Predicting Soil Fumigant Acute, Sub-chronic, and Chronic Air Concentrations Under Diverse Agronomic Practices

S. A. Cryer, I. J. van Wesenbeeck, B. A Houtman

SOFEA© (SOil Fumigant Exposure Assessment system) is a recently developed stochastic numerical modeling tool for evaluating and managing 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 appropriate field/numerical observations. Weather information, field size, application date, application rate, application type, soil incorporation depth, pesticide degradation rates in air, tarp presence, field retreatment, 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 profiles. Multi-year simulations are conducted using random field placement in all agricultural capable areas as well 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 risk assessments. Both current and anticipated/forecasted fumigant scenarios can be simulated to provide risk managers the necessary information to make sound regulatory decisions, and SOFEA has been successfully used for regulatory decision making in California. Algorithms used by SOFEA to refine exposure predictions for soil fumigants on a local or regional basis are discussed, and comparison of simulation results to regional air monitoring measurements are presented.

INTRODUCTION

Nematodes are soil dwelling organisms that eat and live in (or on) plant root cells during part of their life cycle. Consequently, large root galls leading to crop death and/or substantial yield reduction occur. Soil fumigants, used to control soil born pests such as nematodes, typically have high vapor pressures and thus the propensity to volatilize from soil into the atmosphere. These high vapor pressures account for efficacy once injected into soil, but may give rise to potential off-site exposure for individuals in the neighboring vicinity. Proper characterization of fumigant exposure is an important stewardship issue since future use of a variety of different fumigants will likely increase as the soil fumigant (methyl bromide - MeBr) is phased out as mandated by the Montreal Protocol of 1987 (UNEP, 1995).

An example of the intricacy for air dispersion scenarios is given in Figure 1 for a representative California (CA) region near Santa Cruz, CA. California has surveyed land into 6 mile x 6 mile townships. Within each township, the area is further subdivided into 36 equal sub-areas called sections (1 mile x 1 mile). Chronic exposure for the soil fumigant 1,3-Dichloropropene (1,3-D) is managed in part by limiting the total amount of 1,3-D mass that can be applied per year in a given township. This mass limit is known as the township allocation and is mandated by the California Department of Pesticide Regulation (CDPR). A recording procedure, known as the California Pesticide Use Records (PUR), is used to document the amount of any pesticide applied to a field, the field size, location, application date, and the depth of application. PUR is now administered and tracked for 1,3-D by the California Crop Data Management System (CDMS). When the current township allocation is reached, no further applications of 1,3-D are allowed. However, not all townships utilize 1,3-D at the current allowable allocation level. In addition, cities, mountains, and oceans constrain where nematicide treated fields (source terms) occur and thus these variables must be accounted for within a given air shed. This paper describes the technical algorithms of SOFEA and provides a comparison of 1,3-D simulated results against air monitoring measurements.

Figure 1. Townships and land cover south of the city of Santa Cruz, CA

MATERIALS AND METHODS

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, agronomic practices, and acute through chronic exposure levels. Time averaged transient air concentrations via a numerical model can be used in exposure procedures for risk determination for unlimited numbers of use scenarios.

Air Dispersion Model

The Industrial Source Complex Short-Term model (ISCST3, 1995) 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. However, these same receptors will continue to receive contributions from other fields for which the given receptors are outside of the other field's buffer zones.

Air Shed Domain

GIS input is required for a single township or up to a 3x3 township domain. This information must include land cover such that ag-capable land can be quantified. Elevation and population information are optional. The complex terrain algorithms of ISCST3 can take advantage of elevation changes within specific regions. Receptors can be placed uniformly in the central township or the entire 3x3 domain. Source terms can be placed external to the central 3x3 up to a domain of 23x23 townships (19,000 mi^2). The user need only specify the annual mass applied to any township within a 23x23 township domain.

Parameter Representation

Stochastic portrayal

Air concentrations resulting from transient agricultural source terms are also dependent upon meteorological conditions, application timing, and so forth. 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 can include 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. Thus, an ISCST3 input file was exported from Excel that was based upon appropriate selections from Crystal Ball PDFs (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.

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 quality 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.

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 that yields 1296 receptors per township (11,664 receptors within a 9-township simulation domain). Receptor height was 1.5 m above the soil surface to mimic the breathing height of an adult.

GIS Data Layers

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]. 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.

Actual examples of GIS data layers used in the numerical system are provided for township M15S04E and surrounding townships located near Monterey California. Elevation, land-cover type, and population data for M15S04E are provided in Figures 2-4, respectively. Left-side graphics found in Figures 2-4 represent the finer resolution of the data found in the data bases. The discretized data (10x10 per township) for direct input to the numerical system is given by the right side graphics obtained by spatially averaging the more refined data into a coarser grid. SOFEA was designed using a coarser grid system for users not having GIS capability when data would have to be input by hand.

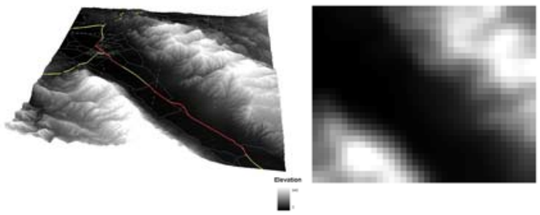

Figure 2. Digital Elevation data for Monterey township M15S04E and surrounding 8 townships. Graphic on right is discrete data used in modeling for the 9-township region.

