer single valued, but rather a discrete distribution is generated from which exceedence probabilities and return frequencies can be calculated (e.g., 1-in-100 year exposure potential, and so on).

Stochastic variables in this analysis included the pesticide application rate, application date, depth of incorporation, tarp presence, shank or drip application, field size, weather year, and pesticide degradation coefficient in air. This air quality modeling work is in accordance with the policy established by the U.S. EPA for Air Quality Models (USEPA, 1995) and follows the guidelines set forth by U.S. EPA for Monte Carlo Analysis (USEPA, 1997).

The MS Excel add-on program Crystal Ball (Trademark of Decisioneering, Inc.) was used to transform ISCST3 from a deterministic model into a stochastic/deterministic system. Crystal Ball allows all spreadsheet cells to be expressed as probability density functions for Monte Carlo simulation (Appendix I). Thus, an ISCST3 input file was exported from Excel that was based upon appropriate selections from Crystal Ball PDFs that are derived from actual agronomic data. Excel, Crystal Ball, ISCST3, and Visual Basic Applications (VBA) programs were coupled to allow the transparent integration of the Monte Carlo component for the ISCST3 model such that multiple simulation years with parametric uncertainty are now addressed.

1.2.3 Crop Selection

Fumigants are used on a variety of agricultural commodities. Each commodity/crop is potentially unique, with different application, agronomic, and management practices. The crops chosen can be based upon current or future forecasted fumigant uses, and currently up to five different crop types can be considered. Predominant crops where soil fumigants are used include tree and vine (TV), field crops (FC), nursery crops (NC), strawberries (SB) and post-plant vines (PP). The contributions of a soil fumigant to air borne concentrations from each crop are easily extractable by keeping the crop types/parameters unique during simulation. This aids in determining appropriate Best Management Practices (BMP’s) by crop type.

1.2.4 Receptors

Receptors are specific (x,y,z) locations in the simulation domain where air concentrations are calculated. Receptors are uniformly spaced as dictated by the user. For simulations reported here, there are 36 equally spaced receptors per township section, yielding 1296 receptors per township (11,664 receptors within a 9-township simulation domain). Receptor height for these sample simulations are 1.5 m above the soil surface to mimic the breathing height of an adult.

1.2.5 GIS Data Layers

Many data bases and GIS software exist to extract appropriate information for SOFEA if the user so desires (Figure 3). SOFEA is not a GIS tool but rather uses GIS information that has been assembled using GIS Software such as ArcView (Trademark of ESRI, inc.). Land cover information is obtained by Landsat Thematic Mapper images (30-m resolution) that contains 21 unique land classifications [available from the National Land Cover Data (NLCD) database at http://landcover.usgs.gov/natllandcover.html]. Elevation information is obtained from the USGS Digital Elevation Models (DEM) data at 1:24,000 scale . Population information is given by census blocks and populated with data from the 2000 US Census.

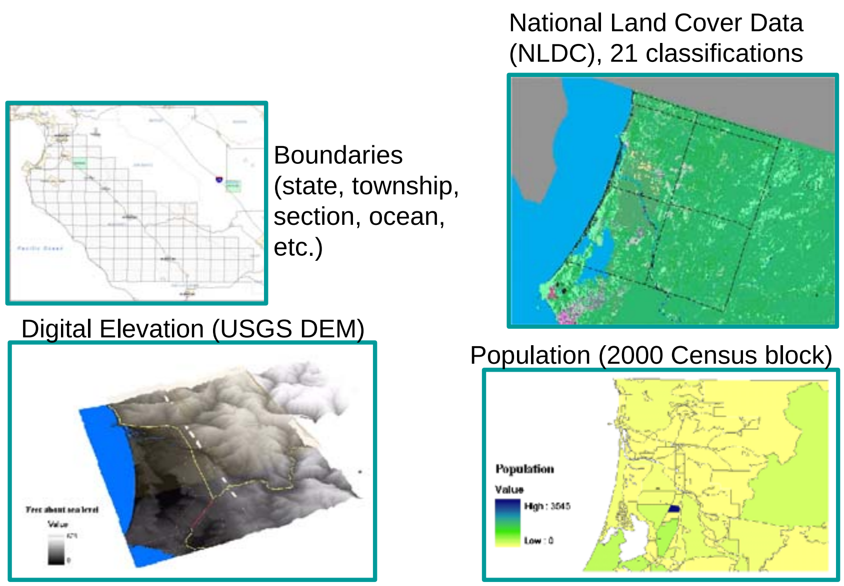


Figure 3. Example of the public domain data bases available to the user of SOFEA

1.3 Purpose of this User's Guide

This guide is intended to assist user's of the SOFEA model to input appropriate data, conduct a simulation to predict distributions of soil fumigant concentrations in air within a defined air shed, and analyze the results. SOFEA input and output is facilitated via a VBA interface that utilizes EXCEL spreadsheets and Crystal Ball probability distribution functions (PDFs). User's can create inputs based on actual field data and use information, or generate hypothetical distributions of use parameters such as field sizes, application rates and timing, depth of injection etc. This guide will lead the user through all the required and optional input parameters that can be varied, and the potential outputs that can be generated.

Details of SOFEA algorithms can be found in the companion programmers guide (Cryer, 2004). In addition, references are provided for peer reviewed literature articles or 3rd party user manuals (eg. ISCST3) for more detailed technical explanation and theory of the modeling components.

Most inputs can be specified as either discrete values, or as PDFs. If possible, PDFs should be used since this will utilize the Monte Carlo capabilities of the SOFEA modeling system and encompass uncertainties and variability in model inputs. Cells colored in green in the input screens indicate cells where Crystal Ball input assumptions (PDFs) have been defined (see Figure 4).

The model is capable of generating fumigant concentrations for each receptor in the simulation domain (up to 11,666 receptors have been simulated in a 9 township air shed), averaged over specific time intervals (24-hr and yearly) or periods specified by the user. For example, the user could use the default maximum 24-hour averages, and annual average concentration distributions, and specify the maximum 60-day average for the purpose of assessing acute, sub-chronic and chronic risk to exposed populations.

This User's Guide consists of a series of screen dumps of the EXCEL™ input and output screens in the SOFEA© model. Following each screen dump figure is a description of the inputs and parameters for that particular screen.

2.0 System Requirements and Directory or Folder Structure

SOFEA will run under a Windows™ XP or Windows™ 2000 operating system. A minimum of 1Ghz CPU speed and 1 GB RAM are recommended. Simulations will complete faster and be less likely to run out of memory the more RAM a computer has.

Crystal Ball™ 2000 Professional version (CB) must be installed on the computer where SOFEA will be implemented. CB must be checked as an add-in via the tools>add-in menu of MS Excel. In addition, once SOFEA has been downloaded, the user needs to verify that the appropriate CB libraries have been added. This is accomplished from the Microsoft Visual Basic editor through the tools>references menu. One can get to the Visual Basic editor from MS Excel via tools>macro>visual basic editor or by tools>macro>Macros to get a dialog box of all macros, highlight one of the macros (it doesn't matter which one) and select edit (see Appendix 1 for details).

The following directory structure is critical for SOFEA to run properly.

The model should be placed in a directory called "SOFEA". Subdirectories "bin" and "weather" need to be contained with the "SOFEA" directory. Yearly meteorological information in the format required by ISCST3 must reside in the weather directory. In addition, the naming convention for weather files must include some type of chronological sequence in the naming convention (i.e., Newberry2001.met, Newberry2002.met, etc.). The folder "bin" contains all executables (ISCST3, OPT2) and is where the ISCST3 input and output files are written to.

A detailed installation Guide is contained in Appendix 1.

3.0 PDF Parameter Inputs

3.1 Agronomic data

The screens shown in Figures 4a,b,c,d allow the user to input agronomic information and a reference fumigant mass allocation for a township (area of 6 miles x 6 miles) for the simulation domain. The model can simulate up to 5 different crops or crop groups. The input spreadsheet defines crop groups as Tree and Vine (T&V), Field Crop (FC), Nursery Crop (NC), Strawberry (SB), and post-plant (PP). Although specific crops or crop groups are named in the model input, the user could define any type of crop or group under any of the specified categories. The potential to define up to five separate types of crops or crops groups (including 1 T&V group) was included to maintain flexibility in the model system and allow users to specify unique agronomic PDF's for widely different crop types, if necessary.

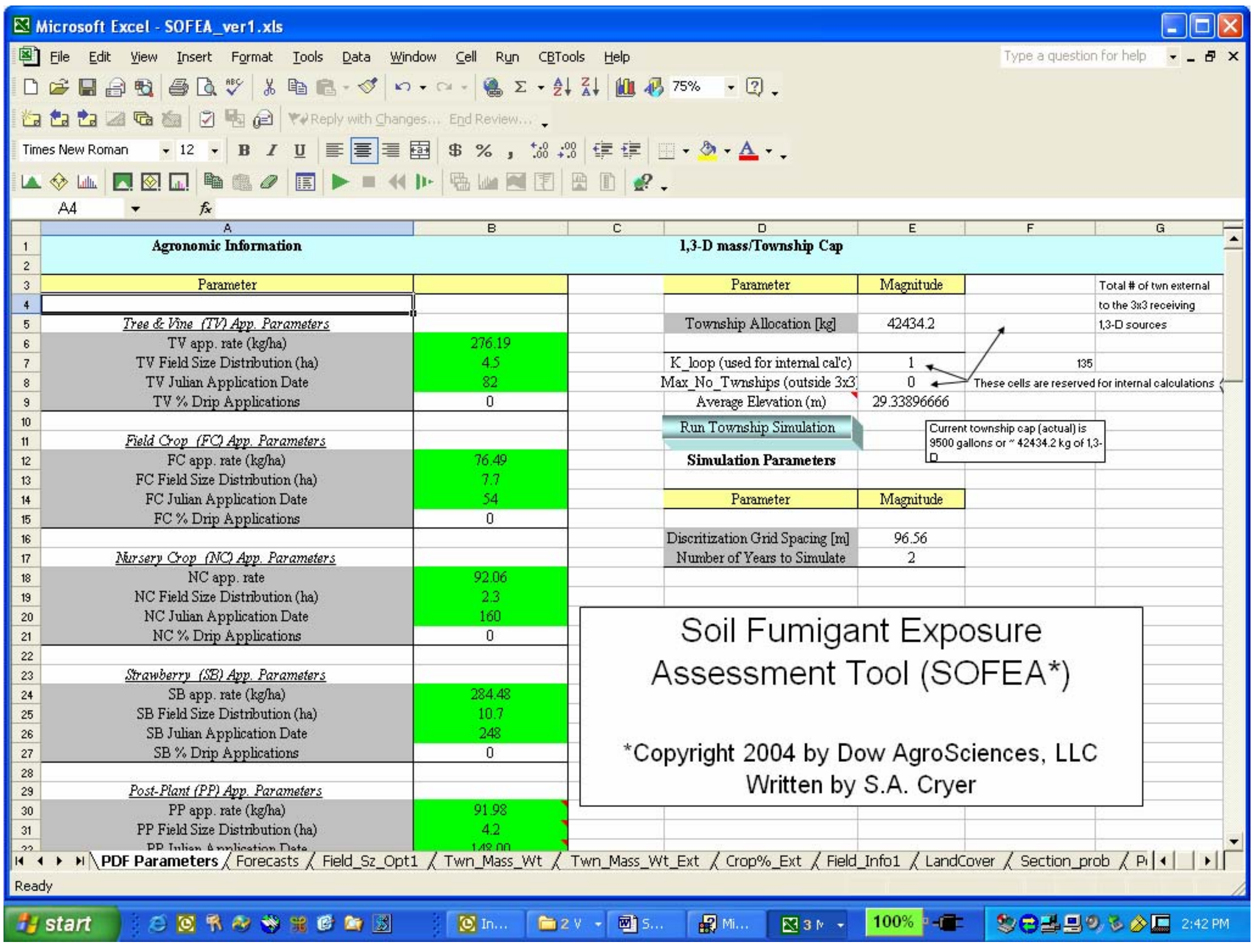


Figure 4a. PDF Parameters Worksheet.

For each crop or crop group, the user must specify a scalar value or PDF as follows:

Cell	Parameter
B6, B12, B18, B24, and B30	application rate (kg/ha)
B7, B13, B19, B25 and B31	field size (ha)

B8, B14, B20, B26, and B32	Julian application date
B9, B15, B21, B27, and B33	% drip irrigation

If a scalar is defined, then this value will always be selected. *However, a PDF is resampled for each year of simulation*. Sample Crystal Ball PDF's for field size, and application rate, date and depth are shown in Appendix I.

If no drip applications are made for a particular crop or crop group, then "0" can be entered for this parameter. Applications to tree and vine crops (T&V) are assumed to occur only once every 20 years. This is assumed to be a conservative estimate of how often tree and vine crops (eg. grapes, citrus, tree nuts etc.) may be replaced. Once a T&V field is placed within the simulation domain, no other fumigant applications will take place on that piece of land for 20 years. Conversely, for field crops and other annual crop groups, fields can be retreated annually, as specified by the user (see Figure 1d). Data for the agronomic PDFs can be obtained from sources such as CA DPR's Pesticide Use Record (PUR) database.

Also entered on this screen is the maximum total mass that can be applied annually within a given township, or simulation domain. For example, if the maximum allowable mass of fumigant that can be applied in a township annually is 100,000 kg, then that value would be entered in cell E5.

Cell	Parameter
E5	maximum allowable mass of fumigant in township
E7, E8	reserved for internal calculations and no user input is required.
E16	discretization grid spacing. This value is defaulted to 96.56 m and is typically not necessary to change.
E17	The number of years to simulate

The authors have found that typically 10-15 years of simulation are sufficient to reach a 'plateau' the fumigant air concentration distribution for the purpose of chronic risk assessment (ie. additional years simulated will not result in a significant change in the air concentration distribution, see Appendix 2).

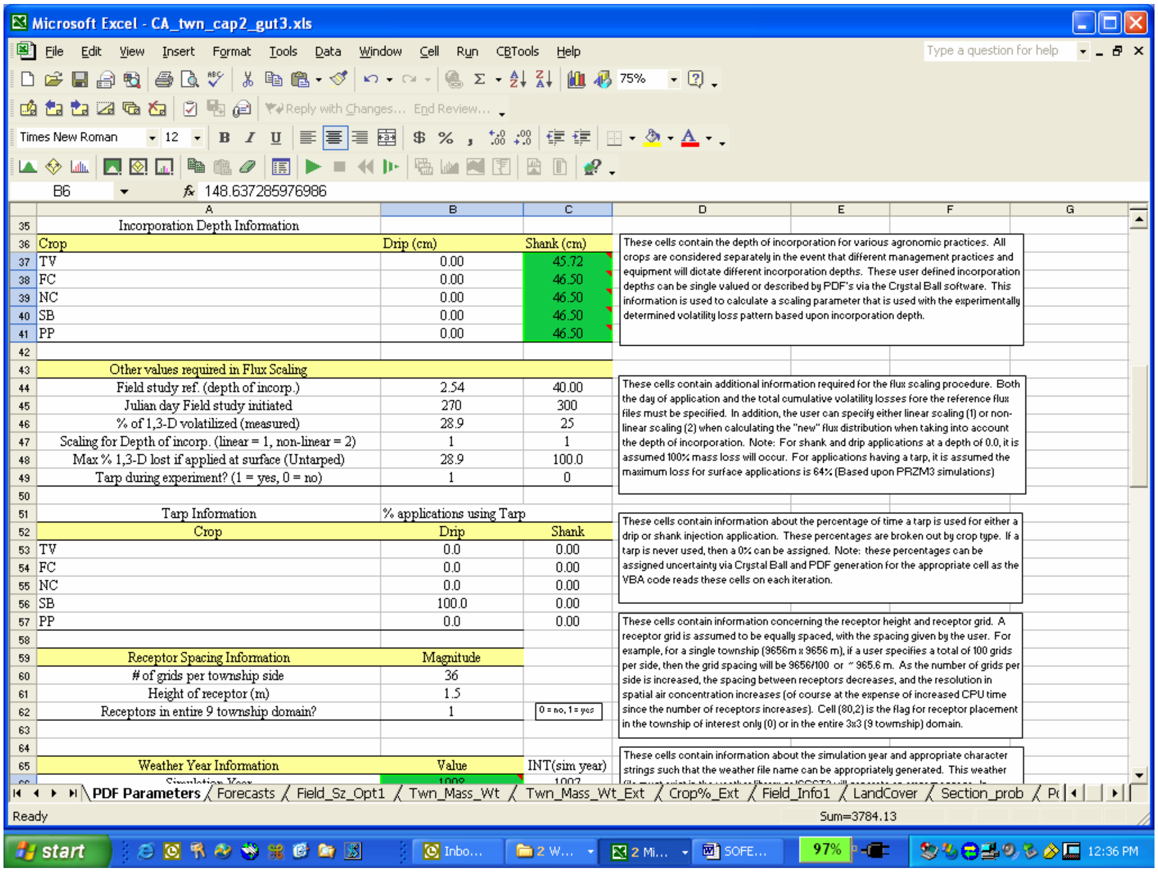


Figure 4b. PDF Parameters Worksheet continued

Cell	Parameter
B37 – B41	discrete value or PDF of drip irrigation depth for each crop
C37 - C41	discrete value or PDF for shank injection depth for each crop

For example, drip irrigation applications may always occur at a specified depth (eg. 2 inches), or could vary from surface applied drip to deep buried drip. Similarly shank injections may vary in depth depending on the type of crop.

Research has shown that the amount of fumigant that escapes from the soil is dependent on the depth of injection of the material. Thus, a flux profile (mass loss of fumigant as a function of time after application) for a reference depth is required as input into the model. An example of a field measured flux profile for a soil fumigant is shown in Appendix 3. This flux profile can be adjusted up or down depending on the depth of application relative to the reference depth. The scaling adjustment of the mass loss profile can take on a linear or non-linear form (Appendix 2). The choice of the scaling function depends on the best professional judgment of the user, based on available lab or field measurements, or theoretical physical understanding of the fumigant in question. Scaling of the reference flux profile is discussed further in Section 12.0. The user must specify several key parameters related to the reference flux profile for drip and/or shank applications in cells B44 to B49 and/or cells C44 to C49, respectively. These parameters include the actual depth of the application used in the reference field study. The Julian date of the reference field study, the total mass of fumigant flux measured, the type of scaling, the theoretical maximum percentage of fumigant flux loss if applied at the soil surface with no tarp, and finally whether the field experiment was conducted with or without tarp.

Cell	Parameter
B44, C44	Field study reference depth of incorporation for drip and shank
B45, C45	Julian Day field study initiated for drip and shank
B46, C46	measured % of fumigant volatilized for drip and shank
B47, C47	scaling for depth of incorporation (linear=1, non-linear=2)
B48, C48	tarped during field study? (yes=1, no=0)

The user must then define the percentage of applications where a tarp (agronomic film or plastic mulch) is used for drip or shank applications for each crop or crop group (Cells B53-B57 and C53-C57).

Cell	Parameter
B53, C53	% of T&V applications made using tarp for drip and shank
B54, C54	% of FC applications made using tarp for drip and shank
B46, C46	% of NC applications made using tarp for drip and shank
B47, C47	% of SB applications made using tarp for drip and shank
B48, C48	% of PP applications made using tarp for drip and shank

3.2 Receptor Grid

Information on the receptor grid must be entered in cells B60-B62. Receptors are points in space where the model will simulate concentrations of the fumigant and capture the results based on the output intervals specified by the user (Figure 4b). These cells contain information concerning the receptor height and receptor grid. A receptor grid is assumed to be equally spaced, with the spacing given by the user. For example, for a single township (9656m x 9656 m), if a user specifies a total of 100 grids per side, then the grid spacing will be 9656/100 or ~ 96.56 m. As the number of grids per side is increased, the spacing between receptors decreases, and the resolution in spatial air concentration increases . Cell B62 is the flag for receptor placement in the central township of interest only (0) or in the entire 3x3 (9 township) domain.

Currently, the default for a CA township with dimensions of 6 x 6 miles is 36 receptors per township section (1 mi x 1 mile) which results in 1296 (36 x 36) receptors per township and thus 1296 values of annual average or maximum 24-hour air concentrations. Receptor grids can be made denser or sparser depending on the needs of the user. The user should keep in mind however that CPU and memory requirements increase proportionally as the number of receptors in the simulation domain, or the size of the domain, is increased.

Cell	Parameter
B60	# of grids per township side
B61	Height of receptor (m)
B62	Receptors in entire 9 township domain (yes=1, no=0)

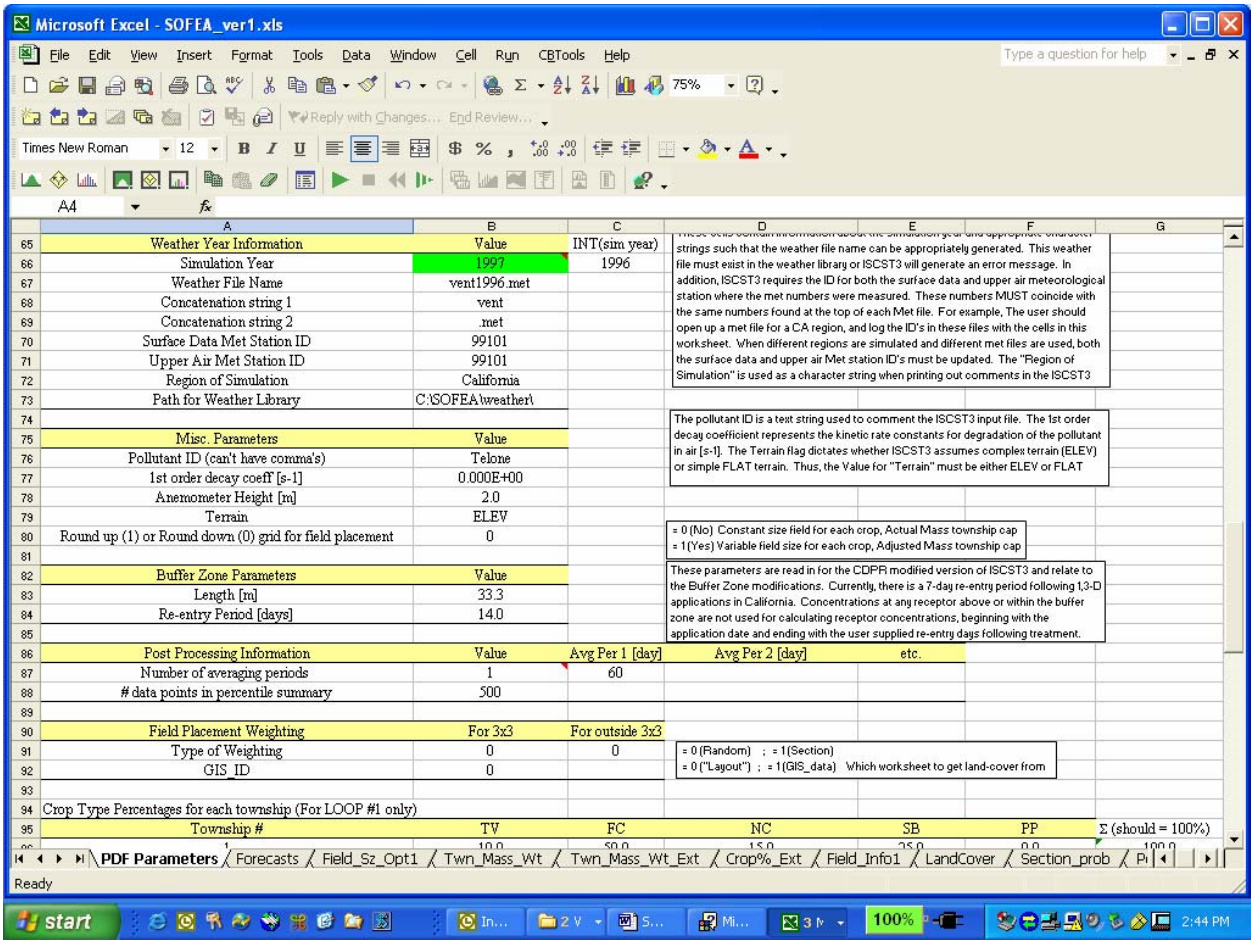


Figure 4c. PDF Parameters Worksheet continued

3.3 Weather Year Information

Meteorological data required by ISCST3 include hourly air stability class, wind speed, air temperature, wind direction, and mixing height for the air shed. Example sources of weather data suitable for use with ISCST3 are the EPA Support Center for Regulatory Air Models (SCRAM) website and the California Irrigation Management Information System (CIMIS) website. Cells B66 to B73 contain the weather information parameters needed to run the model. Cell B66 contains the simulation year. This can be set as a Crystal Ball assumption if multiple weather years are available. For example if weather years 1995-1999 are available, the cell can be set as a uniform distribution such that weather years 1995-1999 will be randomly selected with equal probability. The year must be incorporated in the naming convention if multiple years of weather are to be sampled. Typically, a uniform distribution is assigned to the weather year such that each year in the weather library has an equally likely chance of being selected for the current year of simulation.