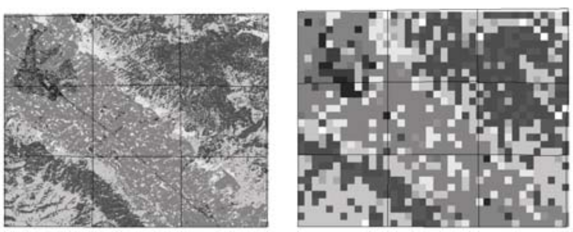

Figure 3. Land cover data for Monterey township M15S04E and 8 surrounding townships. Graphic on right is discrete data used in modeling for the 9-township region.

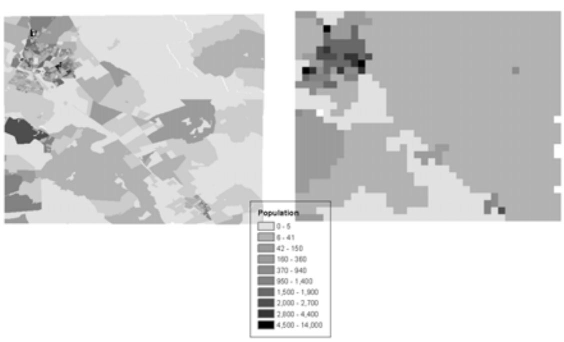

Figure 4. Population census data for Monterey township M15S04E and 8 surrounding townships (left graphic). Graphic on right is discrete data used in modeling for the 9-township region.

Meteorological Data

Meteorological data required by ISCST3 include hourly air stability class, wind speed, air temperature, wind direction, and mixing and ceiling height for the air shed. Multi-year meteorological data for a variety of locations can be found at the USEPA Support Center for Regulatory Air Models (SCRAM, USEPA, 2001) website or through state specific organizations such as the California Irrigation Management Information System (CIMIS). Each weather year has a user supplied probability of being sampled (typically a uniform distribution is assumed).

Source Placement

Transient source terms for simulation are nematicide treated fields where pesticide volatility can occur. Source strength and location are based upon experimental (or numerical) observations, management practices, agricultural capable land, and historical information. Much of the required data is geo-referenced and amenable to Geographical Information System (GIS) overlays and extraction.

The total number of source terms selected is a function of the field size, application rate, and the total amount of pesticide mass allowed in a given township (e.g. township allocation). No further source terms are allowed once the township allocation is met. However, management practices such as application rate, application date, depth of incorporation, field size, and so on vary in a current year for each field of a specific crop type. In addition, once a tree and vine field location has been selected, this area is restricted from use for all additional years of simulation since perennial crops (such as vines or orchards) productivity life span is large. A new fumigant application is typically not reapplied until after the orchard/vineyard is destroyed.

Random Placement

Sources within a township can be placed randomly or weighted to specific township locations. Randomly placed fields within a township have a uniform probability of being placed within any ag-capable land found in the township. Agricultural (ag) capable land is defined as all land excluding urban areas, water bodies, barren, rock, quarries, and wetlands. The constructed numerical system assumes a maximum of 100,000 iterations when attempting to randomly place fields within a township.

Section Weighting

Certain sections within a township (1/36 township area) traditionally apply larger quantities of soil fumigant than in other township sections. Receptors in such sections will register higher chronic soil fumigant air concentrations due to the spatial intensity of fumigant use. For numerical implementation, the user specifies the probability of each section receiving source terms (the sum of the section probabilities for each township equals one). Fields are placed randomly within the appropriate section at frequencies governed by the section probability (but are still constrained by agricultural capable land). This present's a "worst-case" scenario for each year of simulation such that field locations can be quite dense in a single section. No other pesticide is rotated throughout the simulation cycle (i.e., all fields are always treated with the same fumigant) for each consecutive year of the simulation.

Overflow of source terms to surrounding sections

It is possible the number of treated fields can exceed the usable land area in a given township section for a given simulation year. This can occur if the section has a large percentage of non-ag capable land, a majority of the township mass goes into relatively few sections, and/or when the total amount of pesticide mass (township allocation) is large. Once a field is placed, this area is unusable for additional applications of pesticide during that year since a crop is now growing (most soil fumigant applications are made pre plant). Thus, a “cookie cutter” scenario arises as different field sizes are randomly placed within a section (Figure 5). There may be the possibility that a sufficiently large field cannot be placed in a given section, although the overall remaining ag-capable land is of sufficient area. In these cases, a spill-over/overflow algorithm was developed. On subsequent iterations, if a small field size were selected, the algorithm would first try to place the field in the user-defined section before any overflow occurs to maximize the treated area in a user specified section.

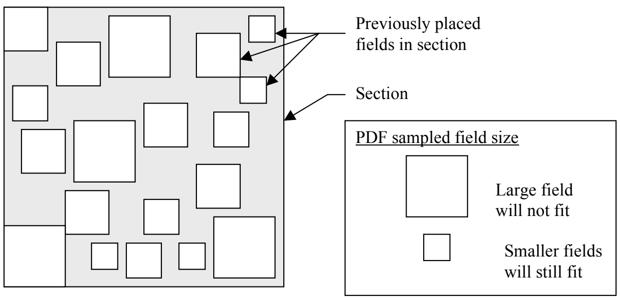

Figure 5. Illustration of field placement within a section/township where not all land can be utilized.

The user has defined section probabilities for treated field assignment within a given township section if section weighting is specified before the onset of a simulation. These section-weighting probabilities can be based upon historical records or expert judgment. The methodology is illustrated in the example found in Figure 6. The difference between Fig. 6 (a) and 6 (b) is that for 6 (a), all user defined section overflows don’t impact (border) other potential overflow sections. In Figure 6 (a), the user has specified three township sections having non-zero probabilities of receiving a treated field (dark cells).