The cells in this section contain information about the simulation year and character strings such that the weather file name can be appropriately generated. This weather file must exist in the weather library or ISCST3 will generate an error message. In addition, ISCST3 requires the ID for both the surface data and upper air meteorological station where the met numbers were measured. These numbers MUST coincide with the same numbers found at the top of each meteorological (*.met) file. When different regions are simulated and different Met files are used, both the surface data and upper air Met station ID's must be updated. The "Region of Simulation" is used as a character string when printing out comments in the ISCST3 input file.

Hourly weather files must have the following format:

YYMMDDHH, Direction [9X], Speed [9X], Temp [7X], Stability [3X], Urban Mixing Height [7X], Rural Mixing Height [7X]

The first line of the weather file must contain the surface station ID (eg. 99056) and upper station ID (eg. 99876) and the weather year (eg. 1993), as shown in the example below:

```
99056   1993  99876   1993
93 1 1 1   282.80     2.94 279.0 5    320    320
93 1 1 2   302.80     3.71 279.3 4    320    320
93 1 1 3   330.90     3.91 279.5 4    320    320
93 1 1 4   321.00     4.00 279.4 4    320    320
93 1 1 5   317.90     4.90 279.4 4    320    320
93 1 1 6   317.60     4.98 279.7 4    320    320
93 1 1 7   330.10     5.48 279.6 4    320    320
.
.
.
```

HINT: *Weather file creation – In an* Excel *spreadsheet set all column widths as required above, then do a "Save As" .prn file, name extension as ".met"*

Model inputs required for weather information

Cell	Parameter
B67	Weather file name
B68, 69	these cells are filled automatically by concatenating cell B67
B70, 71	The surface met station and upper air met station ID's must be entered here and must match the met station ID in the first line of the weather file (see example above)
B72	Region of simulation
B73	Path for weather library

3.4 Miscellaneous Parameters

The pollutant ID is a text string used to comment the ISCST3 input and output files. This parameter may not have comma's. The 1st order decay coefficient represents the kinetic rate constants for degradation of the pollutant in air [s^{-1}]. The Terrain flag dictates whether ISCST3 assumes complex terrain (ELEV) or simple FLAT terrain. Thus, the Value for "Terrain" must be either ELEV or FLAT.

Cell	Parameter
B76	Pollutant ID (eg. Telone) May not have comma’s
B77	1st order decay co-efficient in air (s^{-1})
B78	Anemometer height in surface weather station (m)
B79	Terrain (ELEV or FLAT)
B80	Round up (“1”) or round down (“0”) grid for field placement

3.5 Buffer Zone Parameters

This section allows the user to specify a width of buffer zone and a re-entry period for treated field. Once the model chooses field locations all receptors over the treated field and within the specified buffer distance from the treated field are turned off; that is they do not contribute to concentrations of airborne soil fumigant, from the time of application until the specified time period lapses. After the specified re-entry period (typically specified on the product label for most soil fumigants), receptors on the treated field and within the specified buffer distance are once again turned ‘on’ and can contribute to overall fumigant concentration. The model can be used to test the effect of different buffer distances on the air concentration distribution and subsequent exposure to non-target populations. Details of this methodology are found elsewhere (Johnson, 2001).

Cell	Parameter
B83	Width of buffer zone (m) is typically included on product label
B84	Re-entry period (days) is typically included on the product label

3.6 Post Processing Information

The user can specify averaging periods in addition to the default annual average air concentration distribution that is automatically generated by this model. For example, the user may wish to examine the air concentration distribution of 48-hour maximum values, and maximum 60 day average values in the simulation domain. The user would then specify “2” averaging periods in Cell B87, and “2” day in Cell C87 and “60” days in cell D87. Additional averaging periods can be added, however to date the model has not been tested with more than 2 additional averaging periods. Also the user should be aware that memory requirements increase as the number of averaging periods is increased.

Cell	Parameter
B87	Number of averaging periods
C87	Length of averaging period #1 (days)
D87	Length of averaging period #2 (days)
E87	Length of averaging period #3 (days) etc.
B88	# of data points in percentile summary

3.7 Field Placement Weighting by Section

Depending on the level of detail of historic use data available, or the hypothetical use scenarios a user may wish to evaluate, the user can specify either random field placement within the simulation domain (or within agricultural capable areas, of land use data is available), or section specific weighted field placement. The section weighted field placement means that fields are only placed in sections within a township that are specified by the user, and furthermore that the amount of fumigant mass placed in the sections will be apportioned according to the 'section weights' that are entered by the user in the worksheet "Sect_Prob" (see Figure 7).

If land use data is available, the user may elect to use this information to guide the placement of treated fields. The user can enter information on land use, population and elevation. Land use information defines land as urban, agricultural, water, mountain, etc. Elevation data can be used by the ISCST3 model when it is run in the complex terrain mode. Finally population data can be used for higher tier risk exposure and assessments to correlate fumigant concentrations with exposed populations. GIS data is entered in the GIS_data worksheet (Figure 12). Further information on populating that worksheet is contained in Section 14.0.

Cell	Parameter
B91	Type of weighting for central 3x3 twps (0=random, 1=section)
C91	Type of weighting for twps outside of 3x3 (0=random, 1=section)
B92	GIS_ID (0= "LandCover", "Population", "Elevation", 1=GIS data)

GIS_ID determines which worksheet SOFEA will extract data the GIS data from. Worksheets "LandCover", "Population", and "Elevation" will only typically be edited if GIS data is not available and the user is entering input 'manually'.

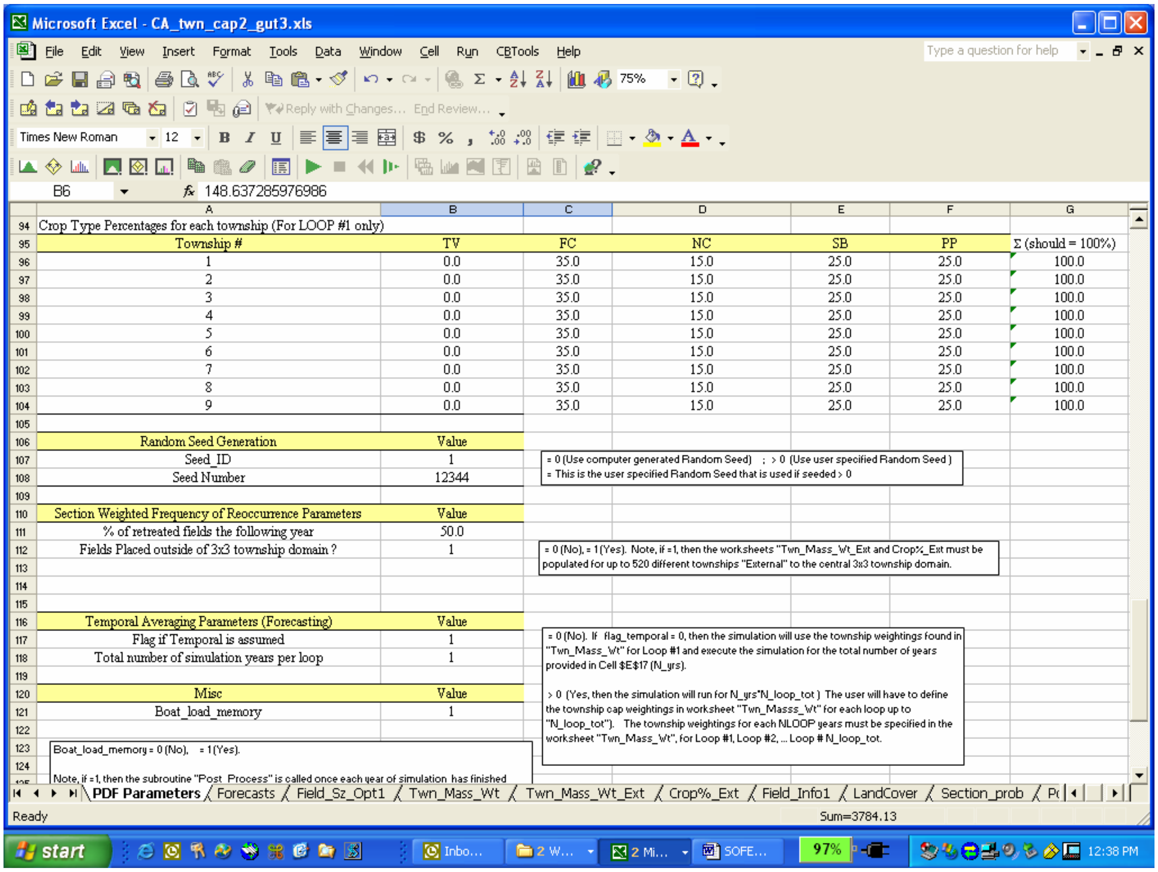


Figure 4d. PDF Parameters Worksheet continued

3.8 Crop type or crop group percentages for each township (Loop #1 only)

Cells in this section are populated for the measured or hypothetical distribution of crops or crop groups within each of the 9 center townships (3x3 grid) being simulated. Township numbering follows the system of the example shown below.

Twn 7	Twn 8	Twn 9
Twn 4	Twn 5	Twn 6
Twn 1	Twn 2	Twn 3

Cell	Parameter
B96 – B104	% of T&V crops in townships 1-9, respectively
C96 - C104	% of FC crops in townships 1-9, respectively
D96 - D104	% of NC crops in townships 1-9, respectively
E96 - E104	% of SB crops in townships 1-9, respectively
F96 – F104	% of PP crops in townships 1-9, respectively
G96 - G104	*No input required*. This cell is calculated and is simply provided as a check that the sum of percentages of each different crop within a single township should add up to 100%.

If the user wishes to change the distribution of crops within townships over the course of a multi-year simulation, then additional parameters, structured the same as for loop #1, require input (Figure 5). The user can enter different crop type percentages for up to 5 'loops' of variable duration. For example, the user may wish to test the impact of growers moving to different crops is every 2 years for a total of 10 years on the annual average air concentration distribution for a fumigant. Thus the user would enter crop percentages for 5 loops in the Forecasts worksheet, and run the simulation for a total of 10 years (*see also Cell B118*). Additional worksheets that require input if multiple loops occur are "Twn_Mass_wt" (Section 6.0) for township weightings for the central 3x3 townships, "Twn_Mass_wt_Ext" (Section 7.0) for township weightings for townships up to a 23x23 domain (external from the central 3x3), and "Crop%_Ext" (Section 8.0) for the crop percentages within each township (for external townships from the central 3x3).

3.9 Seed Number Generation

A seed value was defined such that the same starting value in terms of random sampling would be initiated. Ideally, a simulation could be re-run and the same values regenerated if the simulation were repeated using the same seed value. Unfortunately, the way Crystal Ball selects a random seed value is different when performing a single step at a time (SOFEA implementation), vs. selecting a series of numbers at a time. Thus, this functionality is currently not available, although the ties to a random seed are still intact.

Cell	Parameter
B107	User defined seed=0, Computer generated seed=1
B108	User defined seed (5 digit number) if Cell B107=1

Section weighted frequency of occurrence parameters

Cell	Parameter
B111	Percentage of fields retreated from year to year (%)
B112	Fields placed outside 3x3 township domain (0=no, 1=yes)

If Cell B112 is "1",that is fields are placed outside the 3x3 township domain, then worksheets Twn_Mass_Wt_Ext and Crop%_Ext must be populated (See below).

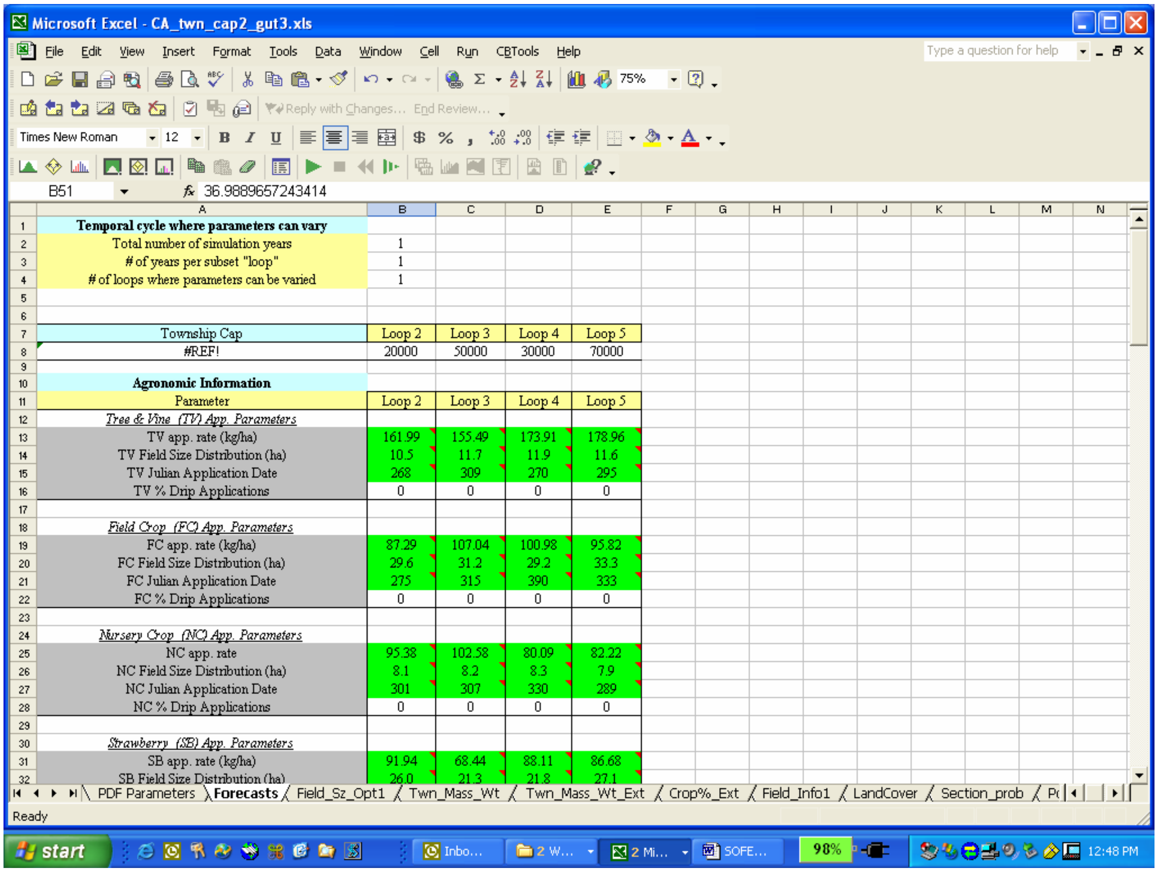
3.10 Temporal Averaging Parameters

If the user wishes to define temporal changes in crop types or distributions for different years of a simulation, as discussed above, then the number of years to assign to additional loops is defined in these cells. If ‘flag_temporal’ = 0, then the simulation will assume only “one loop” and will use the township weightings found in "Twn_Mass_Wt" for Loop #1 and execute the simulation for the total number of years provided in Cell E17 (N_yrs). If ‘flag_temporal’ > 0, then the simulation will run for N_yrs*N_loop_tot . The user will have to define the township cap weightings in worksheet "Twn_Masss_Wt" for each loop up to the total number of loops, "N_loop_tot"). The township weightings for each NLOOP years must be specified in the worksheet "Twn_Mass_Wt", for Loop #1, Loop #2, … Loop # N_loop_tot.

Cell	Parameter
B117	Flag for temporal averaging (1=yes, 0=no)
B118	Number of simulation years per loop
B121	Flag for subchronic post-processsing (=1, then subchronic post-processing of 24-hr data will be done to yield user supplied time interval values (will require a lot of RAM). If = 0, then no subchronic post-processing will be done, but the user will still get the 24hr max and chronic air concentrations for each receptor in the air shed.
B122	Flag for 1,3-D simulation in California. (0 = yes) for all other fumigants in any region and for 1,3-D outside of California (1 = no)

<u>4.0 Forecasts Worksheet</u>

The “Forecasts” worksheet shown in Figures 5a, b, c, d allows the user to specify temporal changes in crop application dates, field sizes and application rates, as discussed above in the section on Crop parameters and temporal averaging parameters. Note that this worksheet must be completed for each township of interest for each loop.



	A	B	C	D	E
1	Temporal cycle where parameters can vary				
2	Total number of simulation years	1			
3	# of years per subset "loop"	1			
4	# of loops where parameters can be varied	1			
5					
6					
7	Township Cap	Loop 2	Loop 3	Loop 4	Loop 5
8	#REF!	20000	50000	30000	70000
9					
10	Agronomic Information				
11	Parameter	Loop 2	Loop 3	Loop 4	Loop 5
12	Tree & Vine (TV) App. Parameters				
13	TV app. rate (kg/ha)	161.99	155.49	173.91	178.96
14	TV Field Size Distribution (ha)	10.5	11.7	11.9	11.6
15	TV Julian Application Date	268	309	270	295
16	TV % Drip Applications	0	0	0	0
17					
18	Field Crop (FC) App. Parameters				
19	FC app. rate (kg/ha)	87.29	107.04	100.98	95.82
20	FC Field Size Distribution (ha)	29.6	31.2	29.2	33.3
21	FC Julian Application Date	275	315	390	333
22	FC % Drip Applications	0	0	0	0
23					
24	Nursery Crop (NC) App. Parameters				
25	NC app. rate	95.38	102.58	80.09	82.22
26	NC Field Size Distribution (ha)	8.1	8.2	8.3	7.9
27	NC Julian Application Date	301	307	330	289
28	NC % Drip Applications	0	0	0	0
29					
30	Strawberry (SB) App. Parameters				
31	SB app. rate (kg/ha)	91.94	68.44	88.11	86.68
32	SB Field Size Distribution (ha)	26.0	21.3	21.8	27.1