All sections within the township that surround the user-supplied non-zero probability sections are initially assigned the same probability value (light cells). If a surrounding section borders multiple user supplied probability sections, then neighboring section probability is defined as the sum of the probabilities resulting from all neighboring sections. Then, each surrounding section probability is scaled by the sum of all probabilities for the sections that border the user supplied non-zero probability sections (Eq. 1).

$$P_i = \frac{NP_i}{\sum NP_i} \tag{1}$$

P_i = probability of a neighboring section receiving a treated field if the primary sections are filled up.
NP_i = Initial probability assigned to neighboring section surrounding a user-supplied non-zero probability section (same as bordering user supplied section).
ΣNP_i = sum of the initial probability’s for all neighboring sections within the township.

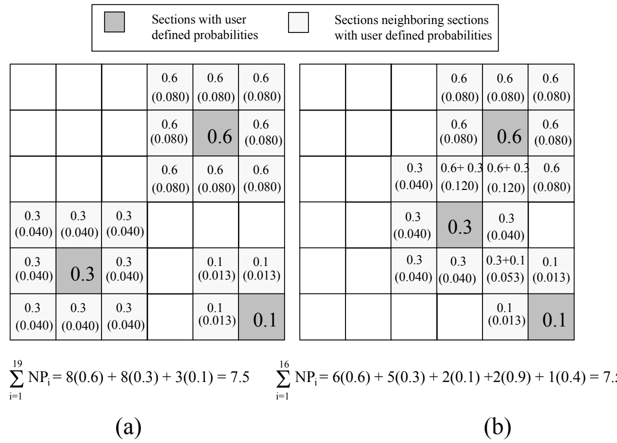

Figure 6. Example of the overflow algorithm for determining probability of surrounding sections that can receive a field if the algorithm is invoked.

For the example provided in Figure 6, the numbers in parenthesis are the actual probability assigned to the section (i.e., original assigned probability (NP_i) divided by ΣNP_i. In this way, neighboring sections near the largest magnitude user-defined section probabilities have the greatest chance of receiving an overflow field once the overflow algorithms are invoked. Similarly, neighboring sections that border multiple user defined sections will have a greater probability of receiving treated fields than the other neighboring sections that do not border multiple user defined sections (assuming the probability is greater). Once a section can no longer accommodate a field, then neighboring sections are used as the overflow area for field placement. If all overflow and surrounding sections fill, then source terms are randomly placed in remaining ag-capable land within the township.

Figure 7 illustrates SOFEA field placement results for both random and section weighting for a 3x3-township simulation domain townships near Ventura, CA. Each small square represents a source term for different crop types. The user specifies a reference allocation for the total amount (mass) of soil fumigant applied to a township. This can be the legally mandated maximum allowable allocation or a specific value for a unique region. Each township is assigned an allocation based upon a user supplied fraction of the reference allocation. For example, a value of 2.0 is 2x the reference allocation. Clustering of fields is due to township sections given a larger probability of receiving a treated field. Township sections at the supplied probability weights of receiving a treated field are the first to fill with source terms. The township allocation weights and the township section probabilities used to generate Figure 7 are given in Figure 8. Field sizes are determined by sampling an appropriate user specified PDF for each crop.

Source Strength

Soil Volatility Flux Patterns

Fumigant mass volatilization from soil can be estimated by field measurements or numerical predictions. Historical fumigant research has focused on field and laboratory measurements (a large time and financial resource commitment). However, numerical models have been used to predict fumigant volatilization for products such as 1,3-D. These include the 2-dimensional USDA model CHAIN_2D (Simunek and van Genuchten, 1994; Wang *et al*., 1998; Wang *et al*., 2000), the 1-dimensional models LEACHV (Chen *et al*., 1995) and PRZM3 (Carsel *et al*, 1995, Cryer and van Wesenbeeck, 2003), and linear approximations (Woodrow *et al*. 2001). Volatility loss from soil predicted by these models (or field measurement) can be specified as transient source terms for air dispersion modeling.

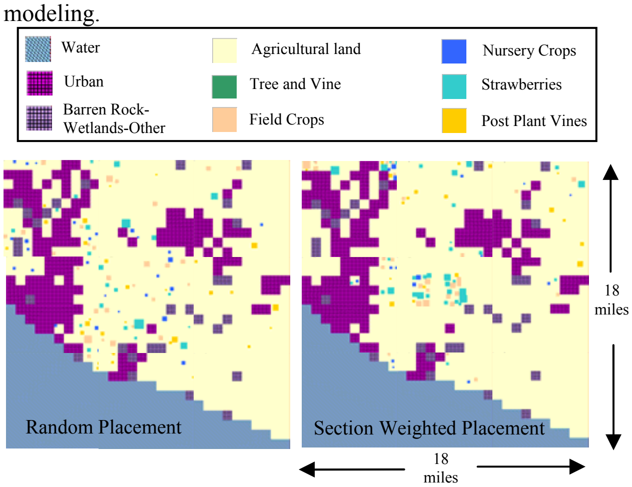

Figure 7. Example random and section weighted field placement (with overflow).

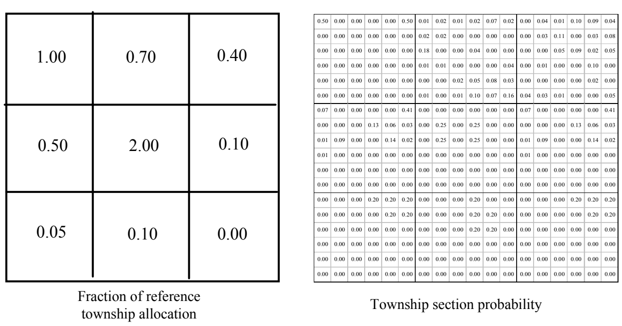

Figure 8. Township allocations and section weighting for a 3x3 township domain used to generate source placement for a single year of simulation for Ventura, CA.

For 1,3-D analysis, an actual field observed flux profile is used. The aerodynamic flux and flux chamber method have been used to measure 1,3-D volatilization from treated fields (Knuteson and Petty, 1995; Knuteson *et al*, 1998). Figure 9 represents experimental observations for 1,3-D volatility losses for a California field-scale study performed by Dow AgroSciences using the aerodynamic flux method. Cumulative loss was approximately 25.0 % of applied for the shank application (bare soil, 45.7 cm incorporation depth). This result is similar to numerical predictions reported elsewhere (Cryer and van Wesenbeeck, 2003).

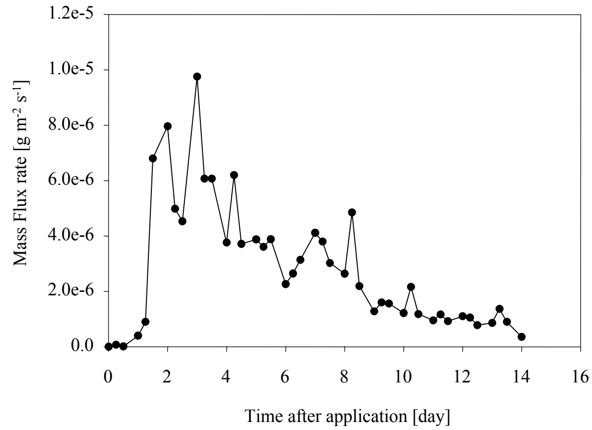

Figure 9. Field observations of transient volatility losses of 1,3-D for shank injection application (rates of 122 lbs 1,3-D per acre.

Application Scaling Factor

Measured flux rates, specific for the conditions at the time of the study, are adjusted based upon depth of incorporation and time of year in an attempt to represent the complete flux response surface. Volatilization losses for the soil fumigant 1,3-D are sensitive to temperature and depth of soil incorporation (Cryer and van Wesenbeeck, 2003). A simple procedure to account for seasonal and incorporation depth variability was developed if specific experimental (or numerical) observations are selected as transient source terms for fumigant volatility loss.

The transient flux loss used in the simulations for each field is given by Eq. 2.

$$Flux_i = R * Fr_i * S_{incorp} * S_{yr} \qquad (2)$$

$Flux_i$ = Appropriately scaled hourly flux loss for hour "i" based upon observations of field trial [kg ha^{-1} hr^{-1}]
R = pesticide application rate (kg/ha)
Fr_i = experimentally observed flux rate (reference profile, scaled by experimental application rate for hour "i" [hr^{-1}])
S_{incorp} = scaling factor for depth of incorporation (dimensionless)
S_{yr} = scaling factor for time of year (dimensionless).

The scaling factors for incorporation depth and application timing are summarized below.

Depth of incorporation (S_{incorp})

Volatility losses from a treated field decrease as the soil incorporation depth for the nematicide is increased. Multiple field and/or flux chamber studies have been performed using the soil fumigant 1,3-Dichloropropene (Wang, et al., 2001; Gan *et al.*, 1998; Knuteson and Petty, 1995; Knuteson *et al*, 1998; Wang, *et al.,* 2001). However, only the experiments of Gan *et al* (1998) were designed specifically to investigate the impact of incorporation depth with cumulative flux losses. Data summarized by Gan *et al*. is isolated and represented in Figure 10 with the best-fit linear and exponential curve through the data (where each function was forced to yield 100% mass loss at the 0-cm soil incorporation depth). Although the linear fit is acceptable, the laboratory data clearly indicate a non-linear volatilization loss with depth of soil incorporation.

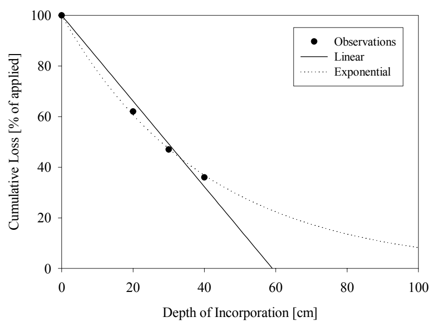

Figure 10. Effect of incorporation depth with 1,3-D volatility losses under controlled, laboratory conditions (Observations from Gan *et al*. 1998).

Figure 11 summarizes independent numerical predictions using the USEPA model PRZM3 and the USDA model CHAIN_2D for 1,3-D volatility losses as a function of incorporation depth. PRZM3 simulations assumed a Metz soil series (sandy loam), while CHAIN2D soil properties were for a Myakka soil (sand). Numerical results corroborate the non-linear behavior for volatilization losses with incorporation depth.

If no tarp is present at the soil surface, than 100% mass loss is assumed for surface applications. If a polyethylene plastic tarp is present, then a default value of 64% of applied is assumed unless otherwise specified (Cryer and van Wesenbeeck, 2003). The rate constant for non-linear scaling (exponential decay) is calculated by fitting a 1st order decay curve through the user defined maximum loss at the soil surface (x=0) and the reference volatility loss via the field study ($x = x_{ref}$). The percent of applied 1,3-D lost is dependent upon if a tarp is present and/or user specified cumulative mass losses. The non-linear approximation has the advantage over a linear approximation since $S_{incorp} \geq 0$ for all incorporation depths of agricultural significance. Either linear or non-linear scaling can be specified in SOFEA.