Figure 5a. Forecasts Worksheet

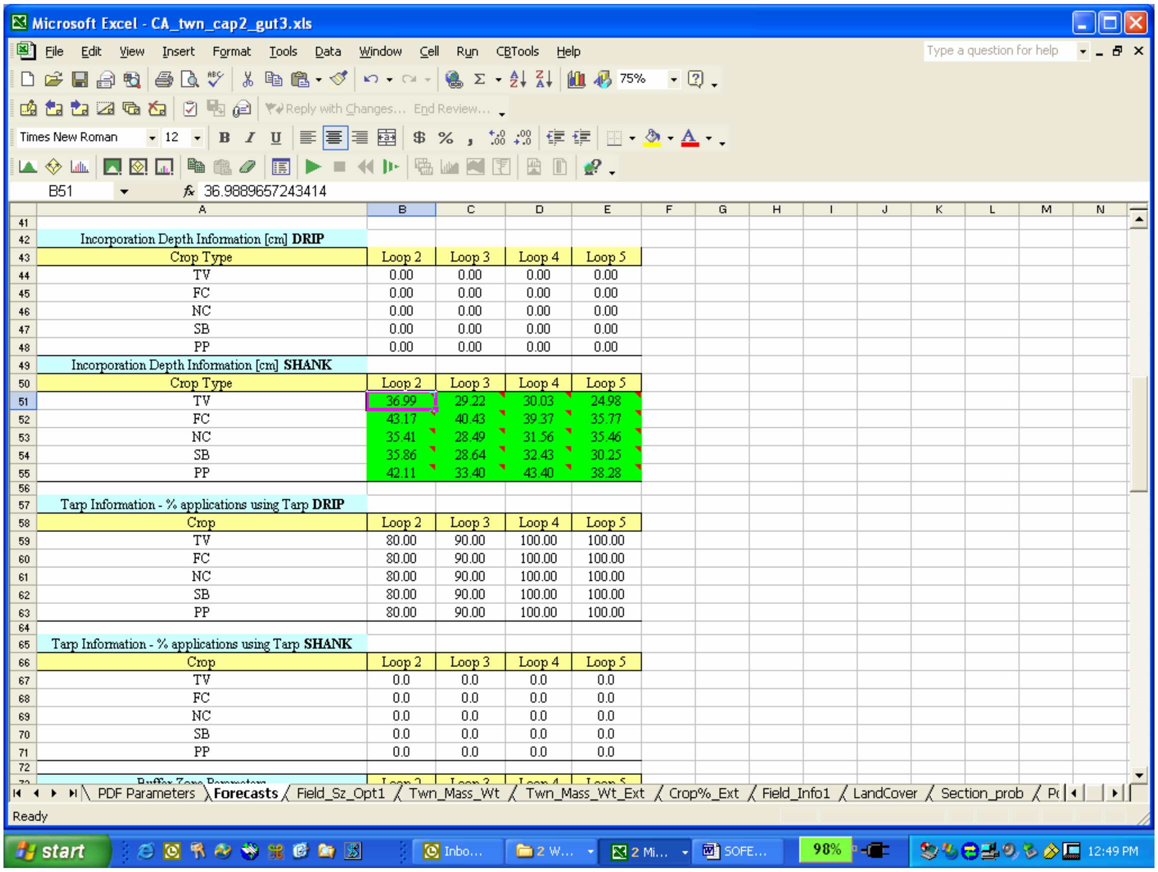
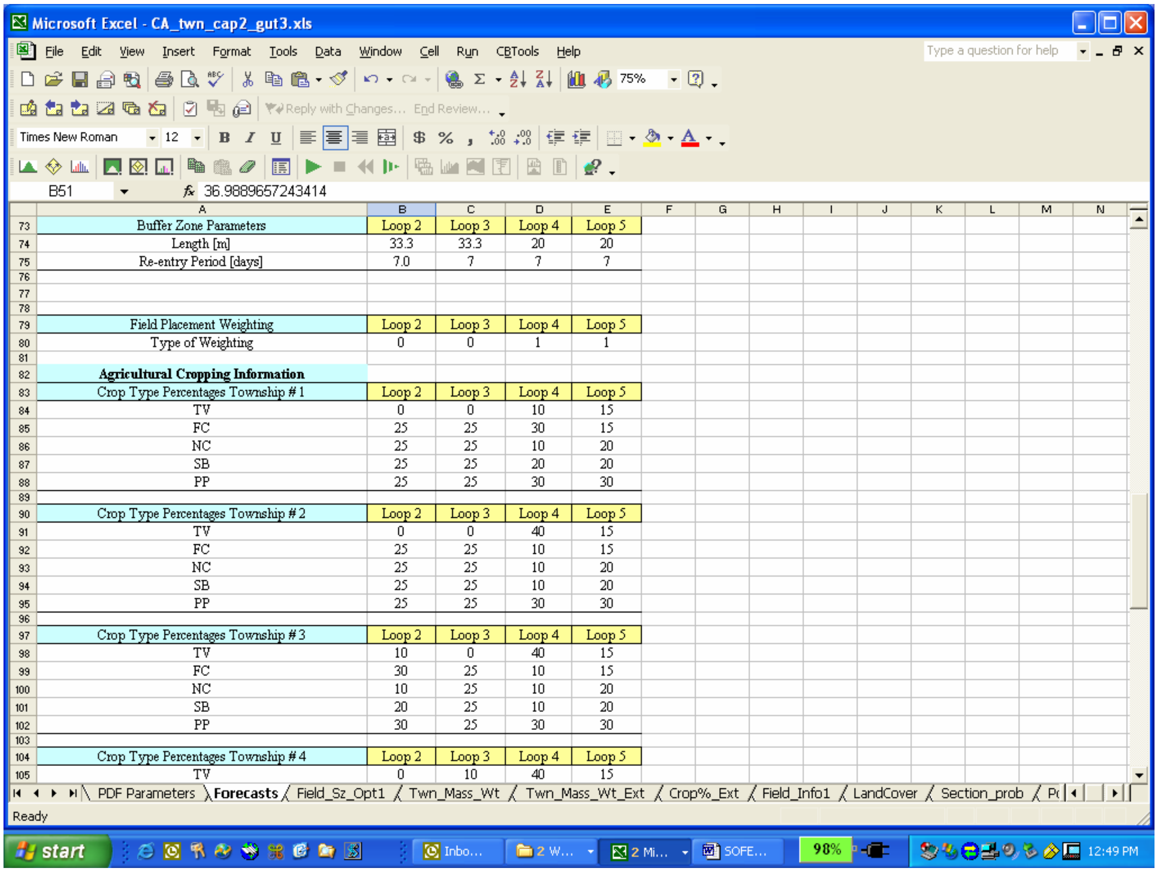
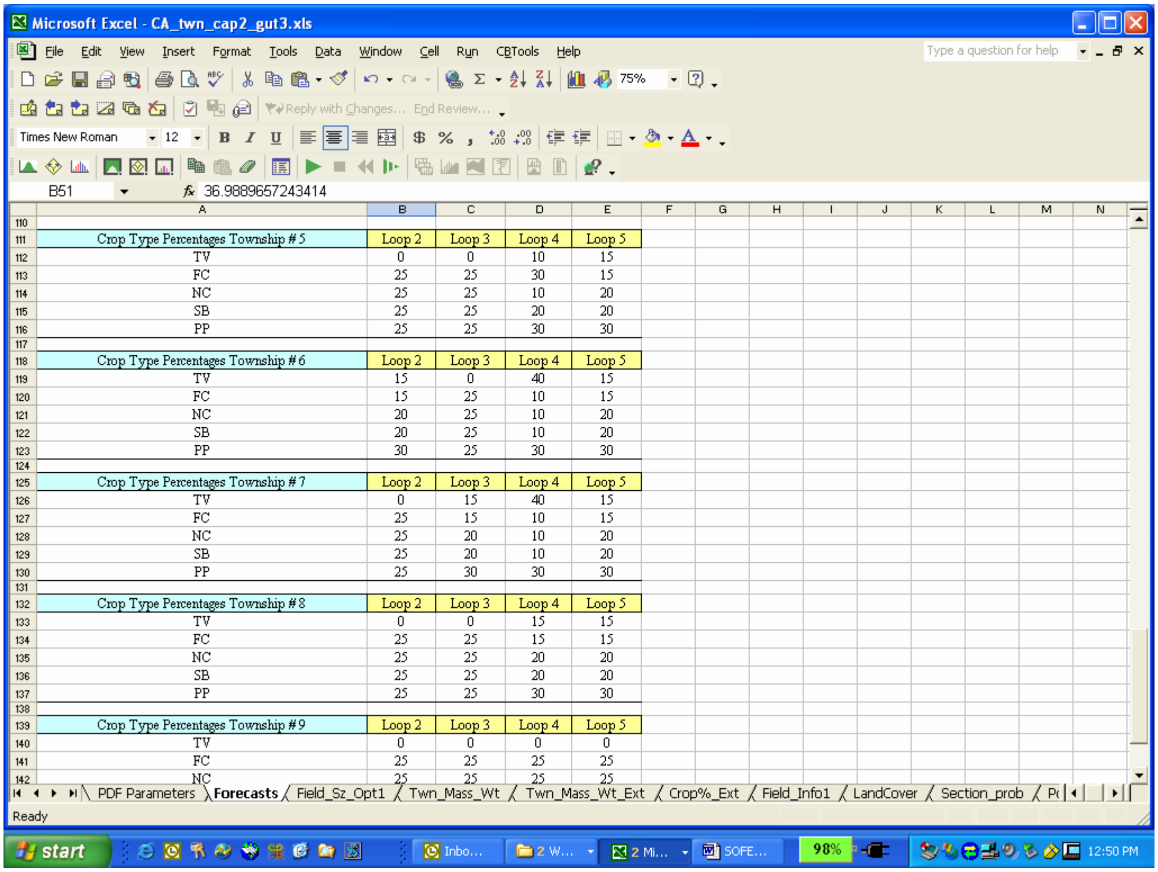


Figure 5b. Forecasts worksheet continued



	A	B	C	D	E
73	Buffer Zone Parameters	Loop 2	Loop 3	Loop 4	Loop 5
74	Length [m]	33.3	33.3	20	20
75	Re-entry Period [days]	7.0	7	7	7
76					
77					
78					
79	Field Placement Weighting	Loop 2	Loop 3	Loop 4	Loop 5
80	Type of Weighting	0	0	1	1
81					
82	**Agricultural Cropping Information**				
83	Crop Type Percentages Township # 1	Loop 2	Loop 3	Loop 4	Loop 5
84	TV	0	0	10	15
85	FC	25	25	30	15
86	NC	25	25	10	20
87	SB	25	25	20	20
88	PP	25	25	30	30
89					
90	Crop Type Percentages Township # 2	Loop 2	Loop 3	Loop 4	Loop 5
91	TV	0	0	40	15
92	FC	25	25	10	15
93	NC	25	25	10	20
94	SB	25	25	10	20
95	PP	25	25	30	30
96					
97	Crop Type Percentages Township # 3	Loop 2	Loop 3	Loop 4	Loop 5
98	TV	10	0	40	15
99	FC	30	25	10	15
100	NC	10	25	10	20
101	SB	20	25	10	20
102	PP	30	25	30	30
103					
104	Crop Type Percentages Township # 4	Loop 2	Loop 3	Loop 4	Loop 5
105	TV	0	10	40	15

Figure 5c. Forecasts worksheet continued



Crop Type Percentages Township # 5	Loop 2	Loop 3	Loop 4	Loop 5
TV	0	0	10	15
FC	25	25	30	15
NC	25	25	10	20
SB	25	25	20	20
PP	25	25	30	30
Crop Type Percentages Township # 6	Loop 2	Loop 3	Loop 4	Loop 5
TV	15	0	40	15
FC	15	25	10	15
NC	20	25	10	20
SB	20	25	10	20
PP	30	25	30	30
Crop Type Percentages Township # 7	Loop 2	Loop 3	Loop 4	Loop 5
TV	0	15	40	15
FC	25	15	10	15
NC	25	20	10	20
SB	25	20	10	20
PP	25	30	30	30
Crop Type Percentages Township # 8	Loop 2	Loop 3	Loop 4	Loop 5
TV	0	0	15	15
FC	25	25	15	15
NC	25	25	20	20
SB	25	25	20	20
PP	25	25	30	30
Crop Type Percentages Township # 9	Loop 2	Loop 3	Loop 4	Loop 5
TV	0	0	0	0
FC	25	25	25	25
NC	25	25	25	25

Figure 5d. Forecasts worksheet continued

5.0 Field Size Optimization

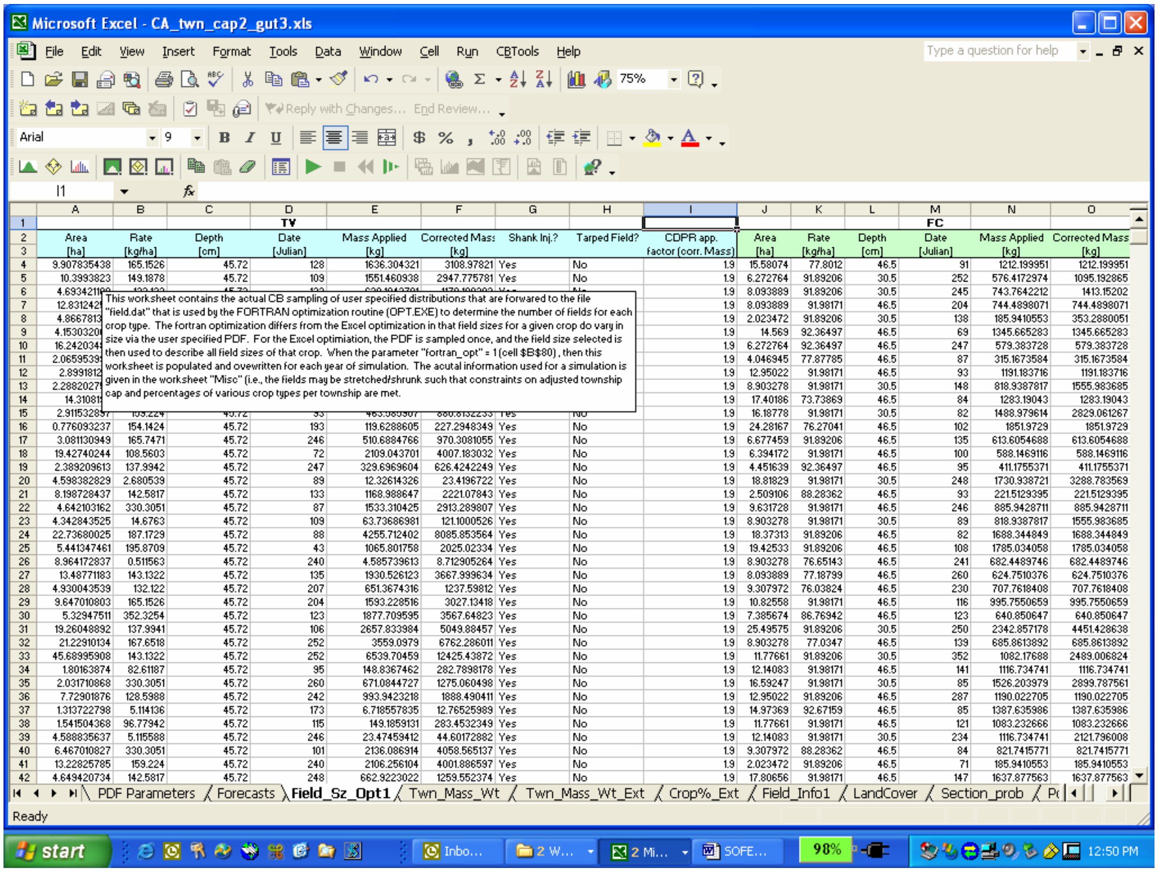


Figure 6. Field_Sz_Opt1 Worksheet

The Field_Sz_Opt1 worksheet (Figure 6) does not require input by the user. The purpose of this workheet is to display the actual field sizes, application rates, application dates etc. that the model chose from the corresponding PDF inputs for each crop type that are supplied in the PDF parameters worksheet. This can be usful to see how the fields were stretched/shrunk by the optimization program to meet constraints on crop percentages and the township allocation. For further details on the optimization procedure, see Cryer 2004.

Cryer S.A., 2004. Predicting Soil Fumigant Acute, Sub-chronic, and Chronic Air Concentrations Under Diverse Agronomic Practices, In preparation.

6.0 Township Mass Weights

This worksheet (Figure 7) allows the user to input the relative amount (weighting) of the maximum allowable fumigant mass that is used for each year of simulation, in each township in the simulation domain. For example, in Figure 4, the central township of interest for Loop 1 (Twp #5) has a “2” weighting, (ie. 2x the maximum township mass entered in Cell E5) in the “PDF Parameters” worksheet (ie. If Cell E5 specified 100,000 kg, then Twp #5 in Loop #1 would be allotted 200,000 kg of the soil fumigant for each year). Similarly fumigant mass for each township in the simulation domain can be entered as a multiple of the value entered in Cell E5. If multiple loops are simulated (Cell B17 and E118 in PDF Parameters), then the township cap amounts for Loops 2-5 must be entered as well.

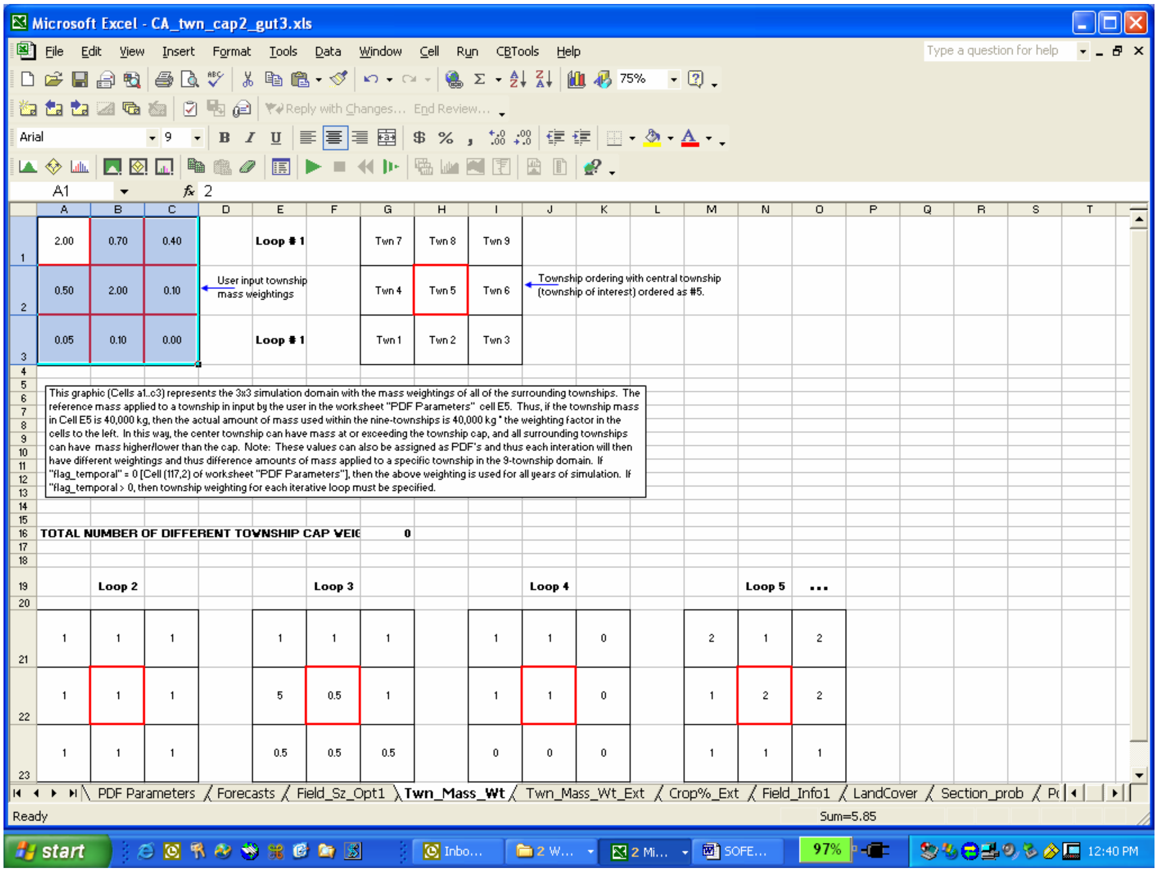


Figure 7. Twn_Mass_Wt worksheet

7.0 External Township Mass Weights

This worksheet allows the user to specify fumigant mass allocations or weightings for simulation domains up to 23 x 23 townships. The reset button resets all township mass allocations to "0". Note that although fumigant applications can be simulated in these townships, receptors (and hence the output air concentration distributions) are limited to the central 3x3 township grid (or the single central township only), as specified in Cell B62 in the PDF Parameters worksheet. NOTE: If township weightings for the central 3x3 townships are defined in the worksheet "Twn_Mass_Wt", then the central 3x3 townships in this worksheet must be zero or null. If values are specified here and in the worksheet "Twn_Mass_Wt", then the actual weight is the sum found in both worksheets for the central 3x3 townships.

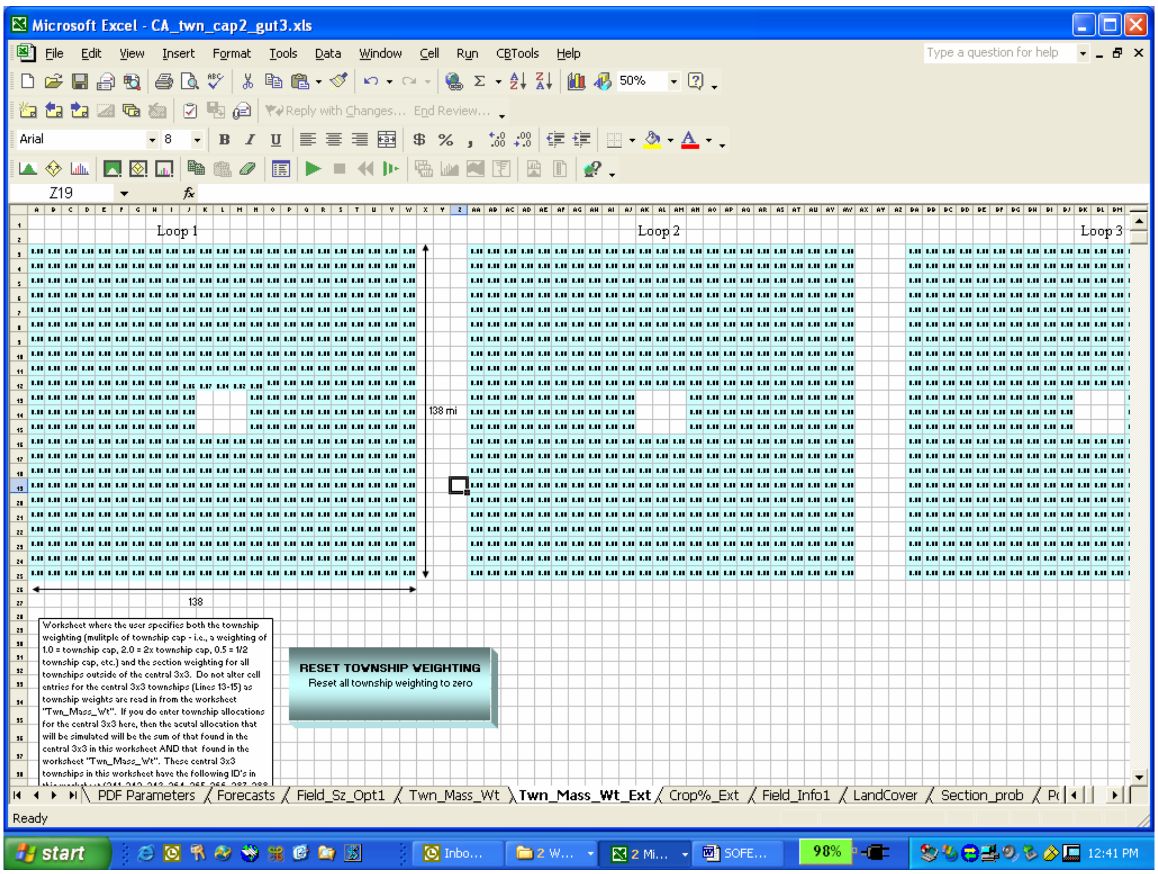


Figure 8. Twn_Mass_Wt_Ext Worksheet

8.0 Agronomic PDF Data for External Townships

This worksheet allows the user to enter crop or crop group percentages for each of the townships in the simulation domain outside the central 3x3 township area.
Note: Township 241-243, 264-266, 287-289 are defined by townships 1-9 in worksheet "PDF Parameters" FOR THE FIRST LOOP ONLY. Thus, any input for these townships here is ignored under loop 1, as source terms for the central 3x3 have already been defined before a call to the subroutine that reads input from this worksheet and subsequently determines the source information for each township represented. All other loops get all of their crop information from this worksheet. Do NOT make any changes to cells that are colored. User should modify white cells only. Peach colored cells denote the central 3x3 townships and should NOT be modified in this worksheet.