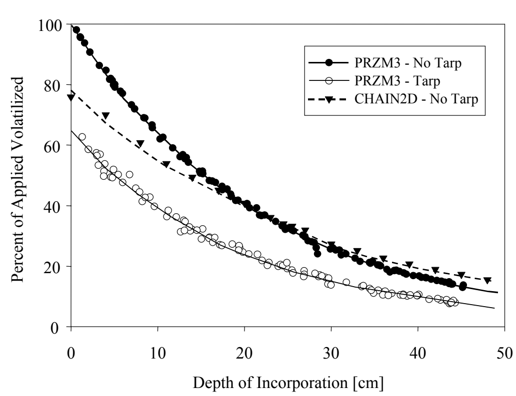

Figure 11. Functional non-linear dependence of cumulative volatilization losses as a function of application depth.

Temporal Representation (S_{yr})

Temperature can affect volatility losses for nematicides since diffusion coefficients are often strong functions of temperature. Temporal scaling for California is broken down into a warm or cool season to account for the greater potential mass loss during warm seasons. The scaling of cumulative mass loss between cool (Sep 22 – Jun 21) and warm (Jun 22 – Sept 21) season emission rates was assigned a factor of 1.6 (B. Johnson CDPR, personal communication, 2001). If the reference field study was conducted in the winter, but for simulation purposes, a summer application was assumed, then the experimental winter flux loss was scaled by 1.6 for a summer time application, with the converse (inverse) also true. If the sampled application date is within the same time frame as the reference field study, then $S_{yr} = 1.0$. Thus, S_{yr} indirectly accounts for gross temperature effects for 1,3-D soil volatility losses from soil for a two-temperature regime year.

Source Constraints

Field Size Optimization

A consequence of the MC analysis is that different field sizes and application rates will be selected for each crop type and for each year of simulation. A method was required to keep the fumigant mass applied to any given township (user specified) as a constant under any condition. Optimization procedures are used such that the township allocation is achieved but constrained by the user supplied percentages for each crop type found within the township being met. User defined field size PDFs are initially sampled to obtain starting values for field sizes for each crop type. The number of fields are determined such that the total mass of 1,3-D for all source terms is constrained at the user specified township allocation and the residual for the crop percent cover is minimized. This results in a Mixed Integer Linear Program (MILP) problem whose optimal solution is obtained using a modified flexible-polygon search procedure (Himmelblau, 1972)

The mathematical representation for the objective function requiring minimization is given by Eq. 3.

$$\Psi = \gamma \sum_{i=1}^{5} \left| T_{pdf_i} - \frac{\sum_{j=1}^{N_i} A_{i,}}{\sum_{i=1}^{5}\sum_{j=1}^{N_i} A_{i,}} * 100 \right| - \left| T_{alloc} - \sum_{i=1}^{5}\sum_{j=1}^{N_i} A_{F_{i,}} \; A_{i,} \; R_{i,} \right| \tag{3}$$

Ψ = Objective function requiring minimization

γ = Weighting variable (100 or 1000) based upon order of magnitude analysis so optimization procedure executes properly under a variety of diverse conditions. By adjusting γ, one can emphasize the crop percent residual, township allocation residual, or both)

$T_{pdf\,i}$= Percent of township ag-capable land that is specifically for crop “i” (from PDF)

T_{alloc}= Township allocation for 1,3-D [kg]

N_i = Integer number of fields for crop "i" (initially unknown)

A_i = Area of a field for crop "i" [ha]

R_i = Application rate for crop "i" [kg ha^{-1}]

i = counter for the 5 different crop types that can be present

The first and second term in Eq. 3 represents the sum of residuals for cropping area percentages and for the township allocation, respectively. Thus, Eq. 3 is a function of two user constraints: the township allocation and the percentages of user defined crop percentages within the township. The numbers of fields for each crop type (N_i) are constrained as integer's ≥ 0. Once the number of fields for a given crop type are known, then the PDF field sizes (A_i) are adjusted (slightly stretched or shrunk) to meet the township allocation constraint. The logic flow diagram used in optimization procedure is given in Figure 12. The parameter γ is used to emphasize one constraint over the other (or to make each constraint of similar magnitude during optimization).

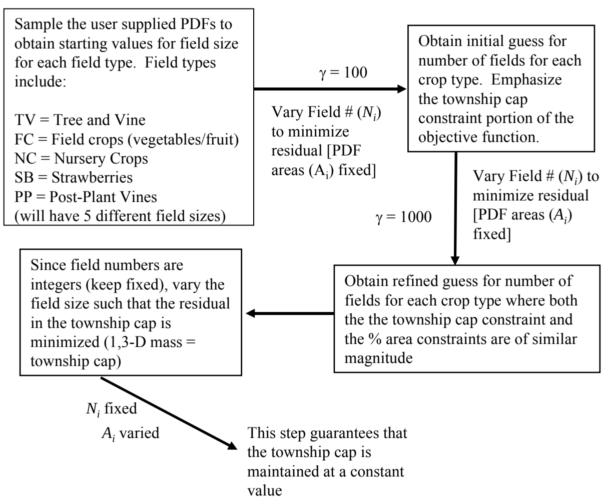

Figure 12. Flow chart for optimization procedure used to determine field sizes for each crop type.

Representative results illustrating how fields are stretched and/or shrunk from using the optimization procedure are given in Figure 13. The small fields remain small and large fields remain large, although the starting and ending field sizes before/after optimization do change. The largest alteration a field can be stretched or shrunk is 20% of it's original PDF sampled value. This approach guarantees every year of simulation will have the same township allocation magnitude.

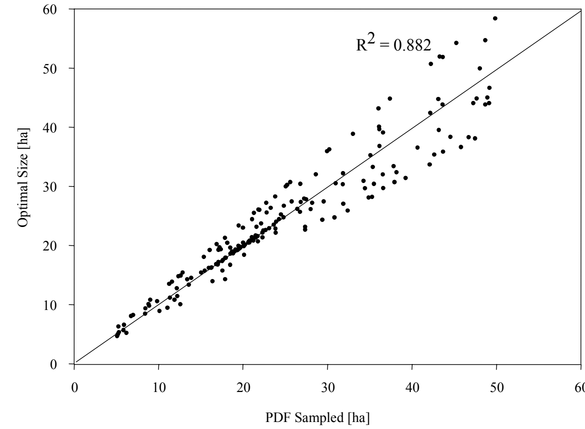

Figure 13. Example of field-size optimization procedure for PDF sampled field sizes.

Raster Grid Resolution

The location for each field is monitored such that no other field can overlap another treated field during the current year of simulation. Due to the discrete nature associated with a raster analysis, the number of surrounding grids a field occupies can be either "rounded" up or down, according to the user preference. Rounding up includes all grids a field comes in contact with, even if there is only slight overlap into a neighboring grid. Rounding down only includes a surrounding grid if more than half of the grid is occupied by the field. Figure 14 provides an example of the procedure in eliminating ag-capable land from further consideration in a simulation year if rounding up or down is assumed. Rounding down or up will give the same result if the field occupies at least 50% of a grid. By specifying rounding up, there will be no possibility for treated field overlap. A small probability of having some fields slightly overlap exists if rounding down is used, although the overlap is at the resolution of the raster grid. However, this may only occur for townships having a large township allocation and high field density in specific township sections. Rounding down can allow for denser field placement within a township section since more ag-land is available for further field placement.

Annual Field Retreatment

It is possible that a farmer can repeatedly treat a field with a soil fumigant for several consecutive growing seasons. The percent of fields retreated from year to year can be specified by the user. For the first year of rotation, fields are placed appropriately (random or section weighted as defined by the user). If a 50% field retreatment is requested, then 50% of the fields from the previous year are randomly selected and marked as fields that will be retreated the following year. Fields that are to be retreated are added with new fields such that properties of retreated fields and new fields meet optimization constraints. This process is repeated for each year of simulation. Retreated fields are not stretched or shrunk during the optimization procedure.

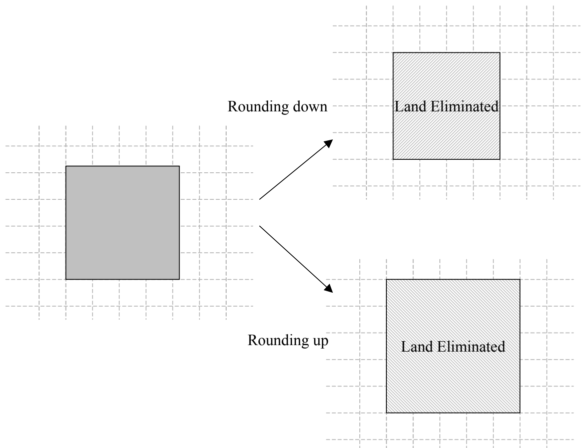

Figure 14. Example of land elimination due to integer rounding associated with field coverage.

Forecasting - Temporal parameter changes

Agronomic practices can and do change over time. These practices can include such things as the percentage of retreated fields from year to year, crop rotation, field size changes, the amount and type of pesticide used, application rates, incorporation depths, and loss of ag-capable land as cities grow. In addition, the ability to explore heuristic rules that may mitigate fumigant exposure is desirable (such as a field cannot be treated 3-years in a row, staggering of sources between township sections in alternating years, and so on). Thus, a system with the ability to forecast an exposure regime was required that could account not only for current scenarios, but future "what-if" scenarios as agronomic practices change. SOFEA offers this flexibility by allowing up to five different parameter change regimes for a multi-year simulation interval. Parameters can included both scalar and PDF values. An example where historical, current, and prospective scenarios are considered in a single simulation is given in Figure 15.

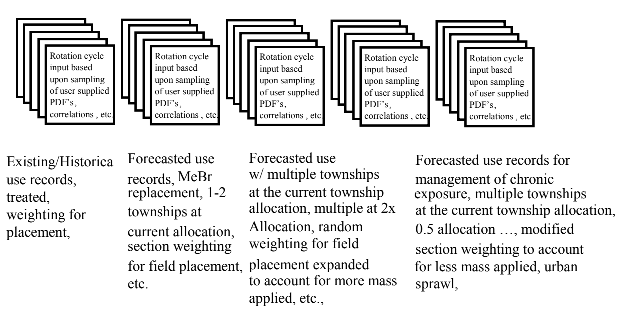

Figure 15. Example of a 5 period rotation cycle, where each period has 5 years of simulation (25-yr simulation).