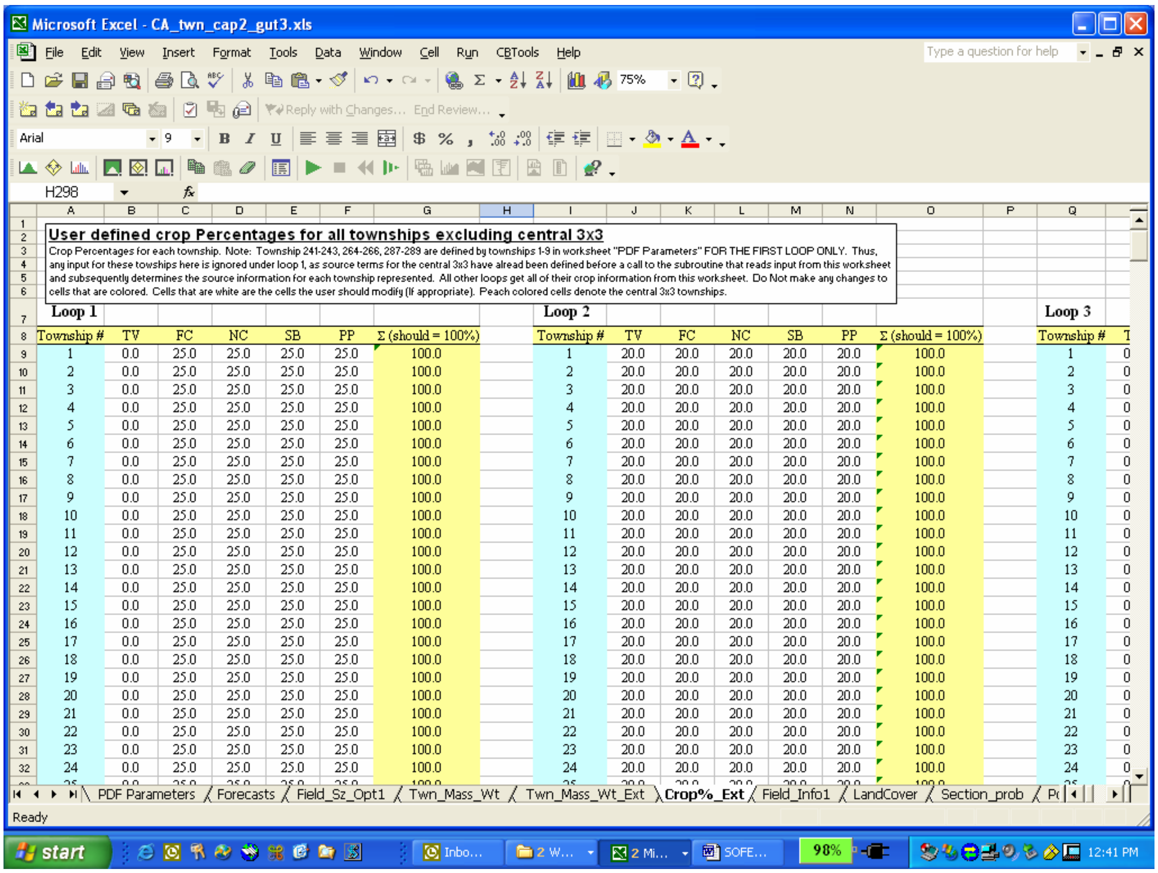


Figure 9. Crop%_Ext Worksheet

9.0 Section Weights

The Section_prob worksheet (Figure 10) allows the user to enter the relative distribution of the fumigant mass within each township, by section. Each township in California is divided into 36 sections, each with a 1 mi2 area. Since CA PUR data is collected on a section basis, it is possible to refine the simulation by locating treated fields by section, as opposed to randomly placing them within agricultural capable areas within the township. Typically, if townships contain 'hot spots', or concentrated areas of high fumigant use, this will have an impact on the highest percentile concentrations in the air concentration distribution.

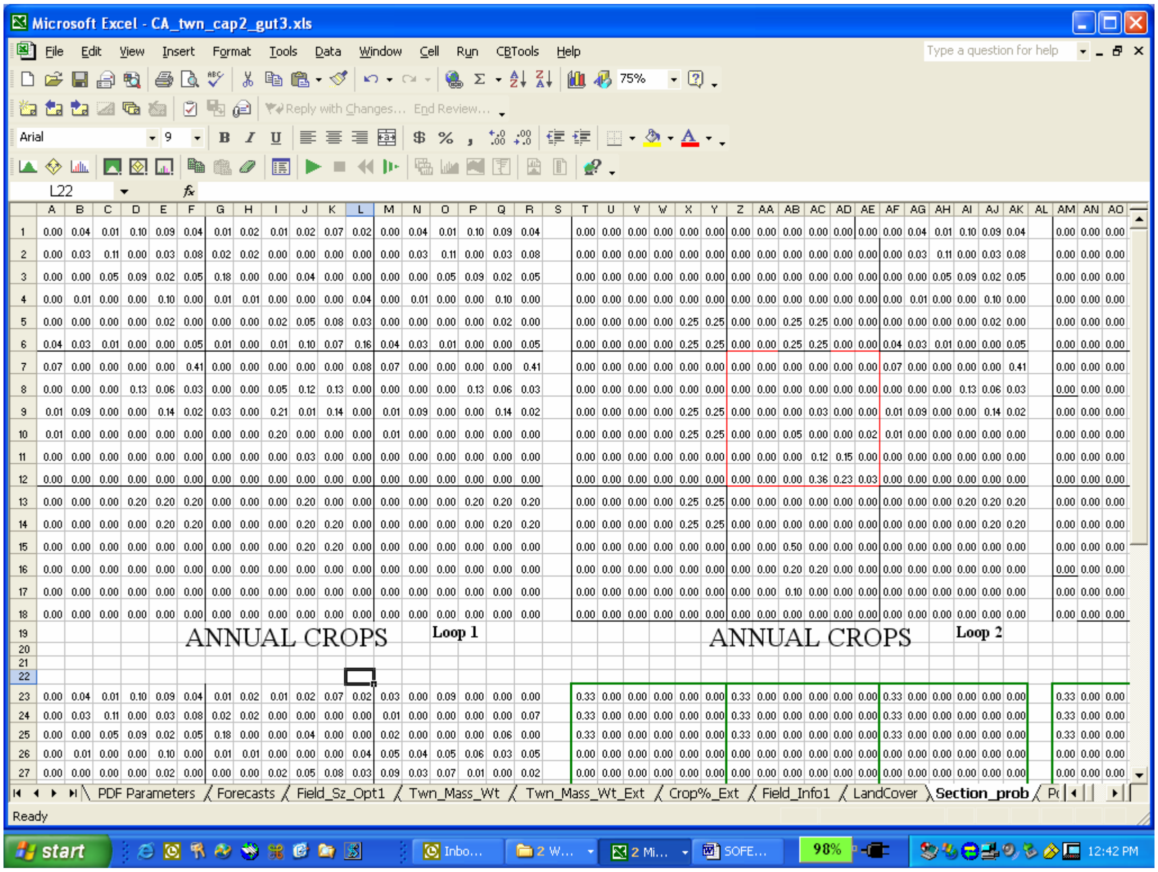


Figure 10. Section_prob Worksheet

10.0 Population data

Population data can be obtained from national census data, converted to raster, and then resampled at an appropriate scale to match the cell grid used by SOFEA. Population data is entered in the "GIS_data" worksheet (Figure 15) and is displayed in the Population worksheet as shown in Figure 11 below.

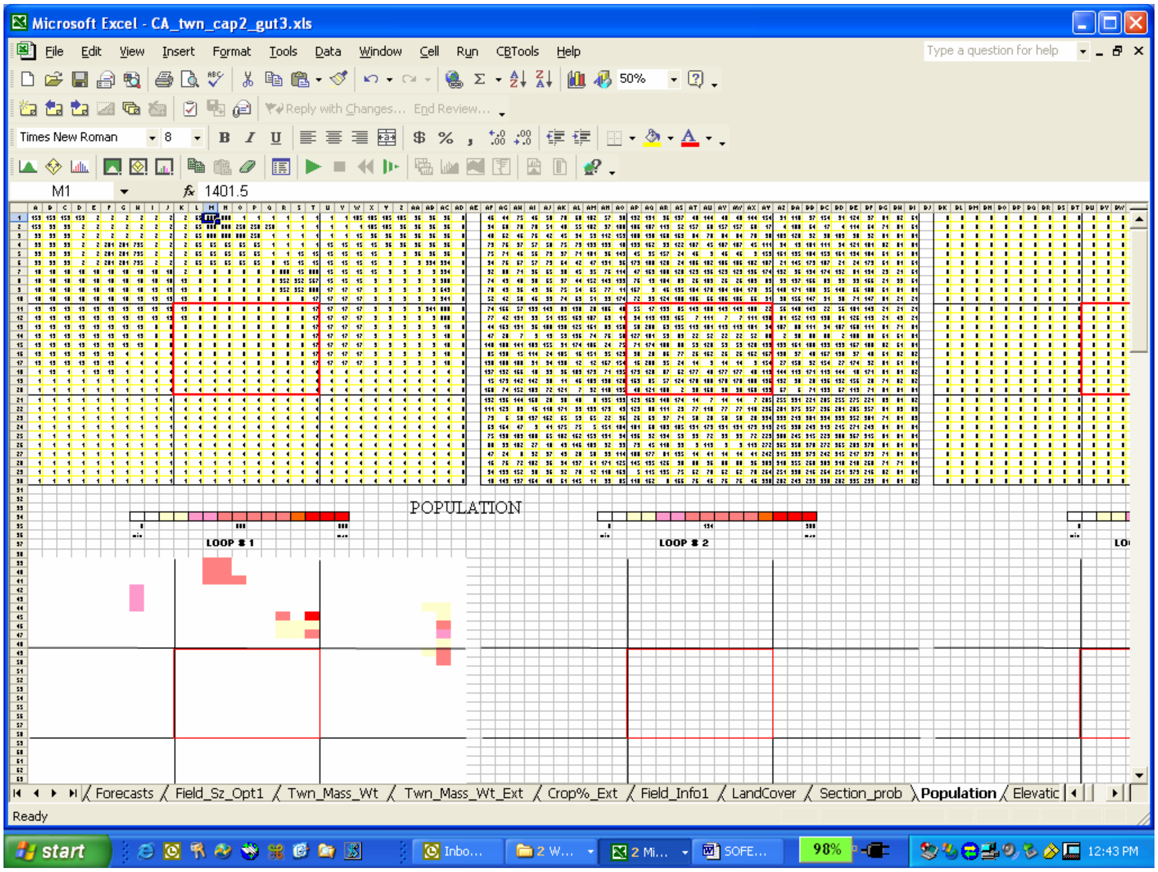


Figure 11. Population Worksheet

11.0 Township Mass Weights

Elevation data can be obtained from the USGS Digital Elevation Models (DEM) and resampled by majority sampling at a lower resolution to match the SOFEA model grid. Elevation data is entered in the “GIS_data” worksheet (Figure 15) and is displayed in the Elevation worksheet as shown in Figure 12 below.

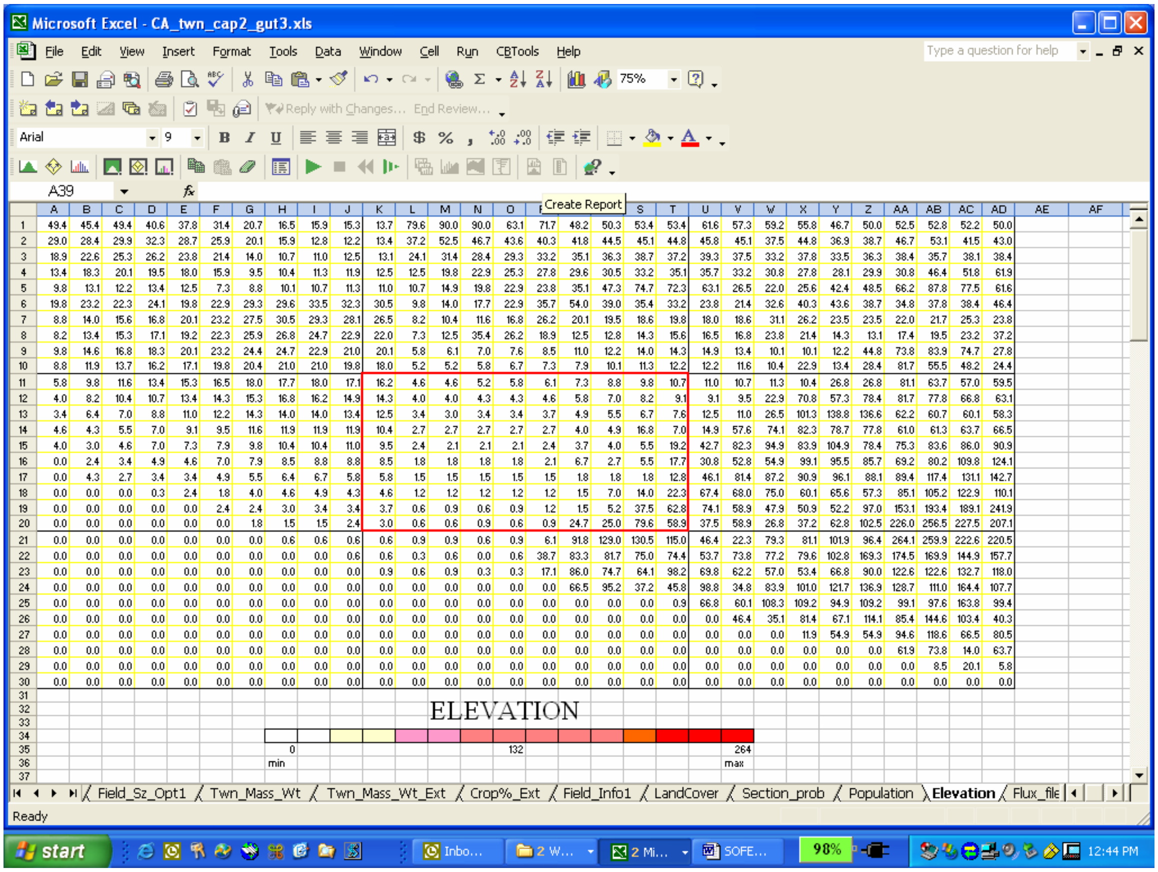


Figure 12. Elevation worksheet

12.0 Fumigant Flux Profiles

The Flux_files worksheet contained the appropriate reference flux files from field experiments or modeling that are used to simulate volatile mass loss from the soil surface after a fumigant application is made.   A flux_files worksheet for 1,3-D drip and shank applications is shown in Figure 13. A sample flux profile for 1,3-D is shown in Appendix 1.

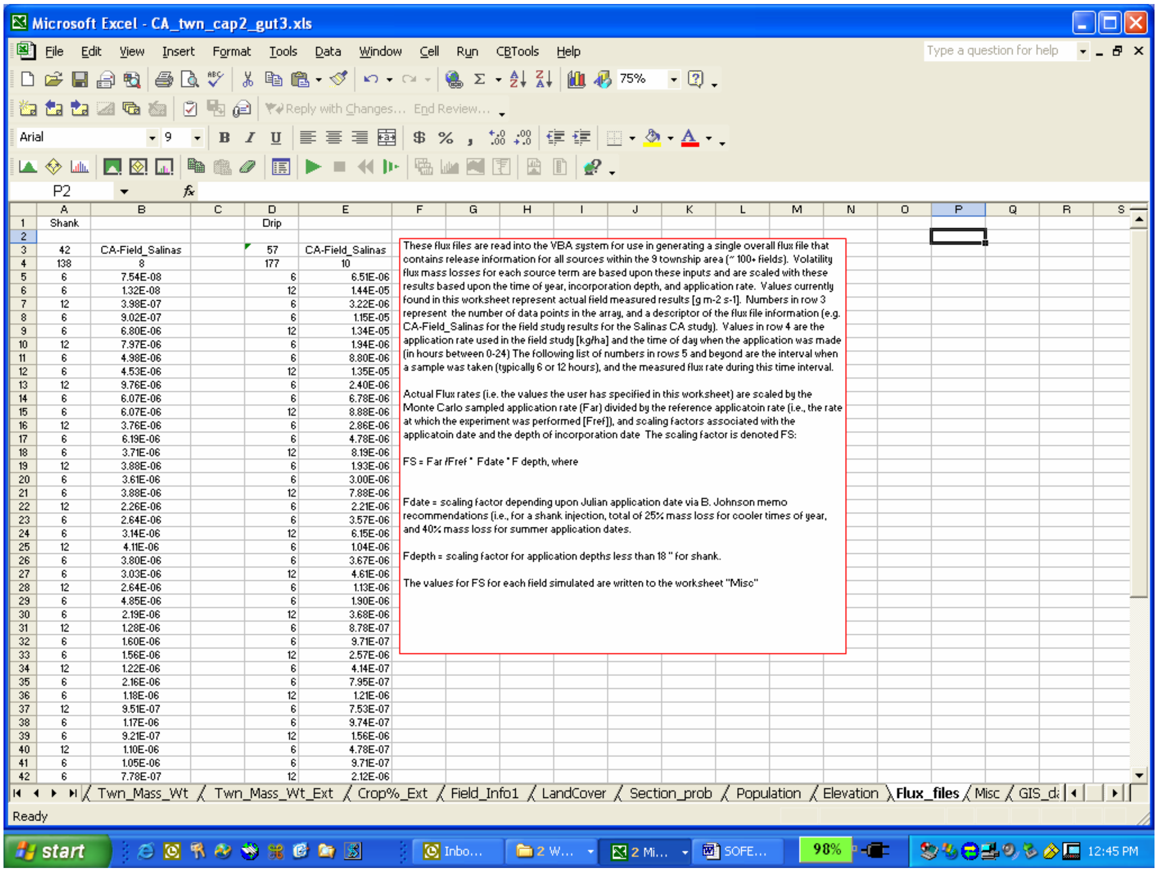


Figure 13. Flux_files Worksheet

These flux files are read into the VBA system for use in generating a single overall flux file that contains release information for all sources within the 9 township area (~ 100+ fields). Volatility flux mass losses for each source term are based upon these inputs and are scaled with these results based upon the time of year, incorporation depth, and application rate. Values currently found in this worksheet represent actual field measured results [g m^{-2} s^{-1}]. Numbers in row 3 represent the number of data points in the array, and a descriptor of the flux file information (e.g. CA-Field_Salinas for the field study results for the Salinas CA study). Values in row 4 are the application rate used in the field study [kg ha^{-1}] and the time of day when the application was made (in hours between 0-24) The following list of numbers in rows 5 and beyond are the interval when a sample was taken (typically 6 or 12 hours), and the measured flux rate during this time interval.

Actual Flux rates (i.e. the values the user has specified in this worksheet) are scaled by the Monte Carlo sampled application rate (F_{ar}) divided by the reference application rate (i.e., the rate at which the experiment was performed [F_{ref}]), and scaling factors associated with the application date and the depth of incorporation date. The scaling factor is denoted FS:

$FS = F_{ar} / F_{ref} * F_{date} * F_{depth}$, where

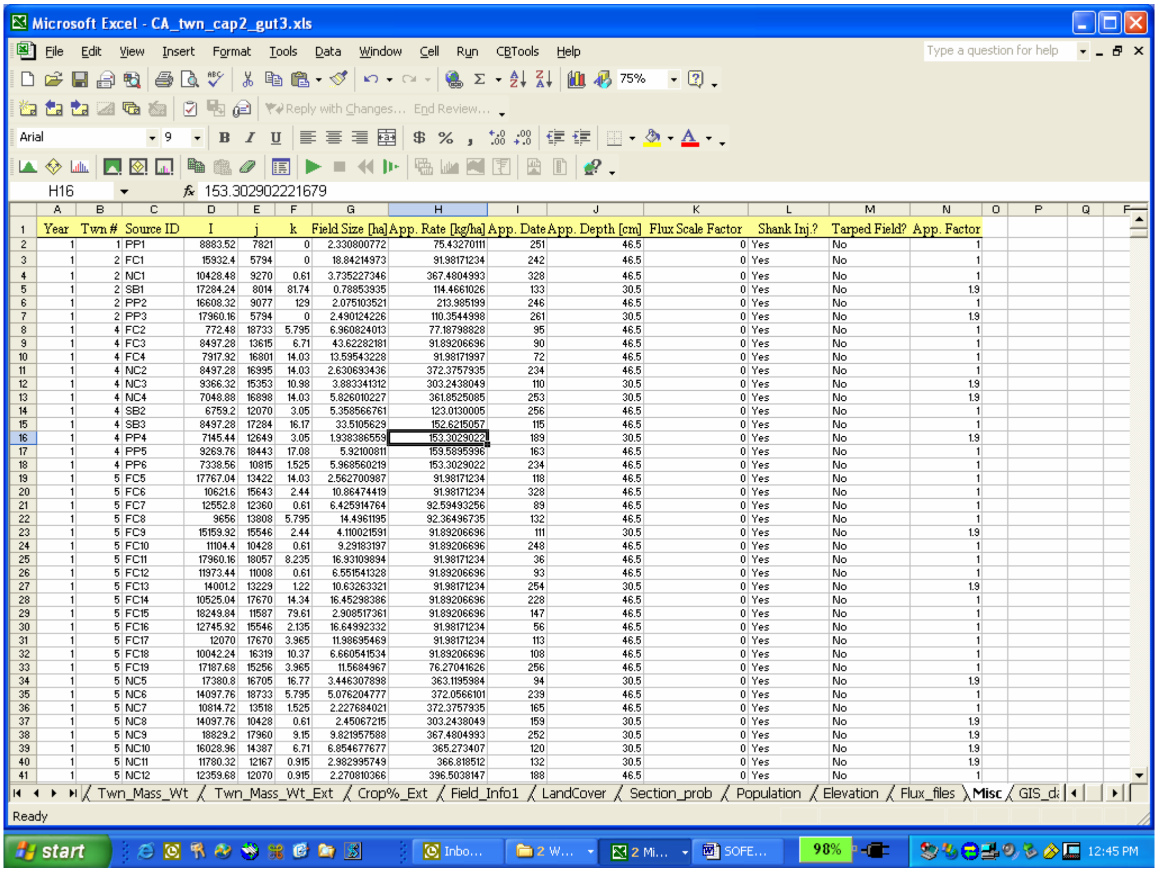
F_{date} = scaling factor depending upon Julian application date via B. Johnson memo recommendations (i.e., for a shank injection, total of 25% mass loss for cooler times of year, and 40% mass loss for summer application dates.

F_{depth} = scaling factor for application depths less than 18 " for shank.

The values for FS for each field simulated are written to the worksheet "Misc"

13.0 Model Generated Agronomic Data

The “Misc” worksheet (Figure 14) contains the Monte Carlo generated field locations, field sizes, application rate, date, and depth, the flux scale factor (FS), the type of application (shank, drip) and the application factor.