Figure 15 represents how the temporal nature of agriculture can now be simulated. A 25-year simulation has been broken down into five different 5-year intervals. The first 5 years represents current conditions (i.e., actual use data that has been collected). The next five years are "near term" approximations to agronomic practices, where input parameters are altered slightly (such as increased use of a fumigant as a replacement for MeBr). The following 15-years incorporate land use/demographics that may occur such as urbanization, ending of the life span of current orchards (i.e., new areas for TV), potentially new BMPs regarding insect resistance management, and so on. The same 25-year simulation can be equally broken up into three distinct intervals (where parameters are statistically different than in other intervals) of 8 years, 8, years, 9 years, and so on, to address parameter assumptions and their impact on forecasting results

Model Output Characterization

Summarized ISCST3 output includes 24-hr maximum, and annual average receptor concentrations. Post processing routines were written and additional averaging periods can be specified by the user (i.e., 15-day, 60-day, and so forth) if sub-chronic exposure levels are desired.

Superposition of Source Terms

The execution time for ISCST3 scales linearly with the number of source terms and the number of receptors. When current township allocations are approached or exceeded, and the field sizes are small, then a relatively large number of sources for the simulation domain will exist. Likewise, the total number of receptors placed within the central 3x3 (9-township) simulation domain can become large as the resolution/spacing (user specified) between neighboring receptors becomes small. Additionally, MC sampling requires an appropriate number of yearly simulations for stochastic response surface generation since parametric uncertainty is characterized through PDF sampling. Thus, a simulation was broken up into yearly events for each crop type to keep I/O and simulation execution time manageable (Figure 16). Simulation results for each crop type were superimposed (i.e., added) on a daily basis for each receptor within the simulation domain. Results can be superimposed since Gaussian dispersion is independent of concentration gradients (i.e., the wind convects the pesticide mass with dispersion as specified by the directional dispersion coefficients).

Figure 16. Superposition of daily simulation results for each crop type for the simulation interval (1-year) for an example having 3-crop types.

Monitoring of 1,3-D in Kern County

The Air Resource Board (ARB) of the California Environmental Protection Agency has been monitoring for several soil fumigants, including 1,3-D, for the past decade. Seven monitoring locations in Kern County had daily air samples taken and analyzed for 1,3-D concentrations during the high use periods in the summers of 2000 and 2001. Table 1 summarizes the sampling locations of ARB. Monitoring in 2000 was from Jul. 19 - Aug. 31, while in 2001, the monitoring interval was from Jun. 30 – Aug. 30. Details and monitoring results are found elsewhere (ARB, 2001, 2002)

Table 1. Descriptor-location and ID's for air monitoring locations in Kern County.

ID	Descriptor-Location-Township
VSD	Vineland School District - Sunset School (M31S29E)
ARB	ARB Ambient Monitoring Station – Bakersfield (M29S27E)
CRS	Cotton Research Station – Shafter (M27S25E)
MET	Mettler Fire Station – Mettler (S11N20W)
MVS	Mountain View School – Lamont (M30S29E)
SHA[a]	Shafter-Walker Ambient Monitoring Station (M28S25E)
ARV[b]	Arvin High School – Arvin (M31S29E)

[a] monitored in 2000 only
[b] monitored in 2001 only

Figure 17 represents the application date (Julian) histogram for all 1,3-D applications made in Kern County in 2000-2001 as documented by CDMS/PUR data. Clearly, the monitoring window of ARB only captured a single mode of the tri-modal distribution. Thus, SOFEA was only executed over the monitoring interval using PDFs generated from CDMS data occurring only during this window.

CDMS data for crop type for the 2000-2001 years illustrate the different agronomic practices occurring within the county and is further summarized over the monitoring time window to yield the smaller pie charts in Figure 18. Thus, for the Kern simulation using SOFEA, a total of three crops were assumed. Simulations using SOFEA [carrots, potatoes, other (peppers, onions, roses)], and the agronomic practice PDFs for input parameters (field size, application rate, date, depth, tarp presence) for each of the three crop types were determined from data summarized in the CDMS data base.

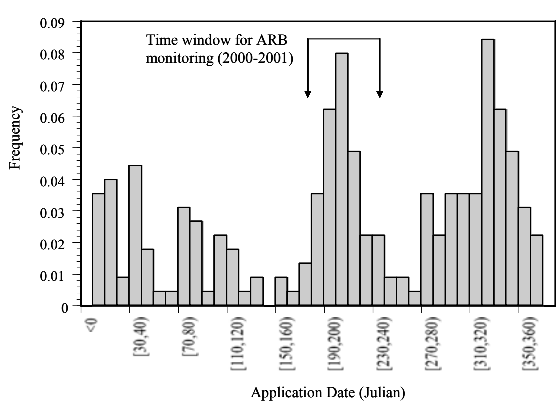

Figure 17. Histogram for 1,3-D application dates occurring in Kern County during 2000-2001.

No weather information in electronic format could be found for Kern over the monitoring time window. Thus, CIMIS weather [1993-1997] for Merced, CA was used as a nearby surrogate.

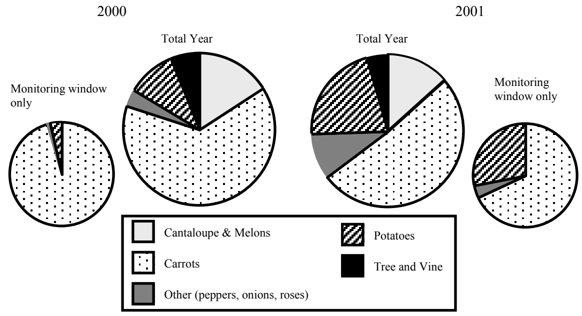

Figure 18. Kern County Crop percentages treated with 1,3-D for 2000-2001.