Year	Twn #	Source ID	I	j	k	Field Size [ha]	App. Rate [kg/ha]	App. Date	App. Depth [cm]	Flux Scale Factor	Shank Inj.?	Tarped Field?	App. Factor
1	1	PP1	8883.52	7821	0	2.330800772	75.43270111	251	46.5	0	Yes	No	1
1	2	FC1	15932.4	5794	0	18.84214973	91.98171234	242	46.5	0	Yes	No	1
1	2	NC1	10428.48	9270	0.61	3.735227346	367.4804993	328	46.5	0	Yes	No	1
1	2	SB1	17284.24	8014	81.74	0.78853935	114.4661026	133	30.5	0	Yes	No	1.9
1	2	PP2	16608.32	9077	129	2.075103521	213.985199	246	46.5	0	Yes	No	1
1	2	PP3	17960.16	5794	0	2.490124226	110.3544998	261	30.5	0	Yes	No	1.9
1	4	FC2	772.48	18733	5.795	6.960824013	77.18798828	95	46.5	0	Yes	No	1
1	4	FC3	8497.28	13615	6.71	43.62282181	91.89206696	90	46.5	0	Yes	No	1
1	4	FC4	7917.92	16801	14.03	13.59543228	91.98171997	72	46.5	0	Yes	No	1
1	4	NC2	8497.28	16995	14.03	2.630693436	372.3757935	234	46.5	0	Yes	No	1
1	4	NC3	9366.32	15353	10.98	3.883341312	303.2438049	110	30.5	0	Yes	No	1.9
1	4	NC4	7048.88	16898	14.03	5.826010227	361.8525085	253	30.5	0	Yes	No	1.9
1	4	SB2	6759.2	12070	3.05	5.358566761	123.0130005	256	46.5	0	Yes	No	1
1	4	SB3	8497.28	17284	16.17	33.5105629	152.6215057	115	46.5	0	Yes	No	1
1	4	PP4	7145.44	12649	3.05	1.938386559	153.3029022	189	30.5	0	Yes	No	1.9
1	4	PP5	9269.76	18443	17.08	5.92100811	159.5895996	163	46.5	0	Yes	No	1
1	4	PP6	7338.56	10815	1.525	5.968560219	153.3029022	234	46.5	0	Yes	No	1
1	5	FC5	17767.04	13422	14.03	2.562700987	91.98171234	118	46.5	0	Yes	No	1
1	5	FC6	10621.6	15643	2.44	10.86474419	91.98171234	328	46.5	0	Yes	No	1
1	5	FC7	12552.8	12360	0.61	6.425914764	92.59493256	89	46.5	0	Yes	No	1
1	5	FC8	9656	13808	5.795	14.4961195	92.36496735	132	46.5	0	Yes	No	1
1	5	FC9	15159.92	15546	2.44	4.110021591	91.89206696	111	30.5	0	Yes	No	1.9
1	5	FC10	11104.4	10428	0.61	9.29183197	91.89206696	248	46.5	0	Yes	No	1
1	5	FC11	17960.16	18057	8.235	16.93109894	91.98171234	36	46.5	0	Yes	No	1
1	5	FC12	11973.44	11008	0.61	6.551541328	91.89206696	93	46.5	0	Yes	No	1
1	5	FC13	14001.2	13229	1.22	10.63263321	91.98171234	254	30.5	0	Yes	No	1.9
1	5	FC14	10525.04	17670	14.34	16.45298386	91.89206696	228	46.5	0	Yes	No	1
1	5	FC15	18249.84	11587	79.61	2.908517361	91.89206696	147	46.5	0	Yes	No	1
1	5	FC16	12745.92	15546	2.135	16.64992332	91.98171234	56	46.5	0	Yes	No	1
1	5	FC17	12070	17670	3.965	11.98695469	91.98171234	113	46.5	0	Yes	No	1
1	5	FC18	10042.24	16319	10.37	6.660541534	91.89206696	108	46.5	0	Yes	No	1
1	5	FC19	17187.68	15256	3.965	11.5684967	76.27041626	256	46.5	0	Yes	No	1
1	5	NC5	17380.8	16705	16.77	3.446307898	363.1195984	94	30.5	0	Yes	No	1.9
1	5	NC6	14097.76	18733	5.795	5.076204777	372.0566101	239	46.5	0	Yes	No	1
1	5	NC7	10814.72	13518	1.525	2.227684021	372.3757935	165	46.5	0	Yes	No	1
1	5	NC8	14097.76	10428	0.61	2.45067215	303.2438049	159	30.5	0	Yes	No	1.9
1	5	NC9	18829.2	17960	9.15	9.821957588	367.4804993	252	30.5	0	Yes	No	1.9
1	5	NC10	16028.96	14387	6.71	6.854677677	365.273407	120	30.5	0	Yes	No	1.9
1	5	NC11	11780.32	12167	0.915	2.982995749	366.818512	132	30.5	0	Yes	No	1.9
1	5	NC12	12359.68	12070	0.915	2.270810366	396.5038147	188	46.5	0	Yes	No	1

Figure 14. Misc Worksheet

The application factor is unique to the Telone (1,3-D) permit conditions in the state of CA. Application factors were derived in order to conservatively extrapolate mass loss form experiments conducted during cool seasons to warmer seasons and to account for increased flux due to shallower applications. The application factor functionality is probably not required for soil fumigants other than 1,3-D. However, the CDPR application factor can be set to 1.0 (all other soil fumigants) through an appropriate input parameter flag found in the worksheet “PDF_Parameters” (Cell B122, see Chapter 4).

The location for a source term (treated field) is represented by a Cartesian co-ordinate system where i,j represents the Northwest corner of the field, and ‘k’ represents the elevation of the field. The township number, the year of simulation, and the Source ID (ie. Type of crop or crop group) are also contained in this spreadsheet.

14.0 GIS data

Population, elevation and land use data is entered in the GIS-data worksheet shown in Figure 15 below.

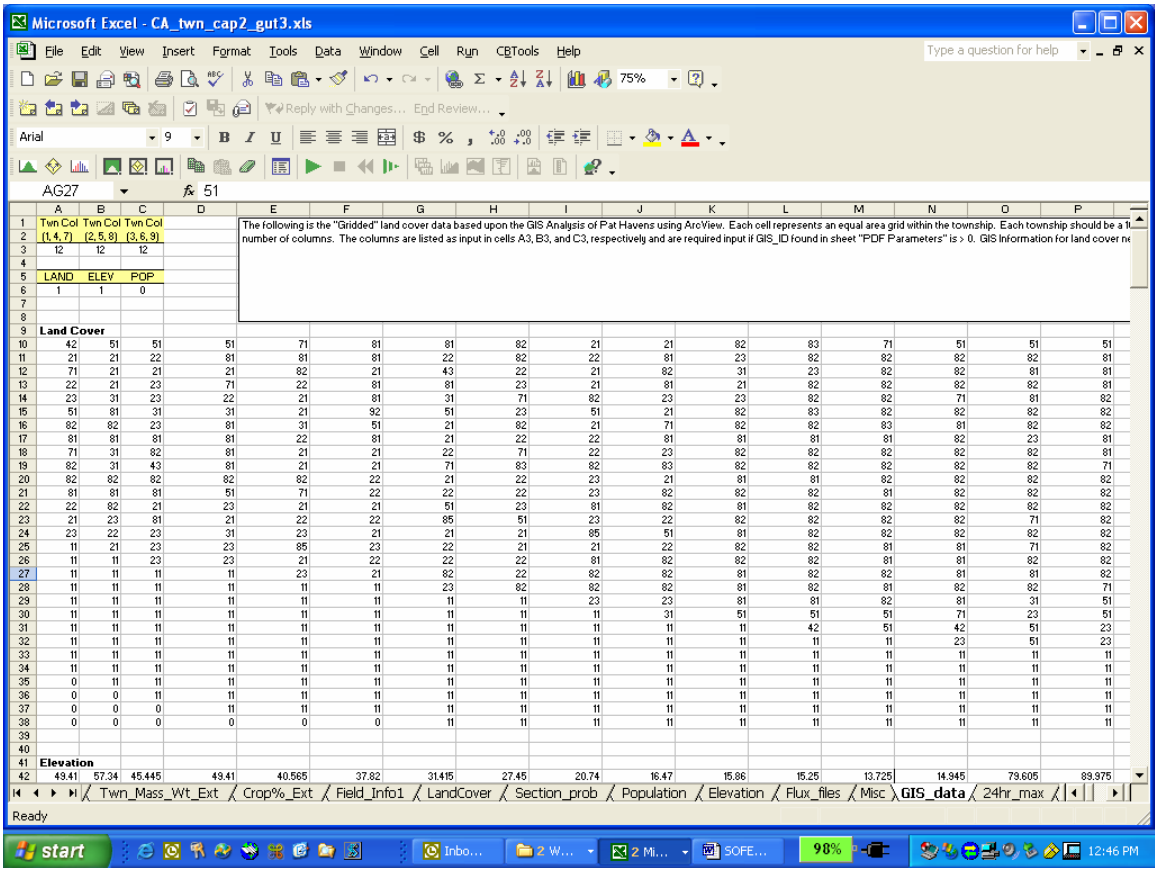


Figure 15. GIS_data Worksheet.

As discussed previously, the data must be resampled to the appropriate grid for use in SOFEA. Each cell represents an equal area grid within the township. Each township should be a 10x10 grid of cells if it were exactly square. However, many CA townships are not exactly square and thus the number of cells in a township may be something like 10x12 (rows x columns), etc. From the analysis of several CA townships, each township is a 10 x *, where townships (1, 4, 7), (2, 5, 8) and (3, 6, 9) all have the same number of columns (*). The columns are listed as input in cells A3, B3, and C3, respectively and are required input if GIS_ID found in sheet "PDF_Parameters" is > 0. GIS Information for land cover needs to start in Row 10, Row 42 for elevation data, and Row 74 for population data. If "PDF_Parameters" is "0", then GIS data is not required.

Table 3. Classification of land cover from the National Land Cover Data (NLCD) database.

Water	
11	Open water
12	Perennial Ice/Snow
Urban	
21	Low Intensity Residential
22	High Intensity Residential
23	Commercial/Industrial/Transportation
85	Urban/Recreational Grasses
Non-ag-land-other-than-Urban	
31	Bare Rock/Sand/Clay
32	Quarries/Strip Mines/Gravel Pits
33	Transitional
91	Woody Wetlands
92	Emergent Herbaceous Wetlands
Land-Assumed-Ag-capable	
41	Deciduous Forest
42	Evergreen Forest
43	Mixed Forest
51	Shrub land
61	Orchards/Vineyards/Other
71	Grasslands/Herbaceous
81	Pasture/Hay
82	Row Crops
83	Small Grains
84	Fallow

15.0 Model Outputs - Air Concentration Distributions

Once SOFEA completes a simulation successfully the following screen is displayed (Figure 16). The dialog box displays the elapsed CPU time in minutes. The user should click OK on this dialog box at which point the output spreadsheet files will update and the data is available for plotting or exporting to another program. It is recommended that the file is saved under another name prior to manipulating the output data. NOTE: When re-opening a SOFEA simulation file that has been renamed, the user should select “Disable Macros” in the dialog box that EXCEL/Crystal Ball displays or the file will not display.

SOFEA will display the “Run_Avg_Twp” worksheet when the run has completed successfully. This worksheet displays the results of the moving average periods (in days) that were specified in the “PDF_Paramaters” worksheet. Other output worksheets are described below.

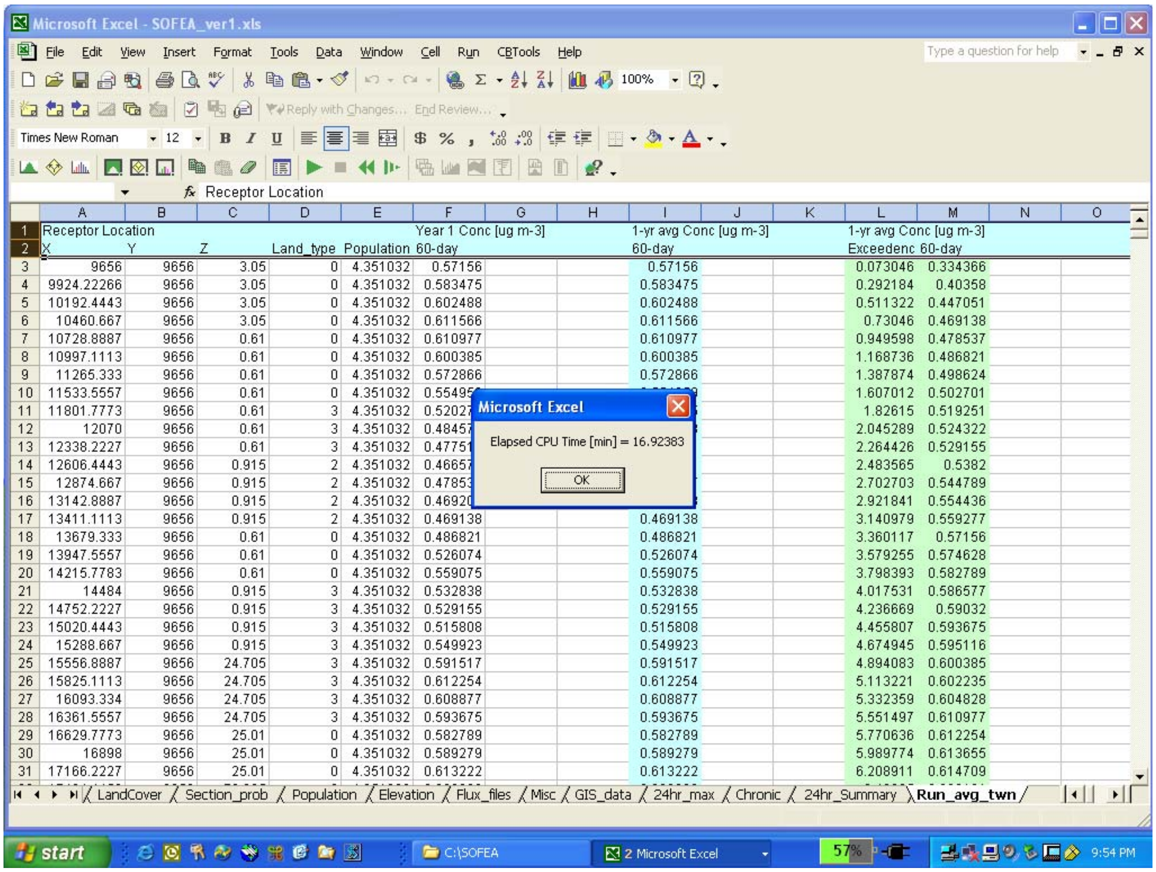
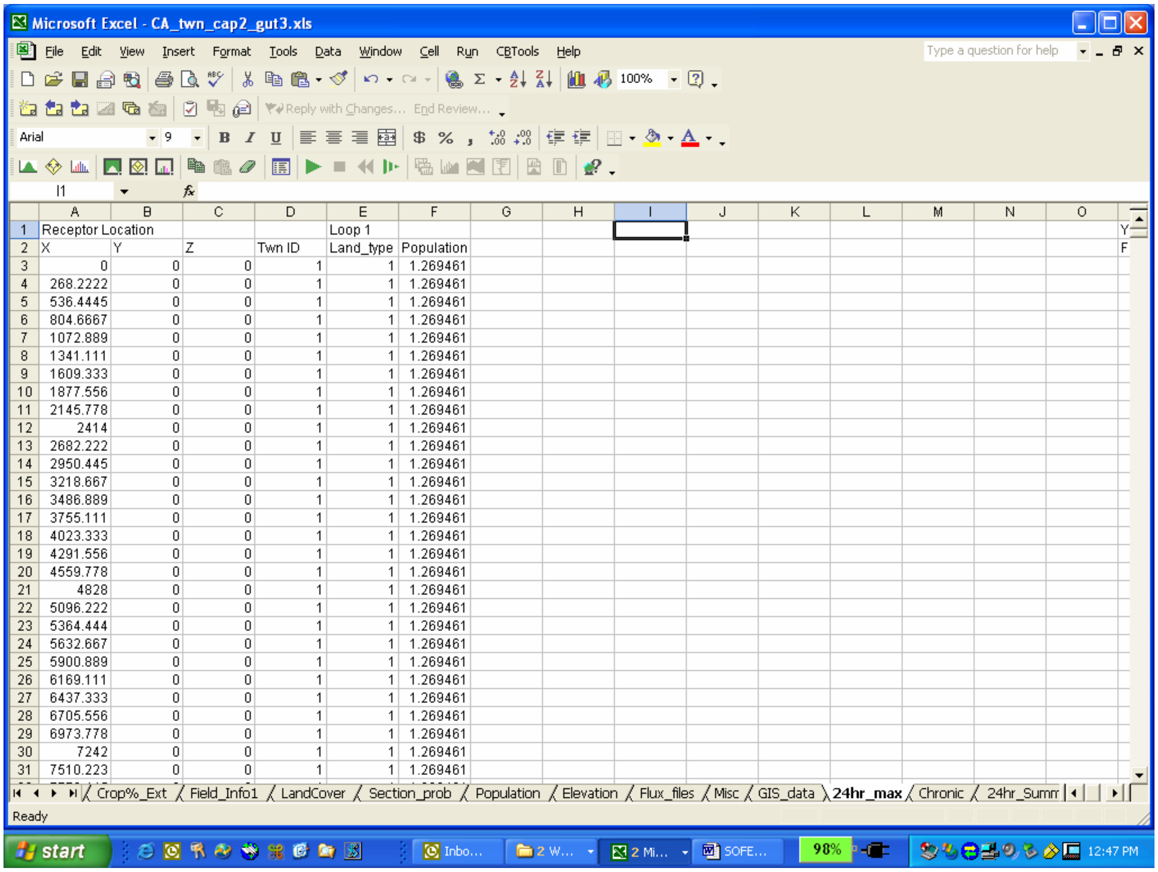


Figure 16. Successful SOFEA run completion screen.

The 24hr_max worksheet (Figure 17 displays the output of the MAXIMUM 24 hour average concentration (ug m^{-3}) observed at each receptor during the entire simulation. Thus, entries for each node/receptor that are summarized in this worksheet may have been obtained at different days throughout the simulation year. The receptor location is given in X,Y,Z co-ordinates (Z is elevation), as well as the township ID (Column D), the land type (Column E), and the population (Column F).



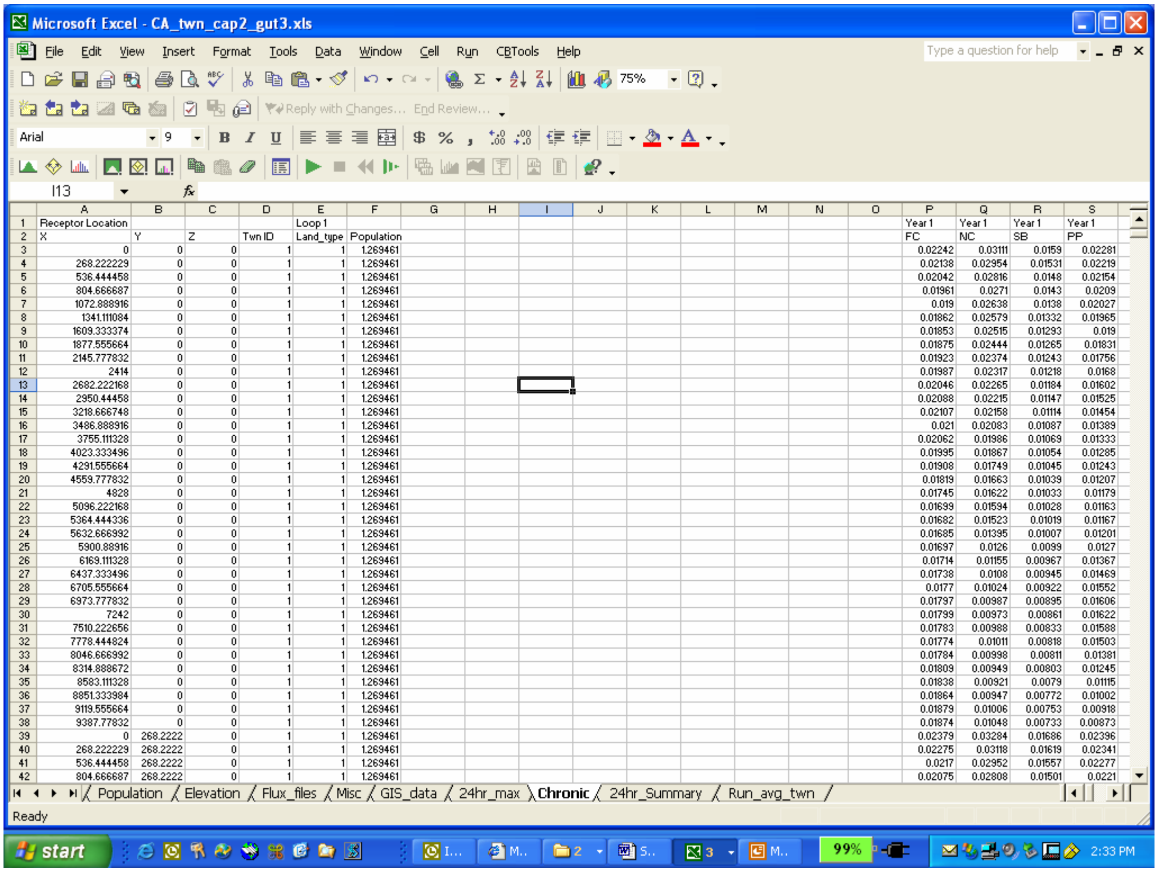
Microsoft Excel - CA_twn_cap2_gut3.xls

	A	B	C	D	E	F
1	Receptor Location				Loop 1	
2	X	Y	Z	Twn ID	Land_type	Population
3	0	0	0	1	1	1.269461
4	268.2222	0	0	1	1	1.269461
5	536.4445	0	0	1	1	1.269461
6	804.6667	0	0	1	1	1.269461
7	1072.889	0	0	1	1	1.269461
8	1341.111	0	0	1	1	1.269461
9	1609.333	0	0	1	1	1.269461
10	1877.556	0	0	1	1	1.269461
11	2145.778	0	0	1	1	1.269461
12	2414	0	0	1	1	1.269461
13	2682.222	0	0	1	1	1.269461
14	2950.445	0	0	1	1	1.269461
15	3218.667	0	0	1	1	1.269461
16	3486.889	0	0	1	1	1.269461
17	3755.111	0	0	1	1	1.269461
18	4023.333	0	0	1	1	1.269461
19	4291.556	0	0	1	1	1.269461
20	4559.778	0	0	1	1	1.269461
21	4828	0	0	1	1	1.269461
22	5096.222	0	0	1	1	1.269461
23	5364.444	0	0	1	1	1.269461
24	5632.667	0	0	1	1	1.269461
25	5900.889	0	0	1	1	1.269461
26	6169.111	0	0	1	1	1.269461
27	6437.333	0	0	1	1	1.269461
28	6705.556	0	0	1	1	1.269461
29	6973.778	0	0	1	1	1.269461
30	7242	0	0	1	1	1.269461
31	7510.223	0	0	1	1	1.269461

Crop%_Ext / Field_Info1 / LandCover / Section_prob / Population / Elevation / Flux_files / Misc / GIS_data / 24hr_max / Chronic / 24hr_Sumr

Figure 17 24hr_max Worksheet

Annual average air concentrations are shown in the chronic worksheet (Figure 18. This worksheet displays the annual average concentrations (ug m^{-3}) for each receptor location (given by X,Y,Z co-ordinates). Contributions from each crop type for each year of simulation are summarized, followed by the overall concentration probability distribution. The location of the final annual average concentration PDF is located at the far right hand side of the spreadsheet, thus, depending on the number of years simulated the user may have to scroll over in order to view the distribution.
Figure 19 shows a comparison of the fumigant concentration in air for all 11,664 receptors contained within the 9 township air shed in Ventura, CA, and for the 1296 receptors within the center township (01N 21W) only. Percentiles of these air concentration distributions can be used for risk assessment. Figures are not generated automatically by the program at this time.



	A	B	C	D	E	F	P	Q	R	S
1	Receptor Location				Loop 1		Year 1	Year 1	Year 1	Year 1
2	X	Y	Z	Twn ID	Land_type	Population	FC	NC	SB	PP
3	0	0	0	1	1	1.269461	0.02242	0.03111	0.0159	0.02281
4	268.222229	0	0	1	1	1.269461	0.02138	0.02954	0.01531	0.02219
5	536.444458	0	0	1	1	1.269461	0.02042	0.02816	0.0148	0.02154
6	804.666687	0	0	1	1	1.269461	0.01961	0.0271	0.0143	0.0209
7	1072.888916	0	0	1	1	1.269461	0.019	0.02638	0.0138	0.02027
8	1341.111084	0	0	1	1	1.269461	0.01862	0.02579	0.01332	0.01965
9	1609.333374	0	0	1	1	1.269461	0.01853	0.02515	0.01293	0.019
10	1877.555664	0	0	1	1	1.269461	0.01875	0.02444	0.01265	0.01831
11	2145.777832	0	0	1	1	1.269461	0.01923	0.02374	0.01243	0.01756
12	2414	0	0	1	1	1.269461	0.01987	0.02317	0.01218	0.0168
13	2682.222168	0	0	1	1	1.269461	0.02046	0.02265	0.01184	0.01602
14	2950.44458	0	0	1	1	1.269461	0.02088	0.02215	0.01147	0.01525
15	3218.666748	0	0	1	1	1.269461	0.02107	0.02158	0.01114	0.01454
16	3486.888916	0	0	1	1	1.269461	0.021	0.02083	0.01087	0.01389
17	3755.111328	0	0	1	1	1.269461	0.02062	0.01986	0.01069	0.01333
18	4023.333496	0	0	1	1	1.269461	0.01995	0.01867	0.01054	0.01285
19	4291.555664	0	0	1	1	1.269461	0.01908	0.01749	0.01045	0.01243
20	4559.777832	0	0	1	1	1.269461	0.01819	0.01663	0.01039	0.01207
21	4828	0	0	1	1	1.269461	0.01745	0.01622	0.01033	0.01179
22	5096.222168	0	0	1	1	1.269461	0.01699	0.01594	0.01028	0.01163
23	5364.444336	0	0	1	1	1.269461	0.01682	0.01523	0.01019	0.01167
24	5632.666992	0	0	1	1	1.269461	0.01685	0.01395	0.01007	0.01201
25	5900.88916	0	0	1	1	1.269461	0.01697	0.0126	0.0099	0.0127
26	6169.111328	0	0	1	1	1.269461	0.01714	0.01155	0.00967	0.01367
27	6437.333496	0	0	1	1	1.269461	0.01738	0.0108	0.00945	0.01469
28	6705.555664	0	0	1	1	1.269461	0.0177	0.01024	0.00922	0.01552
29	6973.777832	0	0	1	1	1.269461	0.01797	0.00987	0.00895	0.01606
30	7242	0	0	1	1	1.269461	0.01799	0.00973	0.00861	0.01622
31	7510.222656	0	0	1	1	1.269461	0.01783	0.00988	0.00833	0.01588
32	7778.444824	0	0	1	1	1.269461	0.01774	0.01011	0.00818	0.01503
33	8046.666992	0	0	1	1	1.269461	0.01784	0.00998	0.00811	0.01381
34	8314.888672	0	0	1	1	1.269461	0.01809	0.00949	0.00803	0.01245
35	8583.111328	0	0	1	1	1.269461	0.01838	0.00921	0.0079	0.01115
36	8851.333984	0	0	1	1	1.269461	0.01864	0.00947	0.00772	0.01002
37	9119.555664	0	0	1	1	1.269461	0.01879	0.01006	0.00753	0.00918
38	9387.77832	0	0	1	1	1.269461	0.01874	0.01048	0.00733	0.00873
39	0	268.2222	0	1	1	1.269461	0.02379	0.03284	0.01686	0.02396
40	268.222229	268.2222	0	1	1	1.269461	0.02275	0.03118	0.01619	0.02341
41	536.444458	268.2222	0	1	1	1.269461	0.0217	0.02952	0.01557	0.02277
42	804.666687	268.2222	0	1	1	1.269461	0.02075	0.02808	0.01501	0.0221

Figure 18. Chronic Worksheet

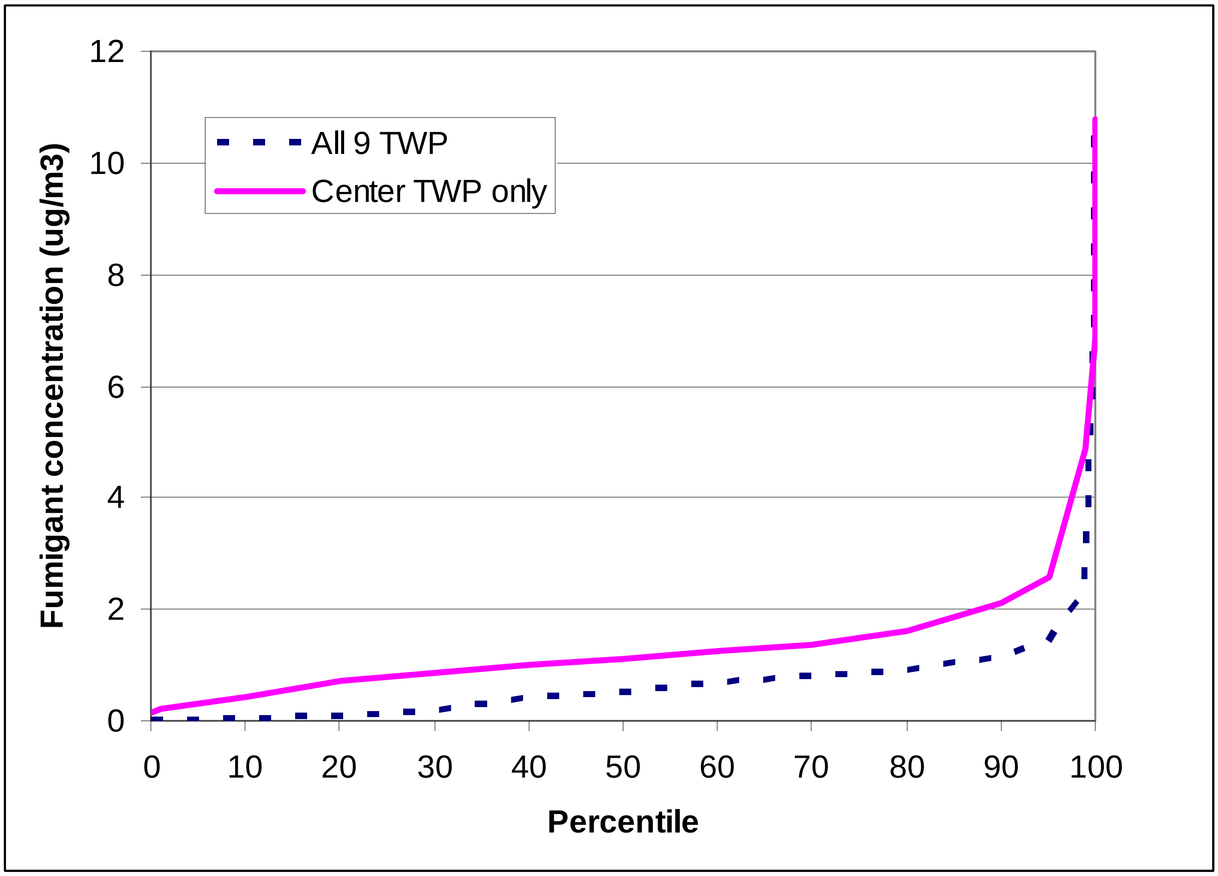


Figure 18. Comparison of fumigant concentrations for 9-township air shed (11,664 receptors), and center township only (1296 receptors) for Ventura County township(01N 21W), CA..

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APPENDIX 1. SOFEA Installation Guide.

SOFEA System Requirements.

SOFEA is a Microsoft Excel worksheet that incorporates VBA macros as the programming language. Thus, an up to date version of MS Excel is required. SOFEA runs the most consistently on PCs having large amounts of RAM (> 1 Gb). SOFEA can run on PC's having less memory than this optimal, but the user may be limited to smaller air sheds, receptor density, source term density, and years of simulation to avoid exceeding memory constraints. CPU time can be excessive for non-optimal PCs. SOFEA has been successfully run under Windows™ XP and Windows™ 2000. It will probably run on earlier versions of Windows, but the user may have to export the macro modules as Basic files (*.bas), and import them back into MS Excel if earlier versions of Windows and Excel are used. In addition, the 3rd party software Crystal Ball 2000 Pro (Trademark of Decisioneering Inc.; www.decisioneering.com) is a mandatory requirement for SOFEA and is used as the stochastic intermediate component for generating probability density functions (see Users Guide for details).

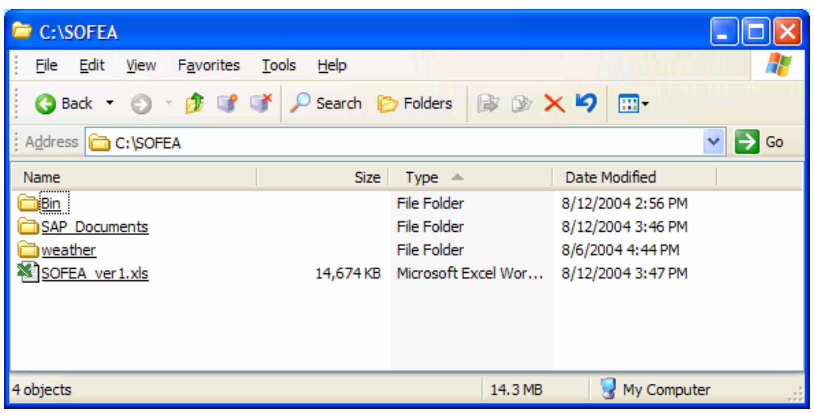
SOFEA offers the potential to link GIS data such as population density, elevation, and land cover to regional simulations. Thus, software such as ArcView (Tradmark of ESRI, Inc.) may prove beneficial. GIS data is not a necessity to run SOFEA as default values can be used or coarse descriptors of GIS information can be input directly into SOFEA without the need of GIS software or GIS expertise.

Installing SOFEA on a PC.

The software will have to be unzipped if downloaded from the Internet. The following installation instructions assume files have been unzipped. To install SOFEA, the user need only install the folder "SOFEA" to their hard drive. This folder can be installed in any directory on a host machine, but for demonstration purposes, the SOFEA folder is installed to the C: drive. If another location is selected, then the user will have to modify the path for the weather file library folder as found in the first worksheet of the SOFEA model.

The content of the SOFEA folder and folder paths is illustrated in Figure 1. Here, the SOFEA folder was copied directly to the C: drive. The model is called "SOFEA_ver1.xls" and is found in the SOFEA directory. Subdirectories under SOFEA include "Bin", "SAP_Documents", and "weather". The "Bin" directory contains all the executables that include the modified version of ISCST3 (ISCST3r) and the optimization program (OPT2). It is in this directory where all ISCST3 input and output files are written. Thus, if a simulation does crash, the user should first look at the ISCST3 error generation messages found in the file called "ISCST3.out" that is located in the Bin directory. The subdirectory "SAP_Documents" contains electronic versions of the Users and Programmers guide, and a concise methodology document that is in preparation for publication submission (8/04). The last subdirectory "weather" contains a library of ISCST3 annual weather files for use in stochastic simulations of SOFEA. The user will have to place all weather files that will be used with SOFEA in the "weather" subdirectory. Example meteorological files for a variety of California areas are provided. In addition, meteorological files specific for ISCST3 for the United States can be found at the SCRAM website of USPEA (http://www.epa.gov/ttn/scram/).

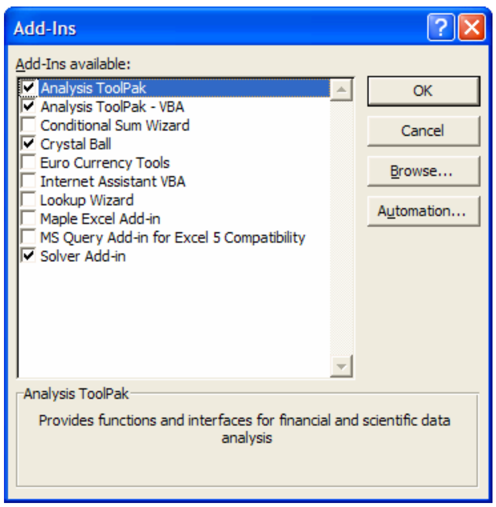
To summarize the directory file system, the subdirectories "Bin" and "weather' must be immediately below the directory where the SOFEA model resides (SOFEA_ver1.xls). This file structure is intact if the user copies the SOFEA folder without making any modifications.



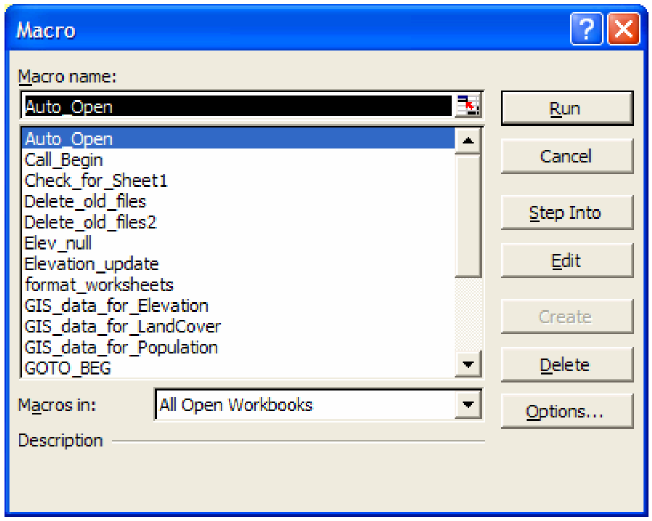
Once the SOFEA folder has been installed, the model is ready to run (or modify inputs and then execute) simply by opening up the MS Excel file called "SOFEA_ver1.xls" (assuming Crystal Ball has been successfully installed).

Crystal Ball Installation

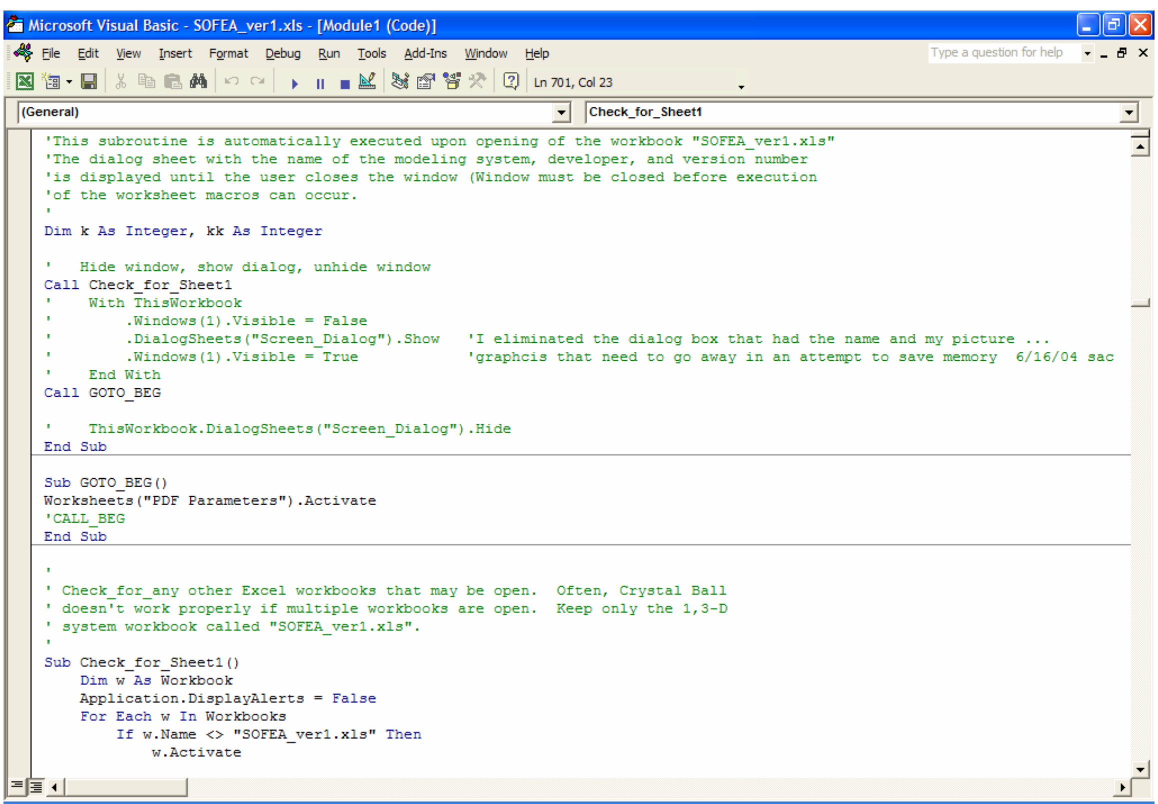
The user will need to follow the Crystal Ball instructions for successful installation of Crystal Ball. However, the user will have the choice of opening up Crystal Ball every time MS Excel is opened (or not). If Crystal Ball is installed, but does not open with Excel, the user can do a search from Explorer, looking for the file called "CB.XLA". Double clicking on this icon will open up Crystal Ball. In addition, the user needs to make sure that MS Excel is linked to the Crystal Ball Libraries. This may only be necessary the first time SOFEA is executed. For proper library linkage, under Excel, the user would select Tools>Add-ins … and the following (or similar) dialog box will appear. Make sure Crystal Ball has been selected.



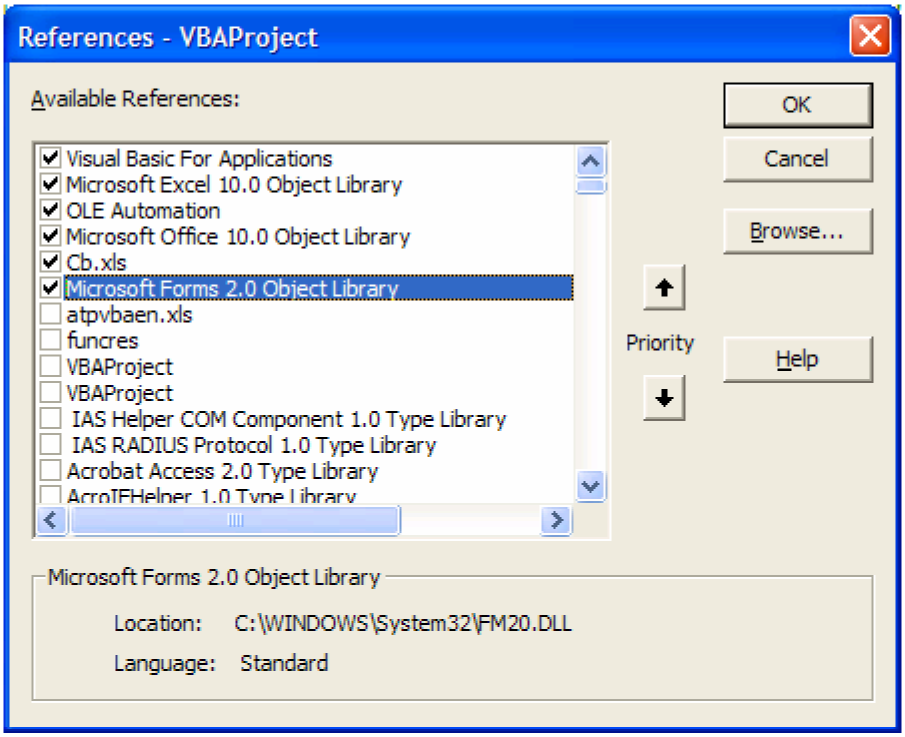
In addition, the user will need to properly verify that the Crystal Ball libraries are linked with the VBA code. This is accomplished via Tools>Macros>Macros …of Excel. The following Dialog box (or something very similar will appear).



This dialog box lists all of the macros for the SOFEA model. Select any macro by highlighting it (it doesn't matter which one) and then select the "Edit" button. Be careful not to inadvertently deleted or modify any VBA code once you're in the edit mode. For example, if "Auto_Open" macro is selected for editing from the above dialog box, the user will get the following via the VBA editor of MS Excel.



From this VBA editor, select “Tools>References…” and the following dialog box will appear.



Again make sure Cb.xls has been selected. If not, make the selection and exit via the “O.K. button”. Once complete, the user can exit the VBA editor via the upper right window button “X” which will return you to the MS Excel worksheet for SOFEA. The user should now be ready to begin a simulation and should not have to repeat these steps again for properly liking Excel to the Crystal Ball libraries.

APPENDIX 2. Examples of Crystal Ball PDFs for agronomic properties.

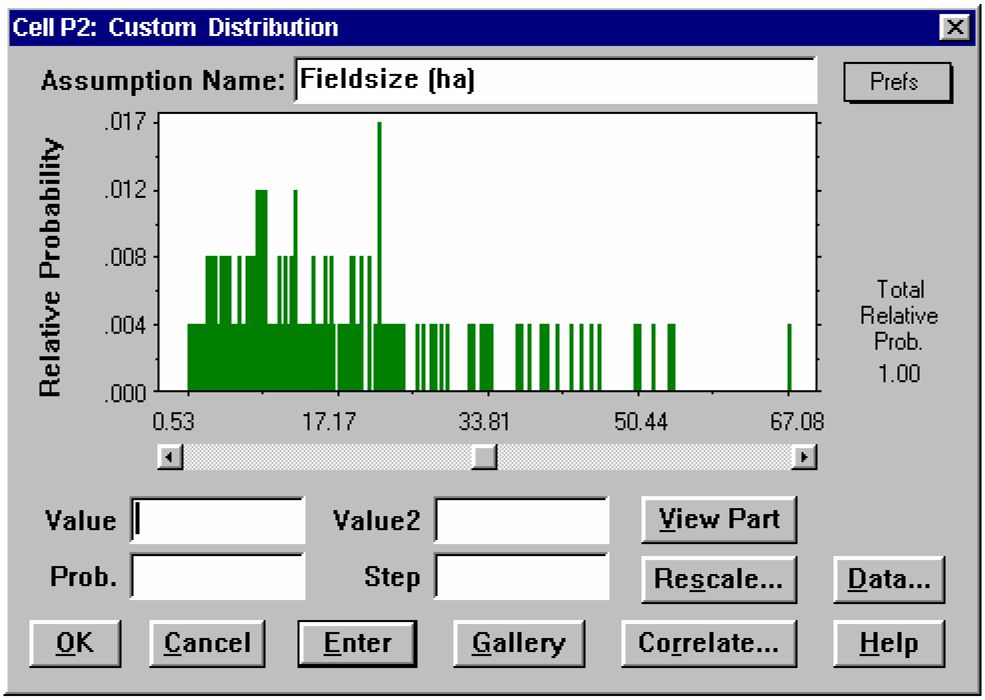


Figure A2.1. Screen shot of Field size distribution used in Merced township cap model run. Taken from CDMS data for 1999-2001.

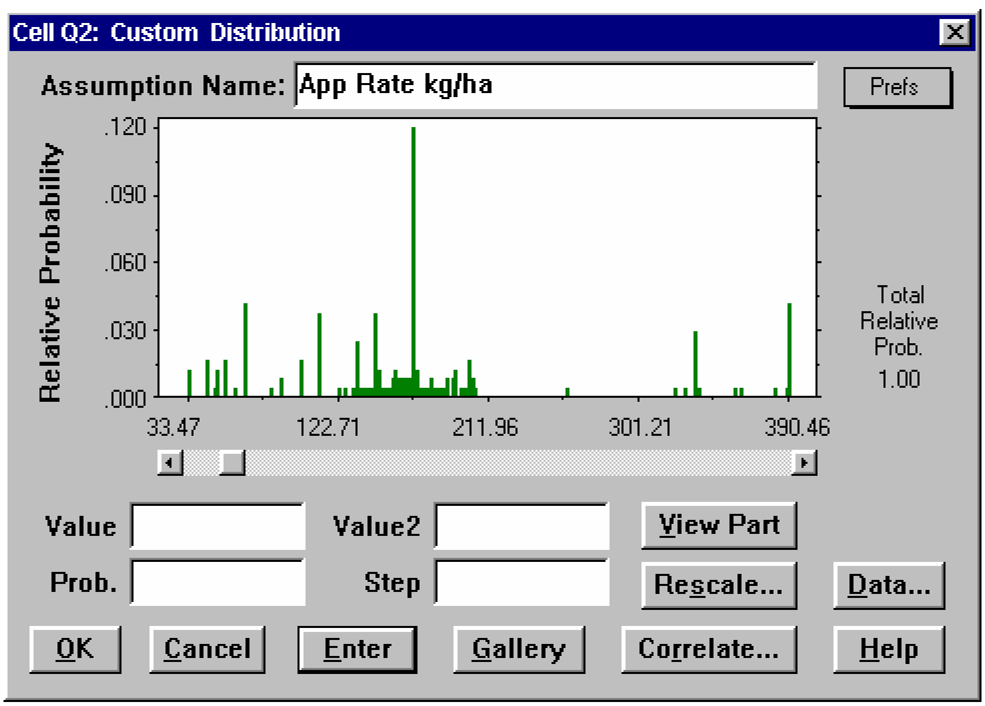


Figure A2.2. Screen shot of Application rate distribution used in Merced township cap model run. Taken from CDMS data for 1999-2001.