Population Based Risk Assessments

Geo-referenced population data can be superimposed on the air concentration data generated by SOFEA to address population based risk and exposure scenarios. Each receptor of the uniform grid within a township is assigned a population density if this information is supplied as an input). An example for a Monterey County chronic exposure simulation is given by Figure 19 where it is evident that the lowest air concentrations occur in/near urban areas where population densities are the greatest. The graphic on the left indicates urban areas, the location of the northwest corner of a treated field, and the township allocation fraction of 1,3-D for a 3x3 township domain. The graphic on the right is a surface plot for chronic air concentrations. The green columns in the surface plot are located at the northwest corner of a treated field and the height is correlated to the amount of 1,3-D mass applied during the year.

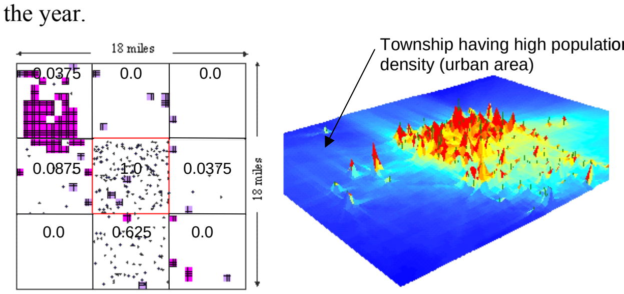

Figure 19. Air concentration results for Monterey 3x3 (central Township 15S04E) represented as a 3-D mesh plot with exaggerated z-axes.

RESULTS

Kern Monitoring Comparison

Township M31S29E had the highest use in 2001 and also the highest reported air concentrations where two of the ARB sampling locations are located (ARV, VSD). ARB monitored values for stations ARV and VSD are used for comparison, along with all receptor values simulated over the time frame for monitoring. A total of 10 yearly simulations were performed, and the air concentrations at each unique receptor on the same Julian day were averaged for township M31S21E only. All townships in Kern county that had reported 1,3-D usage were used by SOFEA to prescribe source terms for that township.

Figure 20 represents the predicted 24-hr air concentrations for the Kern Township M31S29E. Both simulation and monitored (stations ARV and VSD) results are expressed as an exceedence percentage. An exceedence plot represents how often a concentration of a certain magnitude is exceeded. Thus, an exceedence percentile of 95 indicates that 95% of the township receptors had lower concentrations, while 5% had higher magnitudes.

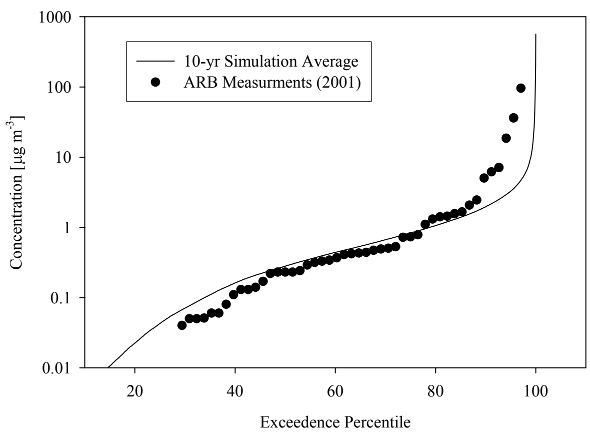

Figure 20. Observed and simulated 24-hour 1,3-D air concentrations in Kern County (M31S29E) over the 2001 ARB monitoring interval (Jun 30-Aug 30).

The use of SOFEA to determine air concentrations for Kern township M31S29E is not a true validation exercise since the proximity of treated fields to the ARB monitoring locations was not known, and the actual historical weather conditions over the monitoring interval were unavailable. However, of interest is the similar order of magnitude comparison that exists between predictions and observations when appropriate township allocations, land and crop type, and agronomic practices have been specified as input parameters. This is indicative of SOFEA to generate realistic concentration profiles using actual and/or representative input parameters describing existing agronomic practices and meteorological conditions. Correct order-of-magnitude simulation results, when compared to monitoring data, suggests the simulation tool adequately captures the appropriate physics and important process parameters to yield meaningful acute and chronic concentration predictions. ARB monitoring data also indicate year-to-year variability in air concentrations, suggesting sites receiving high concentrations of 1,3-D one year can have a lower concentration the following year. A stochastic approach that can account for this variability, like the one presented here, is mandatory for determining/estimating lifetime exposure potential to soil fumigants.

CONCLUSIONS

Simulations used to predict soil fumigant air concentrations should reflect actual or projected use as accurately as possible to avoid overly conservative exposure predictions that would inhibit or restrict the availability of fumigant tools for growers. A comprehensive numerical tool now exists to explore the ramifications of temporal changes in fumigant use in the agricultural regions of California and throughout the United States. Advances in database compilation, GIS systems, CPU processor speed, and the use of scientific programming now allow exposure resolution/refinement to be made on a level that has been historically difficult to achieve. Comparison of 1,3-D air monitoring measurements with simulation results illustrate correct trends and appropriate order of magnitudes are attainable. Having a predictive tool is especially appealing for regulatory risk managers and product stewards who often must make decisions when only small amounts of information are available.

Adjustments of the amount of fumigant used in a given region, both spatially and temporally can be simulated to calculate the exposure endpoint and provide the necessary concentration distribution for performing a population based risk assessment [van Wesenbeeck, *et al.* 2004 – this issue]. Thus, the exposure calculation system outlined in this paper can be coupled into a formalized risk assessment procedure where risk to the human population can be addressed. Proper forecasting techniques, anticipated market adjustments, sales projections and so on, will be the focus of further research to explore the viability of alternative soil fumigants to fully replace MeBr. Understanding how various agronomic best management practices affect acute, sub-chronic, and chronic exposure potential is a mandatory requirement for proper stewardship for all nematicides.

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