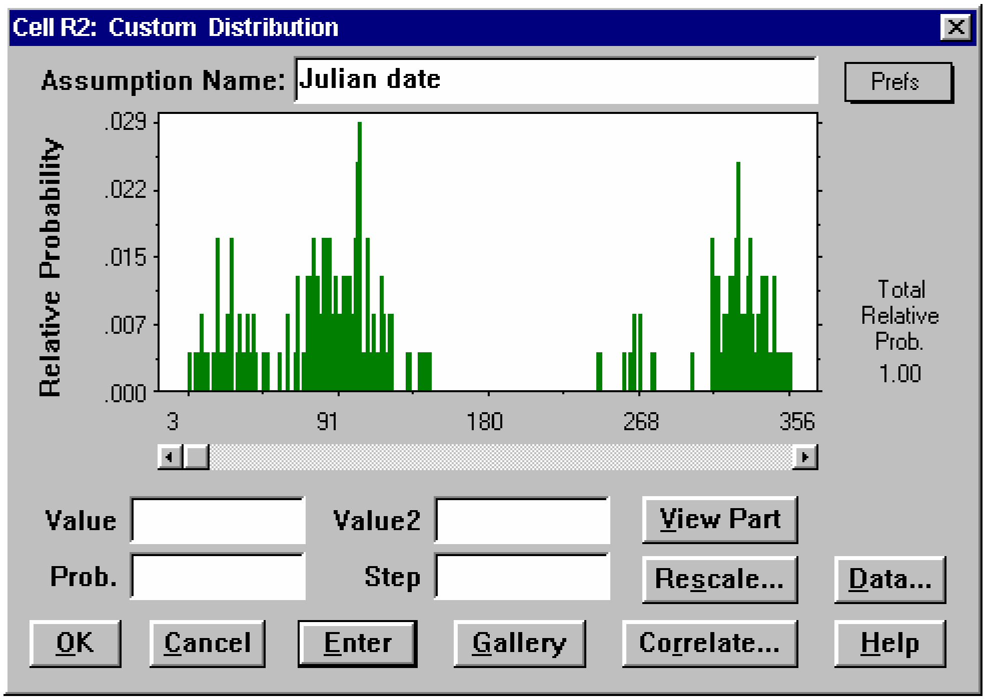


Figure A2.3. Screen shot of Application Date (Julian date) distribution used in Merced township cap model run. Taken from CDMS data for 1999-2001.

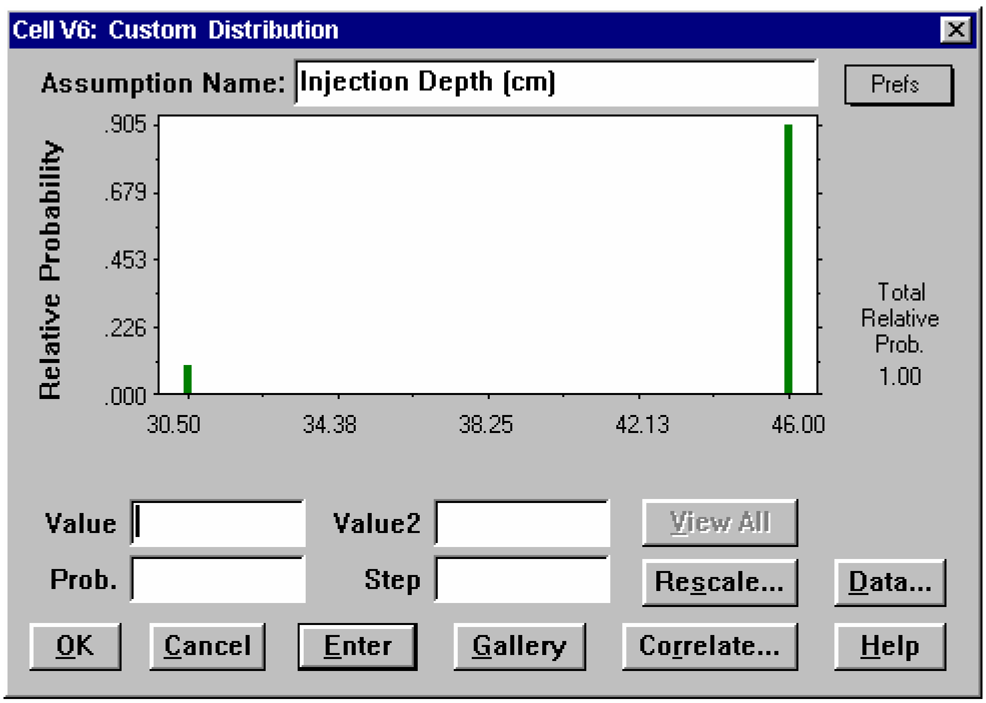
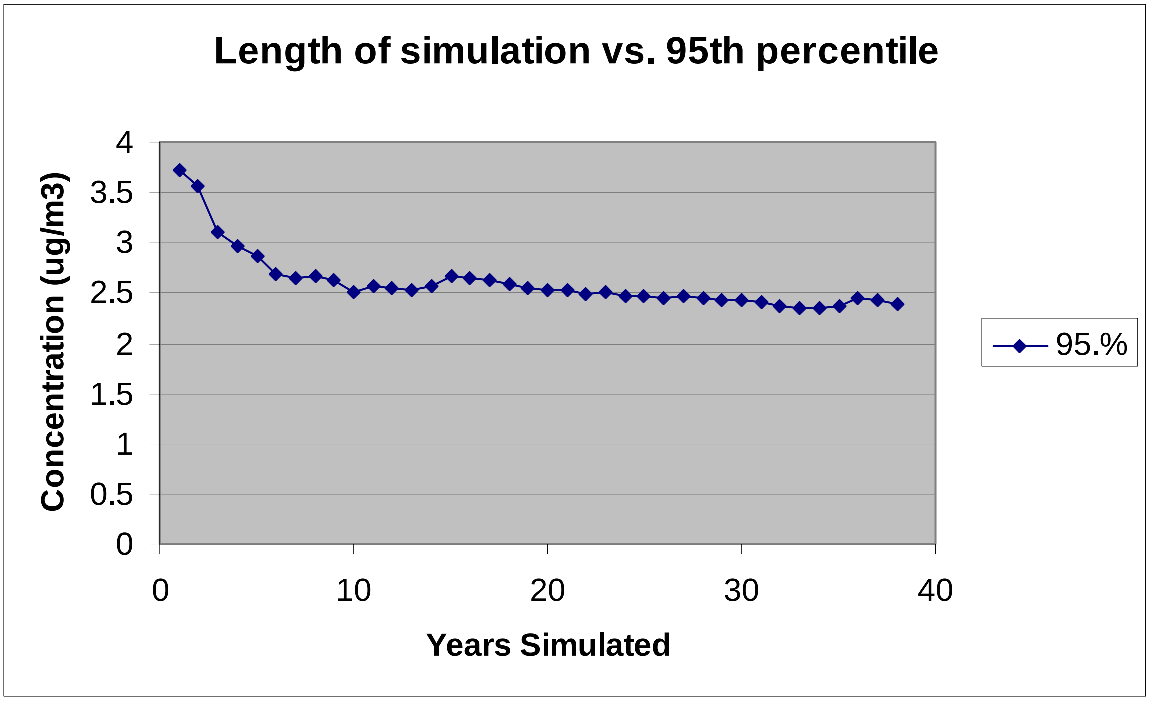
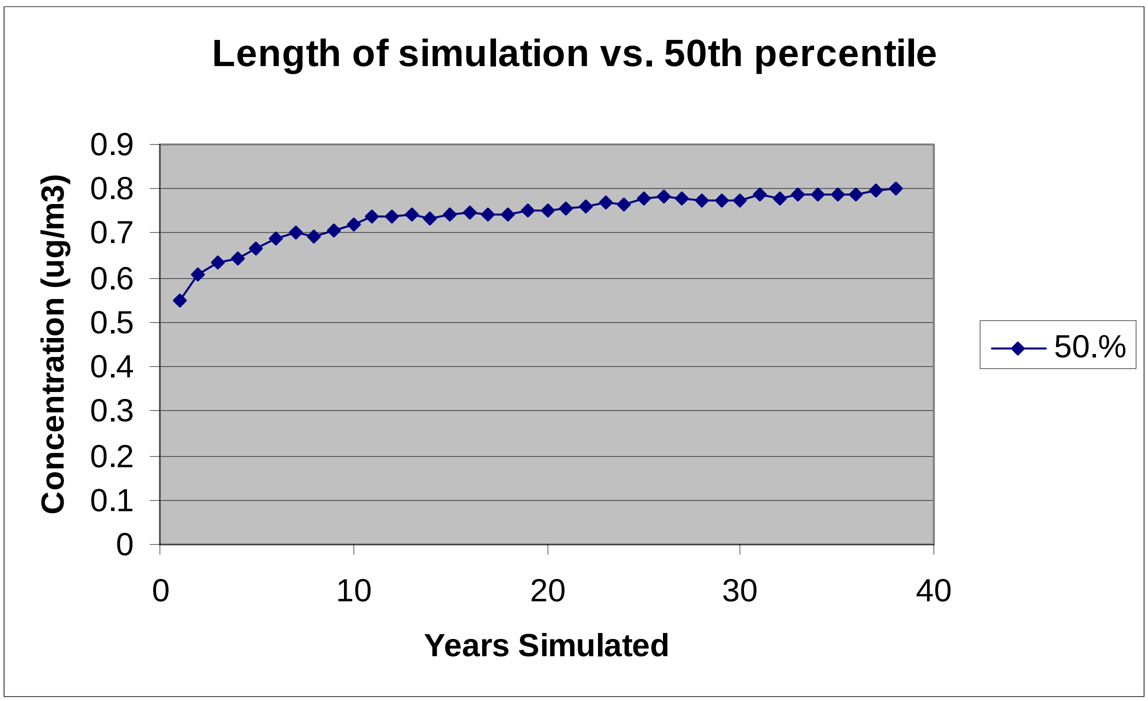


Figure A2.4. Screen shot of Application Depth distribution used in Merced township cap model run. Taken from CDMS data for 1999-2001.

APPENDIX 3. Effect of simulation length on 50th and 95th percentile air concentrations.

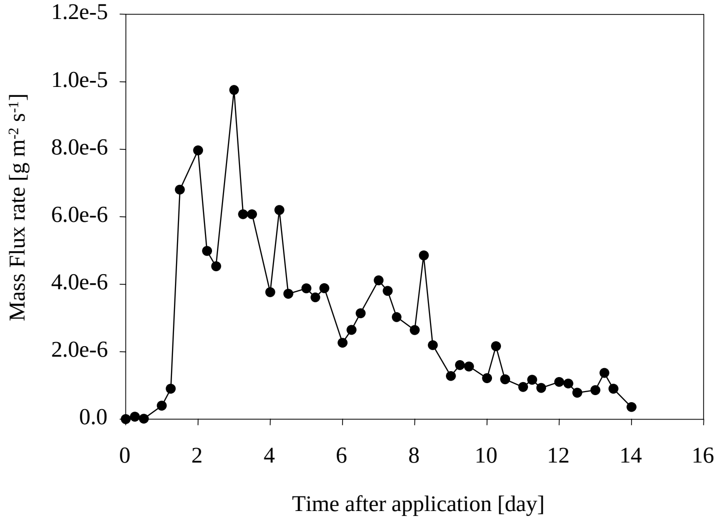
Figure A3.1 Example of 50th and 95th percentile concentrations as a function of simulation time (years).





APPENDIX 4. Example fumigant mass flux profile..

Figure A4.1. Example of field observations of transient volatility losses of 1,3-D for shank injection application (rates of 122 lbs 1,3-D per acre).



APPENDIX 5. Population Based Exposure/Risk Assessment

Population based risk assessments can now be performed using SOFEA since urban areas, population densities, spatial locations for treated fields, and air concentrations are known *a priori* (or simulated). Output worksheets of SOFEA list the spatial location for each receptor (x, y, z), the land cover type, and the population density. Thus, the user has everything required to perform a population based risk assessment. For example, it may be possible that the highest simulated air concentrations occur in the least populated areas. The converse of this could also be true. Thus, receptor air concentrations can be weighted by population densities to deduce the actual risk to the overall population, and not necessarily the worst-case risk to an individual always downwind from a nearby treated source their entire life (both assessments can be made).

Figures A5.1-A5.2 represent contour plots that make use of the spatial locations for source terms, population areas, and application rates. The field northwest corner (x,y), field size, and application rate are found in the summary worksheet “misc”. It is a simple process to use graphics or GIS software to generate contour plots to visualize where high air concentrations reside and the proximity to high population densities regions (i.e., urban areas). Qualitative figures such as A5.1-A5.2 can be quantified since population densities are known for each receptor location assuming this GIS information is available.

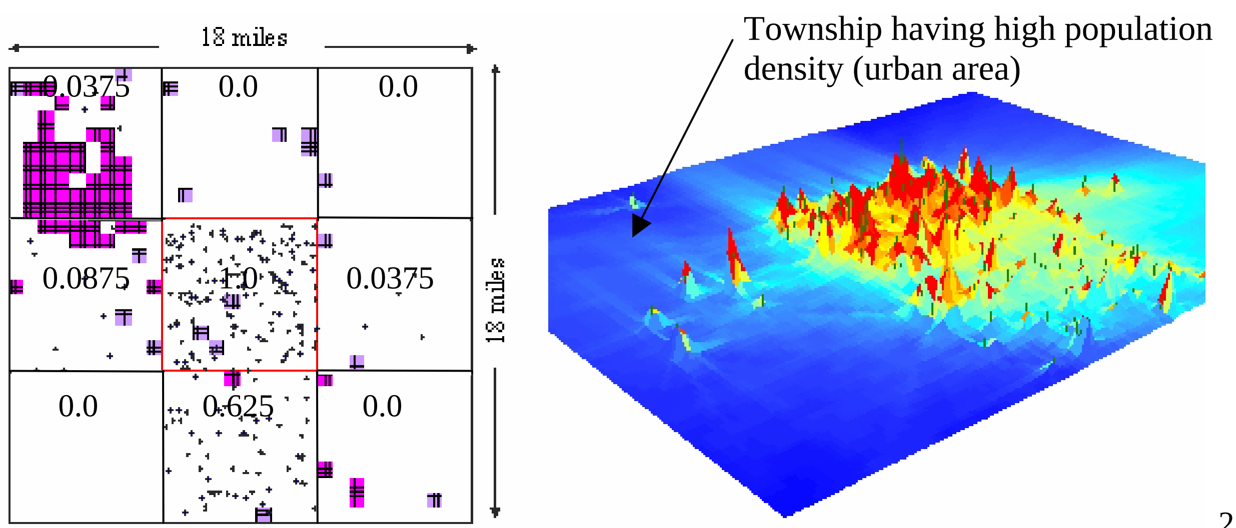


Figure A5.1. Air concentration results for Monterey Township 15S04E and surrounding townships represented as a 3-D mesh plot with exaggerated z-axes. Graphic on left indicates population regions (hatch marks), adjusted township mass per township, and areas where source terms (crosses) were placed in the 3x3 township simulation domain.

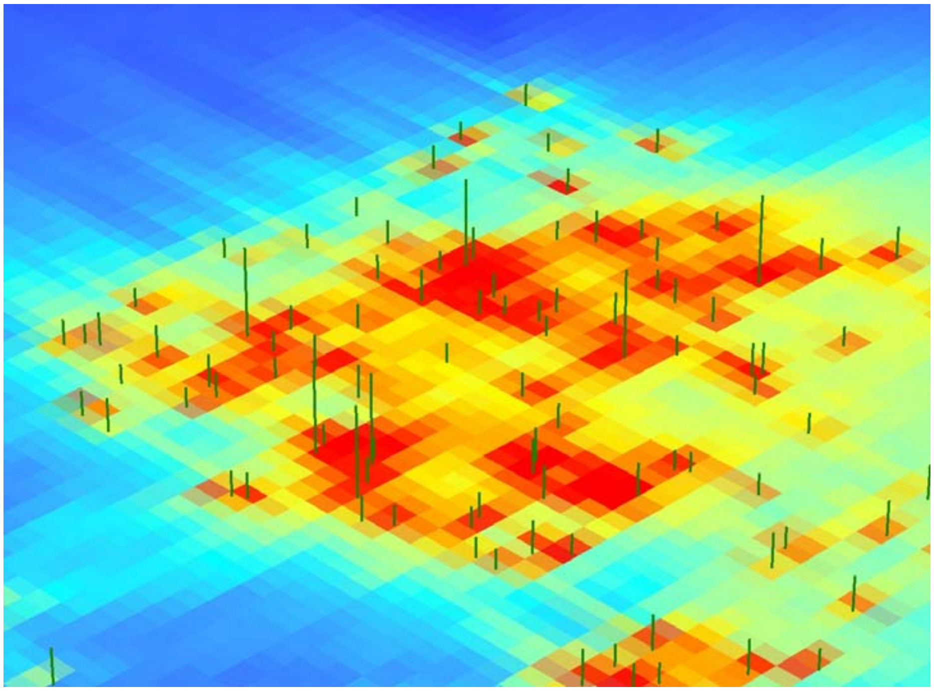


Figure A5.2. Enlargement of air concentration results found in Figure 4.1 represented as a discrete contour plot (no smoothing). Green columns indicate the nouthwest corner for randomly placed source terms, with the column height indicative of the magnitude of soil fumigant mass applied to the field.

APPENDIX 6. Crystal Ball ™ SOFEA Tutorial

Figure A6.1 illustrates the Crystal Ball menu that is added to the MS Excel menu when Crystal Ball is evoked. The circled entries are for the most commonly used functions. For the DAS model (Gamma version), only the first two functions are commonly used, as the run preferences and start simulation buttons are defined and called from the code.

A cell in MS Excel is single valued unless this cell has been defined as an “Assumption” (i.e., a Probability Density Function). For example, Figure A6.2 outlines the procedure for defining a PDF via Crystal Ball (CB). Cell B1 has a single value entry. Highlight Cell B1 and then click on the CB “Define Assumption” button. This will pull up a new window that shows the CB “Distribution Gallery”. The user will highlight a PDF from the gallery and either double click or select “OK”. A new window pops up defining this distribution. For this example, a normal distribution was selected. It is here where the user can make changes in the parameters that define the distribution (for a normal distribution, these are the mean and standard deviation). For this example, it is assumed the mean is 500 with a standard deviation of 25 (Figure A6.3). Once a PDF is assigned then the default color for this cell used by CB is green (Figure A6.4). It should be pointed out that multiple cells can be assigned unique PDFs. There is an upper limit to the total number of PDFs that can be assigned by Crystal Ball, but the DAS soil fumigation model is well under the limit (seem to recollect that 500 assumptions and forcasts can be specified).

Now, the simulation can be initiated by the “start simulation” button. The user defined PDF will be sampled via the user specified descriptions found in the “Run Preferences” function. It is under the “Run Preferences” function where the number of times the PDF is to be sampled, etc. can be specified.

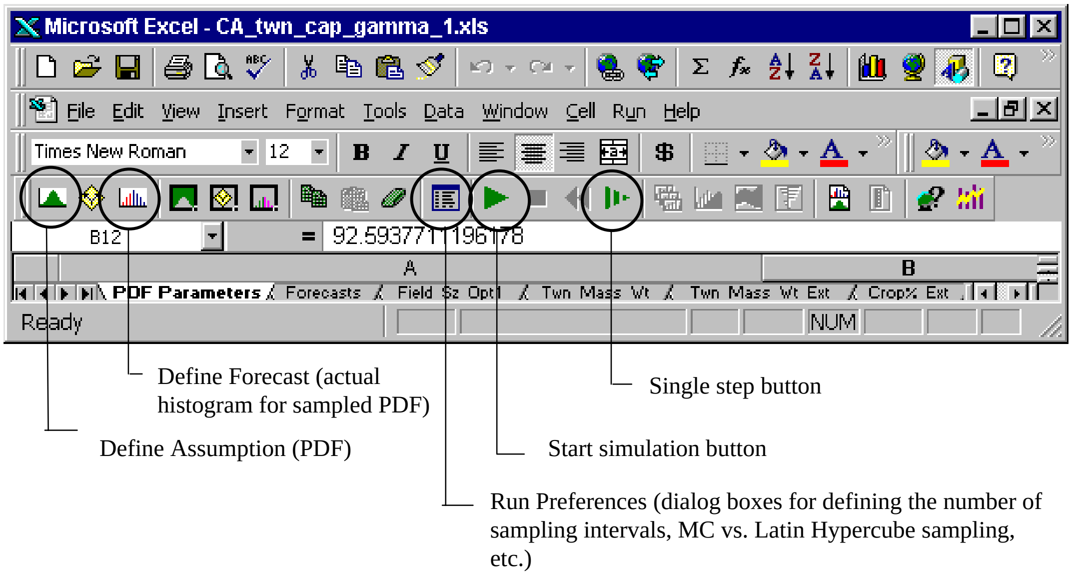


Figure A6.1. Most common menu buttons for use in Crystal Ball.

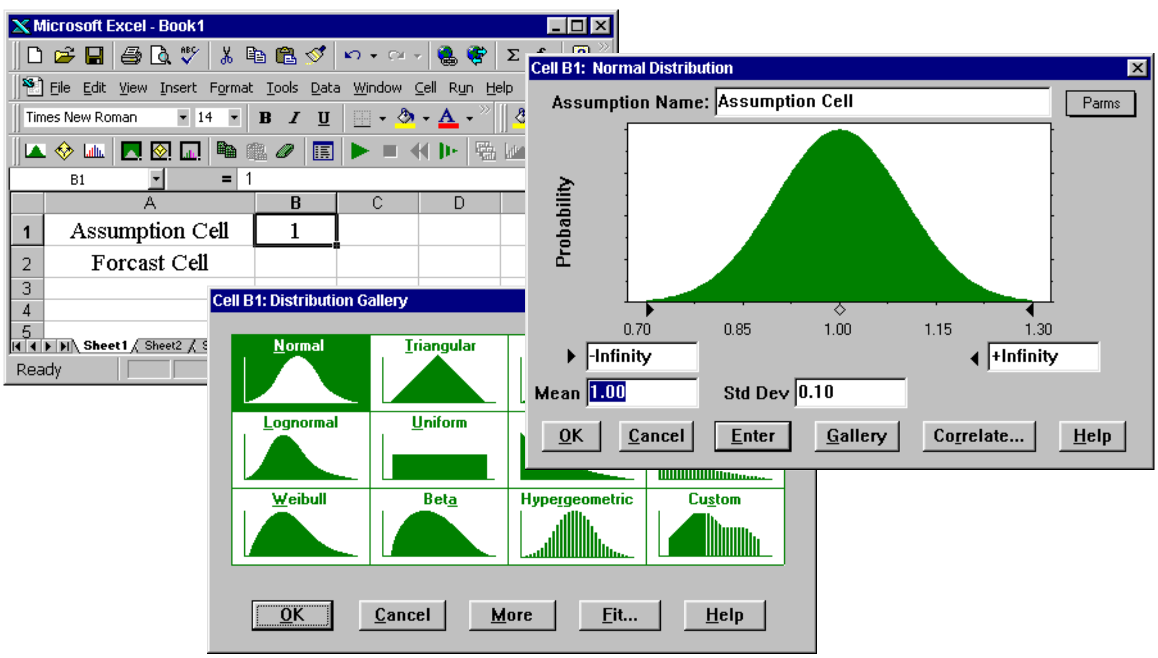


Figure A6.2. Example of using CB and MS Excel to define a cell entry as a PDF.

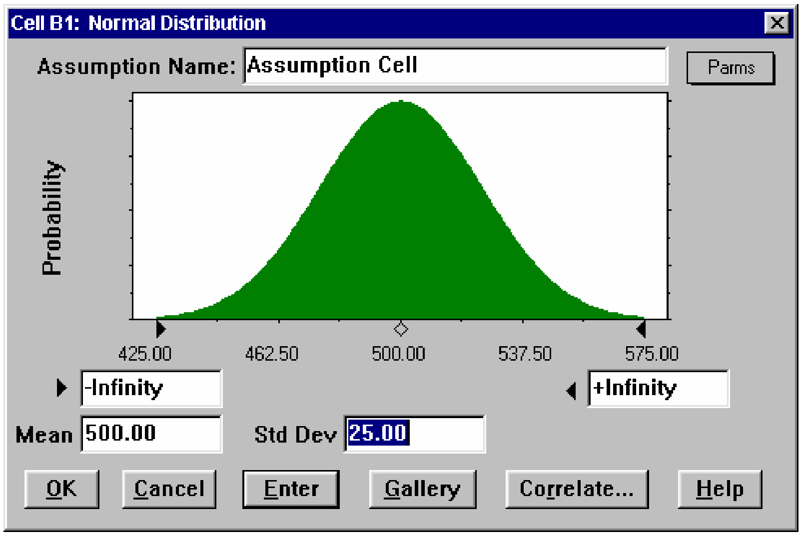


Figure A6.3. Example problem PDF assigned to Cell B1 in worksheet.

Following the simulation execution, the PDF has been sampled a user specified number of times. However, there is no record on what values have been used by the PDF unless

i) these values are written out to a worksheet (via VBA calls as is done in the DAS soil fumigation/exposure model)

or

ii) a forecast cell is defined.

In the latter case, a forecast cell is one that "stores" all of the data entries for each MC iteration. To define a forecast cell for B1 in our example problem, the user would first assign a cell (C1 to equal B1) (Figure 5). Click on the check box to enter this as a MS Excel entry. Then, highlight cell C1 and click on the Define Forecast button. The resulting dialog box that pops up lets the user record bookkeeping information such as the name the user want to give the forecast cell, units, etc. Once the forecast has been defined, the default CB color for the cell is light blue (Figure 6).

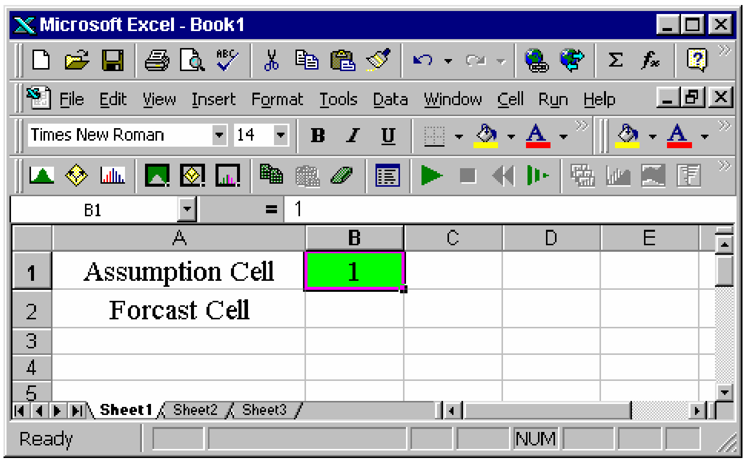


Figure A6.4. Example problem worksheet once PDF for Cell B1 has been defined.

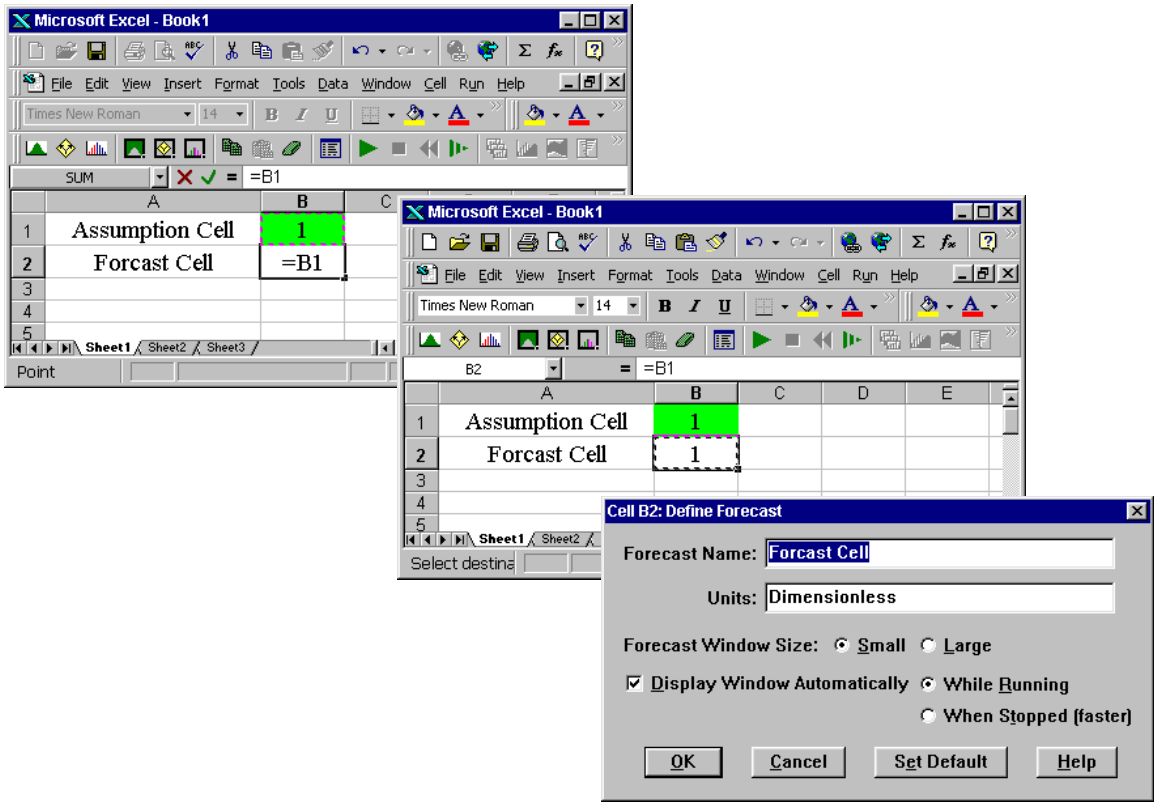


Figure A6.5. Procedure for storing PDF selected values for further post processing and/or model verification.

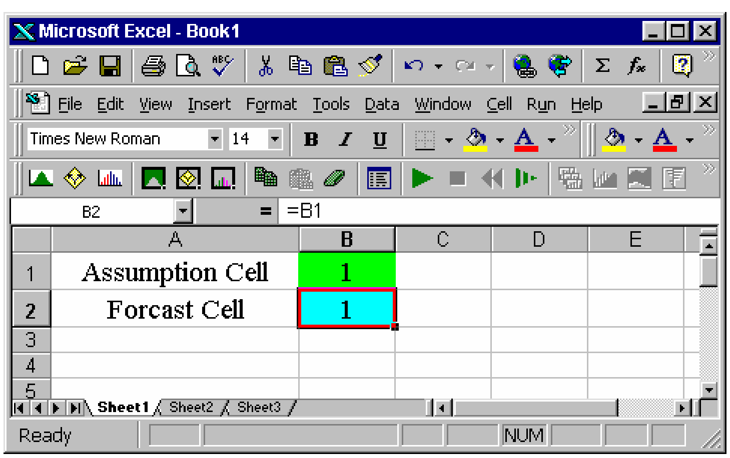
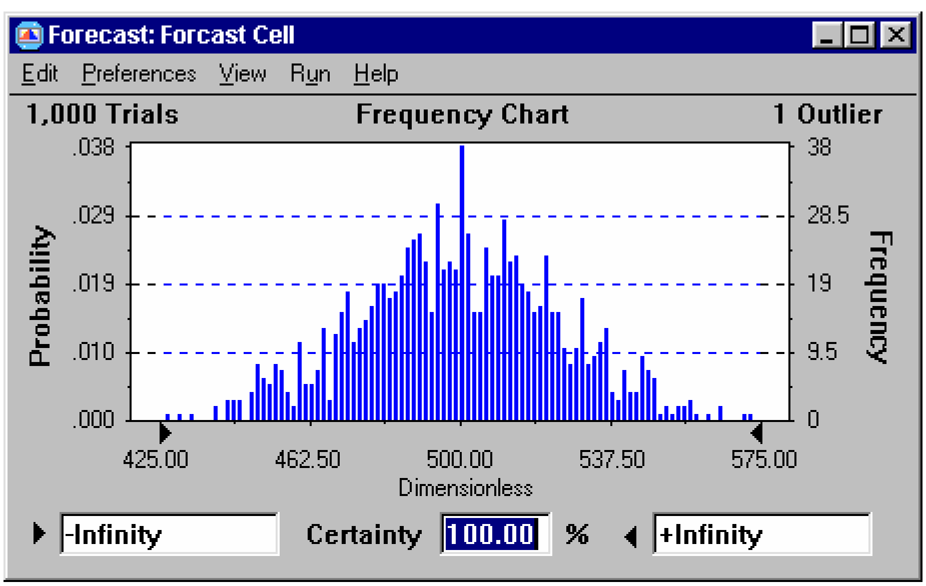


Figure A6.6. Example where both a assumption and a forecast cell have been defined using CB functionality.

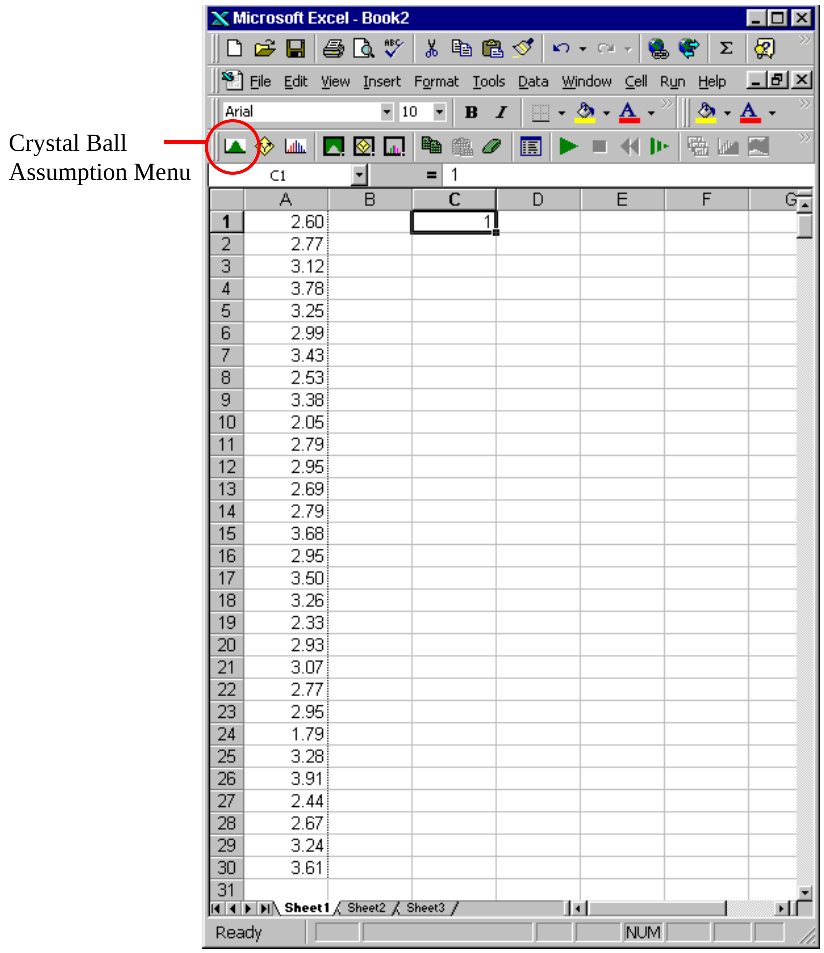
The definition for the type of PDF specified by the user can be obtained by highlighting a CB cell (i.e., B1) and clicking on the CB menu for the CB "assumption". If this were done for the above example, then a normal distribution would arise having a mean of 500 and a standard deviation of 25.

Assuming the user specified a 1000 iteration simulation via the "Run Preferences" menu button, then MC results can be output via the popup window for the "Forecast" (Figure 7) (assuming the user specified the window to be open during the simulation), or results can be obtained via a data dump for forecast values.

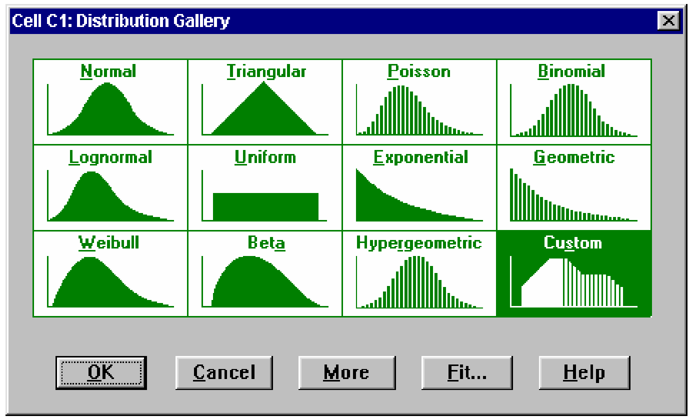


DEFINING CUSTOM DISTRIBUTIONS

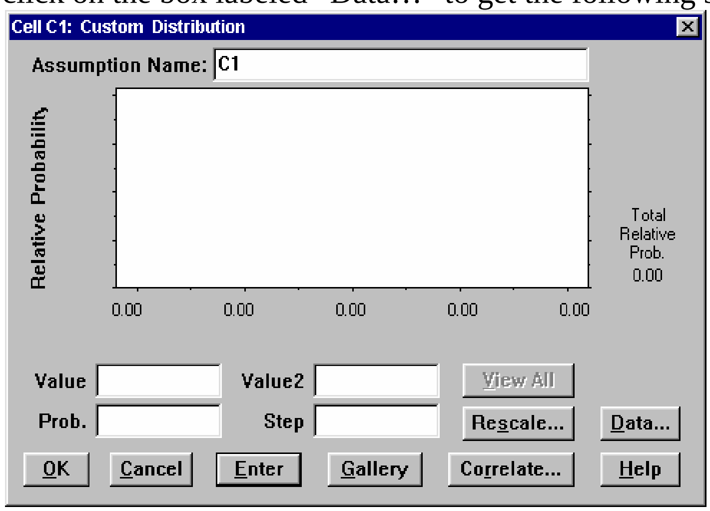
When defining a custom distribution, the user can either type in the values in the CB dialog screen or the user can read in the data from MS Excel. The latter is the example provided, since this is what we did with the CDMS data. Below is a screen shot example of 30 data points (Cells A1:A30) that we'll use to generate a custom distribution. As per crystal Ball methodology, type a number in a cell (It can be any number) and then to to the Crystal Ball Assumption menu to define the cell as an assumption (Cell C1 in this example)



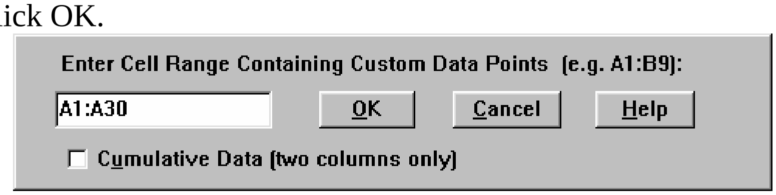
The CB assumption menu will bring up the CB Distribution Gallery. The user should then click on the "Custom" distribution.



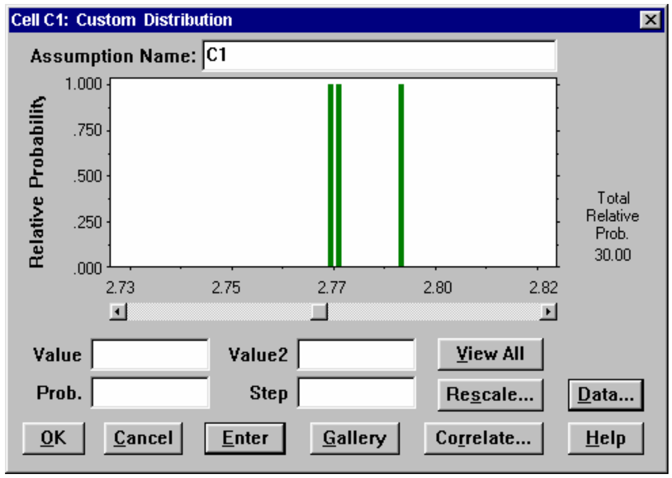
And the user will get the following screen. Here, the user can enter each data point or read in the data from an Excel location. If so, then the user must have "histogram data", it a bin median value and the frequency (probability) of occurring for this bin. We will enter in data from an Excel worksheet So, click on the box labeled "Data…" to get the following screen.



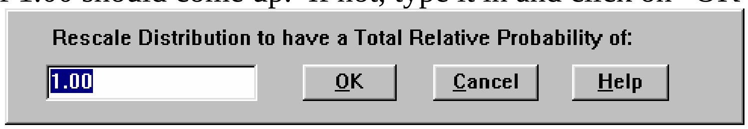
Here, the user must enter the MS Excel Cell locations where the data resides (in our example, its A1:A30). Then click OK.



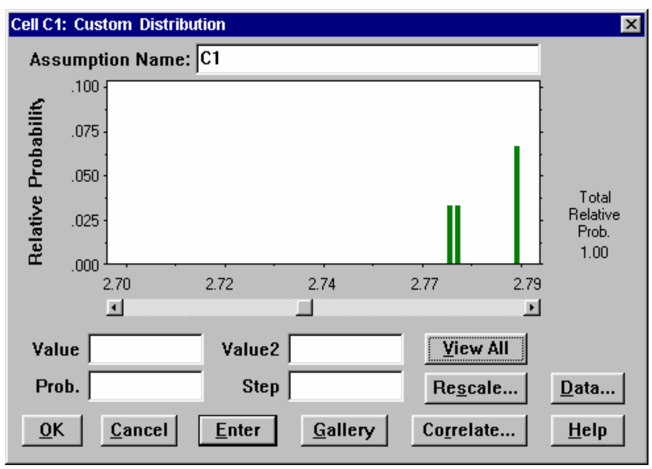
The user will get the following histogram that is based on the data specified. A few things to point out…. Note the "Slider" bar below the histogram graphic. For this example, the screen only shows part of the distribution. The second thing is that The user must now scale the data such that the total relative probabity is 1.0 (i.e., what we now have is a running sum, and since we have 30 data points, the Total Relative Prob. Is 30. Click on the "Rescale…" button to get the following screen.



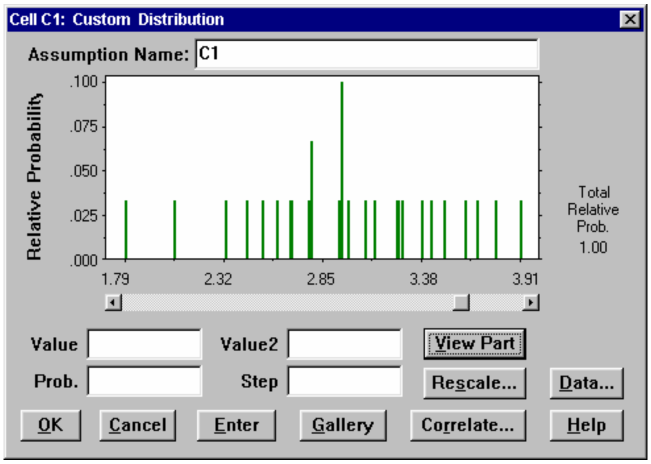
The default value of 1.00 should come up. If not, type it in and click on "OK".



Now notice the relative probability is scaled such that all of the probabilities sum to 1.0.



The user can click on the "View All" button to see the entire distribution as shown below.



When the user click o.k. then the assumption cell (C1 in our example) should now be green. If so, highlight cell C1 and click on the CB assumption menu on the tool bar, the will see the above distribution. This is the distribution that will be sampled for cell C1.

Some more nice to know stuff….. it seems that in CB, the data for a custom distribution must reside on the same worksheet that the assumption is defined (as in this example). This can be problematic on an already cluttered worksheet (such as “PDF Parameters”). To work around this, create a new worksheet that will contain you’re raw data and define the assumption (as outlined to this point). Then highlight the assumption and then go to the “Cell” menu on the MS Excel tool bar. The user will see both a “copy data”, “paste data” and a “clear data”. These are the functions you must use to copy CB PDFs to other locations in the same or new worksheets. Thus, use the Cell> copy data to copy the cell assumption cell, then go to another worksheet (such as “PDF Parameters”) and paste the PDF using the Cell>pasta data command. Thus, the user can have a worksheet that contains the raw data used to generate a custom distribution without cluttering up other worksheets where only the PDF itself is required.

APPENDIX 7. SOFEA troubleshooting guide

Problem:

“Runtime Error 62 - Input past end of File”

Possible Fixes:

This is typically related to the weather files not being formatted correctly.

Make sure the weather file format is as per section 3.3 of the User’s Manual.
Make sure the file has been saved as a *.met (text file).
Make sure the upper and lower met station numbers in the PDF_Parameters” worksheet match the *.met file.
Make sure the directory path for the weather data is correct.

Problem:

“Out of Memory”

Possible Fix:

Reduce the length of the simulation (eg. 20 years to 10 years) or the number of receptors (eg. From 9 twp domain to 1 twp domain).
Try minimizing the number of averaging periods, increase the spacing between receptors, and close all other programs, increase virtual memory of MS products.

Problem:

“Subscript out of range”

Possible Fixes:

Check that the length of simulation (in years) in Cell E17 matches the number of years per loop in cell B118, so that cell C128 is a whole integer number between 1 and 5. (Cell C128 should be 1 of no looping is used).